This way, the neuronal dynamics resulting from an impact on the head could be studied in detail. Also, such models can be utilized to calculate the growth dynamics of tumors, where molecular mechanisms corresponding to tumor growth are correlated with the macroscale mechanics of tumor tissues.

Another important area of research is computational drug design, where mathematical models are developed to mimic the transport and internalization of nanoparticles in cancer cells. Many clinical trials indicate high specificity, however, only 5% of particles typically reach the tumor sites. Transport barriers in the tumor vasculature such as flow barriers, migration of circulating tumor cells, endothelial gaps, etc. add to the complexity of nanoparticle migration, affecting the delivery and particle internalization in tumor cells.

Recent advances in computational power, allow for multiscale simulations that can investigate the influence of a range of parameters in biologically realistic scenarios. High throughput and integrated nanoparticle-design pipelines are possible using the simulation data. Eventually, general design principles can evolve, which when combined with patient-specific data, may provide personalized treatment guidelines for tumors.

Additionally, machine learning techniques can be integrated into in-silico, nanoparticle simulation models such that 'active design learning' is possible. A recent project in our lab focuses on the development of a computational model to mimic the transport and internalization of nanoparticles in lung cancer cells.

We design the molecular models of the surface of A549 cells and functionalized nanoparticles and use coarse-grained and full-scale molecular dynamics simulations to determine the particle internalization pathways in the cells. A variety of drug configurations can be synthesized and tested using such models, meaning a virtual, cost-effective platform for tumor drug design.

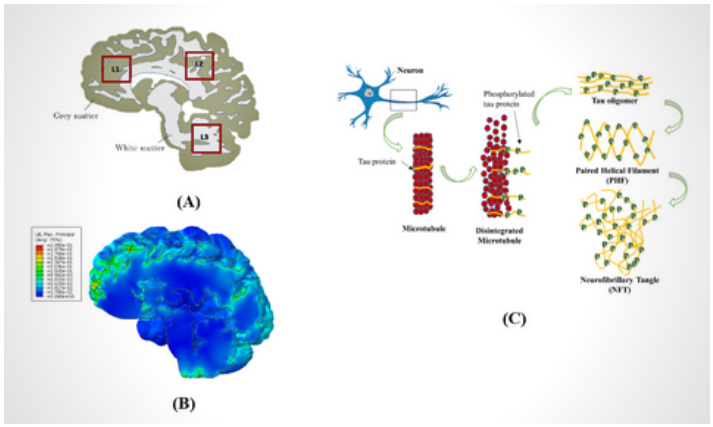

Fig. 1: (A) Segmented white-grey matter and identification of critical strain locations (B) Localized strain in brain sulci (C) Brain strain-induced tau protein aggregation and formation of neurofibrillary tangles (NFT), resulting in neurodegeneration post-TBI

Integrated Computational Engineering

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Integrated Computational Engineering seeks the optimal solution of a system under design or operation considering the detailed analysis of several mathematical models of multiple length scales. This approach has dominated the era of scientific discoveries in the last two decades providing a wholistic look at the problem at hand. The advancements in algorithms in addition to those in hardware have now resulted in a paradigm shift in science and engineering by bringing Data-intensive scientific discoveries to the forefront. At Global Optimization and Knowledge Unearthing Laboratory (GOKUL) in the Department of Chemical Engineering at IIT Hyderabad, we integrate Data Science with Computational Engineering, a much desired and timely need, to solve the problems in Process Systems Engineering using Artificial Intelligence and Machine Learning (AI/ML). Ranging from Surrogate assisted optimization and control to Data-driven uncertainty quantification and sensitivity analysis, the applications are profound.

Computationally expensive optimization of unit processes in polymerization, crystallization, and steel-making, nonlinear closed-loop control of integrated grinding circuits through deep system identification, convolutional generative modeling for wind characteristics emulation, uncertainty quantification in the design of tactical missile systems & large scale expensive optimal control of bioreactors through tailor-made solutions from AI/ML are some instances.

A representation of the ease with which Data Science can be integrated into Computational engineering can be witnessed in the National Supercomputing Mission project at GOKUL that takes up challenges at every level of designing a robust wind energy conversion system and attempts to solve it using Deep Learning **(Fig. 1)**. This work involves the problem of wake modeling in a 200 turbine wind farm spread over an area of more than 400 sq.KM through Large Eddy Simulations for building a neural network-based surrogate that can be utilized in wind farm control under wind state uncertainty.

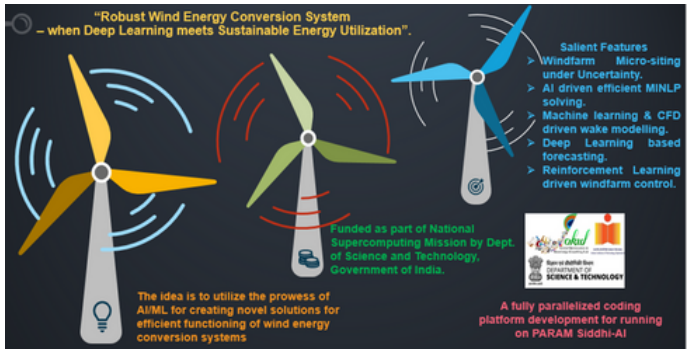

Fig. 1: Representational Image of Robust Wind Energy Conversion System using AI/ ML

The prominence of integrating Data Science with Computational Engineering is such that, it allows for a smooth transition of research in the lab to the product in the industry. In GOKUL, this is evident through some highly ambitious projects with industrial collaborations that include topics such as (i) Steel-Genome: Characterization of Steel through Machine Learning (Fig. 2), (ii) AI-driven solutions for mixed-integer problems mainly for application in a) coal blending in steel plants, b) biofuel supply chains, and c) Climate Change, and (iii) Smart Systems Biology: Screening and Ranking of drug candidates for COVID-19 prognosis through Convolutional Networks and Bio-reactor design and control through Data Science.

