

Artificial Intelligence is transforming how we use computing power to solve complex problems. Incorporating AI tools within Physics Based Models is an emerging area which can enable the solution of so far unsolved problems in many application domains, including energy industry. Machine learning has shown promising outlook to several challenging problems in CFD, such as the identification and extraction of hidden features in large-scale flow computations, finding undetected correlations between dynamical features of the flow, and generating synthetic CFD datasets through high-fidelity simulations. These approaches are forming a paradigm shift to change the focus of CFD from time-consuming feature detection to in-depth examinations of such features and enabling deeper insight into the physics involved in complex natural processes. Machine learning has provided numerous opportunities to advance the field of CFD, including to accelerate the computationally expensive direct numerical simulations, to improve turbulence closure modeling and to develop enhanced reduced-order models.

This symposium is designed to stimulate CFD professional in industry and academia by providing a venue to exchange new ideas and discuss challenges and opportunities as well as expose this

newly emerging field to energy industry. The purpose of this symposium is to provide comprehensive information and insights regarding the role of AI accelerated physicsbased modelling in the energy industry. With a highly impressive agenda and a prestigious lineup of speakers from various sectors. including the industry, academia, and software vendors, this symposium offers a unique

opportunity for experts to share their knowledge and experiences.

The agenda encompasses technical presentations covering a wide range of topics, including but not limited to Scientific Machine Learning, Reduced Order modelling, Physics Based Digital Twin, Multi-Scale Modelling, Physics Informed Neural Network and Hybrid/Fusion Modelling.

AGENDA

05:00 PM – 06:00 PM Closing Remarks followed by Social/Networking Hour

Laurent Alteirac:

Laurent Alteirac began his career in 2001, driven by a passion for innovation. Throughout his journey, he gained expertise across all three core divisions of the company. In the Production Systems division, in the Sand Screen Department, Laurent developed the industry's first intelligent multi-zone completion system, revolutionizing efficiency and productivity beyond gravel pack. A decade later, post Macondo, he validated the industry first API 17G cut and seal subsea landing string valve. Transitioning to the Well Construction division, Laurent developed the first Orion II mud pulse

modulator. In the Reservoir Performance division, he played a pivotal role in creating and patenting Music telemetry, which improved data transmission in oil and gas testing operations. Additionally, in the Digital Division, he commercialized the Valve Commander project, enhancing North America Land stimulation automation. Laurent also contributed to sustainable energy solutions in the New Energy realm delivering the first high temperature geothermal frac plug for the Utah Forge research project. Currently, he serves as the Enabling Technology Development (ETD) Manager. Laurent's academic achievements include two Master's degrees in Engineering: one from Arts & Métiers France and one from Georgia Tech USA. Laurent strives to create performing teams. He is a SLB dual career and has 3 kids.

Title: Pivot for the Future

Madhu Vellakal

Madhu Vellakal is a Solutions Engineering Manager at Rescale. Madhu brings several years of experience in computational science, highperformance computing, analytics, and machine learning to Rescale. He is part of the AI Physics team at Rescale chartered with accelerating the adoption of AI technologies in CAE workflows. He received his Master of Engineering from The University of Illinois Urbana-Champaign and has

authored numerous technical publications throughout his career.

Title: Accelerating CFD Simulations through HPC and AI on Rescale

Abstract: AI Physics powered by NVIDIA on Rescale revolutionizes computation-driven R&D workflows, offering a turnkey, multi-cloud solution built for enterprises and fully supported to accelerate product development. This talk will cover the high-level introduction of AI Physics on Rescale and its potential, along with real-world implementations in various fields including aerospace and automotive industries. The talk will include a demonstration of AI Physics end-toend workflow on the latest GPUs on Rescale.

Dr. Kuochen Tsai

Kuochen Tsai has spent 18 years with Shell as a SME in multiphase, particulate, combustion, and erosion/corrosion modeling. Before joining Shell, he worked for the Dow Chemical Company at Freeport, TX for 9 years in Engineering Sciences. His current interests are in multiphase flows, biomass processing, erosion, flow assisted corrosion and physics-based machine learning. Kuochen has a Ph.D in mechanical engineering from SUNY Stony Brook.

