CONGRESSO DE PÓS-DOUTORANDOS DA USP

Papel e Perspectivas dos Pós-Docs no Brasil (2023)

VOLUME 2

Da Matriz Energética à Indústria Sustentável: Os Novos Cenários da Economia

USP

UNIVERSIDADE DE SÃO PAULO

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Da Matriz Energética à Indústria Sustentável: Os Novos Cenários da Economia

ORGANIZADORES
Celia R. S. Garcia
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USP

A Universidade de São Paulo (USP)

Fundada em 1934, a Universidade de São Paulo (USP) é uma Instituição reconhecida nacional e internacionalmente graças ao talento e à dedicação de seus mais de 5.500 professores, quase oitenta mil alunos e número de funcionários técnico-administrativos superior a 12 mil.

Desde 2003, a USP é incluída entre as 200 melhores universidades do mundo nos principais *rankings* mundiais que avaliam a qualidade das instituições de ensino superior.

No ensino de graduação, são 332 cursos em todas as áreas do conhecimento, oferecidos a quase 60 mil alunos em suas 43 unidades, distribuídas em oito campi localizados em Bauru, Lorena, Piracicaba, Pirassununga, Ribeirão Preto, São Carlos, Santos e São Paulo.

A qualidade da pesquisa e inovação na USP é comprovada pelas contribuições de grande relevância em todas as áreas do saber e pelo interesse aumentado em parcerias por parte de instituições de prestígio dos cinco continentes. Esta ação é alicerçada nos cerca de 2700 profissionais em seus programas de pós-doutorado. Devem ser mencionados recentes avanços na inclusão e pertencimento na USP, pela criação de uma nova pró-reitoria dedicada ao tema.

O sólido sistema de Pós-Graduação da Universidade é o principal responsável pelo seu desenvolvimento científico. Os 264 programas, em todas as áreas do saber, envolvem mais de 30 mil pós-graduandos.

É preciso destacar, também, a atuação expressiva da USP na difusão da cultura e na extensão universitária, atividades que desenvolve em suas Unidades e Órgãos afins, como os quatro museus, parques, centros, cinema, teatro, duas orquestras, grupos de corais, entre outros, e que congregam, a cada ano, dezenas de milhares de participantes, estreitando os laços com a sociedade em geral.

About USP

Founded in 1934, the University of São Paulo (USP) is a nationally and internationally recognized institution, thanks to the talent and dedication of its more than 5,500 professors, nearly eighty thousand students, and over 12,000 technical and administrative staff. Since 2003, USP has been ranked among the top 200 universities in the world in the main global rankings that evaluate the quality of higher education institutions.

At the undergraduate level, there are 332 programs offered across all areas of knowledge, serving nearly 60,000 students in its 43 schools and institutes, distributed across eight campuses located in Bauru, Lorena, Piracicaba, Pirassununga, Ribeirão Preto, São Carlos, Santos, and São Paulo.

The quality of the research developed at USP is evidenced by its significant contributions across all areas of knowledge and the growing interest from prestigious institutions across five continents in forming partnerships. This initiative is supported by the approximately 2,700 professionals in its postdoctoral programs. Advances in Inclusion and Belonging at USP should be noted, with the creation of a Provost Office dedicated to the subject.

The University's strong graduate system is the main driver of its scientific development. Its 264 programs, spanning all fields of knowledge, involve more than 30,000 graduate students.

It is also important to highlight USP's strong presence in cultural dissemination and university outreach, activities carried out through its Schools and affiliated bodies, including four museums, parks, cultural centers, a cinema, a theater, two orchestras, choir groups, among others, which gather tens of thousands of participants each year, strengthening ties with society at large.

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Prefácio

Carlos Gilberto Carlotti Junior, reitor da USP

Tenho muito prazer em fazer o prefácio destas obras, que são resultado dos trabalhos apresentados por nossos pesquisadores durante o congresso "O Papel e as Perspectivas do Pós-Doutorando no Brasil". Estes quatro livros representam registro da importância da colaboração interdisciplinar de nossos pós-doutorandos para enfrentar os desafios globais e promover novas descobertas científicas – tais como as tecnologias de transição energética, incluindo a conversão de etanol em hidrogênio.

Hoje, a USP conta com cerca de 2.700 pós-docs desenvolvendo suas atividades acadêmicas em suas Unidades de Ensino e Pesquisa. O congresso teve como objetivo ampliar a colaboração e promover a integração entre pesquisadores de diferentes áreas, abrindo novos horizontes, fortalecendo projetos em andamento e incentivando o desenvolvimento de novos estudos.

A programação incluiu seis *workshops* dedicados a temas como empreendedorismo, saúde pública e processos de carbono zero, além de palestras de pesquisadores nacionais e internacionais que abordaram assuntos tão variados como "A Crise Contemporânea das Democracias e seu Impacto nas Universidades Públicas", "Invernos e Verões da Inteligência Artificial" e "A USP Contribuindo para a Medicina do Futuro".

Os diversos grupos de pesquisa participantes, formados por pesquisadores e pesquisadoras altamente qualificados, apresentaram 350 comunicações orais e 1.200 pôsteres, organizados em sessões temáticas e multidisciplinares, abordando desafios da humanidade. O evento proporcionou, ainda, importantes desdobramentos, como encontros e interações entre as mais variadas áreas científicas, incluindo agentes políticos públicos e do setor privado.

Merece também ser mencionada a premiação, em oito áreas do conhecimento – Ciências Agrárias, Ciências Biológicas, Ciências Exatas e da Terra, Ciências da Saúde, Engenharias, Ciências Humanas, Linguística, Letras e Artes e Ciências Sociais Aplicadas –, de trabalhos que foram selecionados por três comissões científicas, por meio de um processo em três etapas, sendo a última comissão composta por membros externos à USP.

Com a chegada da economia do conhecimento, as bases do desenvolvimento econômico dos países passaram por uma enorme transformação. Investir em ciência é o caminho que nações desenvolvidas têm seguido na busca por fontes de conhecimento profundo, cujo núcleo se baseia em pesquisa de excelência e inovação. Neste novo cenário, o papel do universo acadêmico como ator imprescindível na geração de conhecimento não pode ser desprezado.

A observação atenta dos ecossistemas de ciência, pesquisa e inovação, por sua vez, revela o enorme potencial dos pós-doutorandos e de seus supervisores para acelerar o desenvolvimento de um país.

O congresso de pós-doutores da USP exemplifica o papel crucial que os pós-docs desempenham no avanço do conhecimento científico e da inovação. A capacidade de tirar o melhor proveito de novas tecnologias depende dos recursos humanos que atuam tanto na academia quanto em setores privados. Um ambiente de apoio e colaboração para os pós-doutorandos beneficia a comunidade acadêmica e contribui significativamente para o desenvolvimento da sociedade.

Ademais, o evento foi uma oportunidade valiosa para reunir pessoas e instituições altamente qualificadas e suas contribuições para o progresso da ciência. A publicação desta coleção diversificada e abrangente de textos científicos vem intensificar o ambiente aberto e estimulante para a condução da ciência em benefício de todos.

Apresentação

Celia R. S. Garcia[1], Raul Gonzalez[2] e Arlindo Philippi[3]

Os ecossistemas da ciência, investigação e inovação são motores essenciais do crescimento de uma nação, estando os pós-doutorados entre os grandes impulsionadores do progresso nestes sistemas. Com a conclusão dos seus estudos de doutoramento, estes indivíduos ocupam uma posição única na intersecção da criação e aplicação de conhecimentos. São os futuros líderes dos mundos acadêmico e empresarial e os pioneiros que avançam sobre os limites do possível. Esse papel vital do Programa de Pós-Doutorado é exemplificado no âmbito da Universidade de São Paulo (USP), uma das principais instituições acadêmicas do Brasil, que em 2023 contava com aproximadamente 2.650 pós-doutores. Estes profissionais compõem a vanguarda da investigação científica, contribuindo significativamente para a reputação da universidade como um centro de inovação e excelência acadêmica.

A importância do Programa de Pós-Doutorado para a produção de pesquisa e para ampliar a vitalidade intelectual da USP foi evidenciada durante um importante congresso realizado de 17 a 19 de outubro de 2023. Intitulado "O Papel e as Perspectivas do Pós-Doutorando no Brasil", o congresso serviu como plataforma para promover, discutir e analisar as contribuições desses acadêmicos para a universidade e para a comunidade científica em geral.

Mais do que um simples encontro de mentes, foi uma demonstração do empenho da universidade para promover um ambiente de pesquisa dinâmico, que prospera com a contribuição desses indivíduos altamente qualificados.

Como resultado do congresso foi gerada uma obra com quatro volumes, cada um deles sintetizando as pesquisas apresentadas durante o evento. Esses volumes trazem a essência de 350 comunicações orais e 1.200 pôsteres, refletindo a amplitude e a profundidade da pesquisa realizada pelos Pós-docs da USP. As apresentações foram organizadas em sessões temáticas e multidisciplinares, cada uma destinada a abordar alguns dos desafios mais urgentes da humanidade. Essa estrutura evidenciou a diversidade da pesquisa na USP e ressaltou a importância das abordagens transdisciplinares nas questões globais complexas. Ao reunir

1. Comissão Executiva do Congresso; Assessora do Gabinete do Reitor.
2. Comissão Executiva do Congresso; Pró-Reitor Adjunto de Inovação.
3. Conselho de Orientação do Congresso; Chefe do Gabinete do Reitor.

pesquisadores de várias disciplinas, o congresso demonstrou como os esforços de colaboração podem conduzir a soluções de caráter holístico e prático para os problemas contemporâneos mais prementes do mundo.

A conferência proporcionou também a oportunidade de promover interações críticas entre diferentes agentes, ampliando a sua influência para além dos limites da academia. Essas interações incluíram compromissos com agentes políticos dos setores público e privado, essenciais para traduzir as descobertas científicas em políticas públicas eficazes e produtos inovadores.

Esses diálogos são cruciais para garantir que os frutos da pesquisa não fiquem confinados às revistas acadêmicas, mas sejam utilizados para impulsionar o progresso e o desenvolvimento da sociedade.

Um dos principais objetivos do evento foi reforçar a interação, a colaboração e a integração entre pesquisadores de diferentes disciplinas. Este objetivo não consistia apenas em incentivar o trabalho em equipe, mas também em abrir novas vias de investigação, reforçar os projetos existentes e catalisar o desenvolvimento de novos projetos. Numa era em que os desafios que enfrentamos estão cada vez mais interligados e globais, essa colaboração multidisciplinar é essencial. As soluções mais inovadoras nascem da convergência de diversas perspectivas e conhecimentos, cocriação.

O programa da conferência foi rico tanto em conteúdo como em diversidade, apresentando seis *workshops* com tópicos de importância crítica para o futuro. Estes incluem o empreendedorismo, a saúde pública e os processos de carbono zero – áreas que não só estão na vanguarda da investigação atual, como também são cruciais para enfrentar os desafios globais. Os *workshops*, complementados por palestras de pesquisadores nacionais e internacionais, trouxeram para a discussão um vasto leque de perspectivas. Temas como "A Crise Contemporânea das Democracias e seu Impacto nas Universidades Públicas", "Invernos e Verões da Inteligência Artificial" e "A USP Contribuindo para a Medicina do Futuro" proporcionaram aos participantes uma visão profunda sobre os rumos da pesquisa e da inovação. Essas discussões ressaltaram o papel fundamental que instituições como as universidades desempenham no avanço do conhecimento e na formação do futuro das sociedades.

A conferência também celebrou a excelência em todo o espectro acadêmico. Foram entregues prêmios em oito áreas do conhecimento: Ciências Agrárias, Ciências Biológicas, Ciências Exatas e da Terra, Ciências da Saúde, Engenharia, Ciências Humanas, Linguística, Letras e Artes e Ciências Sociais Aplicadas. O rigoroso processo de seleção desses prêmios, que envolveu três comissões científicas – sendo a última composta por membros externos à USP –, garantiu

o reconhecimento das mais destacadas contribuições à ciência e à pesquisa, estabelecendo uma referência para futuros projetos de investigação.

A história da ciência está repleta de estudos científicos básicos que conduziram a aplicações após algum tempo. Para deixar clara a conexão entre ciência e benefício da sociedade, permitam-nos mencionar duas moléculas, a Bergenin e a Aequorin.

Bergenin, uma molécula extraída da planta *Endopleura uchi*, é encontrada em várias espécies nativas da Amazônia e tem usos medicinais. No catálogo da empresa farmacêutica Sigma-Aldrich de 2024, o composto Bergenin é cerca de 4.400 vezes mais caro do que o ouro, em peso. Além disso, a extração de ouro está frequentemente associada a problemas socioambientais na mesma região.

As contribuições de Osamu Shimomura, Martin Chalfie e Roger Tsien foram reconhecidas por meio do Prêmio Nobel de Química de 2008. Nos Estados Unidos, na década de 1960, Osamu Shimomura dedicou-se a estudar o fenômeno da bioluminescência na medusa *Aequorea victoria*. Depois de purificar os extratos desses animais marinhos, isolou uma proteína chamada "aequorina". Shimomura também descobriu outra proteína que exibia fluorescência verde, a Green Fluorescent Protein (GFP). A aequorina, por si só, emite luz azul, mas se a GFP estiver presente, é produzida luz verde. Douglas Prasher mostrou que a proteína era fluorescente no nematoide *Caenorhabditis elegans* e na bactéria *Escherichia coli*. A GFP pode ser vista como um farol de luz, abrindo caminho para várias aplicações dessa proteína como marcador biológico. A GFP pode rastrear múltiplos processos moleculares e celulares quando ligada a diferentes proteínas e expressa nas células. Consequentemente, a GFP tem sido utilizada em milhares de estudos que fazem avançar as ciências biológicas e médicas. Roger Tsien e o seu grupo descreveram a estrutura da GFP, desenvolveram proteínas fluorescentes de cores diferentes e várias ferramentas para monitorar funções celulares.

À medida que as nações se esforçam para alcançar a sustentabilidade do desenvolvimento e enfrentar os desafios globais, as contribuições destes pesquisadores, com seus respectivos supervisores, demonstram a relevância deles para moldar um futuro mais brilhante e inovador.

O Compromisso da USP com os Jovens Pesquisadores

Celia R. S. Garcia, Raul Gonzalez e Arlindo Philippi

O Congresso de Pós-Doutorandos da Universidade de São Paulo (USP) é um evento importante que reúne estudiosos de várias disciplinas acadêmicas. Com 1.233 participantes inscritos, esse congresso foi um fórum vital para o intercâmbio acadêmico, permitindo aos investigadores de pós-doutoramento apresentar os seus resultados, colaborar com os seus pares e participar em discussões multidisciplinares. As seções seguintes apresentam uma análise dos dados demográficos dos participantes, do enfoque temático e dos resultados notáveis do congresso.

O congresso contou com a participação de várias unidades da USP, tanto dos *campi* da capital quanto do interior. A Faculdade de Filosofia, Letras e Ciências Humanas (FFLCH) teve o maior número de inscritos, 158 participantes. A Faculdade de Medicina (FM) e a Escola Politécnica (EP) vieram em seguida, com 72 e 67 participantes, respetivamente.

Outras unidades com representação significativa foram o Instituto de Ciências Biomédicas (ICB) e o Instituto de Estudos Avançados (IEA), com 59 participantes cada (Figura 1).

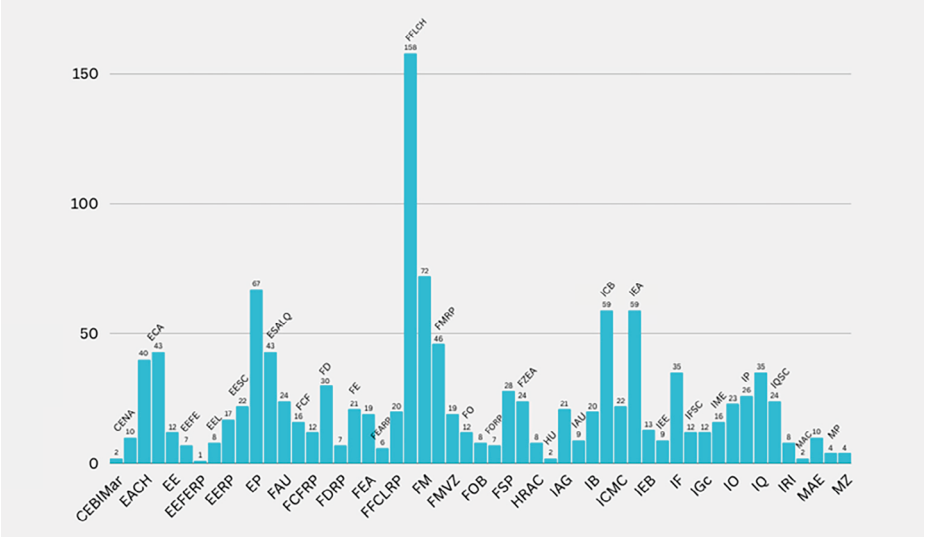

Figura 1 – Percentual de distribuição do cadastro de Pós-docs por Escolas da USP.

Dos 1.233 inscritos, 627 eram mulheres e 580 eram homens, o que revela uma representação de gênero relativamente equilibrada entre os investigadores pós-doutorados presentes no congresso (Figura 2).

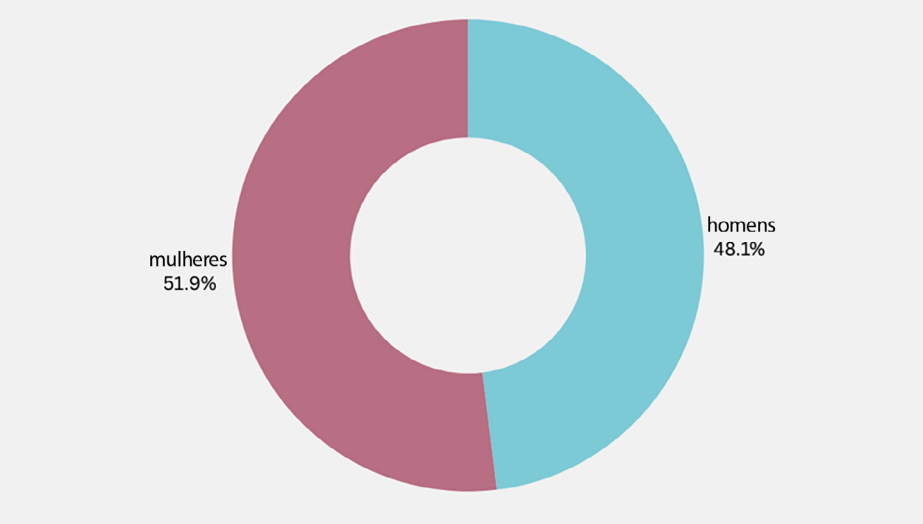

Figura 2 – Percentagem de Pós-Doutorados por gênero dos inscritos.

Para garantir a participação de pesquisadores de fora de São Paulo no congresso, a universidade disponibilizou auxílio financeiro para viagem e hospedagem. Dos 143 indivíduos que solicitaram auxílio para viagem, 108 foram contemplados. A maioria dos participantes (925) era proveniente dos *campi* da capital da USP, sendo 308 dos *campi* do interior. Dezenove participantes se identificaram como pessoas com deficiência ou com mobilidade reduzida, e a organização do evento disponibilizou os serviços de apoio necessários a todos os participantes.

O congresso atraiu investigadores das mais diversas áreas acadêmicas. A área das Ciências da Saúde foi a que registou maior participação, com 374 inscritos, seguida das Ciências Exatas, com 205 apresentações; das Humanidades, com 204 apresentações; das Ciências do Ambiente, com 190; e da Cultura e das Artes, com 136. Destacam-se ainda as Ciências Sociais (166), as Engenharias (108) e as Ciências Biológicas (155) (Figura 3).

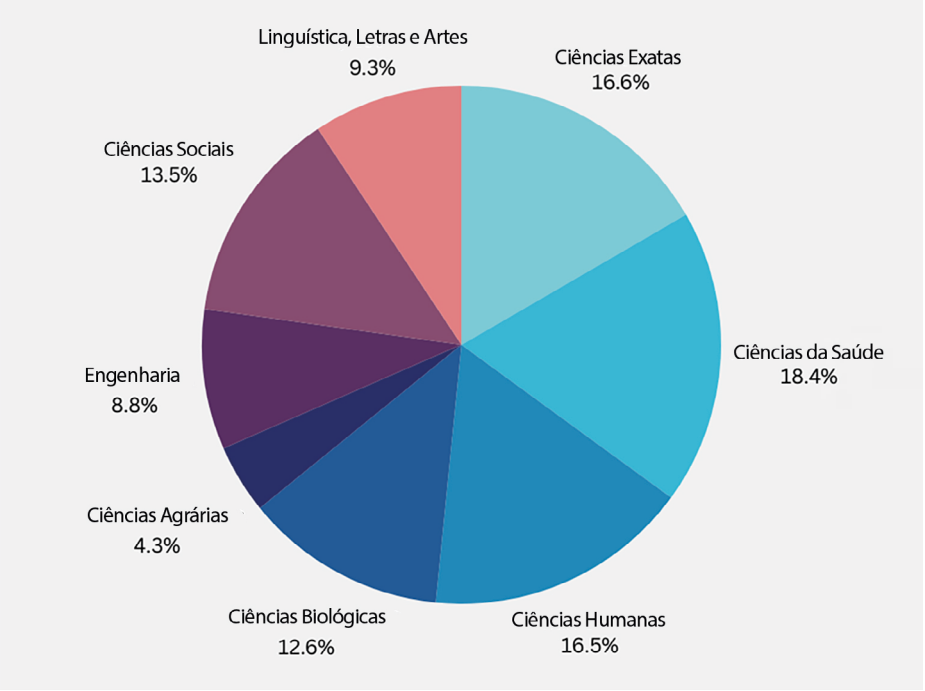

Figura 3 – Distribuição dos inscritos em pós-doutoramento por área.

As apresentações foram agrupadas em torno de desafios globais atuais e revelaram a interdisciplinaridade dos temas e da pesquisa realizada na USP. Foram selecionados 383 resumos para apresentações orais. Esses trabalhos foram divididos entre as diversas disciplinas, com destaque para as Ciências Exatas (65) e Ciências Humanas (64). Ciências da Saúde, Ciências Biológicas e Ciências Sociais também tiveram forte presença, com 61, 51 e 47 apresentações orais, respectivamente (Figura 4).

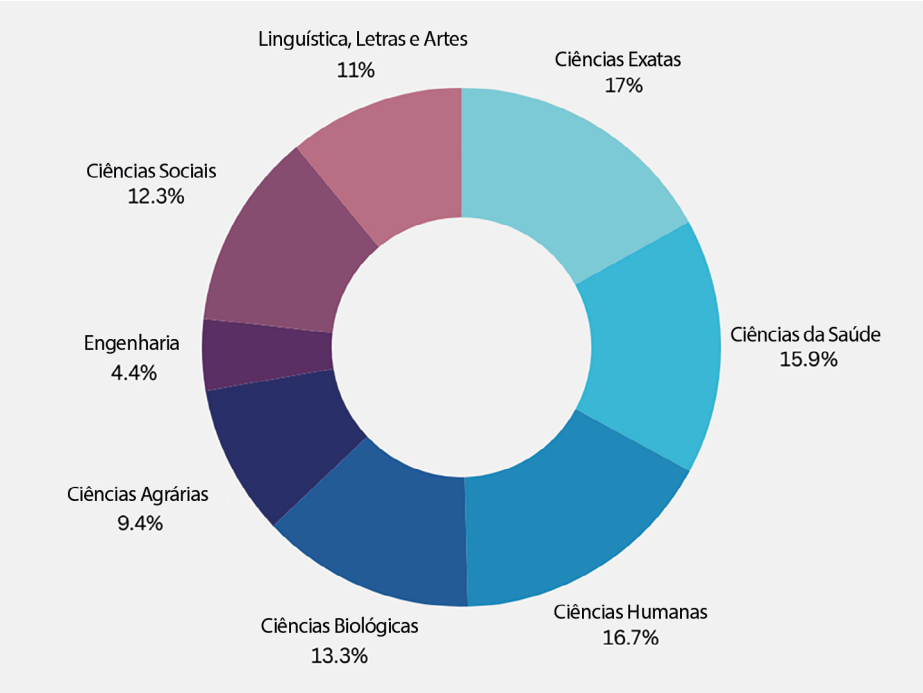

Figura 4 – Distribuição percentual das apresentações orais pelos diferentes domínios.

Oito investigadores em pós-doutoramento foram reconhecidos pelas suas contribuições excepcionais nos seus respectivos domínios. Estes indivíduos foram agraciados com o Prêmio de Pós-Doutoramento. Os premiados foram selecionados entre oito áreas que refletem o vasto âmbito da investigação de excelência no congresso. Na área de **Ciências Agrárias**: Flávia de Oliveira Scarpino Van Cleef, pelo seu trabalho sobre a redução da produção de metano pelos ruminantes. **Ciências Biológicas**: Mateus Vidigal Castro, pela sua investigação sobre a resistência natural à COVID-19. **Ciências da Saúde**: Marlón Juliano Romero Aliberti, pelo seu estudo sobre os efeitos a longo prazo da COVID-19 em idosos. **Ciências Exatas**: Hugo Luiz Oliveira, pelo seu trabalho sobre a modelação matemática da válvula cardíaca Wheatley. **Ciências Humanas**: Fabiana Barbi

Seleguim, por sua pesquisa sobre governança climática e direitos humanos. **Ciências Sociais**: Joana D'Arc de Oliveira, por seu estudo sobre memórias negras e justiça social. **Engenharia**: Raissa Antonelli, por sua pesquisa sobre purificação de água usando reatores eletroquímicos. **Linguística, Letras e Artes**: Cynthia Agra de Brito Neves, pela pesquisa sobre letramento literário em *slams* escolares.

Na mesma linha, a USP apoia diversas bolsas de pós-doutorado: o Programa de Formação em Gestão Acadêmica, com 35 bolsas; o Programa de Eixos Temáticos, 16 bolsas; o Escritório de Gestão Ambiental, 36 bolsas; e o Programa de Gestão da Inovação, nove bolsas em dois programas-chave. Um total de 96 bolsas, com rendimentos mensais compatíveis com os valores das bolsas de pós-doutorado da Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP), foram apoiadas financeiramente pela universidade. Esses pesquisadores foram selecionados por meio de um edital bastante competitivo. Tais iniciativas evidenciam o investimento que a Universidade está a fazer nos jovens investigadores.

A USP dedica-se a promover as carreiras de jovens investigadores. Por meio de iniciativas como o Congresso de Pós-Doutoramento, a USP proporciona uma plataforma dinâmica para a colaboração interdisciplinar e o reconhecimento da excelência da investigação. Com mais de 1.200 participantes, o congresso incentivou a troca de conhecimentos em diversas áreas acadêmicas e premiou os investigadores de pós-doutoramento que se destacaram pelas suas realizações. Além disso, a atribuição de bolsas com valores competitivos em programas pela USP demonstra o seu apoio a jovens investigadores. Entre as iniciativas de longa data, a Universidade incluiu esses pesquisadores nos seus comitês de investigação, ou seja, deu-lhes direito a voto. Estas iniciativas evidenciam o compromisso da USP para capacitar os investigadores emergentes, reforçando o seu papel como catalisadora do crescimento acadêmico e científico e promovendo a próxima geração de líderes científicos e educativos.

Preface

Carlos Gilberto Carlotti Junior, rector of USP

It is my pleasure to write the foreword for these works, which are the result presented by our researchers during the conference "The Role and Perspectives of Postdoctoral Research in Brazil." These four books represent a record of the importance of interdisciplinary collaboration among our postdoctoral fellows in addressing global challenges and fostering new scientific discoveries–such as energy transition technologies, including the conversion of ethanol to hydrogen.

Today, USP has approximately 2,700 postdoctoral researchers pursuing academic activities in its Teaching and Research Units. The conference aimed to expand collaboration and promote integration among researchers from different fields, opening new horizons, strengthening ongoing projects, and encouraging the development of new studies.

Four books, the result of 350 oral communications and 1,200 posters, were presented at the congress, organized into thematic and multidisciplinary sessions, and addressed the challenges of humanity. Thus, the congress drew attention to the multidisciplinarity of research groups formed by highly qualified researchers. The event led to meetings and interactions among various scientific areas, including public and private sector policy makers.

The event aimed to promote greater collaboration and integration between researchers from different areas, open new horizons, strengthen ongoing projects, and encourage the development of new ones.

The program included six workshops dedicated to topics such as entrepreneurship, public health, and zero-carbon processes, as well as lectures by national and international researchers who addressed various topics, such as: "The Contemporary Crisis of Democracies and its Impact on Public Universities", 'Winters and Summers of Artificial Intelligence' and 'USP Contributing to the Medicine of the Future'.

The participating research groups, comprised of highly qualified researchers, presented 350 oral presentations and 1,200 posters, organized into thematic and multidisciplinary sessions, addressing challenges facing humanity. The event also provided important opportunities, such as meetings and interactions between a wide range of scientific fields, including public and private sector policymakers.

Also worthy of mention is the awarding of prizes in eight areas of knowledge – Agricultural Sciences, Biological Sciences, Exact and Earth Sciences, Health Sciences, Engineering, Human Sciences, Linguistics, Literature and Arts, and Applied Social Sciences – for works that were selected by three scientific committees, through a three-stage process, with the last committee being composed of members outside USP.

With the advent of the knowledge economy, the foundations of countries' economic development have undergone a profound transformation. Investing in science is the path developed nations have followed in their search for sources of deep knowledge, whose core is based on excellent research and innovation. In this new scenario, the role of academia as an essential actor in knowledge generation cannot be overlooked.

Close observation of science, research, and innovation ecosystems, in turn, reveals the enormous potential of postdoctoral researchers and their supervisors to accelerate a country's development.

The USP Postdoctoral Congress exemplifies the crucial role that postdoctoral researchers play in advancing scientific knowledge and innovation. The ability to take full advantage of new technologies depends on the human resources working in both academia and the private sector. A supportive and collaborative environment for postdoctoral researchers benefits the academic community and significantly contributes to the development of society.

Furthermore, the event was a valuable opportunity to bring together highly qualified individuals and institutions and their contributions to the advancement of science. The publication of this diverse and comprehensive collection of scientific texts strengthens the open and stimulating environment for conducting science for the benefit of all.

Presentation

Celia R. S. Garcia[1], Raul Gonzalez[2] and Arlindo Philippi[3]

Science, research, and innovation ecosystems are essential drivers of a nation's growth, and postdoctoral fellows are among the major drivers of progress in these systems. With the completion of their doctoral studies, these individuals occupy a unique position at the intersection of knowledge creation and application. They are the future leaders of the academic and business worlds and the pioneers who push the boundaries of what is possible. This vital role of the postdoctoral programs becomes visible at the University of São Paulo (USP), one of Brazil's leading academic institutions, which in 2023 had around 2,650 postdoctoral fellows. These professionals make up the vanguard of scientific research, contributing significantly to the university's reputation as a center of innovation and academic excellence.

The importance of the Post-Doctoral Program for research production and for expanding USP's intellectual vitality was highlighted during an important congress held from October 17 to 19, 2023. Entitled "O Papel e as Perspectivas do Pós-Doutorando no Brasil", the congress served as a platform to promote, discuss, and analyze the contributions of these academics to the university and the scientific community in general.

More than just a meeting of minds, it was a demonstration of the university's commitment to promoting a dynamic research environment that thrives on the contribution of these highly qualified individuals.

As a result of the congress, a four-volume book was produced, each summarizing the research presented during the event. These volumes contain the essence of 350 oral presentations and 1,200 posters, reflecting the breadth and depth of the research carried out by USP's Postdocs. The presentations were organized into thematic and multidisciplinary sessions, each designed to address some of humanity's most pressing challenges. This structure highlighted the diversity of research at USP and underscored the importance of multidisciplinary approaches to complex global issues. By bringing together researchers from various disciplines, the conference demonstrated how collaborative efforts

1. Congress Organizing Executive Committee; Advisor to the Rector's Office.
2. Congress Organizing Executive Committee; Deputy Provost on Innovation.
3. Congress Advisory Council; Head of the Rector's Office.

can lead to holistic and practical solutions to the world's most pressing contemporary problems.

The conference also provided the opportunity to promote critical interactions between different stakeholders, extending their influence beyond the confines of academia. These interactions included engagements with political agents from the public and private sectors, essential for translating scientific discoveries into effective public policies and innovative products. These dialogues are crucial to ensure that the fruits of research are not confined to academic journals, but are used to drive progress and development in society.

One of the main objectives of the event was to strengthen interaction, collaboration and integration between researchers from different disciplines. This goal was not only to encourage teamwork, but also to open up new avenues of research, improving existing projects and catalyze the development of new ones. In an age when the challenges we face are increasingly interconnected and global, this interdisciplinary collaboration is essential. The most innovative solutions are born from the convergence of diverse perspectives and knowledge, through co-creation.

The conference program was rich in both content and diversity, featuring six workshops on topics of critical importance for the future. These included entrepreneurship, public health, and zero-carbon processes - areas that are not only at the forefront of current research, but are also crucial to tackling global challenges. The workshops, complemented by lectures from national and international researchers, brought a wide range of perspectives to the discussion. Topics such as "The Contemporary Crisis of Democracies and its Impact on Public Universities", "Winters and Summers of Artificial Intelligence," and "USP Contributing to the Medicine of the Future" provided participants with an in-depth insight into the direction of research and innovation. These discussions highlighted the fundamental role that institutions such as universities play in advancing knowledge and shaping the future of societies.

The conference also celebrated excellence across the academic spectrum. Awards were presented in eight areas of knowledge: Agricultural Sciences, Biological Sciences, Exact and Earth Sciences, Health Sciences, Engineering, Human Sciences, Linguistics, Letters and Arts and Applied Social Sciences. The rigorous selection process for these awards, which involved three scientific committees, the last one was formed by members from outside USP - ensured that the most outstanding contributions to science and research were recognized.

The history of science is full of fundamental scientific studies that have led to practical applications over time. To make clear the connection between science

and societal benefit, let us mention the discovery of two molecules, Bergenin and Aequorin.

Bergenin, a molecule extracted from the *Endopleura uchi* plant, is found in several species native to the Amazon and has medicinal uses. The compound Bergenin is approximately 4,400 times more expensive than gold by weight, according to the Sigma-Aldrich catalog in 2024. Besides, gold extraction is often associated with socio-environmental issues in the same region.

The contributions of Osamu Shimomura, Martin Chalfie, and Roger Tsien were recognized with the 2008 Nobel Prize in Chemistry. In the United States, in the 1960s, Osamu Shimomura dedicated himself to studying the phenomenon of bioluminescence in the jellyfish *Aequorea victoria*. After purifying the extracts from these marine animals, he isolated a protein called "aequorin". Shimomura also discovered another protein that exhibited green fluorescence, Green Fluorescent Protein (GFP). Aequorin emits blue light, but if GFP is present, green light is produced. Douglas Prasher showed that the protein was fluorescent in the nematode *Caenorhabditis elegans* and the bacterium *Escherichia coli*. GFP can be seen as a light source, supporting various applications of GFP as a biological marker. GFP can track multiple molecular and cellular processes when linked to different proteins and expressed in cells. Consequently, GFP has been used in thousands of advanced biological and medical sciences studies. Roger Tsien's group described the structure of GFP, developed fluorescent proteins of different colors, and developed several tools to monitor cellular functions.

As nations strive to achieve sustainable development and tackle global challenges, the contributions of these researchers, with their respective supervisors, demonstrate their relevance to shaping a brighter and more innovative future. The event served as a reminder of the transformative power of research and the need to continually support and nurture the ecosystems that make this progress possible.

USP's Commitment to Young Researchers

Celia R. S. Garcia, Raul Gonzalez, and Arlindo Philippi

The Postdoctoral Congress at the University of São Paulo (USP) is a relevant event that brings together scholars from various academic disciplines. With 1,233 registered participants, this congress was a vital forum for academic exchange, allowing postdoctoral researchers to present their findings, collaborate with peers, and engage in interdisciplinary discussions. The following sections provide a breakdown of participant demographics, thematic focus, and notable achievements from the congress.

The congress saw participation from various units across USP, both from the capital and interior campuses. The Faculty of Philosophy, Letters, and Human Sciences (FFLCH) had the highest number of registrants, 158 participants. The School of Medicine (FM) and the Polytechnic School (EP) followed with 72 and 67 participants, respectively. Other units with significant representation included the Institute of Biomedical Sciences (ICB) and the Institute of Advanced Studies (IEA), with 59 participants each (Figure 1).

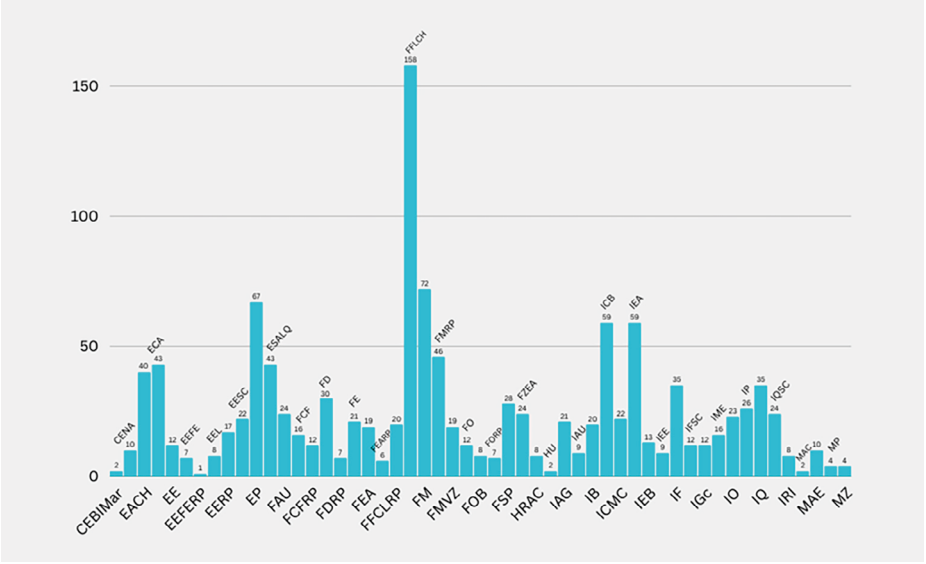

Figure 1 – Percentage of distribution of Postdocs registration per USP Schools.

Of the 1,233 registrants, 627 were women, and 580 were men, highlighting a relatively balanced gender representation among postdoctoral researchers at the congress (Figure 2).

