U.S. DEPARTMENT OF ENERGY | Office of Science

Update on Mathematical Multifaceted Integrated Capability Centers (MMICCs)

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Office of Science

Department of Energy

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History

- **Sep, 2011 Workshop: *A Multifaceted Mathematical Approach for Complex Systems* (Report: Mar, 2012)**

- **New Paradigm:**
  - Holistic approach for increasingly complex systems
  - Broader view leading to strategies that approach entirety of problem
  - Enable large collaborative teams to address problems earlier in process

- **Applied Math Summit, Mar, 2012**
  - Cross-cutting math has been a mainstay of DOE Applied Mathematics
  - MMICCs structure should have clear relevance/impact to DOE mission areas
  - Successful MMICCs will grow entire Applied Math program
  - Applicants should define Grand Challenges

History, cont'd

- **Other key points from Summit:**
  - Multiple applications, mathematical abstractions
  - Defined areas ripe for investment vs current support
  - Center directors
  - Socialization
  - Address long-term mathematical challenges for DOE Grand Challenges
  - Identify research challenges that represent abstractions of the grand challenges
  - Transition to SciDAC Partnerships or Institutes, Co-Design Centers, and/or directly to DOE application scientists

- **FY12 MMICCs solicitation**

History, cont'd

- **First Award**
  - **M2ACS: Multifaceted Mathematics for Complex Energy Systems**
    - *Director*: Mihai Anitescu (ANL)
    - *Institutions*: ANL, PNNL, SNL, U Wisconsin, U Chicago
  - **CM4: Collaboratory of Mathematics for Mesoscopic Modeling of Materials**
    - *Director*: George Karniadakis (PNNL, Brown)
    - *Institutions*: PNNL, SNL, Brown, UC Santa Barbara, Stanford, Princeton, U Wisconsin, Penn State
  - **DiaMonD: An Integrated Multifaceted Approach to Mathematics at the Interfaces of Data, Models, and Decisions**
    - *Co-Directors*: Omar Ghattas (UT Austin) and Karen Willcox (MIT)
    - *Institutions*: UT Austin, MIT, Colorado State, Florida State, Stanford, ORNL, LANL

Center	Yearly Lab Funding	Yearly University Funding	Yearly Total
M2ACS	\$2.600M	\$0.900M	\$3.5M
CM4	\$1.975M	\$1.025M	\$3.0M
DiaMonD	\$0.265M	\$2.235M	\$2.5M
Total	\$4.840M	\$4.160M	\$9.0M

Current Portfolio

- **Second* Award**
  - **MACSER**: Multifaceted Mathematics for Rare, High Impact Events in Complex Energy and Environment Systems
    - *Director*: Mihai Anitescu
    - *Institutions*: ANL, U Chicago, LLNL, Ohio State, PNNL, U Wisconsin
  - **AEOLUS**: Advances in Experimental Design, Optimization & Learning for Uncertain Complex Systems
    - *Co-Directors:* Omar Ghattas, Karen Willcox
    - *Institutions*: UT Austin, BNL, MIT, ORNL, Texas A&M
  - **PhILMs**: Collaboratory on Mathematics and Physics-Informed Learning Machines for Multiscale and Multiphysics Problems
    - *Director*: George Karniadakis
    - *Institutions*: Brown, PNNL, SNL, Stanford, MIT, UC Santa Barbara

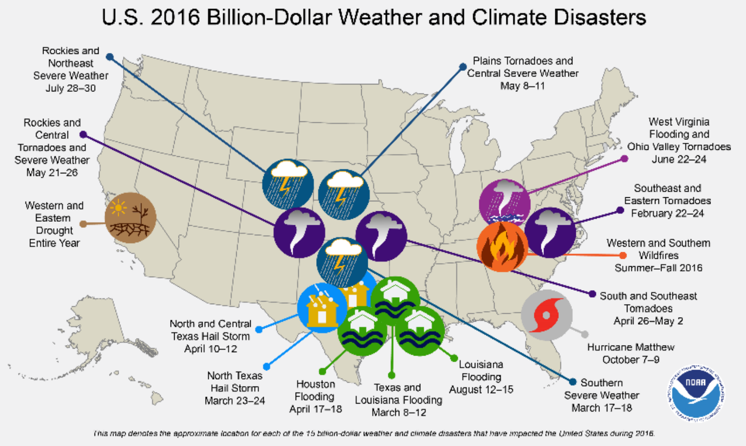
Center	Yearly Lab Funding	Yearly University Funding	Yearly Total
MACSER	$2.0M	$1.0M	$3.0M
AEOLUS	$1.1M	$1.4M	$2.5M
PhILMs	$1.6M	$0.9M	$2.5M
Total	$4.7M	$3.3M	$8.0M