Title: A Flow Assisted Corrosion Model with Machine Learning in a General Pipeline Configuration

Abstract: Pipeline corrosion induced from CO_2 or O_2 is a serious and costly hazard for oil/gas industry. $CO₂$ and $O₂$ are different complex corrosion processes. We developed an innovative hybrid model that combines both the first principal physics and advanced machine learning (ML) method into a single model that can predict multiple corrosion mechanisms involving $CO₂$ and $O₂$. It can significantly speed up corrosion analyses in pipeline geometry in comparison to computational fluid dynamics (CFD). The ML prediction output was used to account for the local effects of mass transfer limitations, which requires 7 variables for a general pipe configuration with bends: average inlet velocity, pipe ID, pipe bend angle, pipe bend radius, CO_2 partial pressure, pH value and temperature. However, the total number of CFD simulations required are significant, further reduction will be helpful in managing the computational costs. It was found that the predicted maximal corrosion rates are only sensitive to flow variables as in most industrial scenarios the corrosion rate is mass transfer limited; thus, the last three reaction kinetics related variables don't need to be parametrized in CFD. This new approach greatly lowered the number of CFD simulations needed to generate data for machine learning. The result is a hybrid model that combines the CFD-based ML flow model with a reaction kinetics based on known stream conditions and is about $10⁶$ times faster than corrosion CFD simulations with acceptable accuracies.

Harpreet Sethi

Harpreet Sethi is a Solutions Architect for Energy at NVIDIA. His work focuses on building AI factories and digital twins for scientific applications using Generative AI and Physics-ML. He received his PhD in Geophysics from Colorado School of Mines and obtained an integrated Masters/Bachelor's degree in the same discipline from IIT Roorkee.

Title: Predicting CO2 Plume Migration in Carbon Storage Projects using Graph Neural Networks

Abstract: Carbon capture and storage (CCS) technology plays a pivotal role in mitigating greenhouse gas emissions and facilitating the transition to a low-carbon future. Effective management of subsurface reservoirs is essential to ensure the safe and efficient storage of captured carbon dioxide (CO₂), necessitating accurate predictions of pressure and saturation over time to evaluate the long-term performance and integrity of CCS projects. Traditional numerical simulations of subsurface reservoirs have proven successful in providing these predictions but involve massive amounts of computational effort and require extensive domain expertise for proper model calibration and validation. Additionally, these models are specific to a particular location, set of subsurface properties, or data resolution. In recent years, Graph Neural Networks (GNNs) have emerged as a powerful framework for analyzing complex data in graphstructured domains and offer an alternative to traditional subsurface modeling techniques. In this work we explore the application of GNNs to forecast pressure and saturation evolution in carbon storage projects with complex geological settings. GNNs can harness the inherent graph structure of reservoirs, where nodes represent reservoir grid cells and edges represent the spatial and geological connectivity between them. The proposed GNN-based framework $-$ a highly optimized version of MeshGraphNet available in NVIDIA Modulus – leverages this graph structure to learn spatial dependencies and temporal dynamics, enabling the model to capture the intricate interplay between pressure, saturation, and geological features. Additionally, these learned

features are independent of graph structure, allowing for the model to be generalized to other subsurface flow problems and breaking a substantial barrier to the use of such simulations in real-world settings.

Anchal Jatale

Anchal Jatale manages the team of application engineers working in Energy, Chemical and Process industry. He is championing the efforts in developing cutting-edge simulation solutions for new clean energy including wind, hydrogen and carbon capture. He has 15 years' experience in CFD modeling and simulations. For the past few years, he is spearheading Ansys Digital twin engagements in O&G and the energy industry. His expertise is in reduced order modeling, system modeling, reacting flow, combustion, multi-phase flow. Prior to joining Ansys, he

received his doctorate in Chemical Engineering from the University of Utah and bachelor's in chemical engineering from Indian institute of technology (IIT), Kanpur.

Title: Leveraging AI/ML with Physics to Accelerate Engineering Workflows

Abstract: The integration of Physics principles with Artificial Intelligence (AI) and Machine Learning (ML) techniques has emerged as a transformative approach to enhance efficiency and innovation in engineering workflows. The foundation of this integration lies in leveraging robust models and simulations (CFD, FEA etc.) that accurately represent real-world phenomena. These models serve as the basis for training AI and ML algorithms, enabling predictive analytics, optimization, and automation within engineering workflows. By harnessing AI/ML, engineers can efficiently analyze vast datasets, discover patterns, and make data-driven decisions that optimize designs, improve performance, and reduce development cycles. This talk will cover different ways of using AI &ML techniques to use simulation together with field data through some relevant use cases.