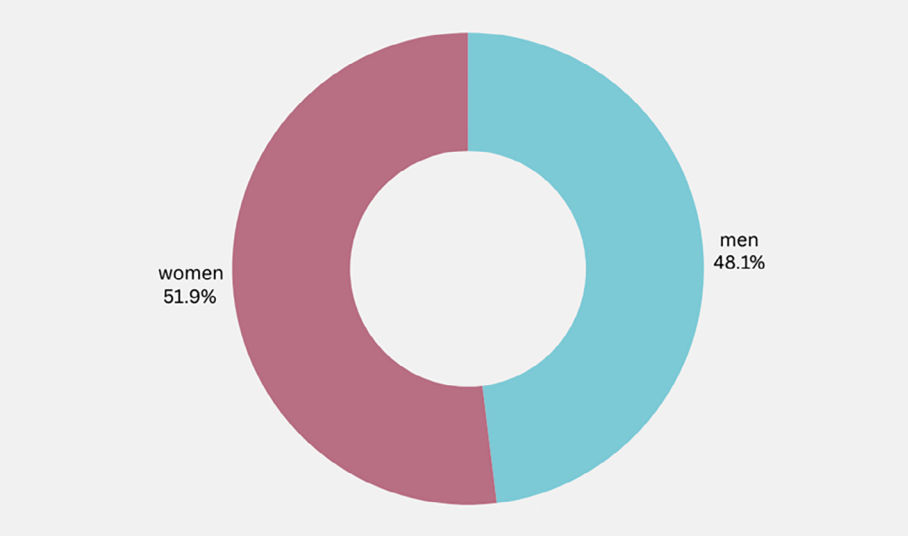

Figure 2 – Percentage of Postdocs by gender distribution of registrants.

To ensure that researchers from outside São Paulo could attend the congress, the university provided financial assistance for travel and accommodation. Of the 143 individuals who applied for travel assistance, 108 were granted. Most participants (925) came from USP's capital campi, with 308 from the interior campi. Nineteen participants identified themselves as having disabilities or reduced mobility, and the event organizers made necessary support services available to all participants.

The congress attracted researchers from a wide range of academic areas. The Health Sciences field saw the highest participation, with 374 registrants, followed by the Exact Sciences with 205 presentations, Humanities with 204 presentations, Environmental Sciences with 190, and Culture and the Arts with 136. Other notable fields included social sciences (166), engineering (108), and biological sciences (155) (Figure 3).

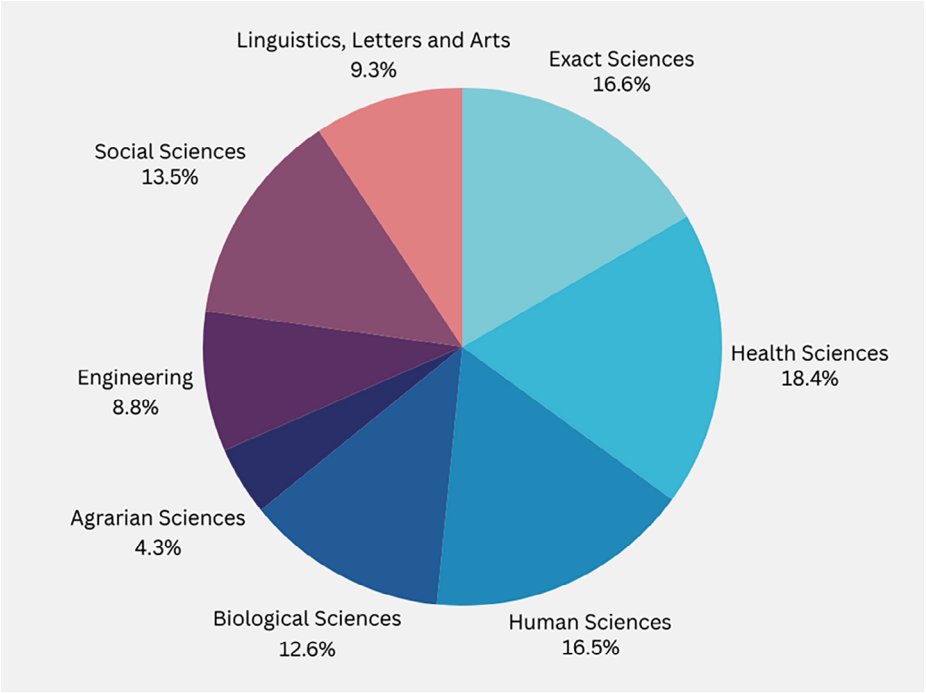

Figure 3 – Distribution of postdoc registrants by area.

The presentations were clustered around current global challenges and revealed the interdisciplinary nature of the themes and the research conducted at USP. A total of 383 abstracts were selected for oral presentations. These works were divided among the various disciplines, with the Exact Sciences (65) and the Humanities (64) leading the way. Health Sciences, Biological Sciences, and Social Sciences also had a strong presence, with 61, 51, and 47 oral presentations, respectively (Figure 4).

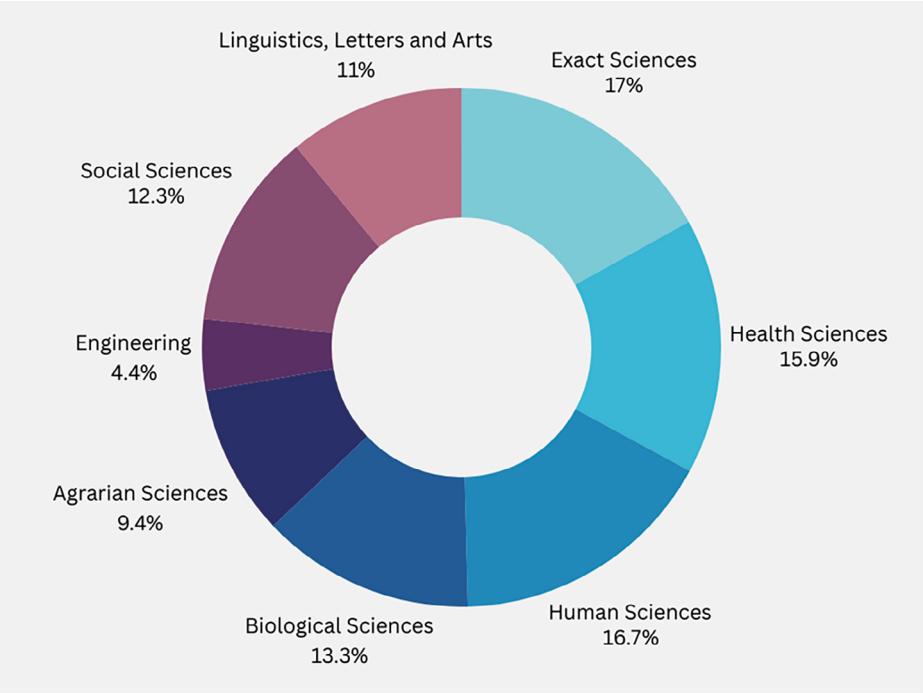

Figure 4 – Percentage distribution of oral presentations across different fields.

Eight postdoctoral researchers were recognized for their outstanding contributions to their respective fields. These individuals were awarded the Postdoctoral Prize. The awardees were selected from eight areas that reflect the broad scope of research excellence at the congress. The awardee was **Agrarian Sciences**: Flávia de Oliveira Scarpino Van Cleef for her work on reducing methane production from ruminants. **Biological Sciences**: Mateus Vidigal Castro, for his research on natural resistance to COVID-19. **Health Sciences**: Marlón Juliano Romero Aliberti, for his study on the long-term effects of COVID-19 in older adults. **Exact Sciences**: Hugo Luiz Oliveira, for his work on the mathematical modeling of the Wheatley heart valve. **Human Sciences**: Fabiana Barbi Seleguim, for her research on climate governance and human rights. **Social Sciences**: Joana D'Arc

de Oliveira, for her study on black memories and social justice. **Engineering**: Raissa Antonelli, for her research on water purification using electrochemical reactors. **Linguistics, Letters, and Arts**: Cynthia Agra de Brito Neves, for her research on literary literacy in school slams.

On the same line, USP supports several postdoc fellowships: the Academic Management Formation Program, 35 fellowships; Thematic Axis Program, 16 fellowships; Environmental Management Office, 36 scholarships; and the Program for Managing Innovation, nine fellowships in two key programs. A total of 96 scholarships, with monthly incomes compatible with FAPESP postdocs fellowships values, were financially supported by the university. These researchers were selected through a very competitive call for applications. These initiatives highlight the investment that the University is considering the young researchers.

The University of São Paulo (USP) is dedicated to advancing the careers of young researchers. Through initiatives like the Postdoctoral Congress, USP provides a dynamic platform for interdisciplinary collaboration and recognition of research excellence. With over 1,200 participants, the congress encouraged knowledge exchange across diverse academic fields and awarded outstanding postdoctoral researchers for their achievements. Moreover, USP's allocation of competitive fellowships across programs demonstrates its support for young researchers. Among long-standing initiatives, USP included them in university research committees, giving them voting rights. These initiatives highlight USP's commitment to empowering emerging researchers, reinforcing its role as a catalyst for academic and scientific growth, and fostering the next generation of scientific and educational leaders.

Sumário

ECONOMIA

The effects of agribusiness spillover in the state of Goiás: analysis of job creation and wage bill

Tânia M. de Freitas[1]

and Silvia F. M. Salustiano[2]; Jesiel S. Silva[3]; Danilo P. Barbosa[4]; Pedro A. V. Junior[5]; Durval D. Neto[6]

Identifying the sectors that promote the economic and social development of a region is an essential process for the elaboration of public policies. The objective of this study was to analyze the main productive sectors, generators of employment, income and economic activity directly or indirectly related to the agribusiness sector with the highest impact value considering the Spillover Effect (ET), developed from the economic activities listed in Table CNAE (National Classification of Economic Activity), through the hierarchy of subclasses, up to the fifth level in the amount of 1332 groupings. The analyzes involve the 246 municipalities in the state of Goiás, which were grouped using the hierarchical cluster methodology (dendrogram). Economic activities were divided into 5 groups, considering their relationship with agribusiness. The results show the municipalities allocated to the respective groups of activities and spatially presented on the map of Goiás, confirming the importance of agribusiness for the economy of Goiás. The present work identified and quantified the importance of agribusiness for the state of Goiás, including its relationship with the local and regional economy. The spillover effects of the segments linked to agribusiness also reverberated over the other sectors of the economy, and in the representativeness in the total of goods and services produced in Goiás.

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Building capacities for public procurement through an innovation laboratory

Maria C. Foss[1]
and Diogo R. Coutinho[2]

The Brazilian innovation system has been structured through leaps and bounds over the past three decades. Budgetary contingencies and discontinuity of public policy programs are, among others, bottlenecks that compromise its effectiveness (Mazzucato & Penna, 2016; Coutinho & Mouallem, 2016). Over time, reforms in public procurement laws strengthened the potential of this legal instrument to catalyze innovation policy goals. But the design, implementation, monitoring, and accountability of public procurement for innovation (PPI) in Brazil still need to improve a great deal due to a lack of expertise, experimentation, and the distrust of new public-private contracts. In general, PPI contracts do not adhere to the default lower-price criteria, and constitute an unusual sui generis public procurement in Brazil's regular flow of public-private contracting. The government control and accountability bodies are seen as bureaucratic instances whose analysis and decisions usually do not recognize criteria for public procurement - such as the uncertainties and technological risks, which are of the essence of PPI - beyond price (Foss & Bonacelli, 2022). In 2015 the Brazilian Federal Accountability Court (TCU) created its innovation laboratory, Colab-i, intending to promote innovation through interaction among government staff, controlling bodies, and society. Colab-i integrates the TCU and conducts activities to train and qualify the government staff, diffusing knowledge about innovation into public service and supporting public procurement for innovation contracts. In 2022, Colab-i launched an open public platform for PPI contracts, providing interactive content focused on the government as a buyer of six kinds of PPI foreseen in the Brazilian public procurement laws (https://inovacpin.org/). The paper aims to analyze the Colab-i case as an enabler to promote and diffuse the contracting for innovation in Brazil. How the activities performed by Colab-i affect the PPI implementation in Brazil? In addition, the article will seek to answer, according to the available data, how the role played by Colab-i rebounds on the court's decisions. The repercussions of the innovation laboratory into the most relevant court of account in Brazil motivates our analysis since it promotes a repositioning of a government actor who is not an innovation public policy maker (Kattel et al., 2018). A possible way to understand Colab-i's role in the

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Brazilian national innovation system is as a novel innovation-friendly enabler in public administration. The paper comprises a descriptive analysis of Colab-i based on documents, including court decisions, laws and regulations, and data collected through semistructured interviews with Colab-i staff. Preliminary findings indicate that the institutional support provided to PPI by prosecutors and government agencies (such as Colab-i) was key in unlocking the negotiation of the public procurement contract for COVID-19 vaccine during the pandemic emergency. The COVID-19 vaccine contract was a pioneer of PPI in the Brazilian health sector, paving the way for a broad and more inclusive approach for PPI. The Colab-i case unveils a new legal and institutional arrangement in the national innovation system, and demonstrates how organizational changes in government bodies can reframe innovation policy instruments (Proksch et al., 2019).

Efficient Breach: between *pacta sunt servanda* and efficiency. An analysis of its applicability in Brazilian Law

Ricardo D. Pizzol

According to the efficient breach doctrine, developed within the Economic Analysis of Law, if the debtor's gain from breach of contract exceeds the amount of damages to be paid to the creditor or if, alternatively, the debtor's cost of complying with the contract exceeds the creditor's benefit in having the performance executed, breach of contract will be the solution that maximizes social utility. For the supporters of this doctrine, breach of contract, under such circumstances, should not be discouraged or punished, as it allows resources to be directed to the economic agent that most values them. The efficient breach constitutes, in both situations mentioned in the previous paragraph, not only a "Kaldor Hicks improvement" but also a "Pareto improvement", since at least one of the agents involved would benefit from the outcome, while the innocent party would remain at least in a neutral position. On the other hand, the most widespread criticism against the doctrine of efficient breach is that it encourages the intentional non-performance of contracts, disregarding the systemic effects that such a practice, if widely disseminated, may have in the long term, in matters of certainty and stability of contractual relationships. After all, would it be appropriate for society to tolerate malice and to encourage the non-performance of contracts? As can be noted, the essential divergence occurs between a strictly "utilitarian" view of the contract, which privileges efficiency through the allocation of goods to agents who value them most (and which, for this very reason, encourages the efficient breach) and a more "deontological" view of the contract, which seeks to emphasize the ethics of fulfilling duties as they were agreed and the impact of this on society in the long term, in matters of legal certainty, trust and reputation of agents (which, for that very reason, tends to reject the doctrine of efficient breach).

Principle of full reparation and compensation for contractual loss of profits and positive contractual interest

Alexandre de M. Guerra

The contribution that is intended to be presented is in the sense of examining the contemporary limits and criteria for indemnification of the injured party in the event of negligent breach of contract. Moving away from the traditional profile strongly attached to the compensation of emerging damages, with the restoration of the innocent party to the state in which it would have been if the contract had not been signed, the contribution that is sought is to examine in which terms, limits and criteria it would be possible to meet to the principle of full reparation in terms of contractual civil liability, covering what the doctrine agrees to call positive contractual interest and indemnification of contractual loss of profits, and providing, especially to jurisprudence and concrete application of the Law, guidelines that can guide the concrete realization of the Law by the State in contractual relations governed by private law.

The history of the State of São Paulo Court of Accounts

Ariel E. Pesso

This research delves into the history of the Court of Accounts of the State of São Paulo (TCE-SP), aiming to answer the question of how its historical development unfolded. The study investigates the TCE-SP's unique legal nature and its expanding role since the 1988 Federal Constitution, which granted the institution autonomy, challenging traditional legal doctrines, particularly the separation of powers. By analyzing diverse historical sources within their respective contexts, including local, regional, national, and international factors, as well as significant legal milestones, the research seeks to shed light on the TCE-SP's historical trajectory. The scarcity of comprehensive investigations in the field of Legal History within the Brazilian scientific community justifies this research. Despite the discipline's resurgence in law school curricula since the 1990s, serious and rigorous studies are lacking. Moreover, the Court of Accounts of São Paulo, despite its century-long existence, remains largely unknown to the population. Therefore, a juridical-historical study on the creation and strengthening of this institution as an external control body is essential, filling a significant research gap. While numerous studies exist on the Union Court of Accounts (TCU), the same cannot be said for the TCE-SP. The research also addresses the impact and relationship of TCE-SP concerning the separation of powers, which is a fundamental principle of the national legal order. Given significant legal milestones, namely the Federal Constitution of 1988 and the Fiscal Responsibility Law of 2000, which granted unprecedented autonomy to Brazilian courts of accounts, by analyzing the TCE-SP's role in this context, the research aims to contribute to a deeper understanding of the institution's influence and challenges over one hundred years. Methodologically, this research adopts a historical approach, employing primary sources (legislation, parliamentary debates, reports, correspondence, specialized journals, etc., covering the period from 1891 to 2023) and secondary sources (such as theses, dissertations, etc.). The methodology aligns with intellectual history, combining institutional history and the history of legal thought. Additionally, the study employs the methodologies of Oral History and Contemporary History, incorporating interviews with TCE-SP's officials, especially the Counselors. In summary, this research project aims to fill the research gap regarding the history of the Court of Accounts of São Paulo, uncovering its historical development, legal nature, and impact on legal principles. By employing a comprehensive historical methodology and addressing the lack of serious investigations in the field of Legal History, this study contributes to the broader understanding of external control institutions in Brazil and their significance within the framework of the national legal order.

Taxation of digital marketing chain

Jacqueline M. da C. U. Braz[1]

Digital marketing refers to communication actions undertaken through the internet, mobiles, or other digital means, with the aim of advertisers disclosing their products or services to potential customers. Today, digital marketing is promoted through real-time biddings to select companies that will advertise in the spaces available on internet. In this context, similar platforms have emerged with different functions to promote digital marketing, including: (i) demand-side-platform (DSP), which serves advertisers, managing their campaigns and sending bids in real time for each bid request received; and (ii) supply-side-platform (SSP), which serves ad spaces owners (publishers) by managing publishers. However, a disclaimer is necessary: The real-time bidding (RTB) and the aggregation of multiple ad networks have not changed the nature of these markets. The only allow transactions to be done in real time with a bidding engine. From this, new challenges arise, such as: (i) understanding the legal transactions entered between these actors in the digital marketing chain; (ii) understanding the contracts signed by them; and, especially, (iii) understanding how these activities, carried out by these actors in the digital marketing chain, should be taxed. It is known that the law is one and indivisible. But the methodological cut is essential for determining the way in which we will approach the object we intend to know, that is, the taxation of activities carried out by the actors of the digital marketing chain, its foundations, and its objective limits. Thus, it is questioned whether they are subsumed under the hypothesis of taxes, especially income tax, social contributions, and consumption taxes. The study does not intend to analyze the subject from perspective of contractual and regulatory law. However, to analyze the object from the tax point of view, it will be necessary to study how digital marketing is regulated in Brazil and in what type of contract are signed by its actors.

1. Universidade de São Paulo.

ADRs and BDRs: legal framework of foreign capital investment

Viviane A. Morais[1]

This research analyzes the normative structure that organizes foreign investment in Brazil in its relationship with the structure of control and ownership of securities representing the share capital of some companies in Brazil that issue ADRs (American Depositary Receipts) and of foreign companies that issue share deposit certificates for circulation in the Brazilian market- BDRs (Brazilian Depositary Receipts). Its main hypotheses are: (i) ADR issues emerged as a secondary strategy for the internationalization of the capital stock structure of Brazilian companies in the early 1990s, especially as one of the legal forms of the privatization process in government- controlled companies; (ii) for private companies, the issuance of ADRs was the response to the oscillation of the supply of liquidity in the internal market and (iii) from the point of view of public finance, the issuance of ADRs composed the intended strategy of forming favorable exchange positions by registration of the acquisition values of such certificates in the national trade balance. BDRs (Brazilian Depositary Receipts) are recent management legal instruments with less use by foreign companies, that lend them to (i) exchange of shares and resolution of corporate issues of companies headquartered in Brazil, controlled by foreign companies; (ii) to organize a way in which some payment institutions resolved the need to offer their customers supposed advantages over maintaining their commercial relationship, without paying attention to the tax disadvantages. The success of placing ADRs in the United Stated market and the failure of the BDR market in Brazil demonstrate how the governing structure of foreign capital promoted (i) the export of liquid resources through the payment of royalties; (ii) the indirect internationalization of the structure of social capital of Brazilian companies and (iii) the attempt to internationalize the control of the Brazilian Payment System in its first phase, capturing payments and creating payment accounts, with the internationalization of the controlling companies of the main companies that operate in this market.

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Consumer protection in digital business

Jesualdo E. de A. Junior

The digital age has brought new business models, such as digital contracts, electronic contracts, digital currencies, encrypted signatures. However, it has also brought new challenges in terms of consumer protection. The proposal of my research is the defense of the integral protection of consumer rights in the digital scenario. In fact, the new business models cannot be refractory to topics such as the strict liability of service providers, joint and several liability of the various economic agents that have acted in commercial relations, clearer and more precise guarantee models, and above all the need for prior and full information of risks to the consumer. The Marco Civil da Internet, the General Data Protection Law, the Marco Civil das Cryptocurrencies expressly touch on consumer protection. However, there are some platforms that have come to enjoy differentiated treatment, such as marketplaces, public transport applications and especially social media content providers. This is exactly the turning point: consumerist norms, as corollaries of fundamental rights, cannot be emasculated or even relativized in the digital landscape.

Cyber risk management – Proposing a model for companies

Germano Fenner
and Fabio Lotti Oliva

In the current work context, organizations are increasingly dependent on information technology (IT) services to carry out their activities. Whether in the process of manufacturing a material, in the commercialization of the product, in the logistics of delivery, in the buying and selling process, IT is involved and, as such, participates in the process. This dependence on IT services has increased considerably with the COVID-19 pandemic, which has accelerated the digital transformation in many companies. Business models that, until then, were centralized, forcing people and technologies to be in the same physical space for their execution, gave way to remote and distributed operations, demanding even more use of IT resources and services. There was an increase in the format of working from home, online education, entertainment through digital platforms, which generated a sharp increase in the time of use and number of users on the internet worldwide. With all this transformation and the little time for companies to adapt to changes, a favorable scenario was created for cybercriminals to exploit the vulnerabilities of organizations, which materialized in data breaches, malware attacks, ransomware, phishing, and social engineering. Companies have sensitive data that, if not protected, will result in losses that can lead to crises and, in more extreme cases, to the bankruptcy of the institution. In this context, the need to protect the business from cyber-attacks arises. Companies need to develop skills to protect themselves and prevent cyber risks from occurring. Thus, the objective of this work is to propose a model for managing cyber risks that the business can use as a measure to increase information security in its operation and work routine.

SUDENE and relations with the United States: Celso Furtado and democratic reformism in the Northeast

Gustavo L. H. Pinto[1]
and Alexandre M. Saes

This post-doctoral research aims to analyze the relations between the Superintendence of Development of the Northeast - SUDENE and the United States from the international policy of the Alliance for Progress (ALPRO) directed to the Northeast region. The study covers the period between the institutionalization of the Alliance for Progress, in 1961, and the Civil-Military Coup of 1964. SUDENE, as bearer of the Master Plans, held an agrarian reform project and an industrial policy of interest to the objectives of the ALPRO. From the documents of the Deliberative Council of SUDENE and the official documents of the United States, it is suggested that the management of ALPRO taken from 1962, with the publication of the Bohan Report, the Northeast Agreement and the installation of USAID in Recife, directed itself to the political struggle of the João Goulart government, financially disfavoring SUDENE's policies. We point out the formation of a power bloc that relates the North American presence in the Northeast, from ALPRO, the political and economic power disputes with the landowner elites (mainly their northeastern governors and deputies) in opposition to the political project and the figure of the economist Celso Furtado. We intend to launch some interpretation clues in relation to the undone fantasy of the democratic reformism of Furtado for the Northeast, positioning SUDENE under analysis in an international perspective in the relations with the United States.

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The impact assessment of extreme events: an integrated approach with computable general equilibrium and risk analysis

Inácio F. de A. Junior[1]

and Eduardo A. Haddad[1]

The research project seeks to develop models to assess the impact of unexpected (and usually extreme) events. Extreme events can be caused by natural disasters (earthquakes or hurricanes), and although it is not possible to avoid them, there is the possibility of trying to reduce their damage. Extreme events can also occur due to changes in climate variables attributed directly or indirectly to human influence. This human influence has implications for the occurrences of unusually severe weather or climate conditions or weather-related events. Another category of disasters is pandemics, such as COVID-19, or wars and armed conflicts. In this context, risks can arise from the potential impacts of these disasters, which cause adverse effects on well-being, ecosystems, infrastructure, and economic assets. Thus, unexpected events affect economic activity and can reduce the productivity of companies and influence the labor demand with implications on migration. The study uses methodologies based on the integration of intensive models in the use of large databases, which allows assessing the impact of disasters. The modeling framework uses an interregional input-output system to calibrate a computable general equilibrium model. This model integrates with economic models that quantify higher-order impacts of the unexpected events focusing on regional and sectoral infrastructure destruction estimates. In addition, the modeling considers the frequency of event occurrence to incorporate the uncertainties coming from the risk analysis into our spatial computable general equilibrium model. The main contribution of the research is the development of an integrated approach that incorporates elements of uncertainty into modeling to evaluate the direct and indirect economic impact of unexpected events. The proposed research project will provide the policymakers with simulations to identify economic vulnerabilities at the regional and industrial level and explore alternatives for mitigating losses in extreme events.

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Recommendations for the adoption of Artificial Intelligence by public sector

Luis F. Guedes[1]

and Moacir de M. O. Junior[1]

The ongoing digital transformation in the realm of work has prompted the OECD to project that automation drive by Artificial Intelligence (AI) will significantly touch one third of jobs. Within the context of embracing emerging technologies, AI emerge as a technology capable of complementing the existing workforce's skills, not without prompting new risks. As AI technology continues to advance, its adoption by government agencies becomes an eventuality. Particularly, tasks driven by processes hold immense potential for automation, thereby liberating public servants to concentrate on more value-added endeavors that are beyond the scope of automation. The present research stems from a theoretical gap identified in the literature concerning AI adoption in the public sector. Given this context and considering the functions of government, our research question revolves around exploring the possibilities and pitfalls associated with the adoption of AI in the public sector. Leveraging a meticulous literature review, we conducted ten interviews with senior executives directly involved in AI projects and an in-depth case study with The Federal Revenue of Brazil. As a result, we identified 66 codes related to the AI adoption, which were categorized into ten dimensions. Furthermore, we observed a disparity in the relative importance of these dimensions when viewed through theoretical and practical lenses. In conclusion, a set of twelve recommendations has been formulated to aid senior executives within the public sector to adopt AI artifacts. These recommendations take into careful consideration associating risks, pitfalls, and expected benefits of embarking upon such endeavor.

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Look at the charitable organization or look at the beneficiary: how identifiability leads to prosocial rewards effectiveness?

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A recent trend in organizations is to motivate employees with prosocial rewards, whereby employees must donate their rewards to charity upon incentive contract. We examine the motivational effects of prosocial rewards size versus donation target under conditions where the pitch is abstract or identified. We develop our hypotheses based on identification model, which posits that, beyond the altruistic act of giving (warm glow), individuals derive utility from the impact or difference that they can make in the lives of victims in need. In a 2 (Prosocial Reward: Small vs. Large) x 2 (Donation Target: Charitable Organization vs. Single Victim Identified) x 4 (Round) mixed experiment design, we recruited undergraduate business students at public Brazilian universities to participate in our study via Labvanced platform. Experiment findings support our hypotheses. Specifically, we find that employees who are rewarded with single victim identified (vs. charitable organization) piece-rate prosocial rewards presented strong emotions with a recipient and high impact perception. Consequently, when employees are assigned single victim identified´ donation target, their effort is higher when incentivized with a piece-rate prosocial reward than a charitable organization´ donation target. Furthermore, contrary to previous research, we show that under large prosocial reward, donation target has a substantial positive effect, but under small prosocial reward, donation target has only a small effect. These findings highlight for incentive system designers the motivational advantage of single victim identified´ donation target relative to charitable organization. Furthermore, we extend the academic literature by showing how tangibility of donation target can influence employees' effort when firms use prosocial incentives.

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Favourable credit to private agents and the local economies in the deprived regions of Brazil: a spatial panel analysis, 2002-2020

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and Carlos R. Azzoni[2]; André L. S. Chegas; Gustavo H. L. de Castro

This article analyzes whether the resources transferred to private economic agents in favorable conditions through Constitutional Funds (CF) impact the GDP per capita of the municipalities of the deprived regions in Brazil. We use data for the period 2002–2019, estimating Spatial Econometrics models to take care of the observed spatial autocorrelation. The disbursement values are low compared to GDP levels, which already anticipates the low impacts of these resources on the economies of the benefited areas. By estimating models that consider the spatial relationships between municipal units, we found positive effects of the resources on the GDP per capita of municipalities one (CF) or two years (BNDES) after the release. Anyhow, the intensity of the effect is very low, which must be associated with the relatively low values disbursed. Another important finding is the existence of spatial spillovers: resources granted to a municipality affect its per capita GDP and the GDP of its neighbors, although limited to the following year, in the case of the Funds. In quantitative terms, the results of the estimates indicate that a 1% increase in the Funds' disbursements in *t* is associated with an increase of 0.0029% in the per capita GDP of the receiving municipalities in *t+1*. This effect is not repeated in *t* +2. To this effect must be added another 0.0009% on neighboring municipalities, composing a total effect of 0.0038%, restricted to the first year. For BNDES disbursements, the effects are quantitatively lower in the subsequent year but last over the following year, so the sum of the effects in the two years is larger than that of the Funds. The conclusion that the resources of the Funds impact the GDP per capita of the beneficiary municipalities and their neighbors is a piece of relevant information for regional policy in the country. The allowance of 3% of revenues from taxes on income and manufacturing products is permanently under criticism in the political arena, as the beneficiary regions remain poor even after 25 years of the existence of the Funds. Our results support the mechanism's existence, as its effect is clearly positive. They do not inform, however, about other possibly better ways of using the money to promote regional development, ways that could expand the effects found in our calculations.

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The beginning of the Brazilian Federal Indigenous Policy: National State, interest groups and the "integration" of the Indian (1910-1930)

Marcelo A. M. de Carvalho

The objective of this project is to investigate the creation, rigging and performance of the first republican federal agency officially responsible for indigenous populations spread across the National territory, the Service for the Protection of Indians and the Location of National Workers (S.P.I.L.T.N.) from 1910, which was later renamed to the Indian Protection Service (S.P.I.) in 1918. We will examine the first administrative steps of this institution, its tutelage policy on indigenous people, competing economic interests over areas traditionally inhabited by traditional peoples and, finally, resistance and criticism of sectors of the republican ruling classes in relation to the actions undertaken by the Service under the command of its most well-known director, the military and sertanista Cândido Mariano da Silva Rondon, all of this in the initial political-ideological environment of the First Republic, where there were groups sympathetic to a process of racialization of the Brazilian State, whether this was permissive or even a protagonist in the ethnic extermination of indigenous groups considered barriers to economic progress on agricultural frontiers. On the other hand, positivist groups and secular organizations that saw in the republican state the exclusive competence to protect and integrate the so-called "uncivilized" peoples in Brazilian society in their effort to modernize and progress and, at the same time, the performance of the Catholic Church's missionary orders an effort not to lose more space and influence with the State where the catechesis of the Indians was still seen by a good part of the conservative ruling classes as a preferential attribution of that traditional religious institution.

Desenvolvimento de modelos de negócios em *startups* de base tecnológica: um estudo sobre *causation*, *effectuation* e *bricolage* na tomada de decisão por empreendedores

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Marcelo C. Pedroso[1]

Nos estudos sobre Empreendedorismo, novas perspectivas teóricas têm emergido, em contraste com o modelo tradicional, tentando explicar as atitudes e a lógica subjacente ao comportamento empreendedor. Como alternativas ao processo de decisão racional do empreendedor, conhecido como *causation*, são propostas na literatura abordagens adaptativas e transformativas, com foco em aprendizagem e experimentação – como *bricolage* e *effectuation*, que parecem se adequar melhor à tomada de decisão sob incerteza. Por outro lado, pesquisas sobre Modelos de Negócios têm observado que os empreendedores muitas vezes enfrentam grande dificuldade para definir um modelo de negócio (MN) que seja viável na primeira tentativa, devido aos altos níveis de incerteza tecnológica e de mercado, e à imprevisibilidade das opções de comercialização. Particularmente nas fases iniciais, os conhecimentos e recursos existentes para lidar com as incertezas são limitados e, assim, os componentes do MN precisam ser criados e revisados em diferentes momentos, pois isso envolve inúmeras tomadas de decisão sob incerteza. Estudos indicam que as lógicas podem ser combinadas e que a ênfase no uso de cada uma delas pode mudar com o tempo, de forma dinâmica. A relação dessas abordagens de tomada de decisão com o desenvolvimento de MNs tem sido pouco explorada na literatura. Este projeto visa investigar a lógica da tomada de decisão, também chamada de *abordagem de empreendedorismo*, usada por empreendedores para design de MNs em empresas nascentes (*startups*). Pretende-se estudar como são empregadas *causation, effectuation* e *bricolage*, no desenvolvimento do MN e do próprio empreendimento, ao longo do tempo. Serão realizados múltiplos estudos de caso longitudinais, em retrospectiva, analisados em profundidade. A ideia é se obter dados sobre o design dos MNs durante o processo de criação de startups, avaliando-se o comportamento do empreendedor no processo. Buscar-se-á com esta pesquisa identificar se os empreendedores alternam entre estas abordagens principais de comportamento empreendedor, no design do modelo de negócio e, em caso afirmativo, entender como isso ocorre.

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Discriminatory variables for value generation for the adoption and implementation of ESG criteria: a comparative analysis between publicly traded companies from USA and Brazil

André L. C. Alves

The present postdoctoral project has ESG as its central theme and, as an object of study, the impact generated on stakeholders from corporate actions. The general objective of the study is to find which variables are discriminatory for value creation concerning to the behavior of companies regarding the adoption and implementation of ESG criteria, based on a comparative analysis between publicly traded companies in the US and Brazil, weaving reflections on the activities developed and analyzing the representativeness of the actions for those who are an integral part of it. It is clarified that companies listed on the New York Stock Exchange (NYSE), and on B3 – Brasil, Bolsa, Balcão.

The impacts of innovation efforts on the performance of the economy in the State of São Paulo between 2003 and 2016: a space-time analysis

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and Julio M. Pires

The main objective of this research is to investigate the impact of innovation efforts on the performance of the São Paulo economy, in a space-time perspective. The analysis being developed georeferences the economic variables according to the spatial distribution of the 645 municipalities in São Paulo, and distributes them annually for the period between 2003 and 2016. Some analyzes demonstrate the existence of positive spatial externalities between territorial factors and the performance of innovation efforts indicators at the regional level. The work by Gonçalves (2005) concludes that technological activity in Brazil presents spatial autocorrelation, taking the regional issuance of patents per inhabitant as an indicator of innovation, indicating an overflow effect. In this, using the calculation of Global and local Moran's I, the author concludes that the quality of the neighborhood is an essential factor in the process of technological spillover. This is in line with the observations of Varga, Anselin and Acs (2003) that the spatial distribution of actors is an essential factor in promoting innovation, given the importance of disseminating tacit knowledge in this process. This explains, among other things, the tendency towards spatial concentration (clusters) of innovation indicators. This promotes a counterpoint to macroeconomic models that assess the dependence of endogenous growth on knowledge generation, but do not consider regional effects, according to the authors. Specifically for the Brazilian case, Moraes et. Al. (2018) found that public and private Research and Development (R&D) expenditures have positive effects on GDP growth and the number of patents filed in the country in the period between 2000 and 2015, through the application of a vector autoregressive model (VAR). These, however, did not consider the distribution of economic variables in the Brazilian territory in the analysis. Casali et. al (2010), using data distributed by states in a panel data model, pointed out that the capacity of regions and states to absorb innovations is crucial for their development, as well as asserting the importance of the regions' ability to generate technology and innovation for its future path. The research carried out by Bahia and Sampaio (2015) deepened the discussion on the relationship between the diffusion of technological knowledge, its overflow, and the regional generation of innovation. The authors concluded that the innovation variable, spatially lagged, showed a positive effect, proving

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the existence of a spatial overflow effect. Factors such as geographic proximity, infrastructure sharing, concentration of skilled labor, sectoral and technological agglomeration of industries, are some of the factors that may be related to the generation of spillover effects. The research proposal that I have been developing in the FEARP postdoctoral program brings some differences in relation to the work carried out in Brazil, one of the main ones being the disaggregation of information by municipality. Centered on the performance of the economy, the municipal approach tends to allow greater detailing of the regionalized effects of the spillover of technological efforts, compared to studies with regional cuts by administrative region, micro or mesoregion. Another differential, compared to published studies, is the performance of bivariate analyses, in which the objective is to evaluate the effect of explanatory variables representative of the innovation effort on economic performance, understood as the generation of added value. Most works have carried out univariate analyses, such as the evaluation of the spillover effects of patents issued on the amount issued in contiguous regions.

A new national port geography: advances, retreats and permanence of the national portsector after 2000's

Edson de M. Machado[1]

Ports are phenomenon rich in spatial, structural qualities, in terms of the network of varied relationships, it is a factor possessing all the geographical qualities (Araújo Filho, 1974). The current globalized economy, characterized by the intensification of the international division of labor and, consequently, the enormous flow of goods between nations, means that transport systems remain continuous targets for innovation. In Brazil, the period marked by the radical evolutions of the port sector worldwide is concomitant with State indebtedness, the depletion of internal financing, and changes in international financing policy. At the same time, there is an incentive and expansion of exports of mineral and agricultural commodities, increasing the demand for port services. All this turned the country's ports into bottlenecks already in the 1980s, but which only started to be seriously faced from the 2000s onward, with the return of more voluminous investments through growth acceleration programs (PAC I and II and PIL), together with the new port legislation and public-private partnerships. These programs and the new legislation are creating what can be characterized as a new national port map. This new port map has been materializing mainly due to the vertiginous expansion in the movement of grains and ores through the ports of the North and Northeast, starting to attract and move cargo previously directed to the ports of the Southeast and South. In the case of grains, the movement growth was 482% between 2010 and 2020. Regarding iron ore the Northeast increased its share in the total movement from 30.2% in 2010 to 52.8% in 2020 (Brasil, 2021a). We investigated this process by analyzing the evolution of the Brazilian port issue and correlating it with national and global events. Therefore, we used a bibliographic review, survey and analysis of official data, technical visits and in loco observations. We resorted to the theory of socio-spatial formation (Santos, 1982).

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Sugar and industrialization (16th-19th centuries)

Joana de M. Monteleone

The history of sugar is essential for the formation of Brazil as an independent nation. Sugar was present throughout Portuguese colonization and is still an essential elementof the Brazilian economy today. Sugar production has a well-established bibliography while sugar consumption is yet to be done. In this research, it is the consumption of sugar that interests me and its overlap with Brazilian culture. It is also important to thinkabout who has always produced sweets, establishing a national confectionery with remarkable characteristics.