MACSER

Multifaceted Mathematics for Rare, High Impact Events in Complex Energy and Environment Systems(MACSER)

Goals:

- By taking a holistic view, quantify the occurrence and features of rare, high-impact events and design and optimize energy systems that withstand such events and recover from them.
- Address the mathematical and computational complexities of extreme space-time statistics of environmental events and its impact on analyzing, planning, and operating the energy infrastructure



Location of the 15 weather events in 2016 with more than $1B in damages. A large part due to energy infrastructure damage (NOAA)

Integrated Novel Mathematics Research:

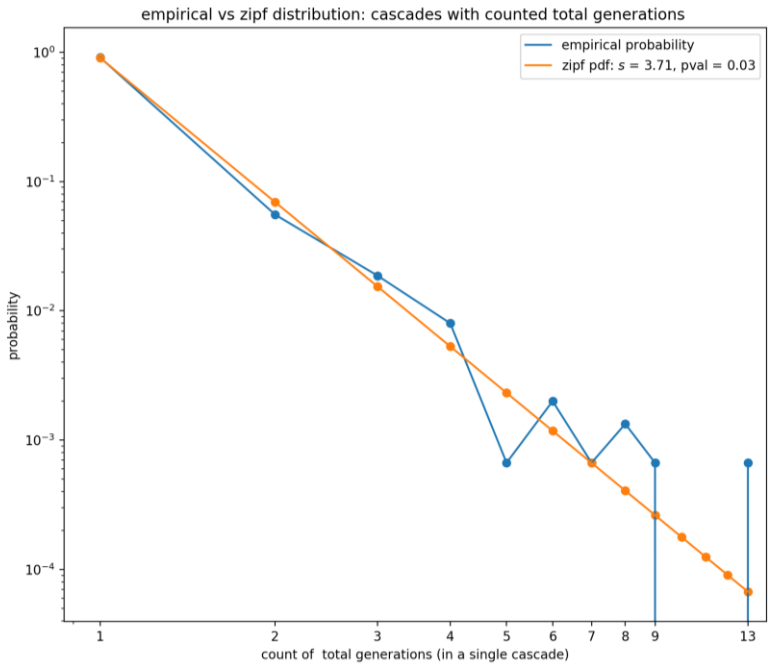
- *Statistics of rare space-time events* that characterize distributions of extremes and efficiently sample from them.
- *Novel formulations for optimization under uncertainty* that best balance worst-case and probabilistic energy systems requirements.
- *Advanced optimization algorithms* that employ model reduction and decomposition to address the feature and rare event complexities.

Long-Term DOE Impact:

- Development of new mathematics at the intersection of multiple mathematical sub-domains.
- Addresses a broad class of applications for complex energy systems, such as :
  - Limiting the probability of cascading failures such as the 2003 blackout.
  - Planning an energy infrastructure that is robust and resilient to rare weather events.

