References:
1) Prabhakaran D., Jeemon P., and Roy A., 2016, "Cardiovascular diseases in India. Current epidemiology and future directions," Circulation, 133(16):1605–1620.
2) Anand M., Rajagopal K., and Rajagopal K. R., 2003, "A model incorporating some of the mechanical and biochemical factors underlying clot formation and dissolution in flowing blood," J. Theor. Med. 5(3–4): 183–218.
3)Mann K. G., 2012, "Is there value in kinetic modeling of thrombin generation? Yes," J. Thromb. Haemost. 10(8): 1463–1469.
4)Susree M., Panteleev M. A., and Anand M., 2018, "Coated platelets introduce a significant delay in onset of peak thrombin production: Theoretical predictions," J. Theor. Biol. 453: 108-116.
5)Morris P. D., Narracott A., von Tengg-Kobligk H., Silva Soto D. A., Hsiao S., Lungu A., Evans P., Bresslof N.W., Lawford P.V., Hose D.R., and Gunn J.P., 2016, "Computational fluid dynamics modeling in cardiovascular medicine," Heart, 102(1):18-28.
6) Ameenuddin M., and Anand M., 2020, "A mixture theory model for blood combined with low-density lipoprotein transport to predict early atherosclerosis regions in the idealized and patient-derived abdominal aorta," J. Biomech. Eng. 142(10):101008.r the 2022 year!

Experience with Dr Mohan & Group

Mikhail A Panteleev
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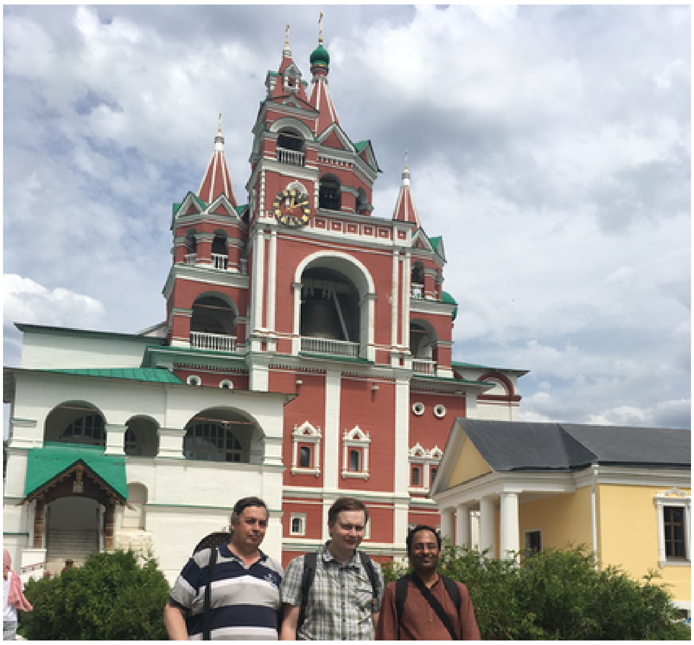
Russian Academy of Sciences

We have been collaborating with Professor Dr Anand Mohan from the Department of Chemical Engineering, IIT Hyderabad for many years on a number of subjects, ranging from joint research on blood coagulation to the establishment of new systems biology journal. I am particularly fond of the study that was pioneered by Dr Modepalli under Anand's guidance and published in J Theor Biol. It was focused on the mystery of the interaction between procoagulant platelets (which has been fascinating to me for more than a decade) and blood coagulation cascade.

It was great fun to be a part of this study, and I am very happy that this opportunity not only deepened our collaboration but also allowed Anand to travel to Russia so that we could meet even beyond the scope of just collaboration. My best wishes to the Anand lab and IITH for the 2022 year!



(L-R) Prof Alexey Lobanov, Mikhail A Panteleev & Dr Anand Mohan During Dr Anand Mohan visit to Moscow, Russia in June 2018

Integrated Computational Engineering

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The need for multiscale understanding of materials and phenomena is well established recently and has applications ranging from aerospace design to DNA biology. Integrated computational engineering refers to the design of materials and understanding of scientific, engineering phenomena through multiscale computational techniques. This means virtual materials design, including virtual testing and virtual processing. Integration of modelling tools (coarse-grained/atomistic, computational thermodynamics, and phase-field) are normally employed to simulate the microstructural development of materials during processes. The relevant applications of such multiscale models are present in various fields and include evaluation of carbon nanotubes, the composition of superalloys, cancer metastasis, etc.

The computational biomechanics lab in the department of biomedical engineering is focused on the development of multiscale computational techniques for a detailed understanding of soft tissue mechanics in the human body. The evolution of tissue microstructure during physiological processes can be determined by computational models that integrate the features of macro and micro-nano scales. An effort on modeling neurodegeneration resulting from traumatic brain injury is underway, where brain strain data computed from a continuum-based finite element model is coupled to a neurobiological computational model in order to assess protein aggregation and death rate of neurons post-traumatic brain injury (TBI) (Fig.1).

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.

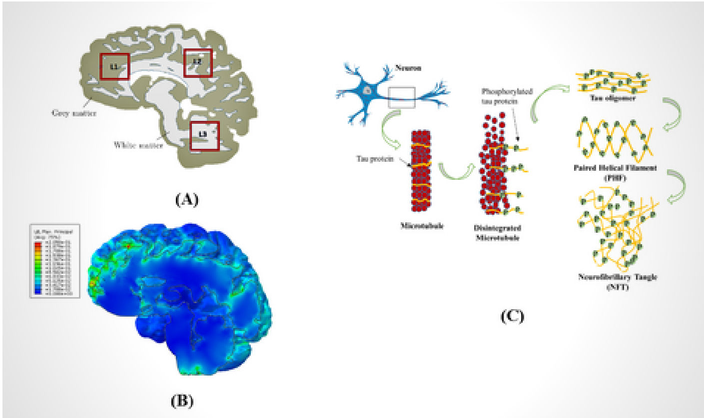

Fig. 1: (A) Segmented white-grey matter and identification of critical strain locations (B) Localized strain in brain sulci (C) Brain strain-induced tau protein aggregation and formation of neurofibrillary tangles (NFT), resulting in neurodegeneration post-TBI

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.

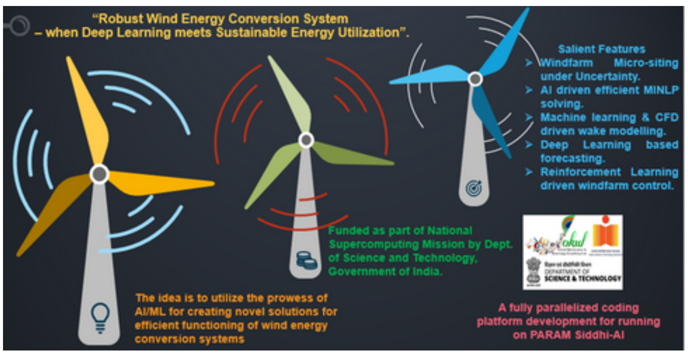

Fig. 1: Representational Image of Robust Wind Energy Conversion System using AI/ ML