The writing of the Empire: the correspondence of the governors of Angola and the project of Novo Brasil

Natalia Tammone

The first half of the 19th century in Portugal can be defined as a time to make the liberalism, a period of political, social and economic instability in which the structures of the Portuguese Ancient Regime were evaluated and reformulated. A transformation of this scope could not happen without advances and setbacks, without shocks and instabilities, which must be considered, not only as a society in transition, but also as the dynamics of that society. Although we can endow the 19th century with a sense of transformation towards liberalism and the end of the monarchic regime, we cannot fail to analyze the synchrony and understand the agents in the light of their own time. In this context, Portugal's relations with the Empire changed due to internal and external conjunctures, resulting in the transformation of the colonial structure centered on the relationship with Brazil and on the role of the metropolis as an outpost for colonial trade with Europe. From Brazil's independence, Portuguese intellectuals and statesmen began to project a "new Brazil", formed in the African colonies, mainly Angola, which would promote the economic recovery and future prosperity of the metropolis. The applicability of the colonial project can be apprehended from the perspective of the colonial administration. For this, we used the correspondence between the General Governors of the African provinces and the Ministers and Representatives of the Portuguese Government in the metropolis. The so-called 'governors' correspondence, preserved by the Arquivo Histórico Ultramarino, registered the day-to-day minutiae of the governors' work, such as the promotion of troop soldiers, construction and repair of public buildings, entry and exit of vessels from the port, as well as projects and plans for colonization as a whole, the aims of the attempted enterprises, and the state of the overseas provinces. The case study of the province of Angola, the largest remaining territory of the Portuguese Empire after the independence of Brazil and for being the place where the "New Brasil's" project had more strength, analyzed the colonial practices, the direct relations with Portugal and the formation of a type of agricultural colonization.

The condition of work in Brazil: precariousness as a rule

Daniela N. de Sousa[1]

The research, of an eminently theoretical nature, based on bibliographical and documentary qualitative research, has analyzed the condition of Work and the Working Class in the context of precariousness as the predominant mode in the world of work in contemporary Brazil. The processes of precariousness, outsourcing and informality have been essential to the expansion of contemporary capitalism, and in the world context, the increase in labor exploitation is one of the factors triggered to reinvigorate and stabilize the structural crisis and leverage capitalist accumulation. The transformation that took place in the work organization model, making it more and more flexible, has its true face in the new mobility of workers expropriated from control of the production process and made available as mere productive capacity. Currently, the deepening of the separation made between economic property and the possibilities of political intervention, aggravates the conditions of work in Brazil, which is too diversified. They are formal workers, made legal persons, "free from employers", "uberized" and the traditional informal workers. In general, the intensification of exploitation of the labor force is accompanied by lower wages, withdrawal of labor rights, focusing/privatization of social policies, raising the age for retirement, growth of regressive taxes, unemployment and insipid resistance from workers. The research uses the categories of political economy criticism: workforce, exploitation, organic composition of capital and relative overpopulation, as they are central to understanding the current determinations in labor relations and the current model of work organization. This summary presents as main results the characterization of precariousness, outsourcing and informality as structuring forms of the Brazilian world of work. And it indicates, preliminarily, that the market has radicalized flexibilization as a form, and imposed on workers more precariousness and exploitation based on the broad development of productive forces and information and communication technologies.

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Cachaça in the economy of Ilhéus-Bahia: production, export and domestic supply, 1862-1889

Marcelo L. de Andrade[1]

The paper will present the results of research on the presence of cachaça in the economy of Ilhéus-Bahia, during the second half of the nineteenth century, a period when cocoa cultivation expanded in the region. The main sources are post-mortem inventories and tax collection books of the municipal council. The objectives are to understand the dynamics of production, export and domestic supply. Our hypothesis is that sugar and liquor mill owners concentrated the production of the beverage, while traders were mainly responsible for exports and domestic supply. Analyzing the socioeconomic context, the presence of slavery, and the characteristics of the cocoa economy will be fundamental for us to understand the importance of cachaça for the Ilhéus population. The drink was commercialized in several business houses, spread in the town and in the interior of the region, and was an important component for the economy of the mills and for the municipal revenues.

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The innovative vocation gap of the Brazilian bourguesie (1930-2014)

Roberto V. Anau[1]

The research seeks to identify and interpret the problem embodied in the absence of vocations, attitudes, and innovative actions of the Brazilian bourgeoisie from the beginning of the Import Substitution Process (1930) to the present day. It is based on a literature review on industrialization and more recent de-industrialization, interviews with innovation experts and eventually secondary statistics. The mentioned gap may be one of the main causes of the socioeconomic distortions verified throughout the industrialization process, such as the transfer of rural poverty to urban exclusion, balance of payments vulnerability, inflationary trends, and the structural public deficit. The oscillation between Bonapartism and open dictatorship, which characterized the entire period in focus, with democratic intervals always limited, is another distortion related to the problems in focus. It is intended to investigate this gap, its causes and its links with the challenges and incompleteness of Brazilian capitalist development.

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An island in the archipelago: scientific studies and experiments in the sugar production in Bahia in the mid-19th century

Silvana A. dos Santos[1]

This paper aims to analyze the scientific studies and experiments carried out in sugar production in Bahia in the mid-nineteenth century by the *Comissão para melhoramentos da cultura da cana, e do fabrico do açúcar* (Commission for Improvements in Cane Culture and Sugar Manufacturing) of the province of Bahia. The Commission was created in 1852, in the scope of the provincial executive and legislative, with the purpose of investigating the conditions of sugar production in Europe, Cuba, the Antilles and the United States, as well as the means to apply innovations related to agricultural, technical and technological improvements in the Bahian plantation. Based mainly on the analysis of the *Primeiro relatório apresentado à Presidência da Bahia sobre os melhoramentos da cultura da cana, e do fabrico do açúcar* (First report presented to the Bahia Presidency about the improvements of sugarcane culture and sugar production), produced by the American engineer living in Bahia and head of the Commission, John Monteiro Carson, we seek to show, on one hand, that the initiatives to improve sugar production in Bahia were in dialogue with practices carried out in other sugar-producing regions of the world. On the other hand, we aim to demonstrate that although there was inspiration in the innovations carried out in other countries, the knowledge related to agricultural improvement was not imported in a passive way. Through studies and experiments individuals sought to verify the suitability of these innovations to local economic and geographic specificities. In this way, the paper complexifies the reading about the initiatives related to the improvement of sugar production in Bahia in the nineteenth century, placing it in a broader context of agricultural improvement in both peripheral and central regions of the world economy.

1. Faculdade de Filosofia, Letras e Ciências Humanas da USP.

Socioeconomic relations between Brazil and Bolivia: determinations of the category overexploitation of work

Vanda M. M. Souto

This thesis aims to discuss the Brazilian foreign policy of former president Luís Inácio Lula da Silva (2003-2010), with emphasis on the relationship between Brazil and Bolivia. Given the fact that Bolivia is a dependent economy and has a number of unemployed workers, the following question arises: would there be in the relationship between the two countries a sort of sub-imperialism manifested by the transnationalization of Brazilian companies, based on mechanisms dependency of labor overexploitation in Bolivia? It is a historical-concrete research that articulates, theoretically and methodologically, a literature built from the categorial complex called by the Social Sciences "historical-dialectical materialism". The study results from the analysis of the documents of the Itamaraty Historical Archive, the Ministry of Foreign Affairs, the National Development Bank (BNDES) and State Oil Company (Petrobras). Its objective is to measure the conflicts of Brazilian foreign policy based on the works executed by the multinationals and funded by BNDES, in addition to discussing Petrobras' role in the nationalization of hydrocarbons in Bolivia. The results of the research are presented here, relating it to the readings of Ruy Mauro Marini's theory, and we hold the thesis that sub-imperialism has its origin in the own laws of the dependent economy, whose foundations are the overexploration of labor and the transfer of value. From the study of Brazilian foreign policy, the work on the screen brings light to the characterization of Brazilian foreign policy towards Bolivia, which may serve as a parameter for a current critique of capitalism in South America. In this way, the variants of the bilateral relationship were measured and analyzed the more general contexts of each country, realizing that history is always forged in struggles, conflicts and disputes of interest. The relation studied was determined by a dialectical relation between the internal correlation of forces in the nations in question. In fact, what can be measured was the expansion of imperialist monopoly capital in the Latin American continent, including sectors of the Brazilian bourgeoisie. It can be said, therefore, that the internal correlation of forces of each country has set up a scenario in which, although with all the elements pointing to it, one can not speak of Brazil's sub-imperialism in relation to Bolivia between 2003 and 2010, in this way, Brazilian foreign policy focused on regional economic integration was adequate for the expansion of imperialist capital.

Complex networks and machine learning for hidrological risk management

Douglas D. de C. Braz[1]

and André C. P. de L. F. de Carvalho[1]

The energy market in Brazil has evolved a lot since its implementation at the end of the 1990 years. This expansion has been accelerated mainly in recent years due to the increasing number of investors and increasing liquidity, making operations in this market more frequent and dynamics. In addition, the implementation of the Brazilian Energy Trading Counter (BBCE), an environment where market agents can buy and sell energy for sale or deliver it to their customers, has provided a significant increase in the volume of financial data and series of historical data. In general, energy prices in the Brazilian market are dependent on rainfall patterns, since power generation plants are predominantly hydroelectric. As a consequence, volatility tends to be related to short-term products traded in the market, mainly those within the current year. There is a gap in the scientific literature on the application of Machine Learning algorithms for forecasting trends in this emerging market. The use of intelligent techniques within the decision-making process in the capital market is not recent. (Trippi & Turban, 1992). A large number of applications have been created, through Artificial Neural Networks, with the objective of predicting the behavior of time series (Zhang *et al.*, 1998, Silva *et al.* 2014, Silva *et al.* 2015). Although most works focus on predicting the price trend in the financial market, it is possible to apply some of these tools in the electricity markets, considering their particularities. In addition to price trend forecasting, another approach widely used in the literature is the analysis of existing relationships between the behavior of financial market time series. Many researchers seek ways to extract information from dynamic environments to analyze them through the topological perspective of complex networks, known as Financial Networks or Stock Networks. Some works in the literature use this information from Financial Networks to manage investment portfolios (Castilho, 2019). In this context, the main objective of this Postdoctoral project is to propose strategies based on Machine Learning to predict price trends in the Brazilian energy market, as well as to propose methods using Financial Networks and Portfolio Optimization to reduce the investment risk in the hydrological market. In addition, this work has as a secondary objective the analysis of the financial return of automated purchase and sale execution strategies (algotrading) that use the proposed approaches as input for investment decision making. The complexity of this problem makes room for several researches in the area, where there is a strong relationship between Hydrological Risk Management, Computer Science and Quantitative Finance.

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Proposal of 55 agendas: the Economic Axis and the Sustainable Development Goals

Andrea F. Young

and Ariaster Chimelli; Cláudio P. M. Filho

The planet is going through a transition process, involving various aspects of our lives. The Thematic Axes Program, the Dean's Office initiative, aims to disseminate research that contributes to achieving Sustainable Development Goals (ODS). The 17 objectives establish commitments to environmental protection and reducing climate change impacts. The challenges demand coordinated actions, ranging from policies to structural reforms to increase the efficiency of public spending. The state members of ONU must eradicate hunger, guarantee housing for the poorest and improve services such as health, sanitation, garbage collection, transportation as well as disaster reduction measures. According to Economy Axis, a series of measures are needed, and a list of 55 agendas has been proposed. To move forward, it will be necessary to produce and generate income from industries that do not pollute, replacing the polluting energy matrix with a clean matrix, renewing the infrastructure, investing in small producers and micro-entrepreneurs, investing in the integration of agriculture with ecosystems, and above all, not burning the forests. It is important to end deforestation, preserve indigenous reserves, and ensure that the resources and services provided by nature are optimized to guarantee the sustainability of ecosystems, and consequently, the Brazilian economy increase. Ensuring sustainability depends on technological, educational, and cultural advances, without social and racial discrimination, through a network of opportunities, businesses, jobs, and decent work.

Políticas públicas de apoio ao desenvolvimento da inteligência artificial e lições para o Brasil

Leonardo M. Lins[1]

O presente projeto tem como objetivo realizar uma análise comparada das ações que China e Brasil estão promovendo para reorientar sua produção dentro do paradigma produtivo da quarta revolução industrial e analisar as oportunidades e desafios que se colocam em um momento de intensa reorganização das cadeias produtivas em todo o mundo. Atualmente, Estados Unidos e China são os países líderes no desenvolvimento e difusão de inovações tecnológicas relacionados à Inteligência Artificial, que possuem adoção ampla não só em termos produtivos, mas com grandes implicações sociais. Para o Brasil, é importante observar como os países líderes estão formatando suas estratégias de competitividade e criando arranjos institucionais para o desenvolvimento tecnológico, tanto para emular melhores práticas, bem como buscar se inserir de forma qualificada em cadeias de valor que possam trazer benefícios científicos, tecnológicos e competitivos para o país. Portanto, o projeto busca entender o que há de novo na formulação de políticas públicas de apoio à ciência e tecnologia e quais arranjos institucionais podem servir de exemplo para que o país acelere o desenvolvimento e adoção de tecnologias relacionadas à inteligência artificial entre as empresas. Será dada especial atenção aos aspectos da conectividade dos países, entendida como a infraestrutura básica que dá suporte ao desenvolvimento amplo da inteligência artificial, e a como os países em questão estão buscando elevar as capacitações digitais das empresas para competir dentro do paradigma da quarta revolução industrial.

1. Instituto de Estudos Avançados da USP.

Economia e democracia: mesma luta – Paul Singer e a transição democrática

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No início dos anos 1980, o Brasil passava por uma grave crise econômica, cujos principais aspectos foram o aumento da inflação e a dívida externa. As seguidas cartas de intenção assinadas pelo governo Figueiredo com o FMI impunham uma política econômica de austeridade, que agravava a situação social do país. Neste contexto, a crescente mobilização política ocorrida no período expôs a força dos grupos "de baixo", que não estavam dispostos a aceitar a transição "lenta, segura e gradual". Assim, a transição democrática foi marcada pelo cruzamento de uma crise econômica e, contraditoriamente, pela luta popular pela redemocratização. Esse período foi objeto de análise detalhada do economista e militante socialista Paul Israel Singer. Nosso trabalho tem como objetivo analisar as interpretações de Paul Singer sobre o período em questão, sobretudo o vínculo que o autor estabeleceu entre aspectos políticos e econômicos, e que remete a seus estudos e reflexões sobre repartição de renda, desigualdade e estrutura de classes no Brasil. Veremos como, a partir da questão da inflação, Singer tece uma análise sobre a política econômica adotada pela ditadura e pelo governo Sarney e quais alternativas a democratização abria para a condução da economia. Além das obras publicadas pelo autor, também utilizamos como fontes documentos do Partido dos Trabalhadores de cuja elaboração Singer participou. O trabalho é composto de quatro seções: uma introdução, em que apresentamos um panorama da conjuntura do país àquele período, bem como da trajetória de Paul Singer; a interpretação de Singer sobre a inflação brasileira no início dos anos 1980; a redemocratização e a construção de uma política de "pacto social"; e a conclusão.

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Mafic and felsic magmatism in the Serra dos Carajás region and their relationships with IOCG type mineralization events: applications of geochronology and isotopic geochemistry in mineral exploration

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Nine samples of mafic and felsic dykes were provided by the company VALE with the objective of identifying zircon and baddeleyite in order to obtain U–Pb geochronological ages, in addition to expanding and improving information about petrographic descriptions, geochronological data and U–Pb isotopic geochemistry. Pb in zircon and baddeleyite, Pb–Pb and Sm–Nd in whole rock and lithogeochemistry already existing in the study area comprised by the project, in particular the mafic and ultramafic dykes. These samples were taken from the mines of Sossego, Sequeirinho, Salobo, Azul and Paulo Afonso, in the Mineral Province of Carajás. However, due to delays caused by the COVID-19 pandemic, responsible for the closure of laboratories that only returned to normality at the beginning of last year, the results of these analyzes were only ready in recent months, and some of them are still in the initial analysis process and interpretation. Firstly, a bibliographic survey was carried out on the geochronology and isotopic geochemistry data obtained in the study area. These data are present in two tables and in a geochronological map, in addition to graphs with U–Pb zircon data and Sm–Nd and Pb–Pb whole rock data aiming to identify points where there is a concentration (or not) of these data and how the geochemical and geochronological results to be obtained by this project will fit into the general scenario of understanding the formation of these rocks. These data were obtained with a process of samples preparation, in which them were pulverized for whole rock (Pb–Pb and Sm–Nd values) and zircon (U–Pb ages and values) concentrations. There was also conducted a petrographic description, in which there is a predominance of gabbros and amphibolites in the samples composition. Although baddeleyite was not found during the mineral separation stage, it was possible to identify Neoproterozoic, Mesoproterozoic, Paleoproterozoic and even Archean ages of these dykes using zircons. These zircons were also analyzed and described individually for a more reliable zircon ages diagrams data. Right now, these results are being interpreted and analyzed, with the intention to determine the relationship of these dykes with the Carajás Mineral Province, especially with the IOCG mineralizations located in the study area. This information will compose the final report of the project and later a paper in which all information gathered and interpreted will be available for the scientific community.

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A Jacobi-type Newton method for Nash equilibrium problems with descent guarantees

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Most algorithms for finding a solution of Nash equilibrium problems consist of solving a nonlinear system given by optimality conditions satisfied by local minimizers of each player's problem. This approach does not make use of the minimization structure of the problem, often leading to saddle points or maximizers. We present a Newtonian algorithm that takes into account the minimization structure of the problem with the goal of finding more often true solutions in the non-convex case. The idea is an expansion on the Jacobi-type strategy, where instead of minimizing the quadratic approximation of the objective function parameterized by the other player current decision, we minimize the objective function parameterized by a prediction of the other player's action. Together with a backtracking procedure for computing the stepsize, we present a Newtonian Jacobi-type algorithm with descent directions for each players' parameterized functions, establishing global convergence and favoring minimizers over non-desirable stationary points.

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The role of interest groups in Brazil-Africa cooperation: the case of More Food Program

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In Brazil, the first movement on behalf of business sectors happened during the government of Dom Pedro I and was intermediated by his mistress, Domitila de Castro, who later became the Marquise of Santos. In 1827, her former father-in-law, Felício Moniz Pinto Coelho da Cunha, wrote to Domitila to ask her to intercede for him with D. Pedro I in order to help him sell his ore mines in the province of Minas Gerais. Cunha was aiming at the British as potential buyers. In the letter, he promised to pay the emperor's lover a commission corresponding to 50% of the sale value, which would be overpriced. This study aims at analyzing how interest groups performed in the negotiation and implementation of More Food Program in African countries. For this purpose, interviews, field research in eleven Mozambican municipalities and telegrams exchanged between Brazilian and African countries were rescued and analyzed under a new perspective. It was possible to identify the role of three interest groups in the negotiation and commercial rapprochement between Brazil and Mozambique – the Brazilian government itself, recipient countries in Africa and the private sector. Furthermore, private sector investments in Brazil-Africa cooperation have great support from the Brazilian federal government and converge with the demands of partner countries.

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ENERGIA

Development of CoNekT Bioenergy to mine expression data of bioenergy important crops

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CoNekT Bioenergy (http://conekt.cena.usp.br) is a web platform based on CoNekT for mining expression data from plants of importance in bioenergy, such as sugarcane. It hosts tools for analysis of expression profiles, condition-specific expression, co-expression networks and modules, and comparative transcriptomics. We have populated CoNekT Bioenergy with expression data of several C3 and C4 plants, mostly grasses. Most genomics and transcriptomics reference data were retrieved from Phytozome or were assembled by our group. RNA-Seq datasets were recovered from NCBI's SRA. Sample metadata were retrieved from NCBI using Biopython and then pre-processed using SpaCy. Then RNA-Seq datasets fitting the following criteria "bulk", paired-end, strand-specific, literature-associated were downloaded and filtered. Salmon was used to quantitate transcript expression levels for each sample as TPM. Expression networks were reconstructed with the LSTrAP's implementation to calculate Pearson correlation coefficients (PCC). Importantly, the current version of CoNekT Bioenergy harbors a sugarcane pan-transcriptome and individual transcriptomes of several cultivars, making it particularly suitable for analysis of this important crop. We recently incorporated ontologies to the platform (e.g., Plant Ontology), controlled vocabularies that enable standardizing sample description and facilitate comparative analyses. We also improved reproducibility by adding a 'data resources' page, sample provenance, and extra download options. Our team is working on a Snakemake workflow for automated data pre-processing, alternative gene expression normalization methods, analysis of plant promoter regions, and on the implementation of semi-automated strategies using Large Language Models for improving sample annotation.

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Fabrication and characterization of planar superconducting tunnel junctions

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Research on superconducting materials has been very intense over the past 100 years, resulting in an overwhelming number of materials that present perfect electrical conductivity. Given this enormous collection of known superconductors, it has become necessary to group together materials with similar features, giving rise to the superconducting families of cuprates; iron-based; conventional materials; etc., and guiding the choice of materials for potential applications. A solid knowledge on the so-called superconducting order parameter is essential to classify a given superconducting material within a family. One way to directly probe the superconducting order parameter is to conduct tunneling spectroscopy measurements at low temperatures, well below the superconducting temperature. To the best of our knowledge, this technique is not currently available in any laboratory or facility in Brazil. In this work, we aim to implement the experimental technique of tunneling spectroscopy using planar tunnel junctions. One of the experimental challenges involved in such implementation is to fabricate reliable, and reproducible, Metal-Insulator-Superconductor (M-I-S) planar tunnel junctions. In a close collaboration with the Laboratório Nacional de Nanotecnologia of CNPEM, we are currently working on a set of M-I-S junctions using the well-known Nb as the superconducting electrode. The results of the preliminary characterizations of M-I-S junctions, as well as junctions builtwith unconventional superconductors, will be discussed in light of the symmetry of the superconducting order parameter.

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Interaction control based on Markov jumps applied to an exoskeleton robot

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Impedance control techniques for robotic devices are used in physical interaction tasks and are increasingly being studied in control and robotics. In these applications, robots are subject to constant energy exchange with the environment, i.e., other robots, unstructured terrain, or humans. In this context, standard fixed gain controllers are insufficient to obtain suitable performance metrics and to ensure system stability. This is because interaction environment dynamics are often unknown and can undergo abrupt behavior changes, e.g., exogenous inputs and/or unexpected parameter variations describing the dynamic model. In this postdoctoral research, it is proposed to investigate robust impedance control alternatives that take into account dynamic variations in the interaction environment, considering an exoskeleton robot in physical interaction with humans. The time-varying human dynamics is modeled using Markov chains, and stochastic jumps associated with behavioral changes in interactions are considered. Therefore, we propose a novel transparency controller based on discrete-time Markovian jump linear systems to minimize the human-robot interaction forces of an exoskeleton robot during walking. Our model-based stochastic control approach describes a gait cycle as an event-dependent Markov chain and uses a given transition matrix to switch between them. An IMU-based Kalman filter is used to perform real-time human state estimation and gait phase detection. The robustness and effectiveness of the proposed controller are demonstrated with experiments on a lower-limb exoskeleton driven by series elastic actuators.

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Modelling of hydrogen and volatile fatty acids production in an acidogenic anaerobic fixed-bed reactor using a dispersion model

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Research related with biohydrogen is increasing over the years due to the eminent necessity of renewable sources of energy. Hydrogen is receiving particular attention due to its high heating value and because it produces only water during the combustion. In this context, the development of mathematical models may contribute to a better understanding of the metabolic pathways involved in processes, thus facilitating the simulation in other scenarios. In this work, a mesophilic (25ºC) anaerobic fixed-bed reactor (AFBR) used for hydrogen production from glucose (2 kgCOD m^{-3}), operated during 60 days, was modelled. This reactor presented 3.5L of total volume, 0.7m of length and was composed of three parts, an influent (0.1m), a bed (0.5m) and an effluent zone (0.1m). To model this system and describe the concentrations over the time and along the reactor height, a dispersion model was built assuming a fixation coefficient for the microorganism inside the reactor in an innovatively way. Analyzing the experimental data, hypotheses about the metabolic pathways were put forward: glucose → acetate + H_2, glucose → lactate, glucose → acetate + ethanol + H_2 and glucose → butyrate, lactate → butyrate + H_2, lactate → acetate + ethanol + H_2, lactate → propionate. It was assumed diffusion-convection in the influent and effluent zone and diffusion-convection-reaction in the bed zone. The model was implemented in the software Matlab R2021b and the solution of the partial differential equations system was carried out with the method of lines (MOL). The model was able to predict the experimental data for substrate consumption, volatile fatty acids and hydrogen production during the reactor operation time and along the reactor height, indicating that the metabolic pathways and the MOL adoptions were assertive.

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Experimental study on droplets breakage of oil-water emulsions (o/w) across a variable pressure drop device

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Emulsions occur in several industrial applications covering different engineering fields, such as pharmaceutical, food, cosmetics, and petrochemical industries. Especially in the oil-gas industry, emulsions are observed in most of the processes, including crude oil extraction, transport, and refining. The injection of water in mature wells, which is a technique recurrently employed to increase crude oil productivity, favors the formation of emulsions during the oil extraction stage. In offshore environments, the effluents from the extraction process are usually treated; however, this operation is challenging in such conditions due to limited space and the inherent difficulty in separating stable oil-water emulsions (O/W). Currently, there are several investigations focusing on emulsion separation, however, this type of study necessarily requires the production and characterization of emulsions with a certain droplet size distribution (DSD). The present study presents an experimental evaluation of the emulsion production process in a mixing device ("mixing tee") and oil droplets breaking in a variable pressure drop device (globe valve). Both devices are part of an experimental facility developed for this study. The emulsion was produced by injecting water in crude oil with API Gravity of 21.31, dynamic viscosity of 229.83 mPa.s, density of 0.9216 g/cm^3, surface tension of 30.9 mN/m, and interfacial tension of 22.0 mN/m (proprieties at 20°C). Emulsion characterization was performed through measurements of oil and grease content (TOG) and also of droplet size and its distribution (DSD). The stability of emulsions was also evaluated through measurements of the Oil and Grease Content (TOG) over time, which were obtained for the following time intervals: i) 0 min (online), ii) 15 min (after the experiments in the glass separating funnel) and iii) 60 min (after the experiments in the glass separating funnel). The results show that the DSD decreases by increasing the pressure drop (ΔP) at the flow restriction device.

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Effect reinforcing carbides on the microstructure and abrasive wear behavior of white cast iron

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In the current study, three white cast iron (WCIs) alloys were manufactured with 14 wt% Cr and the addition of ~3.0 wt% Nb, ~3.0 wt % Mo and a combination of ~1.0 wt % Mo–2.0 wt Nb. The alloys were melted at 1500 °C in an induction furnace and casting was performed at 1350 °C in a mold of sand and phenolic resin. The blocks were cast in a Y- shape. The samples were extracted and prepared by metallography and etching to reveal the microstructure was performed with 10% sodium metabisulphite ($Na_2S_2O_5$). The samples were analyzed by optical microscopy (OM), scanning electron microscopy (SEM), quantitative metallography, hardness, microhardness, and abrasive wear using a SiC slurry. The MO results demonstrated that the alloys presented a microstructure composed of austenite dendrites, surrounded by a combination of eutectic carbides and austenite, presenting a typical microstructure of hypoeutectic WCIs. Additionally, the SEM data demonstrated that the addition of ~3.0 wt% Mo resulted in the production of carbide Mo_2C with a lamellar morphology, while the addition of ~3.0 wt% Nb led to the production of carbide NbC with a nodular-spheroidal morphology. On the other hand, the combination ~1.0 wt% Mo–2.0 wt% Nb produced the MC carbide composed mostly of Nb-containing bound Mo with a like-flake morphology. As for hardness and wear performance, the ~3.0 wt% Nb alloy showed the best performance, with a micro-abrasive wear performance approximately 30% higher than the ~3.0 wt% Mo alloy and 12% higher than the ~1.0 wt% Mo–2.0 wt% Nb alloy. The NbC and MC carbides reduced the mean free path for material removal by wear, protecting the matrix by blocking and preventing the progression of continuous micro-cutting and grooves.

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Bibliometric analysis of axial flow in rod bundles

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The investigation of single and two-phase flows in rod bundles is important, considering the significant role that nuclear energy plays in the energy portfolios of many countries. Furthermore, nuclear energy has the potential to substantially reduce CO2 emissions in the coming decades, given its reliability and low CO2 output. The present analysis goal is to provide a comprehensive overview of the current state of art on studies involving axial flow in rod bundles, which are tightly packed arrays of rods surrounded by flowing liquid coolant, within the context of nuclear applications. Besides delivering relevant and reliable statistical analysis that encompasses influential publications and research directions. The adopted approach involves bibliometric analysis, which relies on the occurrence and citation of available publications. This method incorporates quantitative analysis of attributes such as publications, citations, keywords, contributors, and publishers. The Scopus and Web of Science databases were selected for data retrieval, resulting in 754 publications after eliminating duplicates and applying exclusion criteria. The findings of this study indicate that the annual publication rate of articles exhibits a peak in 2018 and 2019, with growing interest in the field since 2010. The breakdown of approaches utilized in the studies reveals a higher number of experimental papers in comparison to numerical and theoretical studies. The most cited papers are categorized into flow-induced vibration, fluid dynamics, heat transfer, and two-phase flow. The analysis of keyword co-occurrence reveals distinct clusters related to different thematic areas. Furthermore, this study identifies the top contributing countries in terms of publications and citations, with China leading in published papers and the studies from US being the most cited ones. In conclusion, this study demonstrates the increasing interest and relevance of research on rod bundles in nuclear applications. It emphasizes the interconnectivity of various aspects such as flow dynamics, heat transfer, and vibration, and underscores the necessity for comprehensive models that encompass these parameters. The bibliometric analysis provides a valuable overview of research progress in this field and can serve as a guiding reference for future studies in thermo-hydraulic analysis of rod bundles.

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CFD application in Healthcare Facilities: evaluation of ventilation and air contamination risk mitigation

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Healthcare Facilities have specific demands for Building use, which include spatial organizations according to function, personal protective equipment recommendations, and ventilation and air conditioning systems to ensure a lower risk of infection and cross-contamination. The Covid-19 pandemic has raised an important question about indoor air quality: air renewal rate, location of diffusers and grilles, and spatial layout can influence the virus transmission. This research aims to study the air circulation and the risk of aerial infection in a healthcare facility sector in the city of São Paulo. The operational conditions will be modeled through computational fluid dynamics (CFD) simulation. The healthcare facility's physical configurations will be observed, and environmental parameters will be collected on-site with proper instrumentation. Then, one will carry out a model validation for CFD simulation, proposing design guidelines for indoor air quality and thermal comfort, including the potential use of natural or hybrid ventilation in non-critical spaces to increase energy efficiency. The CFD numerically estimates the air movement with the finite volume method, as the output data are provided at each point or at a specific volume, allowing the analysis of environmental conditions in different ventilation conditions. From the computer simulations, we will investigate the ventilation efficiency through air distribution visualization (air velocity and indoor air temperature), obtaining indicators such as the risk of infection and the mean age of air. The results will provide guidelines for new or refurbished healthcare facilities design to reduce the risk of contamination for healthier and comfortable environments.

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Integrated appraisal of sugarcane biorefineries for green hydrogen productionin the Brazilian case

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While the energy supply in the World was around 11.8% of renewable energy in 2018 (IEA, 2018), the Brazilian primary energy mix of renewable sources achieved 48.4% (139,099 Mtoe) in 2020. Renewable energy mainly consists of sources such as sugar cane products (19.1%), hydroelectric (12.6%), firewood and charcoal (8.9%), wind (1.8%), solar (0.3%), and other renewable sources (5.7%). According to the total electricity supply by energy source, it can be noted that renewable energy contribution was about 85% as shown in Fig. 1, in which hydroelectric, biomass and wind energy sources are the most significant contributors with 65.2%, 9.1%, and 8.8% respectively. Biomass includes firewood, sugarcane bagasse, black-liquor, and other primary energy sources (BEN, 2021).

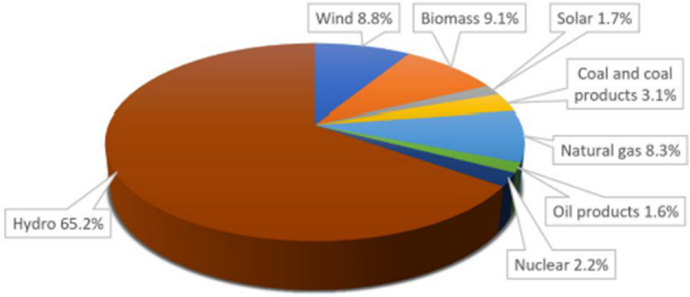

Figure 1. Total electricity supply by source for the Brazilian mix in 2020 (BEN, 2021).

Regarding biomass, 615 units of power plants were installed, totaling a 16.2 GW installed capacity, of which 415 of them use sugarcane bagasse as fuel feedstock (ANEEL, 2022). Thus, the installed capacity of electricity generation by using bagasse biomass was 11.7 GW in 2020, 60% higher than the installed capacity in 2011. In the world, about 1.8 billion tons of sugarcane are annually produced, and Brazil is the largest global sugarcane producer (Negrão et al., 2021), which is responsible for 38% of global production. It is expected Brazil will continue to be the main producer of sugar and sugarcane- based ethanol in 2028

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(FAO, 2019). The industrial processing of sugarcane is usually used to produce electricity, ethanol, and sugar, in which a one ton squeezed sugar cane might produce around 730 kg of sugarcane juice (BEN, 2021). Cavalett et al., (2016) mention that the whole plants contain 7.4 GJ primary energy per ton of cane stalks. Sugarcane products have a key factor in Brazilian economic development because these not only can be transformed in self-producer power plants for electricity generation or in distilleries for ethanol production but also supply raw materials for the industrial sector such as the food and beverages sector and the paper and pulp sector. In terms of energy consumption of sugarcane by sector, sugarcane bagasse consumption in the energy sector represents about 49.3%, agriculture and livestock demand less than 1% that corresponds with hydrated ethanol used as fuel in agricultural airplanes for agrochemicals and fertilizers application. Moreover, hydrated ethanol (12.7%) and anhydrous ethanol (6.6%) are used to attend to the energy consumption of the highways transportation sector. Finally, the industrial sector's energy consumption is 22.1% (BEN, 2021). A 6,565 Mtoe (76.4 GWh) energy of sugarcane bagasse produces 38.8 GWh of electricity, accounting for 5.2% of the national electricity generation that is about 621.2 TWh. Most of the sugarcane energy transformation is generated in the Southeast and the Center-west regions of the country with 66.0% and 21.4%, respectively. Furthermore, sugarcane bagasse plants usually operate as combined heat and power (CHP) plants, allowing to increase the energy utilization factor of the power plants. At least a 50% of thermal efficiency is achieved in sugarcane bagasse thermal power plants, which value is higher than conventional power generation plants with fossil fuels.

Electronic nose from organic thin-film transistors for water analysis

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In this work, organic thin film transistors (OTFT) with bottom gate bottom contact (BGBC) structure on glass, with organic dielectric and semiconductor, will be manufactured to use them as gas sensors in the detection of 2-Methylisoborneol (MIB) and Geosmin (GEO) in water. Glass substrate will be used to deposit NiCr: Au layers by DC sputtering. Then, the gate, source and drain electrodes will be obtained through consecutive photolithography and wet corrosion processes. Solutions of the organic dielectric PVP and the crosslinking agent PMF will be prepared in a ratio of 1 to 5, both dissolved in PGMEA with a concentration of 25 wt%, which will be deposited by spin coating, without filtering over the gate electrodes. With the organic semiconductor PBTTT-C14, solutions in DCB with a concentration of 10 mg / mL will be prepared, stirred with a magnetic bar, heated in a hot plate for at least 1 h and without filtration before deposition by spin coating. In this film, a thermal treatment on hot plate will be practiced to cause the formation of terraces, structures that improve the electrical performance of the devices. The devices used as gas sensors must show variations in the $\mu_{p,\ tri}$ of ~ 50%, in the I_{ON} of ~ -30% and in the V_T of ~ - 50% in the presence of UR.

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Sustainability applied to multi-domain network slicing: promoting energy efficiency in network slices

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In the current scenario of massive connectivity, in which people, companies, institutions and organizations use the most varied devices to exchange information, carry out commercial transactions, or simply keep in touch with other people, computer networks are configured as a means of sustain this new environment. To meet this demand, computer networks have evolved both in technology and in the way resources are made available, becoming more agile with the creation of software-defined networks, multiplying services through the virtualization of network functions, and ensuring the quality of services and guaranteeing the levels of contracted services using techniques such as, for example, network slicing. In this sense, in recent years, there has been great interest from academia and industry in the network slicing technique, with the emergence of several proposals for architectures aimed at slicing multi-domain networks, important standardization initiatives, as well as the investigation of several efficient solutions for slice management, usually using machine learning and artificial intelligence techniques. Seeking to present the state of the art of artificial intelligence and machine learning technologies employed in network slicing techniques, considering the orchestration tools, and the quality of service parameters, this research aims to elucidate the gaps in the definitions of management policies energy efficiency of virtualized and shared computing networks that lead to sustainability in these networks.

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Two-dimensional (2D) swirl Topology Optimization of Labyrinth seal for application in compressors

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Labyrinth seals are the most popular and oldest mechanical sealing solution in the industry and play a key role in the prevention and reduction of fluid emissions. In the last decades, the improvement of the Labyrinth seal in multi-stage pumps and compressors attracts great attention. Due to the very high number of geometrical parameters (e.g., seal cavity depth, seal tooth thickness, and tooth tip clearance) and difficulties related to determining their effects on labyrinth seal performance, Topology Optimization is a feasible approach to achieve the best design with the highest efficiency. Thus, this work presents a Topology Optimization formulation for the design of the labyrinth seal by using a 2D swirl flow model. The model is developed based on the Reynolds Averaged Navier–Stokes equation considering axisymmetric and highly turbulent flow with flow rotation around the shaft (fluid flow in labyrinth seal), and a multiobjective function is defined to minimize the leakage and enhance the sealing performance. Then, the Topology Optimization formulation with a 2D swirl flow model is coupled and implemented in COMSOL Multiphysics (based on the finite element method) and solved using a Sparse nonlinear OPTimizer (SNOPT) solver. Numerical results are post-processed to obtain the optimized configurations. Then prototypes are fabricated via a 3D printer and experimentally validated on a test rig. The results and experimental validation show an improvement in the performance of the labyrinth seal.

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Multiscale simulation of wind farm performance in stable conditions in the AWAKEN experiment

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Numerical weather prediction (NWP) models are progressively being used at very-high spatio-temporal resolutions to simulate the interaction between the atmosphere and wind turbines. A major scientific goal is to accurately represent real wind farm performance. Nighttime stable boundary layer phenomena, such as low-level jets (LLJ), are even more challenging from the wind turbine operation and numerical modeling viewpoint. This decade, NWP models, such as the Weather Research and Forecasting (WRF) model, have been progressively employed at very-high spatio-temporal resolution to resolve microscale turbulence (large-eddy simulation, LES). Wind turbines are often represented with the generalized actuator disk (GAD) approach. This methodology is known as WRF-LES-GAD, and has grown popular in the last three years and has demonstrated effectiveness in simulating farm performance during frontal passages, single turbine wakes in complex terrain and blockage effects. The American Wake Experiment (AWAKEN) is a multi-institutional scientific effort funded by the US Department of Energy (DoE) that investigates the interaction between the atmosphere and wind farms. An unprecedented field campaign that includes radars, ground- and nacelle-based lidars and SCADA data, among other instruments, is currently being executed within a cluster of wind farms located in the Southern Great Plains (SGP), in Oklahoma. Here, our main goal is to simulate the real performance of a two-row subset of the King Plains wind farm (the most instrumented wind farm in AWAKEN) under the complex scenario of a southerly LLJ episode and investigate the physical mechanisms that modulate it. The AWAKEN SCADA data, profiling and scanning lidar observations will be used to fully characterize the farm performance, boundary layer wind, turbulence, stability, and wakes. Preliminary results from our simulations reveal long wakes that qualitatively resemble the observations, but future simulations will employ higher resolution to better resolve turbulence in stable conditions.

