

COMPUTING@PNNL PRESENTS

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GlaxoSmithKline Technologist-in-Residence



Translational challenges in computational math: changing boundaries at multiple scales

As high-performance computing and data analysis methods become more ubiquitous and more specialized, work increasingly requires use of combinations of software tools that implement a variety of sophisticated mathematics. As a result, realizing the full potential of a new mathematical approach can require changing the associated software stack, as well as organizational processes and culture. In this talk, Jay Bardhan will illustrate some of these translational challenges at various scales, using examples from his work in academia and industry.

About Jay Bardhan

Bardhan's academic research focused largely on modeling interactions between biological molecules and their solvent environment. He broke open the "black box" of continuum PDE models for solvation electrostatics, enabling PDE-constrained optimization methods for drug design and molecular engineering and exploited boundary-integral equations (BIEs) to identify a new, much more accurate continuum model. In industry, Bardhan focused largely on the challenges of translating mathematical advances from validation to widespread application. He has helped biologists make the most of advances in methods for analyzing single-cell proteomics data and has explored how methods for secure and private data analysis can improve health care. Bardhan is currently a member of the Beyond Innovation team at GlaxoSmithKline (GSK), where his role as Technologist-in-Residence is to assess technologies emerging on the 5-10 year time horizon, and to scope and manage projects arising from such assessments. He received his Ph.D. from Massachusetts Institute of Technology (MIT), where his graduate research on numerical algorithms for drug design and protein engineering was supported by a Computational Science Graduate Fellowship (CSGF) award. He has worked at Argonne National Lab, Rush University Medical Center and Northeastern University.

Monday, September 30
11:30 a.m. - 12:30 p.m.
CSF/Mural (1508)

All staff invited