While each of these areas is computationally intensive with up to NP-hard complexities, the ideas from Data Science enable a real-time solution that provides a unique perspective offering multiple degrees of freedom to solve the problem intelligently. At GOKUL, we walk the path of a Computational Chemical Engineer empowered with the prowess of Data Science to explore new frontiers in Process Systems Engineering.

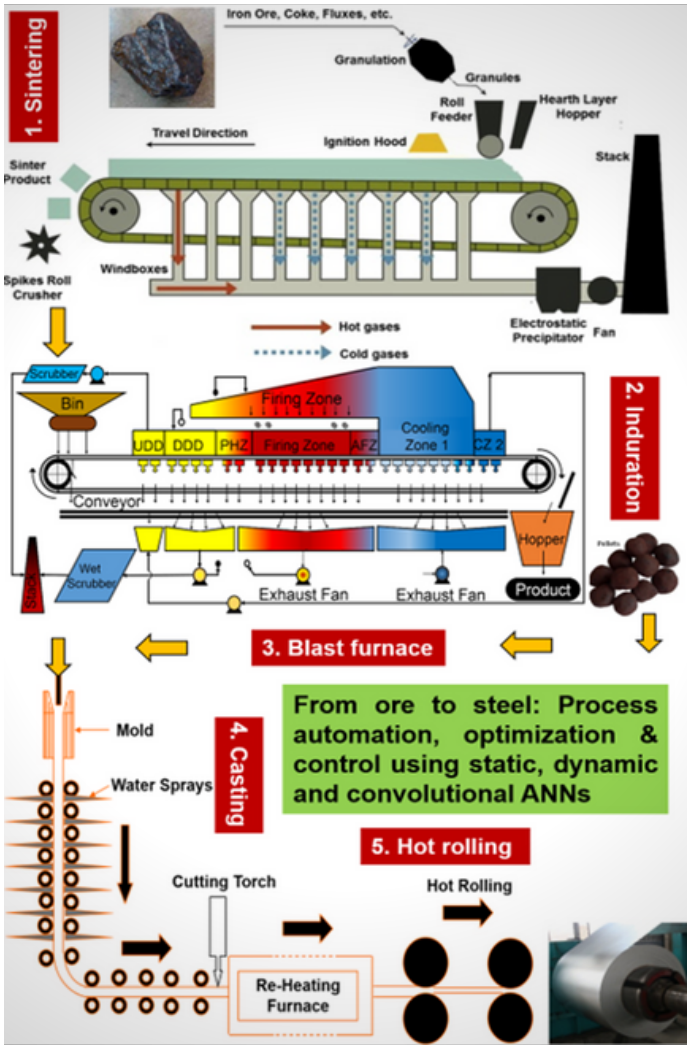

Fig. 2: From ore to steel: Process automation, optimization & control using static, dynamic & convolutional ANNs

Development and application of computational models for modelling particulate flows in Mineral Processing

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Most mineral processing unit operations involve fluid as a medium while separating the particles based on differences in their size, density, shape, and sometimes surface properties in the given slurry feed. Multiphase systems prevalent in minerals processing, usually consist of solid-solid and solid-fluid systems, such as in comminution and classification, flotation, gravity separations, dewatering, and magnetic separation, among several other unit operations. These particulate multiphase flows involve complicated physical processes and complex geometry. The majority of these flows are turbulent in nature. Tumbling mills are the first set of wet-unit operations of comminution circuits, which utilizes large amounts of water while grinding the particles to fine sizes. Dynamics of particles in the presence of water/slurry medium would behave differently than when they are treated in the dry grinding route. Understanding of internal dynamics of the charge and slurry can be of great help in energy-efficient mill design. Grinding efficiency not only depends on the tumbling mill performance but also on the recirculation load that results from the associated classifier with the circuit. Therefore, accurate prediction of classifier flow properties greatly influences the mill efficiency predictions in the given comminution circuit.

Modelling industrial cyclones (Hydrocyclone and DMC) is very challenging due to the existence of a complex flow field that is highly turbulent and varying multi-scale particles. Computational models that solve governing equations in the form of efficient multiphase and turbulence models with appropriate boundary conditions are highly desirable for accurate flow field and particle dynamics thereby affecting performance predictions.

Our group at IITH works on developing a suite of computational models ranging from computational fluid dynamics (CFD), discrete element model (DEM), and coupled CFD-DEM strategies to simulate particulate flows outlined in Fig. 1 & 2. In recent years, our focus research has been to develop and validate the multi-phase CFD models for various mineral and chemical processing units like dense medium cyclones (DMC), hydrocyclones (HC), bubble columns, fluidized beds, and flotation devices. In particular, extensive results have been obtained on the detailed multi-phase flow in DMC/HC devices in terms of air-core resolution, mean and turbulence flow field analysis, turbulent dispersion analysis w.r.to particle classification, and understanding the classification/separation mechanism, see Fig. 3.