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Development of Fe-based oxygen carriers for Chemical Looping Combustion based on Brazilian feedstock

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The investment in systems for CO_2 capture can provide a pathway for the sustainable use of carbon-based fuels. In this regard, chemical looping combustion (CLC) encompasses a process that favors the complete combustion of fuels, and which main advantage is the easy separation of CO2 and water, reducing the energy penalty of gas separation necessary in conventional systems. CLC system is based on the separation of fuel and air reactors and the promotion of oxygen transfer through the use of an oxygen carrier (OC). The OC choice is pivotal in these systems, once it governs the thermodynamical and kinetic parameters of the fuel oxidation reaction. Besides, characteristics such as high surface area, resistance to agglomeration and sintering, negligible carbon deposition, environmental compatibility, and low cost are important to determine OC practical application. Therefore, this study will contribute to the development of Brazilian CLC processes by analyzing OC candidates' structure, chemical composition, textural and thermal properties, and the kinetic parameters of fuel oxidation reactions. To achieve this purpose, there will be evaluated two classes Fe-based OC, considering the availability of this metal in Brazil: (i) mineral samples containing ilmenite, hematite, and other accessory minerals that can affect OC performance; (ii) synthetic iron oxides with different morphologies and supporting oxides (Al_2O_3 and TiO_2).

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P-fertiliser, REE, U and TH production from monazite rich mining waste from Catalão (GO) carbonatitic complex

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The rare-earth elements (REEs) are divided in light rare-earth elements (LREEs) from lanthanum through europium (atomic numbers from 57 through 63) and heavy rare-earth elements (HREEs), which include since gadolinium to lutetium (atomic numbers from 64 through 71). Yttrium (39) and scandium (21), despite lighter, are also considered a HREEs. The REEs demand is constantly increasing due to the new technologies of the "green elements", used to produce a "clean energy", as permanent magnets of wind turbines, electric motors for vehicles, low energy light bulbs and others. The LREEs are specially found in monazite (LREE-bearing phosphate) from carbonatitic and placers deposits. Araxá and Catalão are two known carbonatitic deposits with high contents of REEs in Brazil. Considering that, in the carbonatites, the P-fertiliser and REEs-bearing minerals are associated, it would be interesting find an approach to recovery both in the same mineral processing route. The alkaline leaching is a hydrometallurgy processing to obtain REEs, since the acid leaching is not able to eliminate phosphor, resulting in reprecipitated REEs phosphates and also in the decreasing of the REEs recoveries. Monazite alkaline leaching, is able to produce a trisodium phosphate (a byproduct to the fertilizer industry) and REEs oxides, that will be treated to obtain high REEs recoveries. There are new researches that suggesting good results from bioleaching performed by microorganisms that solubilizing P from lower solubility phosphates minerals. These microorganisms can produce organic acids to solubilizing these minerals. *Aspergillus niger* fungi is an example of microorganism used to solubilize three different sorts of phosphates, one of them, the monazite. Finally, the challenge of this research is to concentrate monazite due to its fine size.

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Impact of the gate work function on the experimental I-V characteristics of MOS solar cells simulated with the Sentaurus TCAD software

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In this work, the influence of the gate work function on the experimental I-V characteristics of TiN/SiN_xO_y/p-Si, Al/SiN_xO_y/p-Si and Al/Mg/SiN_xO_y/p-Si solar cells was investigated with the aid of two-dimensional numerical simulations using the Sentaurus TCAD software. It was observed that the onset of current conduction in the direct operating region of the MOS solar cells occurs at a lower gate voltage for the TiN gate (~ 0.1 V) compared with the Al and Mg gates at values close to-0.5 V. The increase of the gate work function leads to a decrease in the reverse current density (J) levels in the experimental characteristics. The simulation with the Sentaurus TCAD pointed to the same behavior, however, the simulated values obtained differed substantially from the experimental ones, which was attributed to possible differences in the value of the adopted work function that depends on the type of deposition of the films and the post-deposition thermal treatments. The work functions of Mg, Al, and TiN used in the TCAD simulations were 3.7, 4.2, and 4.7 eV, respectively. For Al and Mg gates, the tunneling current mechanism was observed to be predominant through the dielectric when the gate voltage VG is more negative than ~ -0.5 V, with the voltage drop across the device being almost entirely across the equivalent series resistance RS, which means the current proportional to VG more negative than ~ -0.5 V. In the case of TiN, the conduction by tunneling current through the dielectric also predominates, but the downward shift of the J x V_G curve due to the minority carrier generation does not exist. The photovoltaic effect occurs exclusively for Mg and Al gates, where an inversion layer is formed prior to light exposure, which promotes the charge carrier generation current. The usual important parameters of fill factor (*FF*), short-circuit current density (J_{SC}), and open-circuit voltage (V_{OC}) are relatively lower compared to those of commercial outdoor solar cells, but the power generated by the MOS cells reached the mW range, and the efficiency in converting light energy into electrical energy was higher (12.8%) than the typical values found for MOS solar cells for energy harvesting.

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A hybrid model based on wavelets and convolutional neural network for transmission line faults in the power system

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The transmission line faults in the power system play an essential role as the accurate fault location can help manage and restore the electrical network. However, obtaining sufficient faults to train a neural network and extract sufficient information from the fault distance is difficult since a reliable electrical energy transmission system requires that it does not have faults, making it difficult to develop models based on faults in machine learning. Thus, this article presents a model that simulates several faults in transmission lines at different voltage levels. Afterward, daubechies wavelets were used to extract the main features of the current and voltage signals related to the faults. Finally, a 2D convolutional neural network (CNN-2D) is used to predict the distance of the fault from the L terminal. The model has been validated by performance metrics R2, RMS, and RMSE.

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A new approach for calculating the ampacity of directly buried cables with foundations of statistical mechanics

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The ampacity of directly buried cables has been calculated with support from continuous medium mechanics. This mechanics is an extension of Newtonian mechanics, continuously adapted over the centuries for application in engineering. This article presents a new approach supported by Gibbs statistical mechanics. This mechanics departs from the classical theory of ensembles with a formalism suitable for application to engineering problems where entropy manifests itself with intensity: in matter and heat. The results bring contributions to: calculation of ampacity, reconfiguration of backfill geometry, repositioning of cables in the trench and characterization of materials used as backfill.

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Low cost method for monitoring a Photovoltaic System based on the calculation of figures of merit

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Frequent failures in Photovoltaic Systems (PVS) can lead to a significant reduction in energy generation, resulting in financial losses and irreversible wear and tear, contributing to a decrease in the system's lifespan. This study presents a low-cost monitoring method that, based on the data already available in the inverter and the expected simulation of the PVS, calculates the performance metrics, voltage, and current. Using this data, it analyzes the operating conditions of the PVS and, depending on the result, provides real-time indications of the inspection/maintenance actions to be taken by the system manager, identifying possible problems affecting the system. The objective is to reduce inspection costs, which will be optimized and carried out only if the system's performance is below expectations. The method's results were tested by developing software using Visual Studio, a free software, where satisfactory simulation results were obtained.

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Environmentally, socially and economically viable proposal for the production and distribution of green hospital oxygen and hydrogen

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This work shows a new pathway to the production and distribution of green hydrogen (GH2) and green hospital oxygen (GHO2) in a microregion of the State of Bahia, Brazil. The study employs environmental cost accounting techniques to establish the feasibility of the proposed pathway. Specifically, the study considers an alkaline electrolysis of water (AEW) plant powered by a wind turbine set for GH2 production, which will be used as fuel in the transport of GHO2 to cities within the microregion. The study performs a sensitivity analysis of several economic parameters of the investment project, with a lifetime of 20 years. The results indicate that the proposed pathway can supply hospital oxygen to up to 500,000 inhabitants or 1,000 hospital beds. The most favorable economic conditions occur when GHO2 is sold between 4.81 and 5.77 US$/Nm3 and GH2 is priced at 2.50 US$/kg. Under these conditions, a profit of more than US$ 5 million, a payback period between 4–5 years, a rate of return on investment (RRI) greater than 18%, and a return on investment (ROI) greater than 200% were found. Overall, the study demonstrates the feasibility and sustainability of GH2 and GHO2 productions using an AEW plant powered by a wind turbine set in the microregion of Bahia. The proposed pathway provides an environmentally friendly approach to the production and distribution of medical gases, and contributes to the sustainable development of the microregion.

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Undersea separation of CO_2 from natural gas through ionic liquids

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Natural gas (NG) needs to be purified to attend commercial regulations by removal of contaminants such as hydrogen sulfide, water and carbon dioxide. NG purification technologies, which are currently installed on FPSOs, occupy large footprint, present risk of human damage and need additional compression to operate desulfurization, dehydration and carbon capture processes. In this sense, undersea purification of NG has attracted attention recently due to the advantages of operating without personnel and under high-pressure and low-temperature. Among the four main technologies studied to purify NG (adsorption, cryogenic distillation, membranes and absorption), in this research high-pressure absorption using biodegradable ionic liquids (BILs) as solvents for CO_2 removal from methane (CH_4), the main NG component, is being studied. However, one of the main challenges to be overcome is the determination of CO_2+CH_4 mixture absorption in BILs and, thus, the construction of ternary phase equilibrium diagrams. These thermodynamic data can be determined using different approaches already suggested in literature, such as gravimetric and volumetric methods. However, here, a new apparatus is being developed at the High Pressure Laboratory. This device will turn possible the measurement of BIL absorption capacity as well as CO_2 or CH_4 absorption kinetics, plus gas mixture density measurements. In other hand, COSMO-SAC model is being studied to predict CO_2+CH_4+BIL interactions using Aspen Plus software. In this computational part, the main challenge is to provide two properties of BIL for vapor-liquid flash calculations: vapor pressure and ideal gas heat capacity. Finally, it is worth mention this project started in September 2022 and will endure 22 months, where part of this project should be developed in collaboration with the University of Texas at Austin, since it is associated with Center to Center (C2C) program between Research Center for Greenhouse Gas Innovation (RCGI/Brazil) and Center for Innovative and Strategic Transformations of Alkane Resources (CISTAR/USA).

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Coupled 3G – 1G bioethanol production as an alternative CCU technology for improved CO_2 mitigation

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Around 60% of the global oil demand is attributed to the transport sector, which heavily relies on fossil fuels, responsible for about 25% of total greenhouse gas (GHG) emissions, primarily CO_2. Its atmospheric concentration surpasses that of other GHGs, and it can persist in the atmosphere from 300 to 1,000 years, thereby influencing the global climate scenario for a long time. It has become crucial to urgently explore carbon-negative emission technologies to hold the climate change outcome. Brazil is the second largest producer of first-generation (1G) bioethanol, an alternative renewable energy source from sugarcane. According to the National Supply Company (CONAB), the 22/23 harvest yielded around 11 tons of total ethanol produced solely in the State of São Paulo. Yet, the operational units have limited flexibility due to concomitant sugar and ethanol production. It could be overcome by coupling third-generation (3G) bioethanol, a recent and little-explored alternative to previous bioethanol generations that can be produced from photosynthesizing microorganisms' biomass hydrolysate. Sugarcane crops yield around 13% (w w^{-1}) of carbohydrates after maturation. In contrast, an indigenous *Synechocystis* sp. strain obtained from mangroves reached 40% (w w^{-1}) of glucose in a nitrogen-depleted medium without further optimization. Fermentation of its cyanobacterial hydrolysate using an industrial *S. cerevisiae* strain yielded 90,81 ± 3,88% ethanol, which is promising not only to improve ethanol production but could also the CO_2 mitigation if coupled to the already diffused 1G bioethanol technology in Brazil.

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Applying model-based systems engineering (MBSE) in managing microgrids: a practical approach using hardware configurable logic (FPGA)

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Microgrids emerge as a practical, sustainable, and reliable solution to meet the demand of users who, for various reasons, have restrict access to electricity. However, the flexibility of microgrid systems requires considerable creative engineering effort, especially in the design process. In order to combine adaptability to users and good performance, requirements analysis has a leading role in better characterizing, understanding, and specifying the application domain and the problem that the microgrids must solve, and then embodying and identifying solutions to solve the problem. This work seeks to contribute to a proposed method (Orellana Postigo, 2021) inserted in the MBSE (Model-Based Systems Engineering) approach, to model microgrids using IEC 61850 as a reference architecture for the preliminary design. Requirements would be represented in Objective Oriented Requirements Engineering (GORE), using visual diagrams based on the KAOS (Keep All Objectives Satisfied) method, but formally verified using Petri Nets. The preliminary design would be done with matching goals, sub-goals, and algorithms designed in Petri Nets to develop a transfer algorithm for Field Programmable Gate Array (FPGA), thus closing the proposed design cycle.

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Development of a high-efficiency biogas engine for cargo transport vehicles

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The increased demand for energy and the security of its supply have become a concern in recent decades due to strong industrial growth and demand for transportation. The high cost of fossil fuels, as well as the need to reduce greenhouse gas emissions, and pollutants, have made feasible the use of renewable energy sources. Biomass is a source of chemical energy stored in organic matter and its products can be used for biogas production, methane being the main one. The use of biogas for mobility, besides avoiding the release of greenhouse gases, also provides lower carbon dioxide emissions. The proposed research aims monitoring the diesel engine emissions, to perform modeling of gas emissions and support the development of software for emissions control. The engine management will be calibrated to operate with biogas, being diesel emissions the baseline. The intent is to improve emission standards as well as identify energy efficiency. The performance with each of two fuels will serve as a reference for improvement of engine design using biogas, according to the conditions identified for energy efficiency gain and emissions reduction.

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New characterization tool for porosity determination of pre salt core fragments by pycnometry techniques

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Core fragments samples are disregard in routine core analysis (RCAL). The shape and texture of fragmented core samples impair the porosity evaluation by methods commonly applied for preserved core samples. Actually, fragmented samples represent at least 40% of total samples obtained during drilling. Considering that, new methods are pursuit to improve the reservoir characterization. Powder (PP) and helium pycnometry (HP) techniques can be a good alternative for determinate porosity of fragmented samples. HP and PP techniques principle are related to envelope and skeletal densities determinations. The pycnometry set can evaluate porosity, pore volume, skeletal density and envelope density of fragmented samples properly. The advantages of these techniques are short analysis time, simple sample preparation and low complexity of data evaluation. In this study, pre-salt plugs were cut in different format considering the commonly obtained shapes in sidewall coring system. The sample preparation and instrumental parameters of powder and helium pycnometry set were evaluated to assess porosity in irregular core fragments. The main property that influences powder pycnometry (PP) measurement is the enveloper/sample ratio and enveloper particle size. Enveloper material ratio for PP is determined by the maximum height or diameter of the samples. X-ray microtomography and PP analysis present a good correlation for envelope volume determination. The skeletal density of the fragments proves to be dependent of the fragment itself. The porosity evaluation by pycnometry set were compared with analysis of preserved core before cutting and also with mercury intrusion porosimetry (MIP) of the fragments. This study proves the efficiency of the pycnometry association method to evaluate porosity of core fragments with multiple formats. The heterogeneity of the pre-salt deposits affects the results of porosity in fragmented samples. The weighted porosity of pycnometry set analysis for fragments is comparable to RCAL porosity.

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High-impedance faults in power transmission lines: characteristics and detection through zero-sequence current differential protection

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High-impedance faults are short circuits involving the earth in which the fault's resistance is high, and the fault currents have magnitudes similar to load currents. Although more common in distribution, high-impedance faults may also occur in power transmission lines, such as broken conductors in high-resistivity soils and situations involving damaged insulation. From the point of view of the transmission line's protection, high-impedance faults are critical, especially for protection functions such as distance and overcurrent, due to the low magnitudes of fault currents. Furthermore, high-impedance faults can compromise the accuracy of fault locators based on single-terminal measurements. Therefore, this study aims to analyze the behavior of fault current magnitudes at the terminals of a 500 kV transmission line for various resistances and to verify that zero-sequence differential protection can be a potential alternative for aiding this problem.

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Ultimate source of nitrogen for enhancing biomass production and lipid accumulation for biofuel production

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The substantial rise in the world population and diminished fossil fuel energy resources have become a predicament over the past two decades. Finding the best replacement for fossil fuel is a crucial subject as it should be sustainable and renewable. One of the most promising alternatives is microalgae as a source of biofuel production compared to other sources. Under stress conditions, such as biotic or abiotic stresses, microalgae produce lipid in the form of triacylglycerol (TAG). Changes on nitrogen availability have demonstrated to enhance their lipids accumulation. By increasing the TAG accumulation inside the microalgae cells, biomass production declines, which makes it a challenge for scientists to find a way to improve biomass and lipid production simultaneously. Finding a replacement for nitrogen which enhances the lipid production but at the same time does not affect the biomass productivity is the most important dilemma for the industry of biofuel production from algae. Algal cells can directly use amino acids as the source of nitrogen. It has been argued that glutamate may meet the cell requirement of nitrogen, then for lipid production, the cell can use the excess of the ATP and carbon skeleton ketoglutarate, which is needed in the pathway of nitrogen assimilation. Not only glutamate is a precursor of several metabolites production under stress conditions, but also it acts as a signaling molecule which grows the importance of this metabolite in investigating its role in lipid production and stabilizing the growth of microalgae cells. In this study, we were explored the role of glutamate in lipid and biomass production in mixotrophic condition. Using different concentrations of Glutamate, the results showed that after 5 hours of starting the experiment we had the lowest growth in the treatment with 0.5 mM glutamate, and after 24 hours all the treatments showed the same growth rate as nitrogen deprivation. For the lipid results, as it was expected, the control displayed a significantly lowest lipid amount and nitrogen deprivation illustrated the highest levels of lipid which was followed by the treatments 0.5 and 5 mM of glutamate, respectively.

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Critical behavior of hierarchical modular networks of Galves-Löocherbach neurons with different topologies

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Over the last years, many studies have corroborated that neuronal networks with hierarchical modular (HM) topology exhibit self-organized sustained activity better than homogeneous networks, e.g. random networks with the structure of the Erdós-Rényi graph. On the other hand, self-organized criticality (SOC) is a key concept which states that interconnected nonlinear units self-organize into a critical state. In addition, several models have been proposed to explain how cortical networks can reach a critical state through self-organizing mechanisms. However, the network topology strongly influences the critical behavior of the system but the mechanisms responsible for this effect are still unclear. Here we study SOC in HM networks, in which the basic units are stochastic neurons of the. Galves-Löcherbach type. We consider HM networks with three different intramodular topologies: sparse and randomly connected with connectivity ε, sparse and randomly connected with K neighbors per node (both constructed following a top-down approach), and fully connected (constructed using a bottom-up approach). All three systems have two mechanisms that make the critical region an attractor of the SOC dynamics: (i) dynamical gains, which adapt the neuronal firing rates, and (ii) dynamical synapses, which represent homeostatic mechanisms. We characterize the size and duration of avalanches displayed by the model and calculate the crackling noise relation for each topology.

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Uso consciente da iluminação artificial aliada à iluminação natural no campus da Cidade Universitária Armando Salles de Oliveira (CUASO)

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Esta pesquisa irá realizar um estudo para reduzir o consumo de energia relacionado à iluminação artificial em alguns edifícios do campus da Universidade de São Paulo, por meio do aproveitamento da iluminação natural oferecida pela arquitetura do próprio edifício, uma vez que muitos edifícios da Cidade Universitária Armando Salles de Oliveira, o CUASO, localizados na Universidade de São Paulo foram projetados na década de 60-70 por grandes arquitetos que valorizavam a entrada da luz natural nos edifícios. Isso deveria gerar mais conforto visual e eventualmente uma redução no uso da iluminação artificial. A luz natural, além de regular o ciclo circadiano, traz economia de energia dentro dos edifícios se usada de maneira correta. O método que será utilizado para alcançar o objetivo acima será por meio de levantamento de dados da arquitetura dos edifícios (no que tange aos sistemas e recursos/componentes arquitetônicos de captação da luz natural, como janelas, janelas altas, claraboias, átrios e outros), dos sistemas de iluminação presentes nos ambientes (que engloba tipologia de luminárias, lâmpadas, equipamentos auxiliares e a potência consumida), localização dos interruptores, divisão de circuitos, horários de funcionamento e aplicação de uma avaliação pós-ocupação (APO) relacionado ao uso diário dos ambientes. Somado ao levantamento desses dados, serão realizadas medições e simulações computacionais do nível de iluminância proveniente da luz natural nos ambientes escolhidos na situação de céu claro e céu encoberto. O resultado do cruzamento dos dados levantados, simulados e medidos irá gerar uma tabela, que funcionará como uma agenda, com os horários de acionamento e desligamento da luz artificial nas áreas escolhidas ao longo do ano. A implementação dessa agenda, irá gerar uma economia de energia de maneira passiva, sem a necessidade de grandes interferências ou reformas do prédio. Por fim, será produzido um manual dos usuários para que os mesmos sigam os horários de acionamento da iluminação artificial dependendo da estação do ano, e a localização dos interruptores e circuitos dos sistemas de iluminação. É de extrema importância a conscientização de todos os usuários do edifício para que o plano tenha sucesso, pois os mesmos passam a maior parte do dia dentro desses edifícios. A educação ambiental que visa à coletividade deve ser posta em prática de forma de estímulos contínuos ao longo do tempo para que a consciência que existe em seus lares e em ambientes individuais de trabalho seja estendida aos ambientes coletivos.

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The mysteries of gas and dust in nova shells

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Classical novae are thermonuclear eruptions on the surface of an accreting white dwarf that are important contributors to some Galactic abundances. As the ejected gas expands and cools down, the ionized shells can be observed with high angular resolution instrumentation and within a few years of the nova event. The analysis of the expanded shells provides information about the white dwarf and the explosive event, since the quiescent spectra are dominated by the companion star's gas in the accretion disc. Different nova explosions may vary in geometry, composition, and physical properties, including dust formation, resulting in a broad range of observed transitions and spectral line profiles. The consistent presence of emission lines with different ionization energies in the same spectrum suggests non-uniform gas distributions within the shells. Even though the 3D treatment of nova shells has been proved to be a key feature to understand the physical and chemical properties of novae, most of the models and analysis in the literature are uni-dimensional. We will present Integral Field Spectroscopy and high resolution (close to the diffraction limit) imaging data of the dusty novae obtained in different epochs of the nova's evolution, along with 3D photoionization models to provide more accurate constraints on the physical and chemical parameters of both gas and dust in nova shells.

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Particle acceleration by magnetic reconnection in relativistic jets by means of *in situ* three-dimensional MHD-PIC simulations

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and Elisabete de G. Dal Pino[1]; Greg Kowal[3]

The origin of the cosmic rays is still an open question. Observations have shown that magnetically dominated environments (such as the surrounding of black holes and the base of relativistic jets from AGNs, microquasars, and GRBs) produce very high-energy emission (VHE). Especially in Blazars, this emission generally presents high time-variability from days to minutes (in GeV and TeV bands), which implies very rapid and compact emission regions. The most probable mechanism able to explain this high variability and compactness seem to be fast magnetic reconnection in the inner magnetically dominated regions. Our earlier works based on 3D MHD simulations of relativistic jets with test particles, have evidenced that particles are accelerated by magnetic reconnection driven by the turbulence in the flow, from the resistive up to the large injection scales of the turbulence. Particles are exponentially accelerated in time suffering a stochastic Fermi process in the reconnection regions of the jet, attaining ultra-high-energies which are more than sufficient to allow them to produce the observed VHE emission (Medina-Torrejon et al. ApJ 2021; Kadowaki et al ApJ 2021). In this talk, we will show the results of MHD-particle-in-cell (MHD-PIC) simulations following the early stages of the acceleration of a million particles evolving in time with the relativistic jet, which confirm these previous results, demonstrating the strong potential of magnetic reconnection driven by turbulence to accelerate relativistic particles to extreme energies in magnetically dominated flows (Medina-Torrejon, de Gouveia Dal Pino & Kowal, ApJ 2023).

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Modeling ocean-coastal hydrodynamics using Lagrangian particle methods

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Ocean and coastal environments have high socioeconomic values and potential impacts on biodiversity, especially in the context of recent challenges arising from climate change and increased demand for energy sources. Among several factors that influence the safety and sustainable operation of engineering applications in these environments, reliable predictions of the hydrodynamics of free-surface flows are of great importance. With the remarkable advances in high-performance computing (HPC), computational fluid dynamics (CFD) has become an attractive complementary or alternative tool to analytical and experimental methods, and the Eulerian mesh-based methods have been widely adopted. Simulating applications with the presence of free-surface flows, which are characterized by large boundary deformations, is particularly challenging from a numerical point of view, and Eulerian mesh-based models require complex numerical techniques. Due to the easy implementation and flexibility, the mesh-less Lagrangian particle methods opened new perspectives for the modeling of free-surface flow. In these methods, the entire physical domain is represented by a set of nodal points (particles), whose motions are evaluated based on their interactions with neighboring particles, without the need for additional mesh constraints. Within this context, we present the diversification of particle and coupled particle-mesh methods in terms of both their applications, e.g., offshore, coastal protection, renewable energy, and building drainage system, and current challenges.

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Impacts of lithium mining on the energy transition: a comparative study between Brazil and Portugal

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The global energy transition and digitalization drive the search for critical minerals in the context of climate change. However, the supply of these minerals may generate uneven impacts in economically vulnerable regions and different countries. Lithium emerges as a key resource in this debate, especially for batteries used in renewable energy storage. In Brazil, lithium is considered a strategic mineral, with export-oriented projects to increase extraction. In Portugal, holder of the largest known lithium reserve in Europe, exploration is about to begin, which could have significant impacts on these regions. This project investigates the exploration of lithium, analyzing the dynamics in Brazil and Portugal, and seeks to situate this resource in a critical perspective of energy transition. It highlights the importance of considering not only the substitution of energy sources, but also socioeconomic justice and economic dependence in the energy transition. The comparative research between Brazil and Portugal highlights the similarities and differences in approach and socio-economic impacts. Through literature survey and field interviews, this project aims to understand the lithium extraction dynamics and its impacts. The results of this project will be made available on an interactive digital platform created by the researcher, raising awareness about the socioeconomic impacts of lithium mining. In addition, the platform will help in the search for collaborative solutions among the various actors involved in this chain.

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Modeling the energy poverty frontiers: an application of the Water-Energy-Food Nexus analysis for urban sustainability (Phase 1)

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The work carried out makes it possible to advance in understanding the relationships between the main resource demands for urban sustainability (water, energy and food), punctuating the dynamics between their supply, management and end-use variables. In phase 1, the focus of the work considers the local territorial borders (cities and metropolitan regions) and the conceptual gaps already diagnosed (lack of analytical models for public policy managers) and advances to potential solutions ("insights") in public policies and innovations technologies aimed at energy access and energy security, considering their relationship with strategic demands (water and food), to promote full citizenship. In the sequence, aspects associated with analytical and quantitative metrics will be valued, an innovative aspect of the work. The approach to be used is the Water-Energy-Food Nexus (WEFN), with the generation of a versatile analytical model validated by public agents, to be offered to managers of municipal public policies and will allow the generation of an Energy Poverty map for managers public.

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Tracking of mentions of the Sustainable Development Goals (SDGs) in documents

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This article proposes the automatic tracking of mentions of the Sustainable Development Goals (SDGs) and their targets in various types of documents. The aim is to provide an efficient tool for public managers and companies in promoting actions aligned with the SDGs. By analyzing scientific articles, theses, social networks, and newspaper articles, this study quantifies the mentions of the SDGs and creates a document profile without the need for complete reading. This approach enables a quick examination of a large volume of documents, facilitating the identification of specific actions that promote the SDGs. The SDGs represent a global agenda addressing the key social, economic, and environmental challenges of our world. Effective implementation of the SDGs requires the involvement of different stakeholders, including public managers and companies who have a crucial role in promoting sustainable actions. However, identifying and monitoring SDG mentions within a large volume of documents can be a complex and time-consuming task. To achieve automatic tracking, advanced techniques of natural language processing and machine learning are utilized. Specific algorithms are employed to analyze scientific articles, theses, social networks, and newspaper articles, aiming to identify mentions of the SDGs. Through automated processing, mentions are quantified and a document profile is created, eliminating the need for comprehensive reading. This approach enables a rapid examination of documents, facilitating the identification of SDG-related actions. The results obtained from automatic tracking reveal a significant presence of SDG mentions across various document types. The quantification of mentions provides valuable insights into the most frequently addressed goals and targets, offering a detailed understanding of the focus areas. This quantitative analysis equips public managers and companies with valuable information, enabling them to identify areas of opportunity and develop effective strategies to promote the SDGs. The practical applications of automatic tracking of SDG mentions in documents are extensive for both public managers and companies. Public managers can analyze policies, development plans, and government reports to identify actions aligned with the SDGs. Similarly, companies can evaluate their business practices, sustainability reports, and corporate social responsibility strategies, identifying opportunities to contribute to the SDGs. This tool serves as a valuable resource for promoting sustainable development and advancing the SDGs' agenda.

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Study of municipal solid waste potential for hydrogen production in the São Paulo State

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The increasing volumes of non-recyclable municipal solid waste (MSW) that cause problems around the world can be reused to produce a portion of the world's clean energy resources, making them important contributors to sustainable energy systems. In 2021, Brazil generated 225,348 tons of MSW daily, 60.2% (45 million tons per year) of which was sent to landfills, and the rest - 38 million tons per year (corresponding to 39.8% of the total amount collected) - was sent to inadequate disposal facilities (controlled landfills or dumps). Recently biogas and waste gasification have received considerable attention due to they offer the alternative of hydrogen production. Hydrogen has been identified as one of the sources that can facilitate decarbonization due to its ability to store and deliver large amounts of energy without generating carbon dioxide (CO_2) emissions during combustion. This research work presents an estimate of the potential for hydrogen production in the São Paulo State from biomethane reforming and fluidized bed gasification of RDF processes, based on research data on waste generation per capita, number of inhabitants per municipality, and treatment capacity of the technologies available in the state. In order to quantify the generation of methane (CH_4) from the waste disposal in landfills in each municipality, the methodology of the Intergovernmental Panel on Climate Change (IPCC) "Guidelines for National Greenhouse Gas Inventories" was adopted. On the other hand, in the case of gasification, the municipalities of medium size (60,000≤ inhab ≤1000,000) were evaluated. Sao Paulo state presents an attractive market that could be an opportunity for the development of several technologies as well as the study of little explored sources for hydrogen generation. MSW recovery where industry by-products can be sent back into the economy in a circular, low-carbon manner while protecting the basic principles of waste management (waste hierarchy) will be key in the energy transition.

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The CO2 geologic storage capacity of organic-rich rocks: the case study of shale and coal beds from the Paraná Basin, onshore Brazil

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Carbon capture, utilization and storage (CCUS) is a key suite of decarbonization technologies for the hard-to-abate energy and industrial sectors worldwide. According to the Intergovernmental Panel on Climate Change (IPCC, 2005), the CO2 geological storage is the segment of the CCUS technology chain that plays the major role in CO2 mitigation, by injecting significant volumes of CO2 in the subsurface, into suitable geological formations. Potential reservoirs for geological storage of CO2 range from saline aquifers, salt caverns or hydrocarbon depleted reservoirs, which are conventional reservoirs, to coal beds and shale gas reservoirs, classified as unconventional reservoirs. These are characterised by their characteristic low permeability, widespread global occurrence, and by its organic content, which gives these reservoirs a significant CO2 storage capacity through CO2 adsorption into the organic and clay-rich matrix. Furthermore, organic rocks, such as shales and coals, act both as reservoirs and caprocks, configuring a favourable system for the CO2 permanent geological storage. Finally, the aim is that these rocks, that are currently carbon-intensive energy resources, become CO2 reservoirs and, consequently, carbon sinks. In this sense, this project aims to determine the potential for CO2 geological storage of organic matter enriched shales of the Irati Formation and of coal beds of the Rio Bonito Formation, Paraná Sedimentary Basin (Permian), evaluating if these are geologically feasible and safe alternatives to the onshore storage of significant amounts of CO2, captured from stationary sources in the south and southeast regions of Brazil.

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From urban waste to bioenergy and biofertilizers: optimization of biogas production from solid waste and pruning wastein an experimental biogas production unit on the capital campus of the University of São Paulo

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The Experimental Bioenergy and Biofertilizer Production Plant, installed on Campus Butantan of the University of São Paulo, processes the organic waste produced on the Campus, mostly consisting of food waste produced in its restaurants and surroundings, for the production of biogas, converted in electricity, and also production of effluent that can be used as fertilizer, due to its concentration of nutrients. The unit is an experimental and demonstrative plant that can demonstrate the feasibility of a technological packet of environmental and bioenergy services and products in urban areas. The plant has two bioreactors of 430 m3 each, plus a digestate and post-treatment storage tank also measuring 430 m3. With a current capacity to receive approximately 20 tons of waste from kitchens and pruning, the Experimental Plant has a current potential to produce up to 1,500 Nm3 of biomethane per day, which could be expanded to 2,470 Nm3/day. Since the plant started operating, a total of 361 tons of waste have been processed, 189 of which produced on the USP campus. With the processing, around 40,370kWh of electricity were generated. The main objective of the post-Doctoral project are standardizing operating and monitoring procedures for biogas plants aimed at producing electricity, biofuels and other products, such as liquid fertilizers for organic urban wastes. Some products are in progress, such as: (i) adequacy of operating and analysis procedures, (ii) monitoring and support for the development of documentation for the plant's environmental licensing process carried out with CETESB and (iii) characterization and adequacy of the digestate as fertilizer. Is intended with final products, besides the procedures and implementation guides, report the main barriers to the real scale biogas facility implantation in Brazil, especially in urban areas.

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Lattice Boltzmann methods applied to the solution of digital rock problems

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While modern societies are making an effort to transition to greener energy sources, we are going to be dependent on oil and gas for some decades at least. Nowadays, about 60% of all the oil in reservoirs worldwide remains "trapped" inside the pores of the bedrocks. Being able to extract those resources by enhanced oil recovery (EOR) could provide potential societal and economic benefits without the need to explore new oil fields (notice that oil is an important input to the fine chemicals industry). Understanding how brine (water plus salt) and oil flow through the different porous rocks that comprise a field remains a challenge to this day, given the complexity of the task. The flow is affected by the properties of the liquids, like salt or additive concentrations; the rock's properties, such as mineral composition, pore's size, shape and connectivity; to the geological level and the distribution of different rock types. In this work, we focus on the pore (meso)scale and target the description of the flow using lattice Boltzmann methods (LBM). These methods allow to retain information from the microscopic scale and to include explicitly the physical interactions between the different phases interfaces: solid–liquid and liquid–liquid (for both oil and water)). The main goal is to improve LBM codes used in the industry by implementing more physically sounded interaction models, which used in conjunction with digital rock models (extracted from microtomographies of rock samples) will provide more realistic description of the flow inside rocks, and ultimately, a better understanding and analysis of flow simulations results. These, in turn, could provide insights into EOR solutions.

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A combined DFT and machine learning study on the conversion of CO_2 into C_2^+ products

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The conversion of CO_2 into valuable fuels and chemicals has drawn significant attention due to the possibility of tuning the fuel yield and selectivity by changing the catalyst. Regarding this, decades of advances in theoretical and experimental methods have produced a compendium of complex data containing valuable information on materials that can and should be used to optimise reactions. As previously reported, the C–C bond formation is the determinant step to obtain C_2^+ products of higher commercial interest. The C–C bond coupling is usually related to intermediates, such as C* and CO*. The elemental reactions from gaseous CO_2 to these intermediates and side reactions can be used to find the most favourable reaction pathway on different catalysts. The side reactions can lead to usually undesired products such as methane and methanol. As theoretical information from each elemental reaction can be found in the literature for many catalysts, it can feed a dataset and train a machine-learning algorithm. We are also performing DFT calculations to improve the dataset, considering catalysts that already showed good experimental results, mixtures of metals and single- atom supported by usual substrates. The selected catalysts will be both theoretically and experimentally verified. As the solvent and the alkaline metals cations were previously demonstrated to play an essential role in these reaction pathways, they will also be considered.

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Dark matter distribution in exponential growth scenarios

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A new non-thermal production mechanism for dark matter has been proposed recently which results in its exponential growth. The mechanism works provided a small but non-zero initial dark matter number (χ) density exists in the early universe which scatters of the bath particles (ϕ). This scattering generates more dark matter particles ($\chi\phi\,\chi\chi$). The process ends when the scattering rate becomes Boltzmann suppressed, which happens when either bath particles turn non-relativistic or their energies become in-sufficient to generate more dark matter particles. Owing to the dependence on the initial conditions, the solution to the dark matter evolution critically depends on the knowledge of its distribution function/number density at early epochs. In literature, this problem has been solved by considering an initial phase of freeze-in period populating the dark matter number density along with the assumption of the kinetic-equilibrium (either with SM or hidden sector) form of the dark matter distribution function. We consider an initial epoch of freeze-in and inflaton decay processes which produce negligible yet non-zero dark matter density to kick-start the rapid growth production mechanism. In our work, in contrast with the literature, we directly solve for the Boltzmann equation to determine dark matter phase space distribution. We highlight the differences of our approach with the existing literature where the phase space distribution function is assumed to approximately trace the equilibrium distribution. The exponential growth results only in the scenarios where dark matter phase space follows an equilibrium distribution. In generic cases, the growth is slightly faster than exponential.

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Um estudo das barreiras de transporte no mapa padrão não twist estendido

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Entender a formação de barreiras de transporte é uma questão crucial no estudo de física de plasma, felizmente muitas características dessas barreiras estão presentes em mapas simpléticos e que preservam área. Para esses sistemas, o teorema KAM garante a existência de toros invariantes suficientemente irracionais, desde que a perturbação seja suficientemente pequena. No entanto, se a condição *twist* não for satisfeita, a teoria KAM usual não se aplica mais em todo o espaço de fases. Como consequência, surgem novas características que influenciam o transporte de forma drástica. Por exemplo, existem toros *shearless* para os quais o número de rotação tem um extremo local. Esses toros *shearless*, mesmo após sua ruptura, diminuem o transporte de tal forma que se torna uma barreira efetiva de transporte. Barreiras de transporte efetivas observadas em mapas simpléticos não *twist* podem ajudar a entender a formação de barreiras de transporte internas em plasmas tokamak, pois permitem que os pesquisadores vejam como o plasma se comporta em diferentes regiões da câmara de confinamento. Isso pode ajudar a identificar as regiões onde o plasma está sendo mais bem confinado e onde ele está tendo mais dificuldade para ser mantido no lugar. Dessa forma, a fim de compreendermos as características dessas barreiras, utilizamos o mapa padrão não twist estendido. Tal modelo foi proposto por Portela e seus colaboradores como uma expansão local ao redor da curva *shearless* de equilíbrio para um mapa não *twist*, o qual descreve as linhas de campo magnético de um dispositivo de plasma toroidal com um limitador ergódico magnético. Uma vez que as transformações de simetria não podem ser aplicadas, nossa proposta é a utilização do teorema de Slater na investigação dessas barreiras. Tal teorema estabelece que para qualquer intervalo de tamanho δ de uma trajectorial quase-periódica, existem no máximo três diferentes tempos de recorrência: $\Gamma 1$, $\Gamma 2$ e $\Gamma 3 = \Gamma 1 + \Gamma 2$. Além disso, de acordo com o teorema, tais tempos fazem parte da expansão em frações contínuas do número de rotação ω correspondente a órbita. Esse resultado possui uma conexão direta com sistemas dinâmicos pois, barreiras de transporte são um conjunto de órbitas quase periódicas, no nosso caso correspondem as curvas *shearless*. Além disso, tais curvas têm rotação irracional no espaço de fases, podendo ser relacionadas com uma simples rotação de um círculo e consequente ao teorema de Slater.