Jun Zhang

Jun Zhang is a research associate at the Erosion/Corrosion Research Center in the Department of Mechanical Engineering and the School of Cyber Studies at the University of Tulsa. With over 10 years of research experience in both academia and industry, Jun specializes in CFD modeling, cybersecurity in the energy and engineering sectors, fired equipment design, combustion, and particulate flow. He leverages machine learning and AI models to address complex problems across engineering and security domains. Jun has published extensively in leading journals and conferences

and has served on several technical committees.

Title: Predicting CO2 Plume Migration in Carbon Storage Projects using Graph Neural Networks

Abstract: Solid particle erosion affects various industries, including oil and gas, renewable energy, mining, aerospace and chemical engineering. Predicting solid particle erosion is a complex and challenging task that requires a thorough understanding of its underlying mechanisms and patterns. Conducting experiments are often the first approach to investigate erosion but are expensive and time-consuming. Computational Fluid Dynamics (CFD) provides an alternative approach that can simulate erosion with rich physical detail, however, it is computationally intensive and requires significant expertise. Fortunately, decades of experimental work and CFD

simulations have generated a large repository of erosion data. By utilizing machine learning, the hidden patterns within this legacy data can be unlocked, accelerating mechanistic modeling and future prediction efforts. Recent expansion and advances in generative models, particularly, conditional Generative Adversarial Networks (cGANs), allow us to augment existing experimental datasets with physics-informed synthetic data. This augmentation can further improve the accuracy and robustness of machine learning models through better generalization across diverse scenarios. This comprehensive approach, combining CFD, experimental data, and generative models, can significantly enhance the understanding of erosion phenomena and improve the ability to predict and mitigate erosion efficiently and effectively across industries.

Vinicius Girardi Silva

Vinicius Girardi Silva is Technology Development Manager at ESSS O&G, a business unit dedicated to high-end digital tools for the O&G Industry. He has Bachelor's degree in Mechatronic Engineering and Masters in Mechanical Engineering, both from the University of São Paulo and Petroleum Engineer Degree by PUC-Rio. Vinicius' experience spans 12 years in the use of simulation tools and in the development of innovative software technology in the areas of reservoir engineering, drilling, production and flow assurance

Title: Hybrid Model for Monitoring Hydrate Blockage in Producing Wells

Abstract: Hydrate formation in production lines is a complex phenomenon involving a multitude of parameters. While field data and experimental observations are mandatory – one cannot provoke or wait for a hydrate blockage to occur to fine tune simulation models. It is possible to create an alternative, by learning from previous wells, and experiences in combination with physics-based simulations and AI, to create hybrid models. This is especially valuable for online monitoring systems. The technology presented during this talk is a hybrid model, to run in realtime, to quantify the risks of a hydrate blockage in producing wells

Romit Maulik

Romit Maulik is an Assistant Professor in the College of Information Sciences and Technology at Pennsylvania State University (PSU) as well as a joint appointment faculty at Argonne National Laboratory (ANL). He is also a cohire in the Institute for Computational and Data Sciences at PSU . He obtained his PhD in Mechanical and Aerospace Engineering at Oklahoma State University in 2019 and has been the Margaret Butler Postdoctoral Fellow as well as an Assistant Computational Scientist at ANL before starting his current position in August 2023. His research has been funded by the DOE,

NSF and ANL and Los Alamos National Laboratories and he is also a member of RAPIDS, a DOE SCIDAC Institute for Artificial Intelligence. His research group, the Interdisciplinary Scientific Computing Laboratory, studies scientific machine learning algorithm development for various applications in engineering, energy, and the environment.