MACSER Carries out Foundational Mathematical Research for Energy Systems

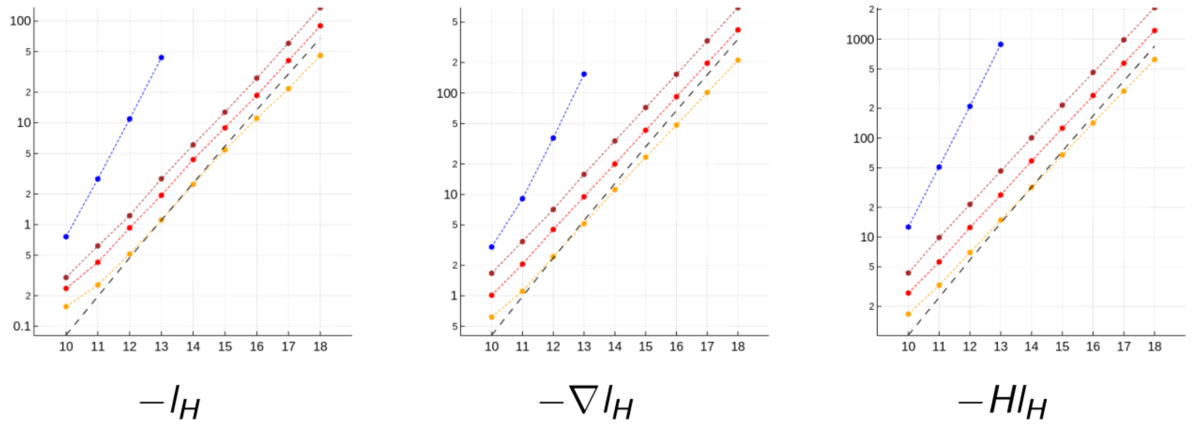
- A novel rate theory analysis for a class of non-conservative stochastic differential equations. In turn this allows a much faster Kinetic Monte Carlo approach to the possibly only practical, first-principles, cascading, blackout probability calculation. The statistics have been validated by real data.
- Optimal data tapers for spectral estimation of space-time data which results in unprecedented combination between the accuracy and artifact reductions.
- Novel importance sampling techniques based on upcrossing statistics of Gaussian processes for highly accurate estimation of tail probabilities in uncertainty propagation for dynamical systems.
- Definition and efficient identification of effective scenarios in multistage distributionally robust optimization. Effective scenarios are the outcomes that affect the optimal solution.
- New smoothing-based approaches for large-scale nonlinear chance-constrained stochastic programs. Allow application of powerful nonlinear programming algorithms and mitigate sampling errors.



Predicted probability distribution for cascades of given number of events follows Zipf's law, *same as real data.* The slope is -3.71; real data is between -2.5 and -3.5

MACSER develops novel algorithms, software and carries out extensive outreach to the mathematical and domain science communities

- Scalable ($O(n \log^2 n)$; classical $O(n^3)$) algorithms for Gaussian processes based on hierarchical off-diagonal low rank linear (HODLR) algebra. As a novelty, the HODLR calculation structure is extended beyond the likelihood calculation to its gradient and Hessian.
- Nonconvex optimization algorithms that are practical and also have best-in-class theoretical complexity.



Quasilinear scaling of HODLR: approximated likelihood, gradient, and Hessian for different off-diagonal ranks. Exact scaling times in blue ($\log_2$ x scale)

- Developed and implemented new asynchronous bundle method for dual decomposition in stochastic optimization with extensive numerical experiments showing strong scaling and improved parallel efficiency.
- MACSER pursued a novel community engagement models where it aims to organize broadly attended events in collaboration with NSF institutes. In 2019 we co-organized with ICERM the “Mathematical Optimization of Systems Impacted by Rare, High-Impact Random Events” workshop with 50+ participants.
- Our research and researchers were recognized for work within or related to our project: a Best Conference Paper at the 2018 IEEE PES (Maldonado, Schanen, Anitescu), SIAM Fellow (Anitescu), PECASE (Zavala), Early Career Award (Kim)

Future Research and Plans

- Blackout-probability-constrained optimization of electrical networks in planning and operations in order to obtain the energy mix that is the least likely to be subjected to a blackout of a given size.
- Extend the analysis of the exit problem for power grid dynamics (underpinning blackout probability calculations) from Brownian noise forcing to (a) fractional Brownian noise and possibly to non-Gaussian noise to better model statistics of renewable power generation and (b) complex event triggering surfaces.
- Investigate the concept of "stochastic flexibility", defined as the capability of a system to maintain feasible operation over a range of uncertain/random conditions. Develop the theory to interpret power grid resilience through the stochastic flexibility index.
- Understand the effect of resolution on extreme event distribution (in the context of space-time environmental forcings) and correct their model and forecast in limited resolution circumstances.
- Carry out novel renormalization-inspired approaches for model reduction in order to express and track complex singularities with limited computational resources.
- Co-organize (with the NSF institute IPAM) the workshop "Intersections between Control, Learning and Optimization" in February 2020.