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New platforms for hard magnets in $Sm_xY_{1-x}Co_5$ system investigated by X-ray absorption spectroscopy

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Hard magnets are fundamental materials for application in memory devices, energy storage and detectors. However, the realization of hard magnets currently demands the use rare-earth (RE) elements whose extraction is highly cost and non-friendly environmental. We propose an alternative route to realize hard magnets using a most friendly environmental and low-cost chemical element based on Yttrium. For this reason, we synthetize polycrystalline $Sm_xY_{1-x}Co_5$ (x = 0 – 1) and investigate their underlying interaction using x-ray absorption spectroscopy (XAS) on the edge of Co and Sm for both total-electron yield (TEY) and fluorescence (FY) modes. Our experiments distinguish high intensity peaks around 1079 eV (1105 eV on high energy) to the Samarium atom edge-$M_{5/4}$ and 789 eV (795 eV on high energy) to Cobalt edge-$L_{3/2}$. The analysis of XAS spectra suggest the softness of the energy- edge absorption with the inclusion of Y. This behavior is related to the spin-orbit interaction reminiscence of the strong interaction between 4f occupied density of states and 3d electrons provided by Yttrium. For the complete series of samples, we can infer the role of itinerant d-electrons and localized 4f-electron to stabilize hard magnetism, magnetic anisotropy and crystal electric field (CEF). The understanding of such fundamental low-energy scales opens a new route for the realization of new quantum materials with double functionality in magnetism and energy harvesting.

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Ab initio study of redox process of $LiNiO_2$ cathode: a spectroscopic analysis

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In this work, we used the combination of DFT + WIEN2k code + LAPW method + GGA + U_{eff} to analyze the redox process of $LiNiO_2$ cathode during charge. We tested three values of U_{eff} in the calculations, 3.0 eV, 4.5 eV, and 6.0 eV to describe the strong Coulomb repulsion between Ni-3d electrons. The best results were obtained when U_{eff} = 4.5 eV. The calculations were performed on a hexagonal 2 x 2 x 1 supercell. To verify changes in the $LiNiO_2$ host matrix during lithium extraction, we propose different structures with different lithium contents ($LixNiO_2$, $0 \leq X \leq 1$). Our results showed the formation of three stable intermediate phases at x = 0.25 and x = 0.50 and x = 0.75 during Li extraction. The total volume change between the phase with x = 1 and x = 0 was approximately 8%. The $LiNiO_2$ exhibited a potential window of 3.43 to 4.34 V and an average voltage of 3.86 V, according to the experimental (3.85 V). For each stable intermediate phase, the X-ray absorption near edge structure (XANES) was calculated. In the XANES calculation, core-role effects were considered, that is, an electron was removed from the 1s orbital of the Ni and O atoms and an electron was added to the bottom of the conduction band. The spectra calculated for $LiNiO_2$, $Li_{0.75}NiO_2$, $Li_{0.5}NiO_2$, $Li_{0.25}NiO_2$, and NiO_2 phases showed that the average Ni oxidation states changes from 3 ($LiNiO_2$) → 3.25 ($Li_{0.75}NiO_2$) → 3.50 ($Li_{0.5}NiO_2$) → 3.75 ($Li_{0.25}NiO_2$) → 4 (NiO_2) during Li extraction. Our results also showed that O also participates in the redox process during Li extraction. There is an experimental debate in the literature on whether oxygen participates in the redox process.

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Towards new Physics at the LHC and beyond

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Since the remarkable discovery of the Higgs boson, the LHC has accumulated a large amount of data that lead to further tests of the Standard Model (SM) and the search for Physics beyond the Standard Model (BSM). So far, all measurements confirm the SM and make it the most precisely measured theoretical physics model over many orders of magnitude in energy. Presently, there is no smoking gun indication of any extension of the SM. From this one can infer several possibilities of where new physics may lie. For example, one can assume that there is a mass gap between the currently experimentally accessible energy scales and the BSM scale. In this scenario, the use of Effective Field Theory (EFT) as the tool to search for hints of new Physics has become customary. Another search strategy is to complement and extend experimental setups to search in yet unexplored directions of particle collisions. A promising proposal for finding new physics is the forward physics facility (FPF) at the LHC during the High-Luminosity era. Hereby, theoretical predictions play a crucial role in estimating the potential of new experimental searches. For one, the far-forward direction in particle collisions is not even fully understood within the SM. For another, the abundant production of particles in the forward direction makes it possible to search for rare decays of some particles into new BSM particles that might leave signatures in the proposed detectors. In both cases, we need to build robust theoretical models to describe the physics behind those processes in order to make predictions for the potential and reach of experimental proposals. In my oral presentation, I would like to shed a light on how the particle physics group at the Instituto de Física de São Paulo contributes to finding signs for new physics in the above mentioned ways.

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Molecular modeling of electronic processes of solar cells sensitized by organic dyes

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In recent years, the search for alternative sources of energy, renewable energies and green chemistry are subjects of prominent role in science. In this scenario, solar cells appear as a promising alternative. DSSCs (Dye Sensitized Solar Cell) are devices that absorb sunlight through dyes and transport electrons through nanocrystalline metal oxide, transforming sunlight into electrical energy. From a theoretical point of view, DSSCs can be modeled considering the following components: TiO2 nanoparticles, organic dyes, acetonitrile solution, iodide electrolytes, triiodide ions and Pt surface, where photophysical and photochemical processes will occur. In the literature, there are several previous studies on DSSCs, but many of them are purely experimental or theoretical works, which use quantum mechanics for the description of photophysical processes but study only some parts of the system, for example the dye in solution or the dye anchored in the nanoparticle or dye with electrolytes, and in general, the solvent is treated as a continuous medium described only by a dielectric constant. A complete description of the photophysical system and processes, with an explicit approach to the molecules involved and the solvent, had not yet been developed, justifying the importance of our work. In our work, we studied each process with theoretical methods considered the current state of the art, focusing on the system as a whole, that is, dye anchored to the TiO2 nanoparticle in acetonitrile solution with electrolytes. The study was only possible due to the hybrid sequential method with quantum mechanics and molecular mechanics (S-QM/MM) developed in our research group in the late 90's and which has been continuously improved until today. This method allows studying systems with many atoms (tens of thousands of atoms) during observation times compatible with solvent relaxation in photophysical processes (on the scale of nanoseconds). As one of our main results, we realized that the proximity of the electrolytes to the dye-nanoparticle system enables an unconventional process, which is the transfer of charge from the electrolyte to the dye mediated by the absorption of photons in the region of 600nm. In this way, we were able to understand and explain the experimental measurement of the efficiency of conversion of photons into current (IPCE - Incident Photon to Current Efficiency) which shows high

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efficiency with the dye NKX-2553, between 60 and 80%, in the region from 400 to 620nm, showing that the photophysical process of light capture at low energies (high wavelength, ~600nm) occurs due to the process of transferring charge from the electrolyte to the dye in the excited state and in high energies (low wavelength, ~450nm) is due to the charge transfer process from the dye in the excited state to the nanoparticle. Some aspects of the photophysical processes of DSSCs still remain open, such as identifying the effects of larger nanoparticles and high concentration of dye per nanoparticle. These questions are the subject of our current post-doctoral research.

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Organic solar cells based on non-fullerene acceptors: fabrication and optoelectronic characterization

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The increase in global energy consumption and its impacts on the environment point to the need of developing and using new energy sources that are clean and renewable. In this sense, photovoltaic solar energy has emerged as a promising source, and organic photovoltaic devices stand as a concrete alternative, as they have already shown (in the laboratory) efficiencies of around 18%, combined with characteristics such as flexibility, lightweight, and low processing cost. These high efficiencies began to be achieved after the introduction of new acceptor molecules, in the last decade, replacing the traditional acceptors based on fullerene derivatives (C_{60}, C_{70}). In this work, we aim to master the techniques for manufacturing high efficiency organic solar cells based on non-fullerene acceptors, and to investigate the physical mechanisms associated with this improved performance. As multilayer devices, not only research on materials for the active layer is relevant, but it is also important to optimize the electrical behavior of the electron and hole transport layers, and to prevent energy barriers for conduction at the layer interfaces. Therefore, we combined traditional techniques for electrical characterization of devices with studies of electrical and photoinduced absorption transients, which contribute to the understanding of the processes of charge extraction and recombination, the latter being the main mechanism responsible for the efficiency loss in these organic solar cells. Therefore, besides mastering the manufacture of these solar cells in Brazil, this work also significantly contributes to the understanding of the mechanisms responsible for their high efficiency, enabling future studies for an eventual further improvement of their performance.

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Present and future constraints on secluded dark matter in the Galactic Halo with TeV gamma-ray observatories

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The dark matter relic density may be governed by the presence of new mediators that connect the dark matter field with the Standard Model particles. When the dark matter particle mass is larger than the mediator's, the pair production of mediators is kinematically open. This setup is known in the literature as secluded dark matter. Motivated by the appearance of secluded dark matter in several model building endeavours, we investigate the sensitivity of TeV gamma-ray instruments in the Southern Hemisphere namely, H.E.S.S., CTA, and SWGO to secluded dark matter annihilating in the Galactic Halo. We exploit the complementarity aspects of these detectors to find restrictive bounds on the annihilation cross-section for different annihilation channels. In particular, for a dark matter particle mass of 2 TeV, H.E.S.S. is able to constraint $(\sigma v) \geq 4 \times 10^{-26}$ cm^3 s^{-1} at 95% confidence level for the $4q$ and 4τ channel, while CTA will be sensitive to $(\sigma v) \geq 7 \times 10^{-27}$ cm^3 s^{-1} and SWGO $(\sigma v) \geq 6 \times 10^{-27}$ cm^3 s^{-1} for the 4τ channel, both well below the thermal relic cross-section. In fact, the combination of CTA and SWGO will be able to probe cross-sections below the thermal relic value for dark matter particles in the whole mass range between 100 GeV and 100 TeV in the $4q$ and 4τ channels, and between 100 GeV and ~40 TeV in the $4b$ channel.

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Investigating Raman scattering of MoS_2 monolayer on Au plasmonic grating

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Two-dimensional transition metal dichalcogenides (2D-TMDCs) have attracted attention because of their unique properties compared to their bulk counterparts, which make them ideal candidates for optoelectronic devices. MoS_2 monolayer (ML) is an example of 2D-TMDCs compound, considered one of this family's most stable layered materials. It is an inorganic semiconductor with a direct gap and high photoluminescence (PL) emission, where the optical response is primarily determined by excitonic transitions. In addition, MoS_2 ML exhibits only three zone-center first-order Raman active modes. It is also possible to observe second-order bands, depending on the energy of excitation. In this study, we investigated the vibrational properties of MoS_2 ML deposited on different fabricated Au gratings (GR) - square and circular geometries. These GR are composed of long sub-wavelength slits with a width of 100 and 50 nm, separated by specific distance in the nanometer range. We examined the MoS_2 ML on both supported and suspended regions inside the GR using confocal μ-Raman hyperspectral imaging. Our results showed that the out-of-plane mode was more intense in the suspended regions than in the supported ones for all geometries and we verified that a broad band around 450 cm^{-1} associated with second-order effects was more pronounced in the suspended regions. Additionally, based on the Raman maps, we analyze the changes in strain and doping properties in each region, observing the influence of polarization – plasmonic effects – and with GR parameters on these properties. In conclusion, our results demonstrate a dependent relationship between the vibrational lattice properties and the characteristics of the Au plasmonic GR.

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Assinatura geoquímica e geocronológica de enxames de diques gigantes associados a tectônica rifte do Atlântico Sul

Antomat A. M. Filho[1]

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A fragmentação do supercontinente Gondwana Ocidental no Cretáceo Inferior foi precedida por importante vulcanismo, reconhecido atualmente do nordeste do Brasil e oeste da África até as Malvinas e África do Sul. No centro-sudeste da América do Sul e contraparte da África, existem derrames basálticos continentais e sistemas intrusivos que compõem a Província Magmática Paraná-Etendeka (PMPE). No nordeste do Brasil, há enxames de diques e complexos de soleiras que formam a Província Magmática Atlântico Equatorial (PMAE). Um dos principais componentes da PMAE é o enxame de diques do Rio Ceará-Mirim (RCM), um sistema de condutos arqueado com cerca de 1.100 km de comprimento. Os dados aeromagnéticos indicam que os diques RCM se estendem do Rio Grande do Norte até o noroeste do Cráton do São Francisco (Bahia), sugerindo uma conexão entre as duas províncias magmáticas. O mesmo ocorre com os diques Riacho do Cordeiro (Pernambuco-Alagoas) e Vitória-Colatina (Espírito Santo), que também indicam continuidade através do Cráton do São Francisco (leste da Bahia). Este projeto de Pós- Doutorado tem como objetivo investigar os enxames de diques Transminas e Vitória-Colatina para estabelecer comparações com os enxames RCM e Riacho do Cordeiro, respectivamente, a fim de confirmar possíveis conexões entre as províncias Paraná-Etendeka e Atlântico Equatorial que juntas reuniriam uma das maiores manifestações magmáticas continentais do Mesozoico.

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Piecewise smooth reconstructions with sharp interfaces in full waveform inversion

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and Antoine Laurain

The Sharp Interface model for inverse problems consists in the reconstruction of coefficients by employing piecewise constant or piecewise smooth finite element spaces. In the context of seismic imaging, this coefficient is called slowness/velocity. In this way the coefficient reconstruction corresponds essentially to reconstructing their discontinuity set. The purpose of this model is to obtain an accurate reconstruction of the coefficient, when it exhibits the same structure in the physical problem. The sharp interface model can be used to refine the results obtained by a piecewise smooth model for the coefficient or can be used as an autonomous reconstruction tool as well. The sharp interface approach differs from the Total Variation (TV) regularization – a commonly used regularization that preserves edges – in the sense that it imposes discontinuity in the coefficients as a constraint instead of a penalization. This easily allows us to include previous information of the geological scenarios which exhibits strong discontinuities. It has been showed that this model conducts to better predictable results and meaningful improvements in the delineation of salt bodies.

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Equivalence between simple multilayered and homogeneous laboratory-based rheological models in planetary science

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The goal of this work is to investigate under which circumstances the tidal response of a strati7ied body can be approximated by that of a homogeneous body. We show that any multilayered planet model can be approximated by a homogeneous body, with the same dissipation of tidal energy as a function of the excitation frequency, as long as the rheology of the homogeneous model is suf7iciently complex. Moreover, we provide two straightforward methods for 7inding the parameters of the homogeneous rheology that would exhibit the same tidal response as the layered body. These results highlight the fact that the two models cannot be distinguished from each other only by the measurement of the second degree tidal Love number and quality factor, and that we do not need the complexity of the multilayer planet model in order to estimate its tidal dissipation. The methodology promises a great simplification of the treatment of multilayered bodies in numerical simulations because the treatment of a homogeneous body – even with a complex rheological model –can be computationally better handled than that of a multilayered planet.

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High-entropy metal-glycerolate as a precursor template of spherical porous high-entropy oxide microparticles

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High-entropy materials have received notable attention concern on account of their unique structure, tunable properties, and unprecedented potential applications in many fields. In this work, for the first time a NiCoMnZnMg-containing high-entropy glycerolate (HE-Gly) particles has been synthesized using a scalable solvothermal method. The HE-Gly particles were used as a precursor in design of porous high-entropy oxide (HEO) microparticles. The morphological and structural characterizations demonstrate that the temperature of the annealing process, and the composition of the metal ions in the HE-Gly precursors play important roles in determining porosity, crystallinity, and phase separation in HEOs. In fact, HE-Gly exhibited a porous structure of spinel HEOs with secreted MgO phase after annealing process at 800 °C, while the annealing process at 400 °C led to a low-crystallinity spinel phase without phase segregation. Overall, this work describes HE-Gly as a new precursor for altering the composition, crystallinity, and porosity of HEOs. This strategy is scalable for potential high mass productions, paving a new path toward industrial application of high-entropy materials for energy technologies.

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Hard carbon nanofibers as a self-supporting negative electrode for sodium-ion batteries

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and Roberto M. Torresi[2]

This project is inserted in the currently relevant context, of global interest, which deals with the development of new alternative energy technologies to fossil fuels, to mitigate the effects caused by global warming. Lithium batteries (LIBs) are currently the most used for energy storage in various applications. However, due to their scarcity, these devices are unable to supply the growing demand for charge accumulators by itself. In this context, sodium ion batteries (SIBs) emerge as a low-cost alternative, based on an element abundant on earth. In this work, we propose the development of negative electrodes for sodium ion batteries, based on hard carbon nanofibers (HCN), which has been considered one of the most promising candidates for this application. The HCN were obtained by the Supersonic Solution Blow (SSB), capable of producing nanofibers with an average diameter below 100 nm (Figure 1a). HCN were obtained using polyacrylonitrile (PAN), which is the state-of-the-art polymer to produce carbon-based nanofibers. The carbonization temperature will range from 1000 – 1400 °C, with the aim of investigating the influence of this parameter on battery capacity. The study will also be conducted using different electrolytes (organic solvents, ionic liquids), and aqueous ones aiming at reducing costs. The initial results observed so far suggest that the temperature has a significant influence on the battery capacity (Figure 1b), due to the organizational change in the molecular structure of the HCN, where the sample carbonized at 1400 °C presents the best Na storage capacity initial.

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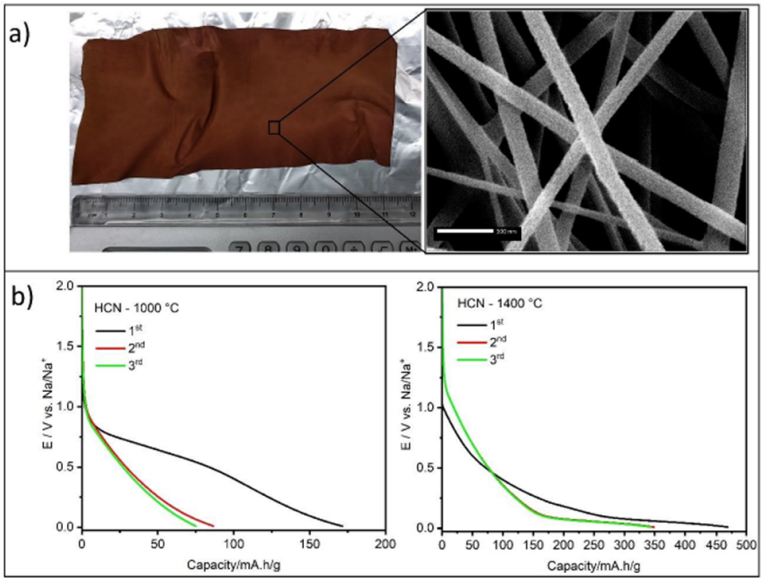

Figure 1 – (a) Photography and SEM of the HCN mats obtained by SSB. (b) Galvanostatic discharge voltage profiles.

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Enhancing CO2 conversion to alcohols: synergistic approach with rhenium and noble metals

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The urgent need to reduce atmospheric CO2 emissions requires effective and economically viable strategies to capture and utilize CO2. Ethanol (EtOH) holds great promise as a direct product of CO2. However, converting CO2 into higher alcohols is a complex process, and careful control of operating conditions significantly impacts product selectivity. In this regard, a study investigated the influence of different temperatures (200°C and 250°C) and CO2/H2 compositions (1:1, 1:3, and 1:4) on the selectivity of EtOH and CO2 conversion. Various catalysts based on Re, iridium, and gold were employed, with Ir-Re catalysts synthesized through wet impregnation and Re-Au catalysts through deposition, followed by in situ reduction. Re/TiO2 demonstrated limited EtOH formation, but the addition of Ir to the catalyst enhanced EtOH/alcohol proportion and methanation rates. Higher temperatures led to increased conversions and methanation, favoring ethane formation in the 1:1 ratio. EtOH exhibited higher selectivity at 250°C, 1:1, and 100 bar (1.4%), yielding the highest EtOH/alcohol ratio. Increasing total pressure and mixture density did not promote higher EtOH synthesis, but it reduced methanation. Introducing water as a solvent in the reaction medium improved selectivity for EtOH in the Ir-Re catalysts on titania, elevating EtOH/alcohol ratios from 2.9% to 4.3% (1:4 ratio) and from 6.6% to 11.4% (1:1 ratio). Substituting Ir with Au facilitated CO formation and resulted in higher EtOH selectivity (3.2% vs. 1.4%) in the 1:4 ratio. Notably, the production of EtOH necessitates the synergy between rhenium and gold metals since monometallic gold catalysts lack effectiveness. Reduction at 500°C yielded the highest selectivity for EtOH (17.2%) among alcohols, with the gas phase exclusively composed of CO.

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Computational fluid dynamics particle resolved in CO_2 hidrogenation

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In recent years, CO_2 hydrogenation has gained significant attention as a promising method for carbon capture and utilization. Computational Fluid Dynamics Particle Resolved (CFD-PR) is a powerful approach to study and optimize chemical reactions and processes involving multiphase systems, offering a comprehensive platform to investigate the complex interaction between particles, fluids, and chemical reactions in these systems using modeling techniques to capture the behavior of individual particles, such as catalyst particles, within the fluid flow, being capable to provide detailed information on particle dynamics, enabling a deeper understanding of the reaction mechanism and catalyst performance. The impact of operating conditions, such as temperature, pressure, and flow rates, on particle behavior and reaction kinetics is also investigated using CFD-PR. This approach, combined with the NGA2 code in OpenFOAM, provides a comprehensive framework for studying the complex interaction between particles and fluid flow. In this work, CO_2 hydrogenation in a fixed bed reactor was simulated using NGA2 code, in openFOAM in order to investigate catalyst particles within the fluid domain. The code incorporated detailed models for particle-particle and particle-fluid interactions, allowing an accurate representation of collision behavior, particle agglomeration, and reaction kinetics. The results showed the ability of the NGA2 code to capture detailed particle behavior, including particle size distribution, residence time, and chemical reactions. Also, it highlights the code's capability to analyze the effects of reactor geometry, flow patterns, and mass transfer on particle behavior and reaction kinetics, which can improve reactor performance, enhance mixing and transport phenomena, and maximize the overall conversion efficiency of CO_2 hydrogenation processes, capturing detailed particle behavior and fluid dynamics, offering valuable insights for process optimization and the development of sustainable carbon capture and utilization strategies.

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Aspen simulation of methanol production via CO_2 hydrogenation catalyzed by $ReOx/TiO_2$

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In the pursuit of a low-carbon economy, the production of green methanol (MeOH) through carbon dioxide hydrogenation (CO_2) has gained significant attention as a potential substitute for fossil fuels. Methanol can be utilized as a fuel or as an additive to gasoline, and it currently finds widespread use as a solvent or as a raw material in various industrial applications. Experimental studies conducted on a laboratory scale have demonstrated promising yields in the direct conversion of carbon dioxide (CO_2) into methanol using catalysts comprised of titanium oxide and rhenium oxide ($ReOx/TiO_2$). The next crucial step towards implementing this technology is to scale up the production of methanol. Thus, the objective of this project is to simulate the production of methanol via CO_2 hydrogenation using Aspen Plus V12.1 software for a plant with a production capacity of 12 Nm3/h. The production of methanol takes place under supercritical conditions (100 bar and 200 °C), catalyzed by $ReOx/TiO_2$. After the reaction, the resulting mixture is depressurized, and the methanol and water produced in the reaction are condensed. The gas phase is then separated from the liquid phase using a gas-liquid separator, and the unreacted gases in the gaseous phase are recycled back into the reactor. The methanol is sent to a distillation system to achieve the required purity level for commercialization. Through process modelling, it becomes possible to predict methanol production, determine the replacement flow of reactants, and aid in equipment sizing. This simulation helps optimize the production process of methanol, ensuring efficient operation and facilitating the transition towards a more sustainable and low-carbon economy.

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Luminescence properties of lanthanide tetrakis – Indandionate complexes as molecular light emitters

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Luminescent coordination compounds based on trivalent lanthanide ions (Ln^{3+}) has further found interesting photonic applications in new technologies, such as optoelectronics, lasers, molecular thermometers, security tags, and biomedical devices. Applications of these materials may be associated with narrow emission bands, which arise from intra-configurational Laporte forbidden 4f – 4f transitions. Furthermore, the Eu^{3+} ion especially can act as a powerful spectroscopic probe and the $^5D_0 \rightarrow {}^7F_J$ transitions are strongly sensitive to small variations in the chemical environment around of the Ln^{3+} ion. This study investigates a series of europium tetrakis complexes that contain tetraethylammonium as counterions, $N(Et)_4[Eu(acind)_4]$, where acind stands for 2-acyl- 1,3-indandionate derivative organic ligands. These compounds were investigated by structural, vibrational (Infrared/Raman), theoretical, and photoluminescent properties, and intrinsic and absolute quantum yields were calculated. The coordination polyhedron of the complexes is described as a distorted triangular dodecahedron close to the D_{2d} symmetry point group. One complex of the series, the $N(Et)_4[Eu(isovind)_4]$, presents an exceptional value of the Judd-Ofelt parameter $\Omega_2 = 73.5\times10^{-20}$ cm^2, the highest value ever reported. Theoretical calculations from the JOYSpectra web platform indicated that the values of Ω_2 are attributed to the symmetry breaking induced by differences in the electronic environment of the ligands. Specifically, within the same ligand, one coordinating oxygen has a polarizability four times higher than the other one. This complex also exhibits a high overall quantum yield (~ 80%) at 300 K and undergoes different and reversible solid-state phase transitions at 367 and 460 K. These phase transitions were characterized by Differential Scanning Calorimetry and Raman spectroscopy. The phase transition leads to significant changes in the profile of the $^5D_0 \rightarrow {}^7F_2$, showing very interesting and promising results for applications such as OLED devices and luminescent thermometers.

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Electrocatalytic N_2 and CO_2 reduction towards plasmon-enhanced urea production

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and Eduardo C. Melo; Paulo F. O. Marques; Susana I. C. Torresi

Nitrogen-rich compounds play a crucial role as important chemical inputs worldwide, particularly in the agroindustry, such as urea. Urea is conventionally produced through the Haber-Bosch process. In this process, N_2 and H_2 react to form NH_3, which then reacts with CO_2 to produce urea. However, this production method accounts for approximately 2% of the global energy consumption due to the high temperature and pressure required for the reaction. Additionally, it contributes to environmental issues, such as greenhouse gas emission. In this work, the co-electrolysis of N_2 and CO_2 was studied as an alternative approach to urea production using $BiVO_4/BiFeO_3$ as a catalyst. The catalyst was synthesized using the sol-gel route, following previously reported methods, and subsequently modified with Ag nanoparticles through ball milling. The resulting material was characterized using various techniques, such as XRD, SEM, TEM, and diffuse reflectance. The catalyst was deposited on carbon paper electrodes by drop-casting to evaluate the co-electrolysis of N_2 and CO_2. Initially, linear sweep voltammetry experiments were performed in 0.2 mol L^{-1} $KHCO_3$ under different gas atmospheres: N_2 and CO_2 mixture, and argon (Fig. 1). The results revealed an increase in current under N_2 and CO_2 mixture, which was attributed to formation of oxygen vacancies in the catalyst due to the ball milling synthesis method. The linear sweep voltammetry was also performed under light irradiation using a 455 nm laser to excite the localized surface plasmon resonance (LSPR) of Ag. The LSPR effect is well known to increase performance of various reactions. Under light irradiation the current was further increase, even at lower potentials in the N_2 and CO_2 mixture atmosphere. The behavior observed under light irradiation might be related to the Ag LSPR excitation, which can be advantageous for urea production. Controlled potential electrolysis experiments are currently underway under N_2 and CO_2 atmosphere, both under dark and light conditions, to quantify urea production and evaluate the enhancement in performance obtained by the LSPR effect.

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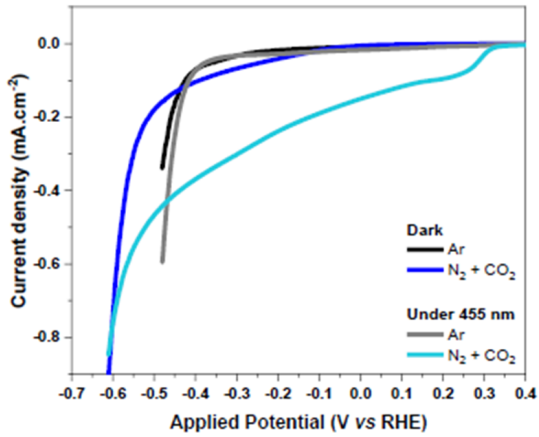

Figure 1. Linear sweep voltametries in 0.2 mol L^{-1} $NaHCO_3$ at 10 mV s^{-1}.

A study of solid-state non-conventional luminescence phenomena through new Light Excited Electronic Paramagnetic Resonance technique

Marcelo C. Portes

Unconventional luminescence phenomena, such as persistent luminescence, are increasingly present and important in society's daily life. However, these many of these luminescent mechanisms have not yet been well established. There is a lot of gray area in understanding how phenomena really work, in particular the actual physicochemical properties of excited states. With the aim of filling some of these gaps and adding a better understanding of luminescence phenomena, in particular those described as unconventional, and their mechanisms, we propose the creation of a new electronic paramagnetic resonance (EPR) technique with in-situ excitation as a powerful and versatile way to elucidate luminescent materials.

Coupling MXenes with metallic nanoparticles: towards plasmon-enhanced electrochemical reactions

Maria P. de S. Rodrigues[1]

and Roberto M. Torres[1]

MXenes are transition metal carbides, nitrides, and carbonitrides with two-dimensional (2D) structures known for their remarkable properties in chemistry, electricity, mechanics, and optics and its applicability across various areas. Recent studies have explored the photothermal and energy harvesting capabilities of MXenes in electrocatalysis and solar cells. However, noble metals remain the leading catalysts for crucial electrochemical reactions like the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). To address this, coupling MXene with metallic nanoparticles in a catalyst has emerged as a strategy to reduce the amount of noble metal required for efficient electrocatalysis. Additionally, metallic nanoparticles such as gold (Au) and silver (Ag) exhibit localized surface plasmon resonance (LSPR) effects in the visible range of the spectrum, which can further enhance the catalytic activity of the material through hot-electron generation and photothermal effect. Coupling MXene and metallic nanoparticles can also expand the catalyst energy harvesting capability, by summing both contributions in their active wavelength range. Thus, in this study we aim to synthesize a hybrid material composed of MXene ($Ti_3C_2T_x$) and gold-rhodium nanoparticles (Au@Rh) for application in the plasmon-enhanced hydrogen evolution reaction (HER). Au@Rh nanoflowers consist of a gold nucleus, exhibiting the localized surface plasmon resonance (LSPR) effect within the visible range of the spectrum, and a Rh shell, which serves as the catalytically active metal in the structure. The $Ti_3C_2T_x$ was obtained through acid etching of MAX precursors, and the resulting structure was characterized using several techniques. The next step involves impregnating the MXene with the Au@Rh nanoflowers to investigate the catalyst activity of the resulting material in plasmon-enhanced HER. The electrocatalyst study will be performed using several electrochemical techniques, aiming to understand how MXene might influence Au@Rh LSPR properties and catalytic activity.

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Development of persistent luminescence glass matrix composites by viscous flow sintering

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and Elaine A. de Mattos[1]; Victor M. P. da Silva[3]; Danilo Manzani[3]; Verônica C. Teixeira[4]; Lucas C. V. Rodrigues[1]

Given the accelerated technological expansion, there are growing interests in basic and applied research in physics, chemistry, and materials engineering focused on the study of new multifunctional materials and technologies for advanced applications. In this work, transparent (colorless) persistent luminescent glass matrix composites (PeL- GMC) were obtained, from the first time to the best of our knowledge, with silicate glass as the host material. 1wt% of persistent luminescence microparticles (PeL-MPs) $SrAl_2O_4:Eu^{2+}$; Dy^{3+} prepared by microwave-assisted synthesis in carbon reduced atmosphere was homogenized with glass spheres of soda-lime-silicate composition. Then, samples with disk-shape were prepared by pressureless viscous flow sintering. Despite the materials' porosity and undesired crystallization upon heating of a silica polymorphic phase, the PeL-GMC are transparent and showed long persistent luminescence (~80 min). Furthermore, we have observed an excellent compatibility between the PeL-MPs and the glass host since no chemical interaction was observed by optical microscopy and optical energy dispersive X-ray (EDX) mapping analysis.

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Ethanol reform for H_2 production in solid oxide fuel cell (SOFC)

Thiago de M. Augusto

Environmental impacts related to the increasing emission of greenhouse gases are a global problem, and studies of decarbonization studies have captured the attention of much scientific research. The development of technologies to decarbonize the Transportation sector, specifically bioethanol, and capable of replacing internal combustion engines with solid oxide fuel cell (SOFC) producing H_2 through internal reforming is investigated by different tools involving simulation, experimentation and analysis. In this project, the goal is to develop Ni-based catalysts, with low noble metals (such as Ru, Rh, and Pd), employing innovative strategies of synthesis and characterization of nanoparticles, evaluated for ethanol reforming and subsequently capable of forming a layer to be deposited on the anode in fuel cells (SOFC).

Multifunctional photoluminescent nanoparticles as amplifiers for $^1O_2$ generation and synergistic enhanced photodynamic therapy

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and Latif U. Khan[2]; Hermi F. Brito[1]; Paolo Di Mascio[1]

The development of multifunctional nanoplatform with integrated diagnostics and simultaneous local therapy, while evading the off-site problems, is highly desired for precise treatment. Since its discovery, singlet oxygen ($^1O_2$) has provoked a great deal of interest in the scientific community, using in a wide area of applications such as cancer therapeutics, antiparasitic and antimicrobial, stereoselective photochemical synthesis, oxidation of organic pollutants in wastewater treatment, and photochemical upconversion. It is also considered a major determinant of Photodynamic therapy (PDT) efficacy. Therefore, this study has a principal objective of nanoparticles-assisted amplification of $^1O_2$ to induce the maximum cellular lethality and concurrently using for synergistic photodynamic therapy (PDT). PDT consumes an excessive amount of oxygen; thus, hypoxia is induced, limiting the treatment's efficiency. Therefore, we also aim to relieve the hypoxic condition by decomposing the H_2O_2, excessively produced in the acidic tumor microenvironments, into O_2 and ROS *via* Haber– Weiss/Fenton reaction. For these purposes, we prepared series of color-tunable CdSe/ZnS core-shell QDs and various $NaGdF_4$:RE^{3+}@ $NaGdF_4$:RE^{3+}, Ca^{2+},Mn^{2+} (RE = Yb, Tm, Er) core/shell upconversion nanoparticles (UCNPs). The CdSe/ZnS core-shell QDs were prepared by new method which exhibited wide-range color-tunability (490–570 nm) as result of interfacial alloying (predominantly exchange of Se^{2-} by S^{2-} anion) without a significant change in the size (from 4.45 to 4. 81 nm) of NCs, as confirmed by XAFS data analysis. The QDs demonstrated efficient $^1O_2$ quantum yields (Φ_{QDs}) of 14, 12, and 18% for CdSe/ZnS (I), CdSe/ZnS (II), and CdSe/ZnS (III), respectively. The QDs were studied in macrophages cells that internalized the NCs *via* energy-dependent endocytosis predominantly macropinocytosis and other lipid raft-mediated endocytic pathways and manifested considerable amount in the intracellular regions without causing cytotoxicity.

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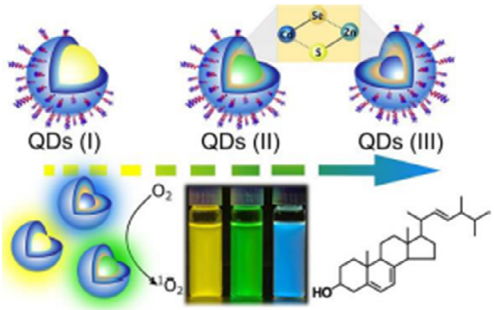

Figure 1. Color-tuning in CdSe/ZnS QDs via interfacial alloying and singlet molecular oxygen generation by the QDs.

The TEM images of $NaGdF_4:RE^{3+}$@ $NaGdF_4:RE^{3+}$, Ca^{2+},Mn^{2+} (RE = Yb, Tm, Er) UCNPs showed spherical shapes and flowers shapes NCs with narrow size distribution and diameters of around 22 nm and 57 nm, respectively. Whereas the core $NaGdF_4:RE^{3+}$ nanoparticles are spherical shape and 10.8 nm in diameter. The detail photoluminescence properties, including upconversion luminescence spectra and luminescence decay curves have also explored in the laboratory. The upconversion emission spectra manifest the dominant blue and green emissions, form the Tm^{3+} and Er^{3+} emission centers, respectively, under excitation with NIR (980 nm) laser. Furthermore, we have also studied the amplification properties of UCNPs conjugated with Rose Bengal photosensitizer (5, 10, and 15 µg/mL) for singlet oxygen generation in water under the 980 nm wavelength laser excitation. Further studies are underway to develop a QDs and UCNPs-based potential nanoprobe for enhanced $^1O_2$ generation and synergistic *in vitro* and *in vivo* photodynamic therapy.

Biofuels production from the catalytic valorization of ethanol: a microkinetic analysis based on first-principles calculations

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The advancement of a sustainable low-carbon economy depends on the development of heterogeneous catalytic materials, particularly in the production of fuels and value-added chemicals derived from renewable biomass. In this regard, evaluating the chemistry and kinetics of chemical reactions at the atomic level can significantly contribute to the screening and selection of efficient materials for catalytic applications. In this study, we focused on the application of computational material science to investigate the role of hydroxyapatite-based catalysts in the upgrading mechanism of ethanol towards n-butanol. Based on experimental observations, the catalytic valorization of ethanol was assumed to follow the Guerbet coupling mechanism, in which the formation of the C– C bond occurs via an aldol condensation reaction. Then, following the formation of crotonaldehyde, two possible hydrogenation routes of unsaturated hydrocarbons were considered for the form butanol: (i) via butyraldehyde and (ii) via crotyl alcohol. According to our findings, both pathways can result in the formation of n-butanol. Furthermore, the hydrogenation can occur via direct H-transfer from ethanol or surface-mediated hydrogenation competing reactions. Concerning the physicochemical nature of the catalyst surface, our analyses demonstrate that Ca^{2+} ions and PO_4^{3-} groups are strongly associated with the identification Lewis acid and Lewis basic sites, respectively. To this respect, the influence of the acid/basic site distribution on the chemical reaction pathways is evident, and a balanced distribution of acidic/basic sites is key for accelerating the C–C bond formation. Overall, our study provides valuable insights into the catalytic valorization of ethanol, highlighting hydroxyapatite as an viable catalyst for biofuels production.