Title: Differentiable Turbulence: Closure as a PDE-Constrained Optimization

Abstract: Deep learning is increasingly becoming a promising pathway to improving the accuracy of sub-grid scale (SGS) turbulence closure models for large eddy simulations (LES). We leverage the concept of differentiable turbulence, whereby an end-to-end differentiable solver is used in

combination with physics-inspired choices of deep learning architectures to learn highly effective and versatile SGS models for two-dimensional turbulent flow. We perform an in-depth analysis of the inductive biases in the chosen architectures, finding that the inclusion of small-scale nonlocal features is most critical to effective SGS modeling, while large-scale features can improve pointwise accuracy of the a-posteriori solution field. The velocity gradient tensor on the LES grid can be mapped directly to the SGS stress via decomposition of the inputs and outputs into isotropic, deviatoric, and anti-symmetric components. We see that the model can generalize to a variety of flow configurations, including higher and lower Reynolds numbers and different forcing conditions. We show that the differentiable physics paradigm is more successful than offline, apriori learning, and that hybrid solver-in-the-loop approaches to deep learning offer an ideal balance between computational efficiency, accuracy, and generalization. Our experiments provide physics-based recommendations for deep-learning based SGS modeling for generalizable closure modeling of turbulence.

Vedanth Srinivasan

Vedanth Srinivasan is the Head of Solutions for Engineering & Design and Go To Market (GTM) at Amazon Web Services. His focus includes modeling, simulations and high-performance computing as well as higher order workloads including model-based system engineering, digital thread and digital twins solutions development. He has over 20 years of experience in development and application of advanced engineering simulation processes across oil & gas, aerospace, automotive and healthcare

industries. He has a PhD in Mechanical Engineering from University of Kentucky.

Title: Using AI/ML to Accelerate Engineering Simulations for Asset Design and Optimization

Dan Probst

Bio: Dan Probst is a Senior Principal Engineer at Convergent Science. He has 15 years of experience with engine research and simulation, with particular emphasis on optimization, simplified models, Machine Learning and AI.

Title: Wind Farm Layout Optimization Using CFD-Based Machine Learning

Abstract: Optimal positioning of individual turbines in a wind farm is an important consideration to maximize total power production. The turbines should be placed in such a way as to reduce wake effects while still satisfying the geometrical constraints of the chosen site. In this work, a combination of Computational Fluid Dynamics (CFD) and Machine Learning (ML) algorithms are used to study the optimal design of a farm consisting of 25 NREL 5MW turbines in an area of 4.8km by 2.6km. The computational domain is 11km by 6km by 1km in x, y, z. The current study employs an ML optimization method consisting of the following steps. In the first step a design of experiments (DoE) is run using CFD to train the ML algorithm. For the CFD simulations required for this study, we carry out simulations of a neutral atmospheric boundary layer (ABL) over a flat terrain, where the turbines are modeled using the refined actuator-disk model (RADM) model with a resolution of 4 m in the rotor regions, while the turbulent scales are modeled using a RANS approach. Next, the generated ML model is employed as an emulator for optimizing the farm layout. Finally, the proposed optimum from the ML emulator is confirmed using CFD simulations. The number of optimal CFD samples in the training DoE is assessed as part of this study. Too few samples and the ML emulator will be inaccurate, but too high a number of samples can lead to prohibitive computational cost. A Latin Hypercude Sampling (LHS) strategy is used to generate the DoE, where smaller DoEs are augmented in succession to increase the training DoE size until an ML emulator of sufficient accuracy is obtained. The DoE size is increased from 75 to 175, then to 275 samples (CFD runs), obtaining an accurate ML model with R^2=0.87. The final proposed wind farm optimum layout is confirmed with CFD to generate high power.

Mothivel Mummudi

Mothivel Mummudi is Industry Director (Pharma/Biopharma) at Tridiagonal Software and manages the development of SimSight - an advanced "Data + Science" analytics platform that enables engineers to leverage the best of physical and synthetic/simulation data for business-critical applications.

Title: Physics-based Digital Twins: Building ROMs Using Python Libraries

Abstract: A digital twin is a virtual model designed to accurately represent a physical object. Computational models (CFD/FEA etc.) are excellent