AEOLUS

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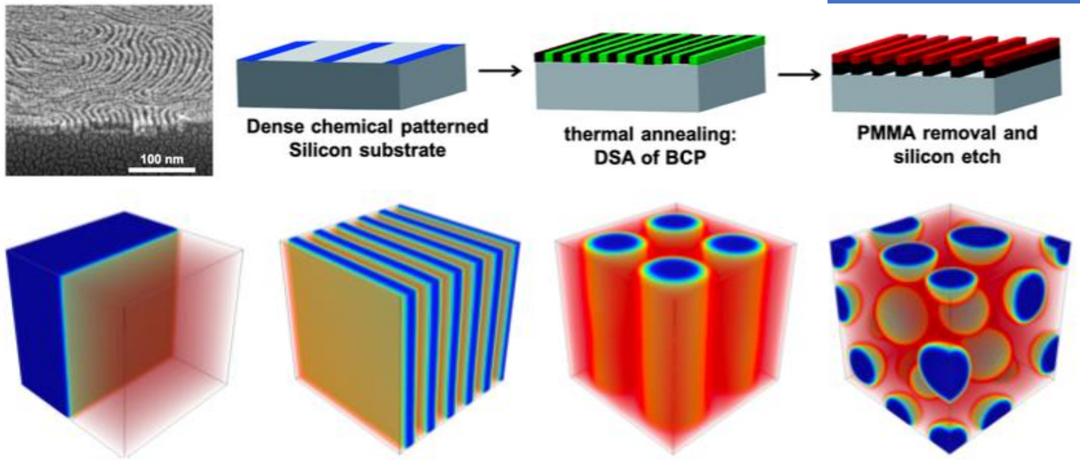
AEOLUS

Advances in **E**xperimental Design, **O**ptimization and **L**earning for **U**ncertain Complex **S**ystems

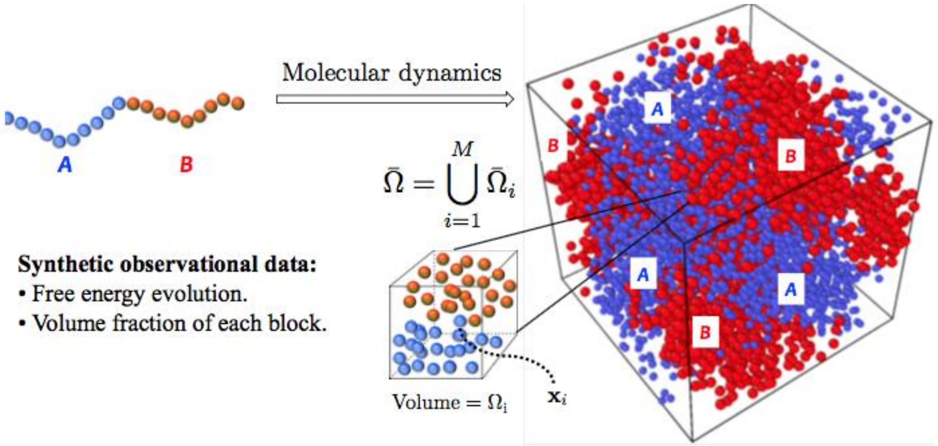
AEOLUS is developing a unified optimization-under-uncertainty approach to
- **learning predictive models from data under uncertainty**
- **optimal design/control under uncertainty**

for complex multiscale systems in advanced materials & manufacturing.

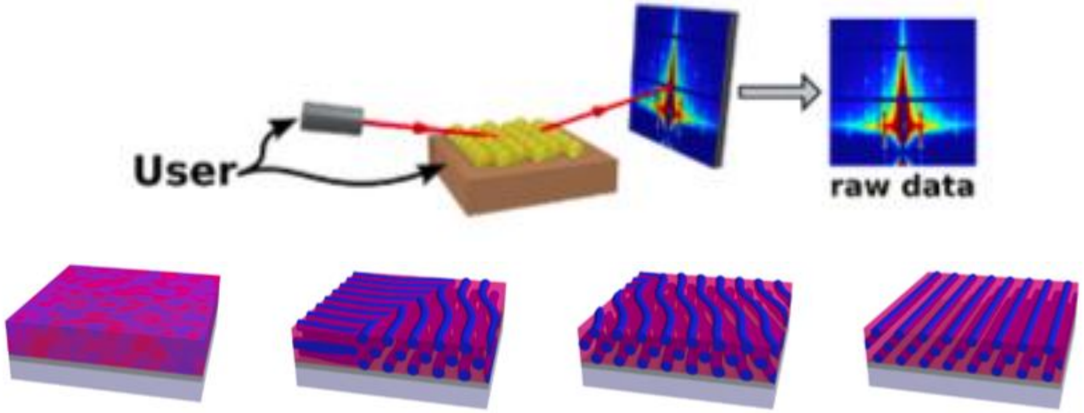
We exploit problem structure (geometry, sparsity, low-dimensionality) to achieve principled, rigorous, & scalable exploration of parameter & decision spaces.