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Lignin oxidation on CuO: (electro)chemical approaches

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Lignin is a macromolecule that is found in biomass, but it has limited industrial applications. It is a byproduct of the pulp and paper industry or bioethanol production and is mainly used for thermoelectricity production. However, lignin is the most abundant renewable aromatic compound which turns it in a promising source of high added value aromatic chemicals. Therefore, there is a high interest in investigating the catalytic depolymerization of lignin to obtain these products. CuO is a potential candidate for heterogeneous catalysis to obtain monoaromatic phenol molecules with ketonic or aldehydic carbonyl, or carboxylic acids in *para* position, at high temperatures of up to 180 ºC and high O_2 pressures. The resulting products may have zero, one, or two methoxy groups, *ortho* to the phenolic hydroxyl, depending on the starting macromolecule's monomeric distribution. Cu oxides are known in electrochemical literature to be good catalysts in alkaline media. This approach can not only find a new way to oxidize lignin, but also provide insights of this catalyst for lignin oxidation. The electrochemical approach produces the same monoaromatic products observed in heterogeneous catalysis, including a similar proportion of functional groups in *para*. The faradaic efficiency was calculated at1.65 VRHE is 28%. The catalyst was electrochemically characterized by electrochemical impedance spectroscopy and capacitive cyclic voltammetry for investigating changes in surface area and oxide characteristics using multi-frequency Mott-Schottky analysis. This analysis showed a decrease in the charge carrier density of this n-type intrinsic semiconductor, which was dependent on the oxidation potential applied. This suggests that these species are involved in the electrochemical mechanism and probably in the heterogeneous one as well. Raman spectroscopy and scanning electronic microscopy were used to compare structural and morphological changes and morphology when the catalyst was applied in (electro)catalysis.

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CO_2 thermocatalytic conversion to higher alcohols using Cu-Fe/UiO-66 catalysts

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Carbon dioxide is a greenhouse gas that plays a crucial role in climate change. In this way, the production of higher alcohols from CO_2 hydrogenation is a very attractive route for producing value-added compounds, and in addition, mitigating this pollutant. In this work, UiO-66 MOF- supported Cu-Fe catalysts were applied in this reaction. Three catalysts were synthesized, containing Cu/Fe weight ratios equal to 1, 2, and 5. The amount of total metal loaded was 30 wt.% for all catalysts. One of the main challenges of this reaction is to convert the main intermediate, CO, into the desired products. The Cu atoms activate the CO associatively, keeping it as the active specie *CO (the asterisk means that the CO is adsorbed on the active sites), while the Fe atoms dissociate it, transforming the CO into the $*CH_x$ active specie. The C-C coupling of these two species produces higher alcohols. The Cu/Fe ratio proved to be crucial in CO_2 conversion and product distribution. The sample of Cu/Fe ratio equal to 5 achieved the lowest CO_2 conversion and highest selectivity toward CO. On the other hand, the sample with a Cu/Fe ratio equal to 1, containing a balanced proportion between Cu and Fe atoms, led to a higher yield for higher alcohols ($2.1\ mol_{EtOH}.kgcat^{-1}.h^{-1}$, with CO_2 conversion of 41.5%) due to its high basicity and good hydrogenation capacity, producing the two active species * CO and $*CH_x$ in abundance and in optimal proportion, depicting the higher C-C coupling ability.

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Inkjet-printed Pt/C co-catalyst on electrodeposited CuS films for enhanced solar-driven hydrogen evolution reaction

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In this work, an inkjet printing method was used to superficially modify CuS films with Pt/C co-catalyst (designated as CuS-Pt/C) for enhancement of photoelectrochemical H2 generation via hydrogen evolution reaction (HER). For such, several Pt/C inks with different Pt loadings (i.e., 30, 50, and 80 wt% Pt) were formulated so to obtain a product featuring suitable jetting performance, compared to a commercial ink for an office printer, as characterised via surface tension measurements. Elemental atomic properties of the Pt/C deposited on the CuS films were investigated by X-ray photoelectron spectroscopy and energy-dispersive X-ray spectroscopy, and the former technique revealed the presence of Pt(IV) which may be bonded to atoms of sulphur and/or oxygen. The photoelectrochemical analysis of the CuS-Pt/C films evidenced optimised activity for the 50 wt% Pt loading (corresponds to approximately 0.0061 mg Pt cm^{-2}) in the Pt/C co-catalyst, that provided a photocurrent density for the HER of −1.49 ± 0.22 mA cm^{-2} at −0.20 V vs. $Ag/AgCl/Cl^-_{(sat.KCl)}$ (0 V vs. RHE), which is ca. 10 times higher compared to that observed for the bare CuS film (−0.14 ± 0.026 mA cm^{-2}). Additionally, the presence of Pt/C resulted in a shift of the HER onset potential of more than 20 mV towards less negative potentials. Such improvements were assigned to the reduction of the charge transfer resistance (2-fold) of the CuS-Pt/C films compared to bare CuS. As evidenced in this study, the inkjet-printing method pointed to be a compelling approach to improve semiconductors' photoelectrocatalytic performance and stands as a promising strategy for large-scale applications.

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Bioengineering of metalloproteins applied in the production of added value products

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The production of value-added products from redox proteins found in nature is limited. This limitation can be artificially overcome by modifying native proteins, or by obtaining artificial apo-reconstituted proteins. In the present study, we intend to contribute to frontier research in the area of metalloprotein bioengineering and to obtain new apo-reconstituted structures. The aim is to modify the structure of proteins with metallic centers to electrochemically produce value-added organic molecules from the electroreduction of CO_2. Since the active site of the redox protein will be modulated, the bioelectroreduction reaction of the H_2O molecule to produce molecular hydrogen is also be investigated. With the completion of this project, it is the transferring of the methods to be developed to the technology sector.

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Theoretical investigation of ionic liquid-based electrolytes for sodium-ion batteries

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The development of high-performance and low cost batteries is one of the initial steps in the chase of a sustainable world. Those batteries are required not only for electric vehicles, but also in the renewable power-plants, which in general are intermittent. Therefore, sodium-ion batteries (SIBs) are promising candidates due to their low cost production and chemical similarities with lithium-ion batteries. In the last years, we have applied molecular dynamics (MD) simulation, density functional theory (DFT) calculations and machine learning techniques, to investigate the ionic liquid (ILs) based electrolytes in SIB, correlating chemical structure, physicochemical properties and electrolyte performance. We have seeing that size, charge distribution and flexibility are key points to improve the IL conductivity, while the use of fluorine-based anions improve the electrolyte electrochemical stability. Moreover, we used MD simulations to investigate the Na^+ intercalation into graphite-based electrode, in which we observed that use of binary electrolytes (IL/glyme) improves the intercalation due to the co-intercalation effect.

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Ni doping in $BaZr_{0.8}Y_{0.2}O_{3-\delta}$ and $BaZr_{0.7}Ce_{0.2}Y_{0.1}O_{3-\delta}$: advancing towards protonic ceramic fuel cells for ethanol

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As an excellent alternative for electric energy generation, the use of ethanol in fuel cells, which can either work as a solid oxide fuel cell (SOFC) or as a solid oxide electrolysis cell (SOEC), has been seen as a significant advance. Competing with the advantages of clean energy and environmental friendliness, provided by these systems, the need to operate at high temperatures (800–1000 °C) instigates efforts to optimize and improve their energy conversion efficiency. Nowadays, most of the conventional solid oxide electrolytes are oxygen-ion conductors, which can only reach sufficient ionic conductivity at high temperatures. Accordingly, the interest in proton-conducting electrolytes has increased due to their relatively lower activation energy and higher conductivity at intermediate-low temperatures (400–700 °C). In this scenery, this work contributes to investigating protonic ceramic fuel cell electrolytes potentially capable of reducing the operating temperature and enhancing the performance of the SOFC and SOEC systems. Herein, commercial protonic electrolytes were modified by doping with Ni 1 wt.%. As expected, these metals acted as sintering aids. Due to their presence, the sintering process occurred at 1450 °C in a time of 6 h. Additionally, densification was observed for the modified materials, whereas the same was not presented by the pristine BZY20 ($BaZr_{0.8}Y_{0.2}O_{3-\delta}$) and BCZY ($BaZr_{0.7}Ce_{0.2}Y_{0.1}O_{3-\delta}$), at the same conditions. Our first conductivity results present that, despite the Ni doping, the conductivity values in dry H_2, were smaller than those obtained in wet H_2. This observation suggests that the Ni improved the sintering process while keeping the protonic conduction of the BZCY, mainly in humidified atmospheres.

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Studies on heteroaromatic organic conductive polymers modified copper electrodes for electrochemical CO_2 reduction reaction

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To mitigate the effects of greenhouse gas emissions on climate change and achieve sustainable clean energy production, it is critical to use earth-abundant and inexpensive catalytic materials in electrochemical energy storage and conversion devices such as fuel cells, water electrolyzers, and carbon dioxide (CO_2) reduction reactors. By addressing the global energy crisis, electrochemical reduction of carbon dioxide (CO_2RR) to multiple value-added hydrocarbon products has gained technological significance for reducing CO_2 emissions and triggering a sustainable solar-fuel-based economy. However, the development of electrocatalysts with high selectivity, stability, and energy efficiency to overcome the activation energy barrier of CO_2, competing hydrogen evolution (HER), and high complexity and diversity of reaction products remain significant barriers to the commercialization of the CO_2RR process. Copper stands out among all metals discovered so far for its ability to generate a diverse range of multi-carbon products, resulting in the formation of 16 distinct products in aqueous media due to its suitable adsorption energy with *CO intermediate and special electronic properties. Nonetheless, the substantial overpotential required, as well as the low product selectivity and instability on pure Cu surfaces, have prompted researchers to explore more effective strategies for tackling these concerns. One of the most promising approaches is to catalytically modify CO_2RR activity and selectivity using organic additives like ionomers or polymer films. As a result, the current study attempted to create a multilayered, N and S-containing, heteroaromatic conjugated conductive polymers on polycrystalline Cu using polypyrrole and polythiophene via a simple technique for increasing C_{2+} product selectivity, such as ethylene. The electrochemical characteristics of the polymer-modified Cu electrodes, as well as the specifics of the qualitative characterization of the CO_2RRs product, were studied using sophisticated online electrochemical mass spectrometry (EC-MS) investigations.

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Theoretical study of the phase transition from perovskite into hexagonal on metal halide compounds

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Metal halide perovskite (MHP) materials have become the most attractive technology in solar photovoltaics, but problems such as the phase transition into photo-inactive structural phases, hinders their deployment. For this reason, energetic analyzes have been performed previously on these compounds by means of *ab initio* calculations. In this work, we studied the perovskite-to-hexagonal structural phase transition by means of Density Functional Theory. We considered seven structures in order to sketch this solid reaction and nine lead halide compounds: $A\mathrm{Pb}X_3$, with A = $\mathrm{HC(NH_2)_2^+}$, $\mathrm{CH_3NH_3^+}$, or $\mathrm{Cs^+}$, and X = $\mathrm{I^-}$, $\mathrm{Br^-}$, or $\mathrm{Cl^-}$. We found that the energy barrier could be modulated by the chemical composition: in $A\mathrm{PbI_3}$, it increases when the volume of the cation in the A-site is decreased, and in $\mathrm{HC(NH_2)_2Pb}X_3$, it increases when the volume of the halogen in X decreases. Further, non-linear variations of the unit cell volumes were obtained, due to the variations of the equilibrium lattice parameters, which led into highly distorted triclinic unit cells. We also tracked the effective coordination number of Pb atoms due to number of broken bonds within the crystals, having a minimum (maximum) in the former (latter) at the middle of the solid reaction for all cases. Finally, an increment on the band gap between 0.3 and 0.9 eV was obtained for all compounds just in the second transition structure (TS), and from the third TS (the one with the highest energy and the middle of the solid reaction) only indirect wide band gaps (> 2.1 eV) were obtained. Our findings pointed out that the applicability of MHPs is reduced once the phase transition take place, but could be hindered by their chemical composition.

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The role of van der Waals corrections in physical-chemical properties of chiral perovskites with different dimensionalities

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The efforts to improve the efficiency generation of clean energies by using perovskites solar cells have had a rapid increase in their power conversion efficiency from 3% in 2006 to more of 25% these days, demonstrating that perovskite materials are promising materials. Particularly, chiral hybrid perovskites (a chiral object isone that cannot be superimposed on its mirror image) have emerged as materials with unique optoelectronic properties and a wide range of applications. These include spin- dependent photovoltaic and photogalvanic responses and chirality-induced photocurrent. However, the effectiveness of these effects depends on the degree of chirality transfer from the chiral cations to the inorganic structure of the perovskites. Although some studies have been conducted on chirality transfer in two-dimensional chiral perovskites, the understanding of this process remains limited for other types of chiral perovskites with varying dimensions. Since chirality resides in organic molecular cations and interactions with the inorganic structure of perovskites are mainly by hydrogen bonds, the long dispersion forces characterized by van der Waals (vdW) interactions play an important role here. To elucidate this, we performed a comprehensive analysis of the impact of vdW corrections on density functional calculations for a carefully selected set of chiral perovskites with various chemical compositions and dimensionalities. We evaluate the accuracy of various vdW corrections, including Grimme's D2, Grimme's D3 with zero damping function and Becke-Johnson damping function, Tkatchenko-Scheffler (TS), TS with self-consistent screening, TS with iterative Hirshfeld partitioning, density- dependent scattering corrections, and the many-body scattering energy (MBD) method. We find that the vdW MBD correction provides the most accurate correction to describe our set of chiral perovskites. The percentage errors calculated for all lattice parameters are below 3%, which is in excellent agreement with the experimental reference. Furthermore, we identify the crucial role of the vdW corrections in accurately characterizing the asymmetric distortions in the octahedral

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structures of zero-, one- and two-dimensional chiral perovskite inorganic structures. These distortions are influenced by the kind of the chiral cations R or S, and their accurate description depends significantly on the long-range scattering forces. Furthermore, our findings indicate that the vdW corrections contribute to increase the binding energy and strengthen the hydrogen bond between the chiral cations and the inorganic structure of the chiral perovskites.

Computational investigation of methane conversion into valuable products

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Methane (CH_4) from natural gas shows promise as a mid-term renewable energy source, providing greener and economically feasible alternatives. To unlock its energy potential, methane must be converted into valuable chemicals like methanol (CH_3OH), formic acid (HCOOH), and carbon monoxide (CO). This conversion relies on catalysts such as metallic substrates, oxides, and zeolites, which facilitate C H activation and dissociation. Our study focuses on the Density Functional Theory (DFT) investigation of CH_4 activation and conversion using various catalyst substrates. We observed that the occupation of *d*-states in 3*d*-TM_{13} clusters (TM = Fe, Co, Ni, and Cu) significantly influences medium-strong chemisorbed systems like CO/TM_{13} and H_2/TM_{13}. Conversely, for weakly physisorbed systems like CH_4/TM_{13} and CH_3OH/TM_{13}, the occupation of *d*-states is less crucial as local polarization and electrostatic effects play a more significant role. Furthermore, our results demonstrate that quantum size effects mainly influence the adsorption energy magnitude of CH_4 activation processes leading to CH_3+H formation in small TM_n clusters ($n < 7$). Furthermore, we uncovered that the activation and dissociation of CH_4 into CH_n+(4−*n*)H species on 3*d*-TM13 clusters occur through a concerted interaction mechanism involving charge transfer, *sp d* coupling, and unpaired electrons. These factors contribute to increased adsorption energy along the dehydrogenation process. Thus, Perac¸a et al. demonstrated that on the $(CeO_2)_{10}$ cluster, CO is the energetically preferred product of CH_4 dehydrogenation, indicating a preference for syngas formation over CH_3OH. However, indirect methanol production remains feasible with this type of material. In our latest work, we explored all possible reaction pathways for CH_4 conversion on TM_{13} clusters. We observed direct competition, in terms of kinetics and thermodynamics, between the formation of CO and CH_3OH, especially in the alkoxy dehydrogenation pathway. However, for the Ni_{13} the formation of CO can be modulated to favor the formation of the *"umbrella"* CH_3O methoxide as a prominent intermediate species. This modulation subsequently decreases the stability of formaldehyde intermediates, effectively suppressing the overall formation of CO. These findings provide valuable insights into the intricate dynamics of CH_4 conversion on TM_{13} clusters, presenting potential avenues for refining the catalytic processes involved.

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The electro-oxidation of ethanol under oscillatory regime on platinum-tin electrodes

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The electrocatalytic oxidation of small organic molecules is of general importance for energy-related issues such as the fuel cells and electrochemical reform. The characteristics that emerge along the catalytic oxidation of small organic molecules critically depend on the coverage and nature of absorbates. The common emergence of current and potential oscillations in these reactions is closely related to the reaction mechanism and implies the overall conversion, and thus on the performance of practical devices. In the present work we study the dynamics of electrochemical oxidation of ethanol under oscillatory regime using tin-modified platinum electrode. Experiments were performed in a classical three electrode cell, polycrystalline platinum flags were used as working electrodes (WE), a graphite stick was served as counter electrode, and a reversible hydrogen electrode (RHE) was used as reference electrode. The investigation was focused on the role played by surface-free sites and the presence of a step with a short-lived specie adsorbed at the electrode surface. To reduce the coverage of poisoning species, and thus to increase the main reaction pathway, chronoamperometry in platinum oxide region followed by potential sweeps or the adsorption of ad atoms, like tin, tin-modified platinum electrodes were used to assess the decrease in coverage of poisonous species. The experimental part includes protocols to invest control the effect of surface coverage using chronoamperometry and cyclic voltammetry, as well as studies under oscillatory regime. The results show that the efficiency of ethanol electro-oxidation is preferred powered, on a less poisoned electrode surface, which is obtained through a self-cleaning process driven by the oscillatory electro-oxidation. These results are rationalized in terms of reaction mechanisms on both platinum and platinum-modified systems.

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Theoretical insights into methane activation on transition-metal single-atom catalysts supported on the CeO_2(111) surface

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Natural gas is a naturally occurring hydrocarbon gas mixture, which the main component consists of methane. Methane activation is absolutely essential in heterogeneous catalysis for future energy needs, as well as a carbon source for chemical feedstock. However, the emission of methane into the atmosphere has the potential to pose a significant environmental risk due to its impact on the greenhouse effect. To address this challenge, there is a growing demand for the development of efficient approaches to convert methane into valuable chemicals and fuels. Single-atom catalysts (SACs) are isolated metal atoms dispersed on a support. SACs exhibit a low coordination environment that maximizes the use of metal atoms and can offer high activity and selectivity. Moreover, ceria (CeO_2) plays a crucial role in heterogeneous catalysis, serving as both a catalyst and a support. Its capacity to reduce Ce^{4+} to Ce^{3+} stabilizes metallic cations, as electrons are transferred from the metal to the support. This mechanism promotes strong metal-ceria interactions, highlighting the diverse and substantial applications of ceria in catalysis. In this context, in this work we performed density functional theory (DFT) calculations using the Vienna *ab initio* simulation package (VASP), with PBE *xc*-functional. To improve the description of Ce *f* -states DFT+*U* method was employed. In order to improve the description of the adsorbed species Grimme D3 vdW correction was applied. The methane C– H bond cleavage was estimated using the bond index-quadratic exponential potential framework (UBI-QEP) on TM/CeO_2(111) systems, where TM are the single-adatoms of Fe, Co, Ni, Cu, Zn, Ru, Rh, Pd, Ag, Ir, Pt and Au. Our findings demonstrate that TM adatoms that donate more electrons to the surface of CeO_2(111) exhibit greater stability, resulting in the reduction of a larger number of surface Ce^{4+} ions. Additionally, CH_3 and H prefer to adsorb on the oxygen surface site that reduces a Ce ion. The strong adsorption of CH_3 suggests a lower energy barrier for the activation of methane. Moreover, our results indicate that the dissociative chemisorption of methane becomes increasingly thermodynamically favorable with the increasing period of the TM adatom.

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Theoretical investigation of the role of mixed A+-Cations in the structure, stability and electronic properties of perovskite alloys

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Experimental studies have demonstrated the importance of the combination of different chemical species at the *A*-, *B*-, or *X*-sites in metal-halide *ABX*3 perovskites to improve the performance of perovskite solar cells (PSCs). However, from our understanding, further efforts at the atomistic scale are required to unveil the role of alloying in PSCs. Here, we performed a density functional theory investigation on perovskite alloy materials, namely, $Cs_xMA_{1-x}PbI_3$, $MA_xFA_{1-x}Sn_{0.50}Pb_{0.50}I_3$, and $MA_xFA_{1-x}PbBr_{2.50}I_{0.50}$ (x = 0.00, 0.25, 0.50, 0.75, 1.00). Equilibrium orthorhombic supercell structures were obtained for all systems with distorted octahedral environments, in which the magnitude depends on the chemical species. Besides, energetically stable crystals, in comparison with the parent structures, were found only for $Cs_xMA_{1-x}PbI3$; even though the remaining alloys presented stronger bonds. Furthermore, we addressed the role of the spin-orbit coupling effects to the electronic structure, which was critical to estimate the power conversion efficiency (PCE) with radiative recombinations, e.g., a PCE exceeding 23 % was obtained. From our analyses, alloys with Cs content stood out as the best photovoltaic material.

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Under the shadow of Aswan: perspectives of economic and technical cooperation between Brazil and the USSR (1962-1964)

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This project aims to analyze the relations between the Soviet and Brazilian governments regarding economic and technical cooperation for the construction of a massive hydroelectric plant on the Paraná River between 1962 and 1964. In Brazil, the period is characterized by severe economic difficulties, political turmoil, and the deterioration of Goulart administration's ties with the United States. On the external front, there is an important initiative by President João Goulart which is largely unknown by scholars. During a meeting with the Soviet ambassador in October 1962, the Brazilian President expressed his interest in a large-scale economic and technical cooperation with the USSR. Goulart mentioned the possibility of aid for the construction of a huge project in the country, similar to the Aswan hydroelectric plant - which was underway in Egypt with Soviet assistance. The talks dragged on over months with no decision in sight. Goulart would return to the topic in October 1963, during a conversation with Ambassador Fomin. The meeting would mark the first time that a Brazilian President would request economic and technical assistance from the USSR for a specific project. The plant would be built at Salto de Sete Quedas on the Paraná River (where, later, the Itaipu plant would be built – the largest in the world when it was concluded). Using Russian, Brazilian, and American sources, this project seeks to understand why the initiative failed. If it had been successful, the joint venture would have a profound impact on the domestic and regional contexts, as well as on Brazil's relations with the USA.

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INDÚSTRIA

Development and analysis on a net-negative emission scenario for Brazilian steelmaking by 2050

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Steelmaking is among the biggest industrial challenges to achieve global warming mitigation goals. While essential for the development in the next decades, current steel production is highly CO_2 intensive, in which fossil coke-fired blast furnaces predominate in Brazil and the world overall. Given specific conditions of Brazilian steelmaking, we proposed a low carbon (LC) scenario based on four strategies: two strategies about increasing well-known routes in Brazil (recycling and biocharcoal) and two strategies about innovative routes (green hydrogen-based direct reduction and carbon capture and storage (CCS)) needed to neutralize emissions by 2050. Our model is based on (e.g.) econometrics, computable general equilibrium model, marginal abatement cost analysis, and IPCC emission factors for greenhouse gases inventory. Preliminary results have shown that Brazil are going to produce 97 million metric ton (Mt) of crude steel by 2050 and steelmaking emissions would surpass 130 $MtCO_2$ in the business-as-usual (BAU) scenario. In the LC scenario, emissions are negative from 2044 and the industry can sink 180$MtCO_2$ until 2050. Such an achievement is only possible by the biocharcoal associated with CCS (BECCS), which works as a carbon dioxide removal strategy and represents 37% of total CO_2 reduction potential in 2050. Although steel recycling through electric-arc furnace contributes to 22% of total potential, it is limited by domestic steel scrap stock forecasted until 2050. LC scenario requires less total energy than BAU scenario; however, its power and biocharcoal demand is sizable: 27,3Mtoe or 78% of steelmaking total energy demand in 2050. Research next steps are related to the accounting for the economic, social, competitiveness and productivity impacts of the proposed LC scenario.

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O ecossistema de empreendedorismo e inovação da indústria criativa brasileira – a conexão entre os atores de impacto socioambiental

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An innovation ecosystem can be described as a complex network of actors with the potential to encourage the emergence of innovative entrepreneurship. This large network of innovation can be divided into sub-areas, such as: academia, business/industrial, investments, support for entrepreneurs and society in general. This postdoctoral research project aims to "Map and describe the entrepreneurship and innovation ecosystem of the Brazilian creative industry and the connection between socio-environmental impact actors". The proponent and his supervisor are experienced researchers in the area of entrepreneurship and innovation and were involved in the projects: "Young Brazilians and Media Practices in a Time of Convergence" from PROCAD n. 071/2013 with UFGRS, UFS and UFPA and "The strategies of marketing and communication in the context of media convergence culture - Young Individual Microentrepreneurs from the Immediate Geographic Region of Propriá - SE" from Call MCTIC/CNPq n. 28/2018 - Universal20. Methodologically, the work will be qualitative, with a case study protocol inspired by Yin's proposal (2014, 2017), as sources of evidence, virtual interviews, document analysis, file registration and physical artifacts will be used. For the theoretical basis, a systematic review of the concepts of Entrepreneurship and Creative Industry Ecosystem and the various actors with socio-environmental impact and cases related to the entrepreneurship and innovation ecosystem will be carried out based on the analysis of publications in the Web of Science database. As an analysis method, the protocol indicated by Bardin (2016) will be used, with the help of the Nvivo 12 software in the analysis of all the investigated content. In theoretical terms, the work will follow the most referenced scientific literature in the world regarding the Ecosystem of Entrepreneurship and Ecosystem of Innovation21 and Creative Industry and in the analysis of the Brazilian case, in the confrontation with authors who also investigated the reality.

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Technological capability model for innovation management for global supply chain enterprises

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As globalization the competition between companies increasingly demands their ability to stay ahead of their competitors who are located far beyond their city, region or country and innovation has become essential for organizations not only to be leaders in their markets, but also to increase competitiveness and, above all, avoid its decline, a world-class innovation management process being vital. The objective of this research effort is to present a technological capability model for innovation managing for global supply chain companies that is adaptable to their realities and aimed at knowledge-intensive industries. To achieve this objective, the research method applied was action research starting with the mapping of the literature to identify the most relevant studies, recognize the state-of-the-art, theoretical propositions and in a collaborative way with the participation of experts and professionals that act, directly or indirectly, in the innovations development, the model is conceived under two evaluation perspectives: the first called technological functions that represent the main areas that have an impact on the success in evaluating strategies, planning, development, execution and in the innovations results in industrial companies and the second perspective that are the competence levels, which at the highest level strongly favour and support innovation in industrial companies, so that organizations can measure themselves, compare themselves with others and, through planning, achieve excellence. Also, as the expected objective is to obtain an indicator through the interaction of the considered items called Innovation Technology Capability Index (ITC Index) as well as a tool that facilitates the application and its dissemination and later the concepts applicability in in the real environment of Fast Consumer Goods (FMCG) enterprises in the Brazilian ecosystem was evaluated.

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Recombinant cellobiose dehydrogenase from Thermothelomyces thermophilus: its functional characterization and applicability in cellobionic acid production

Gabriela Berto

The fungus Thermothelomyces thermophilus is a thermotolerant microorganism and has been explored as source for enzymes with potential biotechnological applications like cellulases, hemicellulases, oxidoreductases and others. Among the oxidoreductases, the cellobiose dehydrogenase (CDH) is an enzymatic class showing great biotechnological interest. Due to this characteristic CDH has been closely studied, however, there are still non-covered particularities related to this enzyme. The functional analysis of a recombinant CDH from T. thermophilus (CDHB) presented the enzyme has a thermophilic behavior and optimum pH in alkaline conditions for inter-domain electron transfer. CDHB showed to be active in cello-oligosaccharides and it was used in combination with recombinant exoglucanases from T. thermophilus (MtCBHI and MtCBHII) to sustainable production of cellobionic acid (CBA) from lignocellulosic materials. Dissolving pulp was hydrolyzed by MtCBHI and MtCBHII in optimized combination and the resulting cellobiose (87.2%) was converted into CBA by CDHB, reaching a conversion of 66.5% in 24 h. Our findings suggest this process is a strategy for CBA production from plant-based material at suitable conversion rates.

Influence of interrupted ageing T6i4-65 on fatigue crack growth of Aa7050 alloy under spectrum loading

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and Carlos A. R. P. Baptista[1]

The application of aluminum alloys encompasses around 70% of the structural components in aircraft, and a better understanding of its mechanical behavior becomes essential for efficient application and ensuring the highest reliability in the in-service structure. Fatigue is the most common failure mode in aeronautical structures. Furthermore, describing crack growth establishes design criteria that incorporate the concept of damage tolerance and constitutes a crucial step in aircraft design. In this context, the aerospace sector fosters research in material fatigue. In this study it was investigated the influence of the interrupted ageing T6I4-65 heat treatment on the fatigue crack growth behavior under variable amplitude loading in AA7050 alloy specimens. The alloy was provided in the form of a 75 mm thick rolled plate in the T7451 commercial heat treatment condition. Subsequently, it was used to obtain the interrupted ageing T6I4 heat treatment condition through a solution treatment (486°C/4h) followed by a two-stage ageing process (145°C/30 min and 65°C/24h). The fatigue tests were conducted using the FALSTAFF spectrum loading and hourglass shaped specimens with a notch was adopted. The crack length was measured by quantitative fractography. It was observed that, compared with the T7451, the AA7050-T6I4 condition presents higher ability of to accumulate plastic deformation. This is related to the favorable combination of higher ductility and strain hardening exponent exhibited by this material condition, that acts in favor of retarding the crack nucleation and early growth from a notch.

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Monascus-derived pigments: sustainable and eco-friendly additives for thermoplastic fabrics and nanoparticle synthesis

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Monascus pigments have gained significant attention across diverse industries due to their natural origin, remarkable stability, and exceptional color quality. In the textile industry, these pigments could serve as eco-friendly alternatives to synthetic dyes, providing fabrics with vivid and naturally derived coloration. Moreover, their effectiveness in enhancing the color properties of thermoplastic materials has been demonstrated. This study delves into the potential of utilizing *Monascus* pigments derived from sugarcane bagasse hemicellulosic hydrolysates as a versatile and sustainable solution for fabric pigmentation. Additionally, it was investigated their application as a catalytic additive in the synthesis of silver nanoparticles, opening new possibilities for the textile sector. Notably, the pigments produced from sugarcane bagasse hemicellulosic hydrolysates exhibit exceptional thermal stability (7.213 Kcal.mol^{-1}). Beyond their role as colorants, these biopigments possess remarkable antioxidant and antimicrobial properties, bestowing textiles with additional active functionalities. The antimicrobial potential of these pigments further augments the performance and durability of textile materials. Furthermore, the catalytic potential of *Monascus* pigments in the production of silver nanoparticles, with a diameter of Dx-(50) 0.0866 µm, unveils fascinating possibilities, presenting a greener and more sustainable process for the development of "*intelligent clothes*" and other advanced textile applications.

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Strategies development for one-way shear and punching shear resistance analyses in bridge slabs

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and Mounir K. El Debs

Menção Honrosa

Most of the shear strength models in the literature deal with the one-way shear capacity of beams or the concentric punching capacity of slabs. However, in the case of loads distributed in small areas and close to the support, frequent loading in bridge deck slabs, an intermediate failure mode between the beam shear and slab punching can occur. In this aspect, several studies were carried out in Europe, but evaluating laboratory tests on a small scale with only a concentrated load close to the support of the slabs. Therefore, most of these experiments do not simulate aspects such as the effect of the combination of concentrated loads and the larger thicknesses practiced in bridge slabs. For this reason, we propose to develop an analytical and numerical study that investigates the one-way shear and punching capacity of slabs under conditions that are more representative of bridge requirements. For this, it is intended, firstly, to calibrate different numerical models of slabs tested in the literature to represent the possible failure mechanisms by shear force that can occur: (i) failure as a wide beam; (ii) eccentric punching failure and (iii) an intermediate failure mode between the one-way shear of beams and punching shear. After validating the numerical modeling strategy, it is intended to simulate slabs with geometry and loading layout closer to professional practice and develop a parametric study with emphasis on the simulation of different combinations of loading, boundary conditions, and slab thicknesses representative of the national practice of design. Based on the numerical study is intended to develop analytical calculation models capable of representing the behavior observed in laboratory tests and that observed in the proposed numerical study. Therefore, the study intends to contribute both to a better understanding of the physical problem and the development of practical design recommendations for professionals related to bridge engineering.

1. Escola de Engenharia de São Carlos (USP).

Cooperative autonomous control of heterogenous vehicle systems

Lucas B. Marcos[1]

and Marco H. Terra

Cooperative vehicle control techniques are increasingly important in several academic and commercial areas, such as smart grids, manufacturing, the automotive industry, and transportation. However, there is still a need to improve the use of these techniques, especially concerning the coordination of aerial and terrestrial heterogeneous mobile robots, which even resulted in the creation of the National Institute of Science and Technology for Cooperative Autonomous Systems – InSac. In this context, this postdoctoral research aims to implement an autonomous, coordinated, and networked control system for land and air vehicles. This system must coordinate the positions and speeds of at least 1 (one) autonomous land vehicle and 1 (one) unmanned aerial vehicle. The development of this control system will be essential to advance research on cooperative autonomous systems, helping to achieve InSac's objectives. It will also contribute to developing scientific initiation, master's, and doctoral projects, functioning as an auxiliary platform for testing new techniques. This post-doctorate was awarded a technical training scholarship, registered in FAPESP process 2021/08103-0, and is associated with research grant FAPESP 2014/50851-0, under the supervision of Prof. Dr. Marco Henrique Terra. It is in the final stages of development, scheduled for completion in August 2023.

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Nano/microfibrillated cellulose with carbon nanotubes applied as interphase/interface in carbon fiber/epoxy composite laminates for aeronautical applications

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and Tita, V.

The reinforcement of polymer matrices with continuous fibers, which constitute the so-called polymeric composites reinforced with carbon fiber (CFRP) have been widely used in the space, aerospace/aeronautical, naval, wind, energy and oil and gas industries due to the growing need to building materials that exhibit high structural efficiency. Improving the interfacial strength between the polymeric matrix and reinforcing fibers, leading to increased overall mechanical performance of CFRPs, has always been a priority for materials scientists, since the interface or interphase between the polymer and fiber reinforcement is extremely important for the transfer and distribution of the applied mechanical load. Furthermore, compared to conventional materials, the reduced weight of using composites results in greater energy savings and efficiency, particularly sought after in the aerospace industry. Cellulose has been one of the most important raw materials used by humans since ancient times and continues to be of great importance in various industries such as paper and clothing manufacturing. It is not a good substitute in many applications due to its unique properties, especially its hydrophilicity and chemical resistance. In addition, there is a new generation of cellulosic materials, generically called nano/microcellulose, among which cellulose nanocrystals (CNC) and microfibrillated cellulose (MFC) stand out, both prepared by low-cost methods involving processes of chemical and physical or physical-chemical extraction. Aiming to achieve advances related to the manufacturing process of carbon fiber composite laminates, the opportunity was seen to invest in the development of a methodology that allows the waterproofing of composite laminates containing MFC/CNT as a compatibilization agent between the reinforcing fiber phases / polymeric matrix. With the improvement of that class of structural composite laminates, it was expected to increase their tenacity and mechanical resistance properties, as well as impact resistance, thus greatly expanding their field of application, mainly in the aeronautical segment.

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Be.Chain: methodology for design applications based on blockchain technology for operations management

Alfredo C. Neto

and Daniel C. do Amaral

Blockchain technology has stood out in recent years for being a solution that integrates the various actors in a business scenario, effectively providing the guarantee of anonymity and traceability issues in a distributed environment. In this way, it records transactional data in the form of a network of data blocks, verified by the network's computers and which, due to this logic, can no longer be erased. In projects of this type, several management points are essential. The context in which the application is involved is highlighted, the definition of the participating actors with roles, responsibilities and common interests, the assets to be controlled, the business process of the context that involves the application, the transactions, the data to be inserted, highlighting the origin of this data, its structure, including data from external systems such as Management Systems, Internet of Things sensors, spreadsheets, among others. You must then define the data model, transaction logic and access control rules of the solution. Within this, can consider technologies that allow the construction of this distributed database, such as hash numbers, block verification algorithms and others that change the form of relationship in a production chain. In this sense, in a real project, it is necessary to define the Smart Contract, the consensus, the endorsement policy, privacy and reliability issues, in addition to the associated service providers. It is understood that technology is difficult to understand and the implementation of real projects goes through issues that, if well defined, facilitate the success of the project. An innovative concept that has been little explored in the literature is the possibility of developing a methodology for creating projects in an easy way and that, if followed step by step, will help in the structuring of projects in the most diverse areas. This research proposes a methodology that assists in the decoding of managerial and technical issues in the configuration of this complicated platform. As a qualitative nature, the research that proposes to carry out a bibliographical survey on blockchain technology and methodologies for the development of technological solutions, also comprises case studies of real projects and the proposal of a generic methodology to be used as one of the ways to describe blockchain-based systems in a language that facilitates development.

New methods for set-based state estimation and fault diagnosis of dynamic systems and applications

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and Guilherme V. Raffo[2]; Marco. H. Terra[1]

Set-based estimation has gained attention in many fields of research and a wide range of applications. This includes state-feedback control, fault diagnosis, robot localization, and parameter identification. In contrast to Bayesian strategies such as Kalman filtering, set-based state estimation methods aim to provide guaranteed enclosures of the system trajectories in applications affected by bounded uncertainties, without assuming knowledge of their stochastic properties. In addition, in view of the required reliability in fault-tolerant control systems, the development of set-based fault diagnosis (FD) methods has gained importance in the last decades. Fault diagnosis aims to determine exactly which fault a process is subject to. Set-based FD methods are usually characterized by robustness and reliability, as diagnosis is often guaranteed. These methods are based on computation with sets, either under concepts such as positive invariance, consistency tests and set separation. Set-based active FD methods allow to determine which fault has occurred, usually by the injection of an optimal input sequence in order to identify the fault, allowing for a faster diagnosis than passive methods. In this context, while set-based estimation and fault diagnosis are relatively consolidated for linear systems, set-based estimation and fault diagnosis of nonlinear discrete-time systems is still an open field. The research project focuses on the investigation of new methods for set-based estimation and active fault diagnosis of dynamic systems. These methods explore the benefits of using constrained zonotopes and possible generalizations as main set representation, which already presented advantages in set-based state estimation and fault diagnosis of a few classes of discrete-time systems in previous works. This will result in improvements and extensions of the previous methods, and the application of these algorithms to practical systems such as joint state and parameter estimation in load transportation using unmanned aerial vehicles, and computation of safe routes for urban air mobility.