candidates for digital twins but are very expensive and almost always require an expert user to maintain/run them. Reduced-order models (ROMs) or surrogate models are computationally inexpensive, simpler versions of full-scale computational models that retain their physical fidelity to a large extent. ROMs provide the dual benefit of physical consistency and computational efficiency. More importantly, due to their simplicity, they enable non-expert users to directly use them and derive benefits. ROMs can also serve as the first ingredient in developing a **physicsbased digital twin** of equipment. Despite the above-mentioned benefits, ROMs have not gained the popularity that they deserve - largely because building them is still done using software that is proprietary and closed-source. Today, most ROMs are built using vendor-provided software tools that are very expensive. We believe that this situation must and can be effectively remedied. In this presentation, we describe methods to build effective and practically useful digital twins - "from scratch" - starting from synthetic data obtained by simulating computational models. We first show how mathematical methodologies such as proper orthogonal decomposition (POD) and its variant "gappy POD" can be used to derive parametric-ROMs for such equipment. We then describe how, using open-source libraries available from the Python ecosystem, one can easily implement these techniques and build/deploy ROMs. The open-source libraries described in this presentation are available readily, are stable and are easy to use. Using these libraries, digital twins/ROMs can be built quickly and deployed readily. Towards the end of the presentation, we also show how once such ROMs are built, they can be deployed to allow engineers to vary process/design parameter values and quickly determine various physical fields such as velocity, energy dissipation rate, shear stress, erosion rates etc. that are of interest to Oil & Gas engineers. A few industrial case studies are presented to illustrate the methods described above and the efficacy of the resultant digital twins.

Dr Chao Xu

Chao Xu is a Research Scientist at Argonne National Laboratory's Transportation and Power Systems Division. His research focuses on computational fluid dynamics (CFD) with detailed chemistry, turbulence and turbulent combustion modeling, as well as reduction and algorithmic acceleration of complex reacting flows for applications in industrial and aero gas turbines, piston engines, industrial burners, and offshore wind. His work leverages leadership HPC to tackle both fundamental and applied

problems in turbulence, mixing, combustion, heat transfer, detonation, and emissions formation related to practical energy and propulsion systems. He is the PI on multiple DOE and industryfunded projects where he collaborates extensively with partners at GE, Solar Turbines, Caterpillar, ExxonMobil, NETL and academia toward the decarbonization of transportation, power generation, and industrial sectors. He is also the lead developer of the reacting flow solver within the spectral element based high-order CFD code Nek5000/RS. He is a four-time Impact Argonne Award receiver (2020, 2022, 2023, 2024) for his innovative and impactful research at Argonne. He is a member of the Propellants and Combustion (P&C) Technical Committee of the American Institute of Aeronautics and Astronautics (AIAA). He received his PhD in Mechanical Engineering from University of Connecticut and his Bachelor's degree in Thermal Engineering from Tsinghua University.

Title: Enhanced CFD Modeling of Hydrogen Mixing and Combustion with Machine Learning

Ani Rajagopal

Ani Rajagopal has been serving as an Industry Process Consultant at SIMULIA since 2019, joining the Worldwide Fluids team following the integration of Exa Corporation. With nearly 8 years of expertise in fluids and thermal sciences, he serves as an expert voice in supporting customers across all industries including Industrial Equipment and Transportation & Mobility. In his role within the Worldwide SIMULIA Fluids team, he focuses on enhancing fluid solutions through physics-testing, and deploying these solutions to optimize customer processes, particularly through automation.

Recently, he has been a key member of the core validation group for SIMULIA's AI/ML initiatives, specifically for fluids-related applications.

Title: Machine Learning-Based Surrogate Model for Computational Fluid Dynamics in Centrifugal Pump Design

Abstract: Centrifugal pumps are used in a large range of applications in the Oil & Gas industries during the production process including extraction, transportation, and refining phases. These pumps typically have a set of vanes, also known as diffuser, surrounding the rotating impeller to enhance efficiency by increasing pressure and reducing flow velocity as the fluid passes through. Therefore, a well-designed diffuser is critical to ensure optimal pump performance.

We propose to use a Design of Experiment through Computational Fluid Dynamics (CFD) in order to train a Machine Learning model allowing to quickly predict the effect of a diffuser's design on the pump's performance. Once trained, this surrogate model approach allows to get information on the main performance indicators, notably the total pressure/head rise by inferring the Machine Learning model, which is much faster than running additional full CFD simulations.