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Artificial rocks obtained from mineral waste

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and Eduardo B. Ferreira

This project aims the development of artificial rocks for ornamental and functional surfaces from the waste of natural rocks processed for ornamental purposes. The mining tailings, according to their mechanical and chemical characteristics, compose a mass that may be transformed into tiles for applications in civil construction, in internal and external environments, as well as countertops or ornamentation. Our main objective is to develop knowledge and technology for these residues, allowing national companies to manufacture new products and increase their sustainability in the ornamental stone sector. A market analysis of consumption and waste generation demonstrates the importance of the national production of alternative new materials using such wastes to increase the sustainability of the ornamental rock sector. The applied methodology is based on the study of the necessary processes to transform these residues into artificial stones by different routes: i) the often suggested glass-ceramic process, which includes the manufacture of glass powder of controlled granulometry, followed by compaction in molds and heat treating for controlled sintering and crystallization; and ii) employing geopolymers, obtained through a chemical reaction between an alkaline solution and different minerals as an alternative to high-temperature burning. Both routes use particle packing optimization to achieve better consolidation and pore minimization. The work is under development. As preliminary results, some material bases were obtained through both strategies (glass-ceramic and geopolymer) from which various materials can be developed as alternatives to natural rocks. The base materials are still expected to be improved. This project gains importance by encouraging the creation of national technology, which simultaneously reduces the environmental impact of waste from the Ornamental Stones Sector and offers an approximation of the mineral extraction sector with the University.

Low frequency acoustic separation of water-in-oil emulsions and oil-in-water microemulsions using Brazilian petroleum

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and Agesinaldo M. S. Junior[1]; Luiz O. V. Pereira[2]; José H. A. L. de Andrade[3]; Marcos de S. G. Tsuzuki[1]

In general, water-in-oil emulsions are generated throughout the oil extraction and production process. They contain asphaltenes and/or resins, which form an interfacial film that encapsulate water droplets, generating stable emulsions. In the stage called primary processing, the emulsified oil is recovered and it must meet technical specifications for the maximum amount of water in order to be sent to the refinery. In addition, the separated water produced must also comply with technical (for reuse) or environmental (for disposal) specifications. Nowadays, chemical, mechanical (barriers), thermal and electrostatic methods are mainly used for oil treatment, but there are records in the literature of the possibility of using acoustic methods for this purpose. The low frequency ultrasound mechanism, when used together with a chemical method (demulsifier), it causes the effect potentiation of the chemical in breaking the emulsions, which is produced by great agitation and/or cavitation of the emulsion generated by the application of ultrasonic energy. Tests employing a separation cell with a central frequency around 20kHz were carried out to treat synthetic emulsions. In tests with water-in-oil emulsions (Fig. 1) the best water separation obtained was 76.5% applying 24.9W for 2 minutes in a synthetic emulsion with water content of 33.3% and 10µl of chemical demulsifier (control without ultrasound: 12%). The technique proved to be promising and can be used in conjunction with other technologies. In the test with oil-in-water microemulsions (Fig. 2) the greatest reduction in oil content obtained was 16.6% applying 31.7W for 4 minutes in a synthetic microemulsion with 3000ppm (parts per million) of oil and 20µl of chemical demulsifier (control without ultrasound: 3.7%). Although the reduction in oil content was low, it is important to emphasize that the treatment of oily water is difficult and essential for the environment, in addition, small/medium-sized equipment that can be easily shipped is needed on offshore platforms.

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Figure 1 - Water separation efficiency

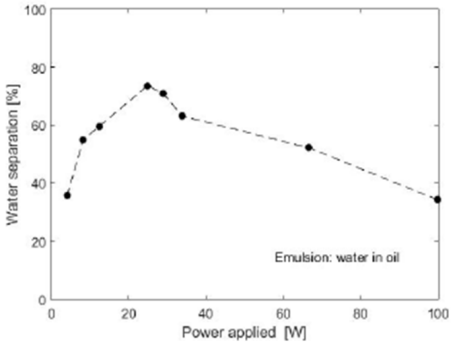
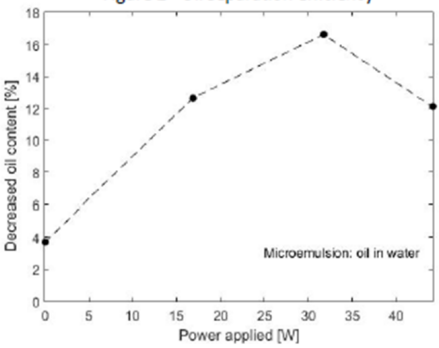


Figure 2 - Oil separation efficiency



A vibration-based structural damage detection strategy using FRFs and machine learning classifiers

Dianelys V. Ruiz[1]

and Cássio S. C. de Bragança; Bernardo L. Poncetti; Marcos M. Futai

In this paper, a damage detection strategy for beam-type structures based on frequency response functions (FRFs) is presented. Five aluminum beams of equal nominal dimensions are utilized in an experimental program under laboratory conditions to obtain experimental FRF data from undamaged and damaged beams. Damages are induced by creating rectangular notches on the beams via saw-cutting. A stochastic finite element model of the beam is developed in MATLAB to construct several training datasets. The damages are modeled by reducing the cross-sectional area at the corresponding damaged elements. Simple damage indexes are utilized as sensitive features. Decision Tree, Support Vector Machines, and Artificial Neural Networks classifiers are trained in the first stage to perform damage detection and localization. Single and multiple damages located at a single zone and more than one zone simultaneously are considered. In the second stage, experimental data not used for training are used for validation. The results obtained at the first suggest that the proposed damage indexes can be used to detect and localize structural damage of beams. Among all classifiers, Artificial Neural Networks is the classifier that best performed. High accuracy is achieved to identify the presence of damage (99.3%) and to detect its location on the beam for some of the training datasets (from 80.0% to 97.1%). In the second stage, the accuracy decreased. However, misclassifications occur mainly for FRF samples at the impact zone, which indicates that the proposed strategy can be efficient to detect damages at locations other than the excitation zone.

1. Escola Politécnica da USP.

Use of organic solvents in the extraction and refining of vegetable oils: investigating physical properties, lipid bilayers, and Gibbs free energies through Molecular Simulation

Lilian C. K. Biasi[1]

and Pedro de A. P. Filho

Molecular dynamics (MD) simulations have been underexplored in the study of lipid extraction and refining, yet they offer valuable insights into macroscopic properties by analyzing the dynamic behavior of individual atoms over time. This study focuses on the application of MD simulations, using a coarse-grained force field (Martini 3), to investigate the substitution of n- hexane with ethanol in vegetable oil production, specifically in the processes of extraction and degumming. The simulations explore the behavior of phospholipid mono/bilayers with and without triacylglycerol in water, ethanol, mixtures of ethanol and water, and n-hexane. The influence of water content on micelle formation during degumming is also explored. The coarse-grained force field allows for efficient simulation of large molecular systems, although it may have limitations compared to all-atom models, particularly in predicting the enthalpy of vaporization and Gibbs free energy of transfer, although these errors are mitigated when calculated relative to the reference value of water. Nevertheless, the force field effectively represents molecular phenomena and interactions in the studied processes. The results indicate that water maintains the integrity of the phospholipid bilayer, while ethanol causes partial disruption and n-hexane leads to complete membrane rupture. Triacylglycerol affects lipid disorder in ethanol but not in water. Micelle formation during degumming is influenced by water content, impacting the volume and number of micelles formed. This study emphasizes the potential of MD simulations in comprehending and optimizing extraction and refining processes in the food industry. These findings offer insights into solvent-lipid interactions and can guide the development of experimental protocols for efficient and sustainable oil extraction and degumming.

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Digital transformation process based on automation and data service: a case study for sustainability projects

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The process of digital transformation propagates throughout the domain of (automated) services and opens up the possibility for cloud services to tend to ubiquitously permeate all human activities, from primary (agricultural) production to assistance and leisure services, passing through for industrial production, fulfillment services and even startups. The diversity of applications creates an even greater demand for theoretical development in service system design methods as well as in the adaptation of these models to the respective domains of application. With respect to design methods the objective is to propose a project cycle (for the digital transformation strategy) in Model-Based Systems Engineering (MBSE) capable of flexibly capturing the demands of users and stakeholders, and trigger the adaptation phase to the application domain with a formal framework. A case study will be the basis for experimentation, linked to the modeling of greenhouse gas emissions in the Amazonian rainforest, a good challenge in terms of complexity and innovation. The design cycle includes the use of requirements analysis techniques, "data lake" treatment, the use (and reuse) of already known processes and of Intelligent Planning (IA Planning).

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Computational modelling for optimization of additive manufacturing processes using machine learning algorithms

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Additive manufacturing (AM) is a technology that enables the fabrication of parts with complex geometries in a relatively short time, offering a rapid and efficient alternative for part manufacturing. It has gained significant prominence in various industry sectors, such as aerospace, defense, automotive, and construction. Among the different techniques of AM, selective laser sintering (SLS) is one of the most widely used due to its speed, ease of execution, and high-quality raw materials. In this technique, a laser device sinters an industrial powder (typically polymer, metal or ceramic) based on a three-dimensional CAD model. However, there are still technological barriers that hinder its widespread adoption, mainly due to the associated operational costs and uncertainties in the mechanical properties of the final part. Another emerging technology that has shown immense potential in the construction industry is 3D concrete printing. This technique utilizes specialized equipment to deposit layers of concrete material based on a digital model, enabling the creation of intricate concrete structures with great precision and efficiency. However, despite the promising capabilities of 3D concrete printing, there are several technological challenges that need to be addressed for its widespread adoption. These challenges include optimizing printing speed (including deposition and nozzle lateral motion), controlling layer thickness, determining the print path, and managing nozzle shape and dimensions. Additionally, ensuring high-quality printed parts with reliable inter- layer adhesion, surface finishing, and understanding the maximum number of printed layers before failure are critical obstacles that require attention. In this context, this research aims to utilize machine learning techniques to address these challenges and optimize the AM processes, with a specific focus on SLS and 3D concrete printing. By leveraging machine learning algorithms, it becomes possible to analyze and optimize printing parameters, such as printing speed, layer thickness, and nozzle path, for both SLS and 3D concrete printing, to improve the quality and reliability of the printed parts. By addressing the technological challenges and optimizing the printing processes for both SLS and 3D concrete printing, this research project aims to contribute to the widespread adoption of these techniques and foster their practical applications across various industries.

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Ultrasound monitoring system of liquid contents applied to oil production separators

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Process monitoring using extraction in more than one dimension through projections obtained by peripheral sensors is called process tomography. For this application, ultrasound sensors can be used to monitor information from objects or fields through which the acoustic beam undergoes some type of interaction. Several ultrasound tomography systems can be found in the literature, for example, for monitoring multiphase flow in ducts, but few are under development. In addition, tomography techniques require sensors to emit along the entire perimeter. The operation of an oil–water separator or any liquid mixture separator can be monitored in a tank in which a mixture of different liquid components flows horizontally. A set of ultrasound transducers should be installed on the vessel wall at different heights in a common stage along the horizontal flow direction. Ultrasound signals are transmitted at different wavelengths through the vessel and are detected between ultrasound transducers. Several acoustic sensors can be placed on the outer wall of the vessel to detect the acoustic propagation generated by different emitters. The acoustic emissions can be processed to generate an acoustic profile to detect the phase shift of a component or other characteristics of the industrial process. However, these applications have limitations in the ability to generate images of the internal volume of vessels from the acoustic emissions detected by the transducers. The image can also be limited by the environmental and structural characteristics of the separators. For this reason, the data acquired through ultrasound measurements for application in process monitoring can be considered incomplete in obtaining images by tomography.

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Contribution to the inspection, monitoring, analysis and diagnosis of railway tunnels with the use of fiber optical sensors

Aline B. Domingues

and Marcos M. Futai

The use of systems like Structure Health Monitoring (SHM) in the monitoring of structures and detection of failures contributes to the accident prevention process and maintenance optimization, thus presenting significant impacts on the lifespan and safety of structures. Based on the simultaneous implementation of various monitoring technologies, SHM's main focus is the detection of damages or abnormal behaviors through an integrated approach with non-destructive techniques. In this regard, this research aims to utilize new promising technologies from the Digital Revolution era for monitoring the structural integrity of railway tunnels in service conditions and proposes to contribute to the SHM of these structures through the utilization of fiber optic sensor (FOS) technology. To achieve this, it is intended to experimentally evaluate a prototype in the laboratory using FOS, propose calibration models between numerical and experimental models, and extend the laboratory evaluation to the application in a real tunnel by defining the sensor instrumentation project up to the computational system for data interpretation and result analysis. The project also foresees the use and application of a digital twin that will link the data from the real SHM twin, inspection data, and computational analyses with the virtual twin. After integrating all the data with the digital twin, it is expected that all the information can be accessed through it.

Aqueous two-phase systems for application in liquid-liquid extraction studies

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and Luis A. Follegatti-Romero[1]

Liquid–liquid equilibria were determined for aqueous two-phase systems (ATPSs) composed by poly (ethylene glycols) (PEG) of different molecular weights (1500 or 4000 or 6000 or 8000 or 10000) $g.mol^{-1}$ potassium sodium tartrate at T= (293.15, 303.15 and 313.15) K with u (T) = 0.05 K and atmospheric pressure. The phase diagrams were obtained using turbidimetry method and Merchuk methodology. Effects of temperature and polymer molecular weight were discussed. Finally, the NRTL activity coefficient model and Othmer-Tobias and Bancroft will be used for correlating tie line compositions. The main objective of this work is to apply the liquid-liquid equilibrium data in the extraction of biomolecules.

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Unlocking the potential of Operational Experience Feedback for organizations

Bruno C. M. Kawasaki[1]

and Fausto Leopoldo

Operational Experience Feedback (OEF) promotes the circulation of information that is useful to pilot production systems. It can also support organizational improvements based on the knowledge of real work combined with horizontal and upward communication flows. However, OEF is commonly hindered by internal communication failures, organizational silence, fear of punishments and lack of confidence in work peers and superiors. Thus, our research goals are to elucidate the barriers to OEF and to identify possible strategies to overcome them. To do so, we initially propose a literature review on OEF, without restriction regarding the field of knowledge. Next, based on complexity theories, we contextualize the need for feedback processes in the evolution of production systems and management conceptions. Finally, we dialogue with psychodynamics of work to discuss organizational silence and the intersubjective skills necessary for OEF. Concerning how to strengthen OEF processes, we suggest the following paths forward: 1) enriching managers' theoretical framework so as to enable them to understand the concept of real work, i.e., what is actually done– which is not restricted to nor described by goals, indicators and prescriptions alone–; and 2) improving the planning of spaces, schedules and performance evaluation systems with the aim of affording discussions on daily work experiences and work rules, as well as developing communicational, intersubjective and listening skills in the organization. For future research purposes, we suggest studies on the real work that makes OEF processes possible.

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Performance of different supports for RWGS reaction

Éder V. de Oliveira[1]
and Martin Schmal; Rita M. de B. Alves

Different solids were synthesized, and the metals Fe and Cu were impregnated as active phases to *reverse water gas-shift* reaction. The scan temperature test was performed to evaluate the activity of them. All catalysts showed high conversions and high selectivity for CO. Only traces of methane were detected, which, the methanation reaction, is the parallel and concurrent reaction with RWGS. Among the catalyst, six of seven showed higher conversion, near the thermodynamic equilibrium of RWGS reaction for temperatures above 600 ºC. Two catalysts stand out for showing high conversions at temperatures superior to 450 ºC. To sum up, all the catalysts developed were highly selective for CO formation, and two of them showed activity close to the thermodynamics equilibrium of RWGS reaction from 450 ºC and the other 4 catalysts showed high activity from 600 ºC.

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Electrical Impedance Tomography: reconstruction by simulated annealing and noise study

Edson K. Ueda[1]

and Rogério Y. Takimoto

Electrical Impedance Tomography (EIT) is a non invasive imaging technique based on estimating the distribution of electrical conductivity in a body when a low amplitude current pattern is applied to the surface of the body and the potentials at some points on the surface are measured using electrodes. A typical EIT setup consists of placing electrodes around the object to be imaged. Then, a low-amplitude current is applied between a pair of electrodes and electrical potentials are measured at all electrodes. This process is repeated n times, applying electrical currents to n pairs of different electrodes, and measuring the electrical potentials. Fig. 1 shows a EIT configuration with 16 electrodes, in which two current patterns are applied J1 e J13.

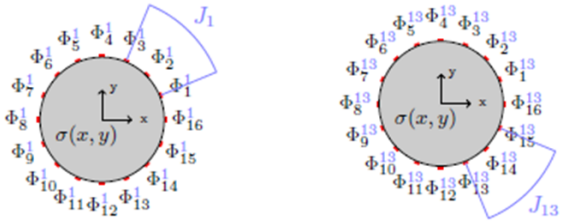

Figura 1: Given a domain with a conductivity distribution $\sigma(x,y)$, the EIT equipment is used to measure the electric potential Φ_j^i at all the $j \in [1,16]$ electrodes for the current pattern injected into the pattern J_i.

The Simulated Annealing (SA) meta-heuristic is used to perform the image reconstruction, in which the distribution of electrical conductivity is determined. This algorithm modify only one parameter on each iteration, and it is verified if the cost function is smaller or not. If it gets smaller, the solution is accepted and a new modification is performed, else the solution can be accepted by the Boltzman probability or be rejected. A modified SA was studied, in which a crystallization factor modifies the probability distribution density contributing to the method to escape the local minima. A benchmark was performed with mathematical function, in which it simulates problems with several local minima and local with zero derivative. This benchmark compared the original

1. Escola Politécnica da USP.

SA, the Adaptive Simulated Annealing and the SA with crystallization. The SA with crystallization performed better for all benchmarks functions, showing its ability to escape from local minima and not depend on the derivative of the function. The goal of this project is to use a deep neural network to make the image reconstruction, however it is necessary to add all the possible sources of noise to create a robust method. A deep neural network is already developed to reconstruct some benchmark tests, in which phantoms with geometric shapes (circumference, square and triangle) are reconstructed. A problem of this developed trained set is that there are no source of noise which is present in real measurements, such as the misplacement of the electrodes, the contour change and the contact impedance. The first and second problem is possible to emulate, however the last one it is not possible to emulate it. A possible solution is to perform the reconstruction of a real measurement with the SA and determine these impedance. Once the real displacement is known, it is possible to get a better solution by adopting the local of the saline aqueous solution as uniform with unknown impedance and only one variable is optimized by the SA for this local. So, once there are less parameters to be optimized, the reconstruction is faster and the cost function is smaller. Fig. 2 shows an real measurement case and two reconstructions, one with the saline aqueous solution not uniform and another one with saline aqueous solution uniform.

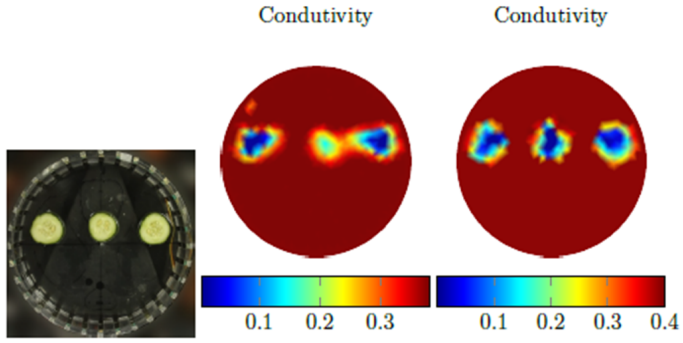

Figura 2: Reconstruction of a real case measurement.

Effect of cellulose-based fillers on vulcanized natural rubber

Flávia L. S. Freitas[1]
and Carla A. Correia[1]; Ticiane S. Valera[1]

Cellulose nanocrystals (CNCs) fillers have exceptional properties and are environmentally friendly nature, making them attractive for several applications. One is incorporating CNCs into natural rubber (NR) compounds to improve properties like elasticity modulus. CNCs can be obtained by different acid methods that promote singular features in interfacial adhesion, according to the type of acid used. This study focuses on characterizing CNCs obtained by hydrolysis using sulfuric acid and less aggressive phosphoric acid. Moreover, the properties of NR nanocomposites containing different concentrations of CNC were analyzed. The results indicated the formation of a zinc–cellulose–rubber complex, leading to a reduction in optimal vulcanization time and an increased cure rate of the NR compound. This effect was particularly pronounced in samples treated with phosphoric acid. The formation of the zinc–cellulose–rubber complex also impacted the morphology and mechanical properties of the composites. The nanocomposites containing CNCs treated with phosphoric acid exhibited significant improvements. Specifically, the tensile strength increased by 90%, elongation at break by 16%, and modulus at 300% strain by 51%. The increased aspect ratio facilitated improved adhesion between the filler (CNCs) and the rubber matrix. Consequently, CNCs treated with phosphoric acid showed promise as an effective means of enhancing the mechanical properties of NR compounds.

1. Escola Politécnica da USP.

Simple formulas for the dynamic response of parametrically excited slender and straight structures immersed in fluid

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In many engineering applications, the use of time demanding computational tools is often employed for the analysis and design of different structures. In turn, analytical solutions of simplified representations of each problem are often used to obtain insights and qualitative aspects of the main phenomena involved. In this work, the problem of a vertical slender beam under the action of an imposed vertical displacement at one of its ends, while immersed in fluid, is considered. This model is suitable for the representation of vertical umbilical cables and exploration risers in offshore operations. The scenario near the known phenomena of parametric resonance is of particular interest in this work. The starting point is the analytical solution presented in Vernizzi et al (2020), which provides good results for the structural response under excitations around the main parametric resonance. In that work, the presented results for the analytical solution are in good match with those obtained with the Finite Element Method (FEM). However, the mathematical steps necessary for the solution are quite cumbersome, requiring the aid of symbolic computation. To make the solution attractive for usage with minimal computational effort and specialized knowledge, a simplified way to obtain the results is herein developed. Using a chosen structural parameter to represent the dynamics of the structure and a series of appropriate simplifications, polynomial expressions in this parameter are obtained as a final form of the analytical solution. Those expressions use tabulated coefficients obtained by the authors, and can be easily implemented on spreadsheet software. The obtained results are in good agreement with many simulations made with the aid of the FEM for different structures from the literature. It is expected that this formulation can be used as a design aiding tool, especially on early stages of design where the evaluation of the effects of variations on the structural parameters is of interest and can demand a great amount of time if performed with more sophisticated models.

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The importance of pegmatites in the demand for Lithium

Hudson de A. Queiroz[1]

In the 2030 national mining policy, PNM-2030, the expression "critical mineral" is defined as a scarce, essential or critical mineral resource for a country. Three situations are understood for the application of the term: the first concerns a resource in which the country is highly dependent on exports, as is the case of agrominerals in Brazil, called NPK, corresponding to Nitrogen, Phosphorus and Potassium. The second situation encompasses those resources associated with the production of cutting-edge technology equipment, which is in growing demand, such as REEs (rare earth elements), Lithium, Silicon, Tantalum, Cobalt, Thallium, Vanadium, platinum group elements, among others. Third situation is that in which a certain mineral resource of the country proves to be essential for its economy. In the CT&I plan for strategic minerals 2018-2022 the REEs, Li and Si, considered "minerals carrying the future" are treated as strategic for the country, due to its growing demand in electronic products and other uses in the high-end technology, in addition to the application in clean energy sources. Observing this scenario of interest in strategic minerals, the first question that can be asked is where to find such resources in Brazil? The geological environments and host rocks in which strategic minerals occur are diverse, but in the southeast Brazil, in particular, the state of Minas Gerais, there is abundance of a type of rock with the potential to host significant amount of lithium ore, very important metal to the energy transition topic, this rock is the pegmatite. Brazil is recognized worldwide for its pegmatites occurrences and one Li-enriched body in eastern Minas Gerais is being characterized in this work in order to understand the distribution of lithium among the minerals of the pegmatite.

1. Escola Politécnica da USP.

Concentration technology and use of bauxite tailings

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and Morgana Rosset[1]; Denise C. R. Espinosa[1]; Fernando G. da S. Araujo

The worldwide quest for increasing the efficiency of production processes and the efficient use of natural resources guides the focus on industrial and mining waste. The bauxite mining tailings, which are usually deposited in tailings dams, have little known chemical characteristics and physical properties. Therefore, this work aims at the physical, chemical and mineralogical characterization and to evaluate the technical viability for the concentration of alumina present in the sample of waste from the bauxite washing. The test methodology used for the concentration covers the steps of sample preparation, homogenization and quartering, purification, technological characterization, exploratory tests to identify the behavior of the material, magnetic concentration tests with different magnetic field intensities and finally concentration tests by flotation. The mineralogical composition of the MRN bauxite tailings sample is mainly composed of kaolinite, gibbsite and iron oxyhydroxides, in addition to other minerals that complete the remaining 5% of the sample. The concentration study demonstrated the technical feasibility of concentrating up to 17.16% of the mass of bauxite waste with a concentration of up to 53.04% of Al2O3. The results achieved demonstrated the technical feasibility of concentrating part of the alumina present in the bauxite tailings, mainly contained in granulometric fractions greater than 0.006mm, demonstrating that the tailings from bauxite mining can, with the use of appropriate technologies, be used as reserves of aluminum ore.

1. Escola Politécnica da USP.

Strategic planning for digital transformation: evolving to Industry 4.0

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Globalized production imposes a new pace on industrial processes, creating challenges for the implementation of new technologies that bring positive results to industrial processes. In this sense, this research aims to develop a "sound" approach, based on the formal modeling of processes, to endorse a strategic innovation plan, respecting the company's level of maturity and readiness to implement technologies aimed at Industry 4.0. The company's current stage will be modeled from the maturity analysis, also including the modeling of the main production objectives, and organizational strategy, defined as an initial requirement of the process. A plan for digital transformation will be generated from this stage, analyzing innovation capacity, readiness, and taking into account the impact on production in addition to risk mitigation. In this way, the research contributes to the process of evolution and modernization towards a model inserted in industry 4.0, based on PIMM 4.0, and on a readiness analysis model. A case study will be applied to at least two companies from the Industrial Pole of Manaus engaged in the Jornada Amazônia 4.0 of the Brazilian Association of Industrial Development (ABDI), with the support of Suframa.

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Non-invasive hidrophone sensor to detecting and monitoring cavitation in pipeline under ultrasound power for cleaning

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The occurrence of growing and fouling formation in ducts of systems operating in the transport of crude petroleum in processing industry is a is one of the main problems during the extraction and processing of oil in the industry causing often non-programmed pause for cleaning the pipelines and equipments leading to a loss of efficiency and production decrease. Beyond to the technical problems of operation, a blocked pipeline can contribute to high financial losses and even make the process unfeasible. Although a plenty of cleaning using ultrasound power transducer in not possible, at least its use combining with detergents containing additives helps to remove encrusted solids since current methods of removal and cleaning are not fully effective, and sometimes inefficients. Currently, studies are demonstrating that ultrasound is effective in removing or even inhibiting encrustations, however, removal is only effective in regions where cavitation is intense. In this sense, it is crucial to know the regions and intensity of cavitation. For this, the development and construction of hydrophones are essential to know the location and intensity of cavitation inside the tubes. For this reason, this study has been proposed the research and development of hidrophones to detect and monitoring cavitation. The results will be compared with those obtained experimentally indirectly from cavitation generated in eroded aluminum sheets when exposed to regions where the phenomenon is more intense.

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Electron beam application to sterilization of wort to optimize process of ethanol production

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The contamination of the wort by microorganisms accounts for 1/3 of the total losses in the plants during the fermentation process for ethanol production. It is estimated that the annual loss for the sugarcane–energy chain, due to the presence of contaminants in the raw material, amounts to approximately US$2.0 billion. For these reasons, the main objective of this study was to develop a new methodology to assist ethanol plants in sterilizing this raw material. Through this proposal, it was possible to evaluate the continuous flow sterilization method of the wort using an electron beam accelerator. For this purpose, an experimental pilot scale unit was built, which included tanks for storing the material before and after sterilization, pumps for homogenization and transport of the wort, solenoid and manual valves, irradiation system, dosimetry and control system, within the facilities of the electron beam accelerator. By studying parameters such as flow rate, dose rate, and radiation dose absorbed by the wort, among others, obtained from the pilot plant, it was possible to assess the efficiency of this new methodology in wort processing, as well as to evaluate the cost/benefit compared to other methods described in the literature, technological development, and economic feasibility for its implementation in the aforementioned plants. It is important to emphasize that the study of the proposed methodology was carried out through a collaboration between ESALQ, POLI, and IPEN. The latter provided and supported the use of the electron beam accelerator allocated at the CTR (Radiation Technology Center). This project was funded through a public/private partnership (EMBRAPII/Sinochem Petróleo Brasil Ltda) via the National Petroleum Agency (ANP).

1. Escola Superior de Agricultura Luiz de Queiroz da USP.
2. Escola Politécnica da USP.
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Preparation and characterization of organogels containing vitamin E for cosmetic application

Renata M. Martinez

and André R. Baby

Human skin is attacked daily by ultraviolet (UV) radiation and pollutants. Such aggressions can promote lipid peroxidation mediated by free radicals in cells, generating DNA damage and inflammatory processes, in addition to endogenous vitamin E depletion. The use of antioxidant cosmetic products has potential for treatment; however, the stability and permeation of these active ingredients may be a limiting factor in their use. Thus, the present work aimed at the development and characterization of organogels containing vitamin E and their dispersions in bigels, focusing on cosmetic application. Bigels were prepared with several combinations of vitamin E–loaded organogels containing 12-hydroxysestearic acid/candelilla wax as organogelators and mineral/vegetable oil as organic phases into acrylic polymer hydrogel. Organogels and bigels were characterized regarding their microstructure, rheological profile and evaluation of efficacy *in vitro* and *ex vivo*. Despite the potential for permeation of hydrophilic and hydrophobic actives through the skin, increased stability and sensory modification, organogels were still little explored in the cosmetic area. The bigels produced were characterized as weak viscoelastic oil-in-water gels, with adequate stability determined by thermal and centrifugal stress. The presence of vitamin E generated little influence on the rheological profile and efficacy *in vitro* and *ex vivo* of the bigels, emphasizing the need for further studies in the presence of stress in the biological sample. Organogels were characterized as weak pseudoplastic gels. The type of organogificator was relevantly influenced in the presence of vitamin E. 12-Hydroxysesteric acid had a reduction in gel strength, while candelilla wax showed increased strength. All phase transition temperatures were reduced in the presence of vitamin E. The results indicated the potential use of organogels and bigels in the delivery of vitamin E for topical application, enabling the development of formulations with stability and modulation of the rheological profile as needed.

Overview of the business and innovation ecosystem in the Midwest of Santa Catarina

Ivanete S. Hahn[1]

and Moacir de M. O. Júnior[1]

Santa Catarina is a reference in the innovation ecosystem in Brazil. Florianópolis, for example, has the highest density of startups per thousand inhabitants in the country – there are five startups for every thousand inhabitants. Blumenau (in the Itajaí Valley) and Joinville (in the North) are also among the ten Brazilian cities with the highest density of scalable, innovative, and technological businesses. However, this is not the case in the midwestern region, which despite having a well-established business ecosystem - is dependent on technologies from other regions, especially from other countries – which affects their competitiveness. This study focuses on answering: How to configure successful business and innovation ecosystems, when there are distances and geographic limitations (in terms of location); cultural (in historical terms/ historical-cultural formation); social (income and wealth inequality)? These limitations are present in most inland municipalities (and are a reality in other emerging economies). The study will be conducted using as a theoretical lens, the Theory of Dynamic Capabilities, and the advanced Paradigm of Knowledge-Based Dynamic Capabilities. In theoretical terms, there is an opportunity to contribute since few studies have specifically addressed the panorama of business ecosystems, and those that have been conducted (e.g. Graça & Camarinha-Matos, 2017; Gupta et al., 2019) do not advance toward the application of these concepts in real business ecosystems.

1. Faculdade de Economia, Administração, Contabilidade e Atuária da USP.

Is there life after oil? The future of O&G companies from the perspective of organizational temporality

Murilo A. Oliveira[1]

Oil and gas (O&G) companies are experiencing unprecedented changes in their history. Despite concerns about climate issues and the future of global energy landscapes, these organizations have a significant role in economic and social development, making them relevant research subjects in organizational studies. This study provides a synthesis of ongoing research on developing strategic orientation for the future of O&G companies, considering their track record in sales efficiency and investments in technology and innovation amidst the impending energy transition. The study design is organized into sequential phases, with a longitudinal examination of the past ten years' financial and innovation indicators available in the first phase of the European Commission's Industrial R&D Investment Scoreboard reports. The second phase, characterized by an analysis of the future adaptation narrative in the official management reports of the researched companies, is supported by a temporality perspective and employs historical rhetoric analysis and the construction of meaning in desirable futures, aided by text mining resources. Preliminary results reveal distinct capabilities in mobilizing processes and actions in developing imagined futures and different orientations toward the future within dimensions associated with clean energy innovation and productive and financial efficiency. In this sense, these organizations possess the ability to project a future temporal horizon aligned with their trajectory. Evidence also emerges of potentially capable companies balancing economic performance with environmental aspirations, which we term "futuristic ambidexterity".

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Implementation of a controllership and compliance department in an innovation company

Guilherme J. de S. Moretti[1]

and Roni C. Bonizio[1]

Organizations, over time, have become increasingly dynamic and complex, with a surprising demand for competitiveness. Which brought the need to improve processes and different types of controls (PIVA et. al., 2017). Thanks to this peculiar scenario, controllership and compliance become strategic areas for the organization. It is then responsible for "informational support, internal control, tax planning, budget preparation and operational measures, also actively participating in the formulation of strategies" (LUNKES et. al., p. 64, 2009). The objective of this study is the construction and implementation of a controllership and compliance department in a Brazilian multinational company, which develops technologies for industrial automation, in the city of Sertãozinho/SP, and the postdoctoral student himself will be responsible for the department. This company is Nova Smar S.A. The development of these areas in an organization has as its main objectives participation in the planning and control of operational and strategic variables, through an effective analysis of the data, which are acquired within the organization, processed by the controllership and transformed into important information for decision making. at all organizational levels. According to Lunkes et. al. (2016, p. 7), "controllership evolved without having its functions and concepts well defined, possibly because it had a practical origin." Its implementation to be successful must cover the organizational culture and use the time necessary for an effective implementation. According to the general objective of the work, this is an applied, qualitative, descriptive research that seeks solutions for a complex and ill-structured problem. How the department will actually be developed and implemented, this is an action research.

1. Faculdade de Economia, Administração e Contabilidade de Ribeirão Preto (USP).

Prosodic units in Portuguese: the treatment of spontaneous speech for natural language processing

Vinícius G. Santos[1]

With the advent of technology, the digital availability of linguistic data has been increasingly encouraged to facilitate its use not only in different areas of Linguistics, but also in related areas such as Natural Language Processing (NLP). As part of the Center for Artificial Intelligence (Inova.USP/IBM/FAPESP), the TaRSila project [https://sites.google.com/view/tarsila-c4ai/] was conceived to overcome the lack of publicly available Brazilian Portuguese speech data for training basic NLP systems (e.g., ASR, TTS). Within TaRSila, we have been conducting the segmentation of spontaneous speech from the academic project NURC-SP, one of the most influential corpora in Brazilian Linguistics. Data are segmented into linguistically motivated prosodic units with terminal and non-terminal values (RASO; MELLO, 2012), whose identification is based on the auditory relevance of acoustic cues (pause, F0, duration, intensity) and their visual inspection in Praat (https://praat.org). It will facilitate, for example, the training of spontaneous speech recognition systems, since the data will exhibit utterances with complete meaning, which will also assist in automatic punctuation prediction. The dataset will have ≈334 hours of transcribed speech, of which a subset (≈40h) has been prosodically annotated, enabling both new linguistic studies (discourse markers, parentheticals, lists, prosodic unit typology etc.) and computational processing itself. The subset data treatment comprises several steps, such as training of annotators ($\kappa \geq 0.8$), forced and phonetic alignment of the original transcription, annotation in multi-level transcription files (.textgrid) (namely, automatic transcription/alignment review, prosodic units segmentation, and manual punctuation), in addition to text normalization. Already partially available [https://hdl.handle.net/21.11129/0000-000F-73CA-C], NURC-SP collection will soon be fully available on an open-access web portal.

1. Faculdade de Filosofia, Letras e Ciências Humanas da USP.

Imbrications between academic and institutional scopes: the terminographic work of a glossary in the field of Aeronautical Meteorology at the Department Of Airspace Control

Rafaela A. J. R. Peixoto[1]

Lexicographic work requires careful criteria to assess term candidates, effectively select terms and, especially, elaborate definitions that are pertinent to the demands of the target audience for which a linguistic product is intended. In terminology and terminography, more specialized characteristics are at stake, which are analyzed based on content selected for the generation and compilation of corpora. In the case of a glossary published by a regulatory institution in the field of Aeronautical Meteorology, this content also has an institutional interface, a pattern reflected in the elements presented in the glossary. In this work, the research developed at the Department of Airspace Control (DECEA) will be presented, for the expansion of a terminological database in the field of Aeronautical Meteorology, based on institutional translation (KANG, 2020; PRIETO-RAMOS; GUZMÁN, 2021; PRIETO-RAMOS; CERUTTI, 2023) and corpus linguistics (TOGNINI-BONELLI, 2001; TAGNIN, 2015) theoretical frameworks. In this sense, the objective is to discuss (a) how the specialized and institutional interfaces are presented in terminographic products of specialized fields; and (b) how the preparation of the glossary took into account these specificities in the process of linguistic analysis of corpus and writing of definitions. The stages of the research were developed as follows: (a) compilation of specialized and institutional subcorpora for the AERMET corpus; (b) analysis of the corpus; (c) selection of candidate terms; (d) study of profiles of specialized and institutional glossaries; (e) search for definitions and information relevant to the specialized and institutional characteristics; and (f) elaboration of definitions. As a result, regarding the specialized and institutional interface, it was found that institutions tend to a normative approach, even when they present more sophisticated stances regarding descriptive perspectives in specialized fields; and, in relation to the preparation of the glossary, the greatest difficulty was to align demands of different audiences, especially academic and professional ones, and maintain the complexity of specialized content disseminated in institutional environment.

1. Universidade de São Paulo.

Hydroxyapatite-zirconia composite conventionally and flash sintered with *in-situ* synchrotron X-ray diffraction

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and João V. Campos[2, 3]; Anderson O. Lobo[4]; Rishi Raj[2]; Eliria M. J. A. Pallone[1]

The combination of bioactivity and mechanical strength exhibited by hydroxyapatite–zirconia (HZ) composites makes them highly promising materials for bone implants. To further enhance their appeal by reducing production costs, exploring alternative more energy-efficient techniques are essential. Flash Sintering (FS) emerges as an innovative method enabling the rapid sintering of ceramics in a matter of seconds and at considerably lower furnace temperatures when compared to conventional sintering (CS). In this way, we investigated and compared the thermal history, crystalline phase evolution, and microstructure of a ceramic composite with 50wt.% hydroxyapatite and 50wt.% zirconia during FS and CS. To achieve this, we performed *in-situ* synchrotron X-ray diffraction (XRD) analysis during both sintering methods of the HZ. Isothermal FS was carried out at 1000ºC with a DC electric field of 500 V/cm and an electric current density of 20 mA/mm^2, applied for 10 seconds. For the CS, a heating rate of 30 ºC/min was used until 1400 ºC for 10 min. To compare the temperature achieved by the sample in both experiments, we used the Pt-standard method to estimate the temperature accordingly with the Pt lattice thermal expansion. The Pt-standard revealed that CS and FS reached similar temperatures (1400 ºC and 1370 ºC, respectively). Intriguingly, zirconia was completely converted from the tetragonal-to-cubic phase, and HAp was completely changed to α-TCP after FS. However, the zirconia phase transformation was not observed for CSed sample, and most HAp remained steady (i. e., only a small portion of it was converted to α- and β-TCP). Regarding the microstructure, needle structures were observed in the FSed sample (suggesting directional crystalline growth), which was not detected in their conventional sintered equivalents. Thus, these results suggest that the electric field applied during FS leads to athermal effects for HZ composite, since both FS and CS samples reached similar temperatures, but showed different microstructure and phase transformation.

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Production of pea protein microgels and their application as pickering stabilisers

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Pickering emulsions are well-known by their higher physical stability compared to conventional emulsions. In these systems, colloidal particles arrange themselves at the interface, acting as stabilizers. However, not every particle can act as Pickering stabilizer and their production remains a challenge. In view of that, the aim of this work was to produce pea protein microgels and evaluate their behavior as Pickering stabilizers. The microgels were produced by thermal treatment, followed by ultrasonication to reduce the aggregates´ size. Then, microgels were characterized and emulsions (10% oil v/v) were produced, varying the concentration of microgels in the continuous phase (1 – 0,25 wt.%). Optical micrography of emulsions were obtained and the droplets size were estimated using Image J. Conventional emulsions stabilized by native pea protein were also produced and compared to Pickering emulsions in terms of physical stability. The microgels presented mean particle size of 232.3 ± 5.9 nm and – 25.3 ± 0.6 of zeta potential. The size distribution curves indicated the presence of aggregates of larger size, which was confirmed by transmission electron micrography. Microgels presented higher surface hydrophobicity compared to native pea protein, with contact angles of 53.2 ± 1.1° and 36.0 ± 3.4°, respectively. The physical stability of emulsions was directly related to the concentration of protein material in the continuous phase. The mean droplet size observed for Pickering emulsions was 25.2 µm, achieving 29.0 µm after storage. Similarly, conventional emulsion presented 27.8 µm mean droplet size, evolving to 30.7 µm after 24 h. With the reduction of protein material in the continuous phase, instability features were observed. For conventional emulsions, phase separation was observed a few hours after emulsion preparation. The droplets mean size decreased with time, pointing to the occurrence of oiling-off. On the other hand, no phase separation was observed for Pickering emulsions, and their mean droplet size increased with time. These results indicate the occurrence of coalescence rather than oiling-off, meaning that pea protein microgels were able to provide stabler emulsions than its native counterpart. In conclusion, pea protein microgels presented as a very promising material for Pickering emulsion stabilization.

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Optical instrumentation at Giant Magellan Telescope

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The current state of the optical instruments and subsystems under development for the Giant Magellan Telescope (GMT) with Brazilian participation is described. We are contributing, along with international partners, to three of the GMT's first light instruments: MANIFEST, GMACS, and AOTC. MANIFEST is a fiber positioner that will expand the field of view for GMT spectrographs, while being able to observe multiple targets at the same time. It is being developed by Australian Astronomical Optics - Macquarie University (AAO-MQU). One of the interfaces of this instrument is accomplished by a Filter Box (FB), that connects MANIFEST to the G-CLEF spectrograph. The FB will filter and transmit light using optical fibers into several science modes to the spectrograph. It must be such that precision radial velocities (PRV) could be performed, aiming at the search of exoplanets. The project is currently in the pre-conceptual phase of development. For this instrument, we are designing the FB optics and optomechanics, as well as executing part of systems engineering for MANIFEST. of the filter box (FB) that will interface. GMACS is a visible multiple-object spectrograph with moderate resolution (R=1500- 5000). The prime contractor for the ongoing Preliminary Design is the Harvard- Smithsonian Astrophysical Observatory (SAO), with expressive Brazilian participation, through IAG and Steiner Institute, in mechanics, optomechanics, electronics, optics, software, and systems engineering. We are assessing the optical elements to refine and ensure the manufacturability and performance of the instrument. Simultaneously, the optomechanics is under development to support and guarantee the optical requirements. The AOTC is the Adaptive Optics Test Camera and it is going to be a support instrument to close the adaptive optics (AO) loop, allowing problem mitigation and testing of the GMT AO system. We are developing the optical and opto-mechanical design of the optics that are going to integrate all the wavefront sensors necessary for the NGAO and LTAO adaptive optics modes of the GMT Infrared spectrographs (GMTNIRS and GMTIFS). The project is currently in the conceptual phase of development.

1. Instituto de Astronomia, Geofísica e Ciências Atmosféricas da USP.
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Electrical structure of the southern Paraná basin lithosphere using magnetotellurics: new constraints to the Paraná-Etendeka magmatism

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and Mauricio S. Bologna[1]

The Paraná basin (PB) evolved on the South-Western portion of Gondwana, one of Pangea's supercontinents formed by the amalgamation of different terranes. PB subsidence began in the Paleozoic and sediments were deposited in five major cycles until the Mesozoic, forming a ~400 My register of tectonic events to which it was subject. In the Lower Cretaceous, the PB was affected by a massive volcanic episode that generated the Paraná Magmatic Province (PMP), one of Earth's largest igneous provinces. It originated prior to continental break-up and the inception of the South Atlantic Ocean. The geodynamic causes for the magmatism are still a matter of debate and new geophysical and geochemical data permit us to constrain possible scenarios as physical parameters of deep layers of the Earth, otherwise inaccessible, are being published. In this study, we use the magnetotelluric (MT) method to yield new constraints to the physical state of the PB lithosphere. The MT is a passive technique based on the electromagnetic induction principle. Natural variations in the geomagnetic field caused by thunderstorms and the solar wind induce current in the Earth. By measuring the electric and magnetic fields on the surface, we can estimate variations in the electrical conductivity in the subsurface from tens of meters to hundreds of kilometers. We focus our discussion on a conductive (<10 Ωm) and long (~800 km) mid-crustal lineament mapped parallel and close to the PB axis, named Paraná Axial Anomaly (PAA). The observed conductivity can be caused by reactions between country rocks and fluids evolved upon crystallization of magma ponded or intruded at the base of the crust, giving indirect evidence for underplating. Moreover, because fluids must rise along fractures and the PAA is also coincident with maximum basalt thickness, the lineament can be an image of the fossil main conduit for magmatic extrusion. This location is possibly related to previous weak zones in the crust created by paleo sutures that could also have controlled the initial basin subsidence.

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High-energy emission from stars and stellar systems

Maria V. del Valle[1]

Since the discovery of cosmic rays more than a century ago the nature of their sources has been an open question. They are mostly high-energy protons and nuclei whose energy spectrum extends over eleven orders of magnitude. Their energy distribution is well described by a power law, the first spectral break is called the knee. Cosmic rays with energies below the knee originate in our Galaxy. These high-energy charged particles are scattered by magnetic fields in the interstellar medium, hence it is not possible to pinpoint their sources. Thus, the quest for cosmic accelerators as well as for acceleration mechanisms mostly relies on photons which propagate along a straight line. The modelling and observation of gamma rays are fundamental for the study of the nonthermal processes that operate in these sources. High-energy gamma rays must come from cosmic rays that are at least as energetic as the gamma rays they produced. Gamma-ray galactic astronomy is therefore fundamental to understand the production of cosmic rays. In particular, the Galactic cosmic rays are thought to be produced mostly in supernova remnants shocks, however open questions exist on the matter. Supernova remnants are bright, powerful sources, but scarce. Other weaker but much more numerous Galactic sources can also contribute to the Galactic cosmic-ray population, such as massive stars. Massive stars modify their surroundings through their powerful winds and strong radiation fields. The fast winds shock the interstellar medium, transferring mechanical power to it. Massive stars are grouped in clusters. Recently, massive stellar clusters are being studied as possible contributors to the Galactic component of cosmic rays. The interacting stellar winds supply large amounts of kinetic energy that could be used to accelerate cosmic rays up to very high energies. In this talk I will present my contributions to the modeling of high-energy processes is massive stars and stellar clusters.

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Paleomagnetic study of the Neoarchean basalts from Carajás Basin, Amazonian craton

Pedro L. G. Martins[1]

and Trindade, R. I. F.[1]; Toledo, C. L. B.[2]; Silva, A. M.[2]; Bellon, U. D.[1]; C. Júnior[3]; Machado, S. M.[4]

The onset of modern plate tectonics, involving subduction and mountain uplift, is a key event triggering the emergence of large continental masses and an oxygen-rich atmosphere, setting the stage for the origin of complex life. But when and how plate tectonics started is still unknown owing partially to the inherent difficulty in studying events that occurred in deep time. Paleomagnetism has the potential to contribute to the discussion by quantifying past plate velocities. Here, we present systematic paleomagnetic study, including the first high-quality paleomagnetic poles and high-precision zircon U-Pb geochronology, of an Archean block of the Amazonian craton for the ~2760-2740 Ma interval. The data were obtained from basalts in the Carajás Basin (Parauapebas Formation), northern part of the Carajás Mineral Province. They occur in extensive successions of massive or amygdaloidal lava flows, with at least twelve cycles and a total thickness of > 370 m. Overall, after inverting all reverse sites, 5 sites in the deeper section yields a calculate paleomagnetic pole of 40.5ºE, -44.6ºS, N = 5 A95 = 6.5º, K = 18.5 (C1), while the remaining sites yield a paleomagnetic pole of 342.4ºE, -54.3ºS, N = 28, A95 = 14.8º, K = 27.8 (C2). The primary origin for the remanence is supported by a preliminary positive baked contact test and rock magnetism. ID-TIMS zircon U-Pb dating constrains the crystallization ages at 2748.67 ± 2.06 and 2742.50 ± 0.75 Ma regarding volcanic mafic rocks. Our results, integrated with geological evidence reveals that the Carajás block occupied low latitudes at the time, and could have been part of the Superia supercraton during the Neoarchean (~2.74 Ga) at equatorial latitudes. The significant change (34.6 ± 12.5º to 3.4 ± 8.5º) in the paleolatitude observed through the lava flow sequence over a relatively short time interval (~10 Ma) suggests that Archean plate motion was much faster than today (>20 cm/year), which supports the idea that the plate tectonic regime is rooted in the early Archean.

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Deep learning for automatic identification of microorganisms grown on solid media

Antonio R. S. Parmezan[1]
and Solange O. Rezende

Microorganisms produce a wide range of bioactive natural compounds with high biotechnological and pharmacological potential, so recognizing their species is crucial. Identifying microbes in laboratories requires considerable time, financial resources, and skilled labor. We propose a framework to automate this task through artificial intelligence, particularly machine learning in the deep learning modality, focusing on analyzing images of cultures grown in Petri dishes. Our framework is organized into four steps: (i) acquisition, labeling, and storage of microorganism images, (ii) image preprocessing, (iii) model training and evaluation, and (iv) deployment of trained models. In terms of deep learning, this research investigates topology selection, architecture parameterization, transfer learning, and model interpretability. Concerning technological results, we are developing the first image database of known and taxonomically labeled microbes. This database is integrated into a prototype computational system that allows users to capture, annotate, store, retrieve, and recognize microorganism images. Our findings and technological products promise to accelerate the pace of microbial biodiscovery studies.

1. Instituto de Ciências Matemáticas e de Computação da USP.

Increasing trust in digital twins

Ana P. Allian
and Elisa Yumi Nakagawa

Digitalizing automated pallet transport systems with digital twins is a growing trend in the manufacturing industry. By creating digital replicas of physical assets, manufacturers can simulate and optimize their production processes, identify and resolve potential issues (production bottlenecks, device failures, energy consumption, and safety hazards), and ultimately improve their overall efficiency and productivity. Often, digital twins from different manufacturers need to interact in complex systems. The goal of this project is to a set of architecture drivers and architecture solutions to ensure trust when dealing with digital twins. The architecture drivers provides the quality requirements to propose the architecture solutions, including standard interfaces protocols to ensure interoperability between different systems, security to help protect the system against potential threats, and data privacy features to help protect sensitive data exchanged between digital twins. We also present a code example of how to implement a trustworthy digital twin architecture in the context of a smart manufacturing considering the architecture drivers identified.

Numerical analysis of Lagrangian schemes for viscoelastic flows

Débora de O. Medeiros[1]

and José A. Cuminato[1]

This work contributes to the study of a Lagrangian scheme applied to viscoelastic models of flows with surface tension and allows the simulation of High Weissenberg Number Problems (HWNP). The constitutive equations are reformulated aiming at investigating the causes of the numerical instabilities that plague simulations involving high Weissenberg numbers presenting a challenge for the study of viscoelastic fluids. The reformulation of the constitutive equations is based on the method of characteristics and intends to improve the numerical stability for high Weissenberg values with no introduction of artificial parameters. The work entails theoretical foundational studies of the proposed scheme, proof that its truncation error may be second-order, and the stability analysis of it in the one-dimensional case. The proposed numerical scheme is applied to the constitutive equations solved together with the Navier-Stokes equations, in the context of the MAC method and free surface boundary conditions with surface tension. Encouraging results are observed for confined and free surface flow problems subject to surface tension effects. This would allow for solving accurately problems in the field of rheology with both industrial and commercial applications.

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Modified Imperfect Repair Model $ARAM_1$ and new PLP parameterization

Jeremias L. T. Lopes

and Vera Tomazella; Francisco Louzada

The Arithmetic Reduction of Age (ARA) class of models has been widely used in modeling equipment maintenance data. However, to use these models, the condition that the system must wear out continuously between failures must be satisfied. This condition implies $\beta > 1$ in the Power Law Process (PLP) often used to fit these data. However, there are several cases where there may be a system improvement between failures, i.e. PLP with $\beta < 1$. In this context, the aim of this paper is to introduce and study a new model of Imperfect Repair (IR) in Reliability. We propose the modified ARA_1 model $ARAM_1$, which enables model systems in the process of reduction or degradation. We also propose a new PLP reparameterization as time truncation to incorporate it into the new model, and thus preserve the original interpretation of the PLP parameters. We evaluated the performance of the parameter estimators through Monte Carlo (MC) simulations. For illustration purposes, we consider the failure times of nine sugarcane harvesters. We compare the fit of the standard model with the ARA_1 model. The results indicated the superiority of the $ARAM_1$ model compared to the ARA_1 in several situations, which illustrates the importance of the proposed approach.

The Tenfold Way: classification of weakly interacting crystalline topological insulators and superconductors

Renato V. Vieira[1]

In it was shown that irreducible free fermion systems can be classified into 10 distinct classes, based on the presence and behaviour of time-reversal and charge-conjugation symmetries. Each class is composed of a space of Hamiltonians compatible with the symmetries, and in it was shown that the spaces of time-evolution operators generated by each class is one of the 10 symmetric spaces of compact type. From these symmetric spaces we can construct ring spectra that represent complex and real topological K-theory. This is at the heart of the K-theoretical classification of crystalline topological insulators and superconductors. In the hypothesis that the systems are free, meaning there is no external potential fields or fermion interactions, is captured by considering the class of quadratic Hamiltonians, a subspace of the Lie algebra of degree 2 elements in the Clifford algebra of field operators, and the associated symmetric space is a quotient of the Lie group corresponding to this Lie algebra. The non-trivial phases of matter are related to Hamiltonians that satisfy the bulk gap hypothesis, ie those with the Fermi energy level contained in a neighborhood disjoint from the Hamiltonian spectrum. In the weakly interacting regime we extend the class of Hamiltonians to even degree elements in the algebra of field operators which don't close the bulk gap. A difficulty in extending the classification to interacting systems is that the Hamiltonians are no longer contained in a Lie algebra, and so the Lie algebra/Lie group correspondence is no longer available. In joint work with Aza and Mu¨ssnich we propose such extensions by relating the classes of interacting Hamiltonians to Murray-von Neumann groupoids of the C*-algebras of observables of the system. As described in the geometric realizations of the Murray-von Neumann groupoids are E_∞-spaces, whose homotopy groups are the K-groups of the operator C*-algebras.

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Assessing logical reasoning abilities in transformer models

Paulo P. A. Silva

Transformer models represent the state-of-the-art approach in natural language processing. They form the basis of language models that are behind popular applications such as Google Translator and ChatGPT. Transformers are remarkably effective at a wide range of natural language processing tasks they are trained on, such as question answering, summarization, and text generation. Curiously, these language models (LMs) also exhibit numerous abilities that emerge unintentionally as a by-product of their general pretraining. Large language models such as GPT-3 and GPT-4, for example, are able to perform complex tasks for which they were not previously trained. Perhaps less obviously, but equally interestingly, encoder-only transformers also exhibit key linguistic and cognitive abilities, albeit implicitly. These LMs have been shown to encode information on things such as tense and number, anaphora, determiner-noun agreement, semantic roles, syntactic dependencies, and relational knowledge. Nonetheless, transformer models have not been extensively studied as regard to their logical reasoning capabilities – fundamental aspect of intelligence, human or otherwise. My work investigates transformers' logical reasoning skills. Particular, I investigate whether they can perform logical reasoning tasks, how generalizable this logical reasoning ability is, how it is structured within their parametrization, and its role in commonsense reasoning. In this presentation, I intend to show my main findings based on probing techniques; i.e., auxiliary classifiers that permit to inspect the information encoded by a model. As those experiments demonstrate, transformers do not exhibit consistent logical reasoning abilities. Instead, they solve logical tasks by leveraging on dataset statistics. They exhibit an impressive behavior on particular datasets for which they are trained on, but a poor performance when attempting to generalize. This shortcoming in logical reasoning problems explains part of the difficulties language models exhibit in structured tasks, such as math and argumentation. Thus, understanding the structure of LMs' logical reasoning is vital for developing robust mechanisms that facilitate the generation of accurate knowledge from databases, structured or not. Furthermore, this understanding may enable us to discern the extent to which LMs' inferences and arguments stem from reasoning versus purely associative memory.

Machine learning based on chaotic transport

Eduardo L. Brugnago[1]
and Iberê L. Caldas

We develop a machine learning algorithm of recurrent neural network architecture in reservoir computing framework. We replaced the reservoir of oscillators, traditionally used in this type of network, for a succession of measurements on systems of interest, namely, non-twist symplectic discrete time systems as the standard non-twist map. Additionally, the artificial neural network was modified and we implement optimizations in order to obtain the most efficient learning. The trained network was applied to control the transport of particles in the same system used as a reservoir, in this way, the machine learning structure acts on itself, causing disturbances in its reservoir according to the control demand. The machine learning control proved to be able to manage the emergence and breakdown of transport barriers, manipulating the shearless curve according to the needs stipulated in the training phase.

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Characterization of membranes for nanofiltration and recovery of Lithium and Boron from produced water

Jeann C. R. de Araújo[1]
and Caetano R. Miranda[1]

One of the challenges in the oil and gas production sector in industrial exploration plants lies in the management of produced water (PW). PW is a byproduct of extraction from underground reservoirs, containing dispersed hydrocarbons, suspended solids, minerals, and dissolved gases. These components can pose a potential contaminant, requiring proper treatment and responsible disposal of PW. Advanced technologies, such as nanofiltration and reverse osmosis separation processes are some of the proposed solutions being evaluated in the industry for efficient PW management. The incorporation of nanostructures into polymeric media has attracted attention as a possibility to obtain membranes for nanofiltration, enabling better control of separation processes and recovery of dissolved components in PW. In this context, this study aims to understand the mechanisms involved in enhancing nanofiltration technologies by applying a methodology to control the synthesis routes of 2D and 3D nanostructured systems. Alongside synthesis processes, the development of a characterization methodology becomes essential to obtain systems with proven functionality and feasibility for large-scale application. From a microstructural perspective, the selectivity properties and incorporation of nanomaterials into the polymeric medium can be altered, thus modifying membrane adsorption and permeation. Starting from computational screenings and materials already applied in electrochemical separation systems, the use of Polyimide (PI) as a polymeric base for constructing membranes with graphene-based nanostructures will be investigated, as graphene has shown potential for boric acid adsorption (boron (B) occurring compound in PW). Another line of analysis aims to improve nanomaterials with enhanced selectivity for lithium (Li) in saline solutions in the presence of other monovalent ions such as sodium (Na).

1. Instituto de Física da USP.

Characterization of optoelectronic devices based on gallium oxide

Marina S. de Medeiros[1]

and José F. D. Chubaci

In this work gallium oxide (Ga_2O_3) samples were deposited at different temperatures using the IBAD (Ion Beam Assisted Deposition) technique. Ga_2O_3 single crystals have α, β, δ, ε and g, polymorphs with free energy of formation in the order of β<ε<α<δ<g. Among different Ga_2O_3 polymorphs, the β phase is the most stable phase with a monoclinic structure and has received significant attention in recent years due to its large band gap, chemical stability and potential for easily scalable bulk crystal growth through a Modified Czochralski method. The reported band gap of β- Ga_2O_3 varies between 4.5- 4.9 eV, which is larger than SiC and GaN. The results obtained were promising. Optical analyzes of transmittance and reflectance were carried out, from which it was possible to obtain the band gap of each of the 5 types of thin films deposited at different temperatures on p-type silicon by Ion Bean Assisted Deposition (IBAD). The values obtained are in agreement with the literature. As for the structural analyses, Raman and X-ray diffraction analyzes were performed. The Raman analysis indicated peaks belonging to Ga_2O_3 and also the presence of a peak for silicon and silicon dioxide. 4-layer optoelectronic devices were built, but the analyzes led to the conclusion that there were 6-layer devices, Al/Si p/SiO_2/ Ga_2O_3/ Ga_2O_3 doped with Al/Al. Photoelectric effect was observed in the IxV analysis, indicating possible use as light sensors and photo resistive memories.

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Experimental-numerical assessment of the mechanical behavior of human hair fiber through force spectroscopy by atomic force microscopy

Raissa L. de Oblitas[1]

and Fernanda de S. Teixeira[1]; Maria C. B. da S. Salvadori[1]; Péter Z. Berke[2]

Mechanical properties of different classes of materials, namely, human hair fiber and Poly (methyl methacrylate) (PMMA), were assessed through force spectroscopy by atomic force microscopy (AFM) in order to obtain its viscoelastic properties. The characterization was done by applying and critically comparing different post-processing methods to (i) computationally generated viscoelastic indentation data and (ii) to experimental load-displacement curves obtained through AFM for PMMA (as a reference material) and hair fiber.

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The solute polarization and structural effects on the nonlinear optical response of based chromone molecules

Rodrigo do M. Gester[1]

and Sylvio Canuto

The solute polarization due to solvent is a an electrostatic quantum effect that impacts diverse molecular properties, including the nonlinear optical response of a material. An iterative procedure that allows updating the solute charge distribution in the presence of the solvent is combined with a sequential Monte Carlo / Quantum Mechanics methodology and Density Functional Theory methods to evaluate the nonlinear optical (NLO) response using the hyper Rayleigh scattering (HRS) of a series of chromones recently identified in Chamaecrista diphylla, an herbaceous plant abundant throughout the Americas and used in folk medicine. From this study, it is determined that from gas to solvent environment, the systems acquire low refractive index (n) and an improvement of the first hyperpolarizability (βHRS), signaling potential NLO uses. It is shown that the octupolar contributions (βJ=3) superate the dipolar ones (βJ=1) and dominate the second-order optical response in both gas and liquid phases, which indicate nontrivial optical materials. Moreover, the solvent environment and structural changes in the periphery can tune significantly the dipolar/octupolar balance, showing a key to control the decoupling between these contributions.

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T2 measurements for moving samples under strong magnetic field gradients

Agide G. Marassi[1]

and Arthur G. de Araújo-Ferreira[1]; Éverton Lucas-Oliveira[1]; Edson L. G. Vidoto[1]; Aparecido D. F. de Amorim[1]; Willian A. Trevizan[2]; Tito J. Bonagamba[1]

Nuclear Magnetic Resonance (NMR) is one of the fundamental techniques used in the oil industry for logging operations and on the laboratory scale to study rock formations due to its accuracy in offering a reliable estimation of oil well productivity. There are two kinds of well-logging operations: Wireline Logging, where the NMR measurements are performed under static conditions, and Logging While Drilling (LWD), where the measurements take place during the drilling process, with the tool translating, rotating, and vibrating relatively to the formation. To understand the behavior of NMR signals measured under LWD conditions, we developed a setup that includes a single-sided magnet, rf probes, and a mechanical system that emulates a relative sinusoidal motion between the sample and the applied magnetic field. Representative rock samples were selected according to their relaxation times, being short, intermediate, and long compared to the oscillation period of the LWD simulator: Fontainebleau, Berea, Portland Red, and Indiana Limestone. The results show that despite modifications observed in the relaxation times distribution, which could lead to a misinterpretation of the geological formation, the total porosity remains unaffected and independent of the sample motion during the NMR measurements, even under severe conditions and using the standard data processing procedures.

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Low Field NMR in Porous Media Applications and Quantum Information Processing

Arthur G. de Araujo-Ferreira[1]

and Agide G. Marassi[1]; Tito J. Bonagamba[1]

Our group has a long history of NMR research and instrumentation, ranging from medical diagnosis applications to high-resolution NMR spectroscopy, low-field NMR petrophysics, and quantum information processing. During this research project, a few of these areas were covered, and this presentation aims to show a few of the contributions in instrumentation for low-field NMR and quantum information processing. NMR relaxometry has many applications in industry and science, from the food industry to geophysics. Most notably, it is a remarkable tool in petrophysics. The use of low-field NMR relaxometry to study rock samples from oil reservoirs is what started and funded this research project. With our extensive expertise in this area, we focused on developing instrumentation to study the application of NMR in unfavorable conditions of the well and logging while drilling situations. In this case, the NMR data is acquired during the drilling process, resulting in very low signal-to-noise ratios. That also requires much effort to develop the necessary signal processing to refine the results and produce usable data, and that constitutes an essential part of the work done in our group. Regarding quantum information processing, NMR is a valuable medium to test and demonstrate practical quantum concepts. Our group has developed over the last decade several NMR experiments demonstrating quantum computation and information concepts using quadrupolar nuclei. Quadrupolar nuclei are those that have nuclear spin high than 1/2. Some of these applications were performed using cesium, which has spin=7/2. These nuclei can be used, for example, to represent a 3-qubit system and perform quantum algorithms that require three qubits. Another possible application of quadrupolar nuclei is using Nuclear Quadrupole Resonance (NQR). This type of experiment is exciting because it does not require high external magnetic fields, and its setup, beyond the probe, requires only a computer and a spectrometer, which can be very portable and relatively cheap.

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Optical technique to sensorial control of the green coffee

Bruno P. de Oliveira[1, 2]
and Jarbas C. de C. Neto

The quality analysis and selection of green coffee beans is currently carried out by the sensory methods in pairs in which the SCAA cupping protocol is followed where the experience is the decisive fact of the results. The evaluators work on the identification and score of 11 sensory attributes, for this it is made the roasting of 300 g of raw coffee in the band of clear toast (10 – 15 min) in a direct flame roaster, does the grinding and division in equal parts in 5 pots, infuses water and let rest for 5 min. Following is the sensory analysis, filling and definition of the sample in triple (1 evaluator for each assessment). This process is carried out by the staff daily and with each new tower and/or coffee batch exchange. The present research is aimed at the application of concepts of artificial intelligence, in which a beam of light is emitted in the raw/green coffee sample, and this interacts with light and emits other wavelengths, these are collected by an optronic system and converted into an electromagnetic spectrum, then AI performs calculations and decisions for the definition and better grouping of the sample. We seek and aim to develop a new analytical form of green/cru coffee, in which we have a greater standardization of the analyses obtained and organization on a national scale of information. This will be done through the qualitative and quantitative measurements that are obtained by the equipment with a consequent organization of the database and provision in the form of service to customers and partners. Finally grouping the samples into 4 large groups of Special, Gourmet, Riado and River coffees.

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Implementing (U-Th)/He thermochronology at the Instituto de Geociências, USP: instrumentation and initial calibration

Alisson L. Oliveira[1, 2]

and Parra, M.[1]; Gautheron, C.[3]; Souza, D. H.[1]

Low temperature thermochronology has become one of the most employed techniques to address the spatial and temporal pattern of tectonic evolution, as it allows the extraction of the thermal history of a rock, particularly at the uppermost kilometers of the crust. In orogenic settings, and less so in cratons, (U–Th)/He has the potential to resolve these histories due to the relatively higher diffusivity of Helium from U-rich minerals. In this project, we are aiming to implement the (U–Th)/He method at the CPGeo – USP (Centro de Pesquisas em Geocronologia e Geoquímica Isotópica – Universidade de São Paulo) using a MAP 215–50 Single Collector Mass Spectrometer coupled with a near-infrared laser for ^{4}He measurements and an Inductively Coupled Plasma Mass Spectrometer for measuring U, Th and Sm. The initial results from standard mineral Durango apatite (reference age 31.1 ± 1.4 Ma) were obtained in collaboration with partner researchers at the Université Paris Sud (UPSUD) and produced dates from 1.8 to 83.8 Ma, with a weighted mean value of filtered data around 30.8 ± 1.1 Ma, in range to reported values for this standard. Additionally, samples from the Central and Eastern Cordilleras, South of the Colombian Andes, were dated at USP/UPSUD and University of Potsdam (UP), independently. Data shows that samples dated at USP/UPSUD (n= 18, av. 9.39 ± 0.75 Ma) agree within errors to dated samples at UP (n= 32, av. 10.32 ± 0.75 Ma). Improvements are still needed, in addition to a first batch of samples completed solely at the CPGeo labs, but the initial data are encouraging. In the next few months, we hope to make this laboratory available for the academic and industrial community as a part of the Multi-User facility USPMulti CPGeo-LTC.

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Sectional number and related topics

Cesar A. I. Zapata

In this talk, we present a construction of foundations of sectional theory in category theory and build bridges between important areas in mathematics. For an arbitrary morphism f: X → Y in a category C, we define a numerical invariant, the sectional number of f, in terms of covers of the target Y. By specializing the category C, we obtain some known invariants as well as several new invariants. For instance, by setting C = The category of topological spaces Top, our definition yields the sectional number of a map which is studied in Algebraic Topology. In addition, we build bridges between important areas in mathematics. For instance, Fixed point theory, Borsuk-Ulam theory, Milnor fibration and Robotics. To study concrete applications of the sectional number in industry and technology. We present a solution for the motion planning problem for a multi-robot system of firefighting and rescue unmanned ground vehicles (UGVs). In the air transport sector, we will present a solution to the problem of aircraft navigation. On the other hand, we will present a study of the complexity and design of solutions to some problems generated by a pandemic, for example, economic and social problems.

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Reconstruction of Voronoi diagrams in electrical impedance tomography

Danilo R. Souza[1]

and Ernesto G. Birgin[1]; Antoine Laurain[2]

The inverse problem of electrical impedance tomography (EIT), also known as the inverse conductivity or Calderón's problem, is an active field of research with an extensive literature; see for a thorough review of the topic. The goal of electrical impedance tomography is to reconstruct the electrical conductivity inside a medium, using measurements of the electrical potential on the boundary obtained by applying boundary currents. EIT is a low cost, noninvasive, radiation free and portable imaging modality with various applications in medical imaging, geophysics, civil engineering and nondestructive testing. In the EIT literature, the conductivity is often supposed to be a relatively smooth, continuous function. However, the case where the conductivity presents discontinuities is important for applications, in particular in geophysics and civil engineering, but also in medicine. In this project we consider the particular case where the conductivity is a piecewise constant function. The domain of definition of the conductivity can then be partitioned into cells such that the conductivity is constant in each cell. In this work we also suppose that the set of cells is given by a Voronoi diagram.

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Relation between some p-groups of class two and exponent p and some Fp-Lie algebras of class two via alternating bilinear maps

Farangis Johari

Let p be an odd prime number. Let Fp be a field of characteristic different from two. Suppose that N2 is the category of finite-dimensional nilpotent Lie algebras of class two over the field Fp and that ALT p is the category of alternating bilinear maps of F-vector spaces. Consider the category EXp of finite p-groups of class two and exponent p. We establish a relationship between the category N2, the category ALT p and the category EXp. Then as an application of this technique, for an odd prime p, we obtain an equivalence between the classification of certain p-groups and n-dimensional Fp-Lie algebras. The problem of the classification of finite p-groups has a long history. Now, we focus on finite p-groups of class two. Among several tools for studying these p-groups, one of the techniques is the use of alternating forms and vector spaces. The relationship between groups of nilpotency class two and bilinear maps began with the works of Brahana and Baer in 1930's (see [1, 2]). This method is the first approximation of the well-established use of the Mal'cev–Kaloujnine–Lazard correspondence (sometimes inadequately referred to as the Baker–Campbell–Hausdorff formula); see [8, Section V.5] and [9, Section 10] for details. A finite p-group G is called special if its center is elementary abelian and Z(G) = G′. The rank of a special p-group is defined by the definition of the rank of its center considered as an elementary abelian p-group. Special p-groups of rank one are called extra-special. Mazur [10] described some special p-groups of rank two for odd primes p, using alternating bilinear maps. In particular, p-groups of class two and exponent p are closely related to vector spaces equipped with alternating bilinear maps. This result plays an important role in the classification of capable p-groups of class two with exponent p. Some researchers characterized some classes of small-dimensional Lie algebras, and several classifications have been appeared in [3, 5, 6] Hence, focusing on the notions of categories and functors, we are interested in giving different aspects for characterizing nilpotent Lie algebras of class two. Throughout the paper, let p be an odd prime number and let Fp be a field of characteristic different from two. In this paper, we focus on the category N2 of finite-dimensional nilpotent Lie algebras of class two over the field Fp. Consider the category p whose objects are alternating bilinear maps B: U U W such that U and W are nontrivial finite-dimensional Fp-vector spaces and the image of B spans W. The rank and the dimension of B are denoted as dim W and dim U, respectively. Consider the category EX p of finite p-groups. We obtain an equivalence between the categories 2, p, and p. Then we show that, for an odd prime p, the problem of classifying groups G of order pn and exponent p with the derived subgroup of order pk is equivalent to classifying the n-dimensional Fp-Lie algebras of class two with the derived subalgebra of dimension k.

Optimization of the first Dirichlet Laplacian eigenvalue with respect to a union of balls

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The problem of minimizing the first eigenvalue of the Dirichlet Laplacian with respect to a union of balls with fixed identical radii and variable centers in the plane is investigated in the present work. The existence of a minimizer is shown and the shape sensitivity analysis of the eigenvalue with respect to the centers' positions is presented. With this tool, the derivative of the eigenvalue is computed and used in a numerical algorithm to determine candidates for minimizers. Overall, for configurations formed by a small number of balls (between 2 and 10), candidates for minimizers of the eigenvalue are proposed and their geometrical properties as well as the appearance of regular patterns formed by the centers are discussed.

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Synthesis and characterization of star-shaped amphiphilic polypeptides based on L-Lysine

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Synthetic polypeptides have been attracted the attention of several industrial and scientific areas as promising biocompatible and biodegradable materials for developing implantable materials, including novel drug delivery systems for DNA, RNA and other therapeutics. In this view of the current technological relevance, star-shaped polypeptides based on L-lysine with controllable sequential blocks of hydrophobic amino acids were prepared by ring-opening polymerization (ROP). These macromolecules are attractive to design new bio-inks and other technologies with electrolytic, amphiphilic, and pseudoplastic rheological behaviors suitable for tissue engineering, pharmaceutics, cosmetics and regenerative medicine.

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Singlet oxygen production by analogues of natural anthocyanin pigments

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Anthocyanins are responsible for most of the red, blue and purple colors of flowers, fruits and leaves of plants. Given the limited structural diversity of the chromophoric moiety of the anthocyanins and the fact that plant extracts generally consist of mixtures of several different anthocyanins, synthetic flavylium cations have been extensively employed as surrogates for unravelling the pH-dependent chemistry of anthocyanins and for the development of strategies for the stabilization of their color. The photophysics of the excited singlet state of anthocyanins and flavylium cations has been extensively investigated both experimentally and theoretically, however, much less is known about the excited triplet states of flavylium cations. In the present work, we address the question of excited triplet state formation of flavylium cations in fluid solution at ambient temperature via measurements of sensitized singlet oxygen formation quantum yields for a series of 14 different flavylium cations in TFA-acidified acetonitrile. Fluorescence quantum yields and lifetimes have been reported for the 14 flavylium cations in dry acetonitrile acidified with 0.1 mol L^{-1} trifluoroacetic acid in order to suppress ESPT in the excited singlet state of the hydroxyflavylium cations. Triplet sensitized singlet oxygen formation was detected for four out of the fourteen flavylium cations investigated, which exhibited significant yields of singlet oxygen formation, demonstrating that, in some cases, relatively long-lived excited triplet states of flavylium cations can be formed in acetonitrile at ambient temperature when ESPT is absent or suppressed by addition of TFA. The other ten flavylium cations produced little or no singlet oxygen, the differences being consistent with the chemical structures and the corresponding photophysical properties of the excited singlet state of the compounds. The current results suggest that excited triplet state formation should be extremely inefficient, if it occurs at all, upon excitation of the flavylium cation form of naturally occurring anthocyanins.

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Peptide-resins derived from Shepherin I: exploring the ability to bind divalent metal ions for column chromatography and in-batch purposes

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Divalent metal ions can bind to peptides containing histidine because, owing to its basic character, the imidazole moiety is a susceptible site to metallic coordination. Our research group has been studying an interesting glycine- and histidine-rich[1,2] peptide named Shepherin I (Shep I) that contains the ATCUN (*Amino Terminal Copper and Nikel Binding*) motif Gly-Gly-His (GGH), is a potent antimicrobial peptide, has the uncommon amino acid sequence G^{1}YGGHGGHGGHGGHGGHGGHGHGGGGHG^{28}, thus six repetitions of GGH, and ability to chelate divalent metal ions. These properties are very important in human health and nutrition, environmental chemistry, and general science. For instance, metal-chelating ability is attractive for use in analytical applications, such as essential metal detection and quantification in different samples. The aim of the present work is to design, prepare and test Shep I derived sequences of variable sizes covalently attached to resins, thus able to bind Ca^{2+}, Cu^{2+} and Zn^{2+}, that can be employed as stationary phases in column chromatography and in-batch analytical applications. So, we designed Shep I-derived short peptides (a tetra- and a pentapeptide) with one or two histidine(s) C-terminally connected to HMBA-PEGA. Such peptide-resins were synthesized by the microwave-assisted solid-phase synthesis at 60ºC. For characterization, small amounts of the peptide-resins obtained were submitted to cleavage from resin without deprotection of His-trityl group, the crude peptides were isolated and analyzed by liquid chromatography/electrospray ionization- mass spectrometry (LC-MS) and acid hydrolysis followed by amino acid analysis. The results indicated that the peptide-resins obtained were the desired ones and provided their peptide contents. Knowing the right substitution degree of the peptides on HMBA- PEGA is crucial for finding the stoichiometry between peptide (therefore, the ATCUN motif) and the metals as well as for the next experimental step of performing quantitative determinations of Ca^{2+}, Cu^{2+} and Zn^{2} monitored by fluorescence spectroscopy and ICP- OS.

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