Vinod Kumar

Vinod Kumar is a Professor and Chair of the Mechanical & Industrial Engineering Department at Texas A&M University - Kingsville and a Co-Founder of deepVein Inc., a startup that develops predictive technologies for the detection, prediction, and tracking of deep vein thrombosis (DVT) and pulmonary embolism (PE) using data-driven and physics-based approaches. Vinod is interested in applying artificial intelligence/machine learning (AI/ML), high-performance computing (HPC), and computational fluid dynamics (CFD)

to investigate complex engineering and health challenges through R&D, innovation, and

entrepreneurship. Vinod brings many years of academic, administrative, and research experience through interdisciplinary collaboration with various DOD and DOE labs, Princeton University, Rice University, and Calysta, a biotechnology company. He has worked on projects involving CO2 sequestration modeling, climate modeling, concentrating solar power simulations, exascale computing, multiphase and multiphysics flows, and compressible and incompressible flows. He has also deployed data analytics, big data, ML, and AI for solving engineering problems and enhancing predictive capabilities. Vinod has extensive experience with multiple engineering software, programming languages, and HPC platforms. He has published multiple papers, patents, and books on my topics of interest and expertise.

Title: The Rio Grande Consortium for Advanced Research on Exascale Simulation (Grande CARES)

Abstract: Understanding the complex physics and phenomena of intricate engineering systems is essential for designing and maintaining reliable, efficient, and economical systems. These systems must be capable of safe operation despite the complex, multi-physics challenges that span multiple scales and magnitudes. The latest advancements in computational and data-driven technologies, coupled with supercomputing infrastructures, offer novel solutions to these engineering challenges. Advanced modeling and simulation (M&S) capabilities enable detailed investigations and can significantly reduce operational costs. However, effectively implementing these technologies requires a workforce with a deep understanding of multi-physics concepts across multiple disciplines and cross-cutting technologies. The CARES team, comprising four universities and Sandia National Labs, aims to address this need through an innovative multiphysics integrator that includes five core research thrusts and a pioneering curriculum. Our goal is to cultivate next-generation scientists and engineers and equipping them with the integrative skills needed to advance M&S. The research focus on developing and integrating cutting-edge computational algorithms using high-performance computing (HPC), machine learning (ML), data analytics, uncertainty quantification (UQ), and other novel computational capabilities

Shubhamkar Kulkarni

Shubhamkar Kulkarni is a mechanical engineer by training with a background in optimization. He was the Product Manager for VisualDoc/Iliad, a multidisciplinary optimization tool developed by Vanderplaats R&D. He is currently work as a Product Specialist in the Engineering Data Science team.

Title: Next Gen AI Tools for Faster Design Exploration

Rupesh Reddy

Dr. Rupesh Reddy is working as a Principal Simulation Scientist in NOV. He has 14 years of experience in cutting edge simulation analysis and design optimization in wide range of applications in areas such as multiphase flows, turbulence modeling, free-surface flows, FSI and fluid-particle flows. He has experience in application of simulation analysis to the design and optimization of the oil and gas equipment's like Multiphase separators, BOP and Downhole tools. Recent years he is involved in developing Hybrid

Digital Twins and Simulation methodologies related to Renewables.

Title: Overview of Hybrid Simulation and Data Science Models

MISSION

Mission of the SPE-GCS Computational Fluid Dynamics Study Group is to provide a common platform for CFD practitioners in Oil & Gas industry to foster knowledge sharing and networking, facilitate discussions, education/learning/training and develop boarder consensus on best practices in the area of CFD modelling for applications including (but not limited to) Near wellbore reservoir modelling, Drilling and Completion, Flow Assurance, Process and Process Safety, Offshore and Deepwater, Refining and Petrochemicals as well as Renewable and Low Carbon Energy.

Scope for CFD modelling is gaining momentum and growing rapidly in Oil & Gas industry. It is important to set proper expectations through good understanding of opportunities and challenges in CFD modeling. By raising awareness and providing a platform for industry professionals to network, this Study Group increases confidences on CFD predictions and influences sound decision making.

To address the growing interest within the SPE community, the CFD Study Group organizes quarterly meetings/webinars/workshops and annual symposium which are knowledge‐sharing events by key industry practitioners, thought leaders, and decision makers. The target audience for these events include oil and gas executives and managers, CFD practitioners, industry professionals, and subject matter experts from operators, service companies, consultants, academia, software vendors, and government labs.

Madhusuden Agrawal

Chair

Mazdak Parsi Treasurer

Kuochen Ts

Mi **Program Coordinators**

Gocha Chochua

Uday Godse

Jason Wang

High Performance Computing Built for the Cloud

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- Matthew Robinson Engineering Systems Admin

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