One target: **Directed self assembly of block copolymers**

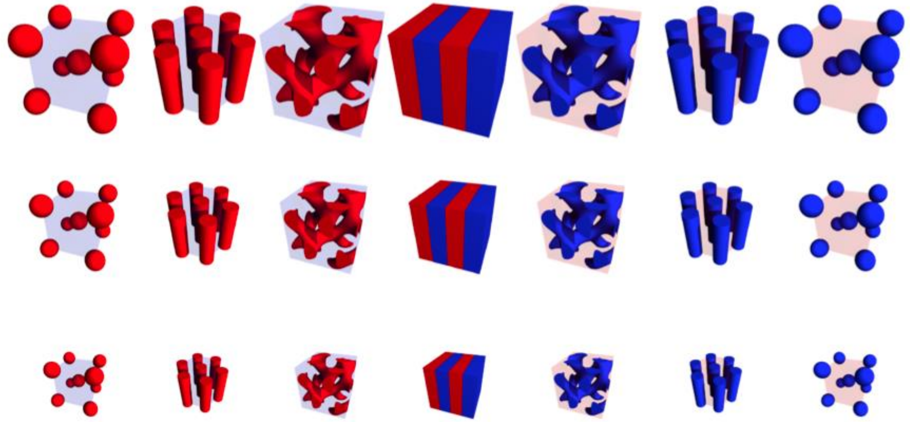


Bayesian inference of phase-field models from fine scale model data



Courtesy NSLS-II (K.Yager, M.Fukuto, J.Hill)

Optimal exptl design to determine most informative experiments



Optimal design & control under uncertainty to achieve desired structure

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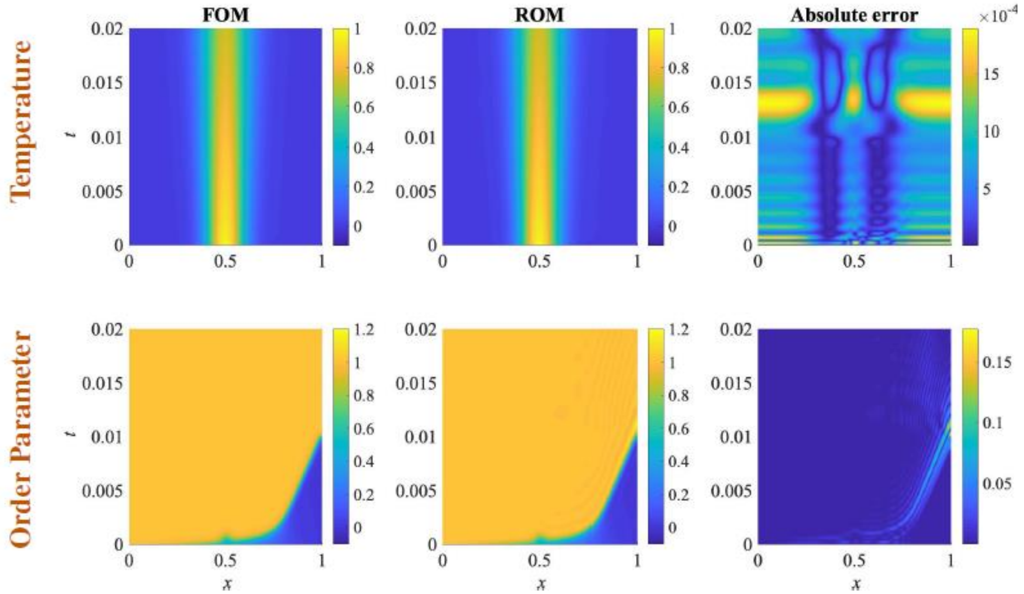
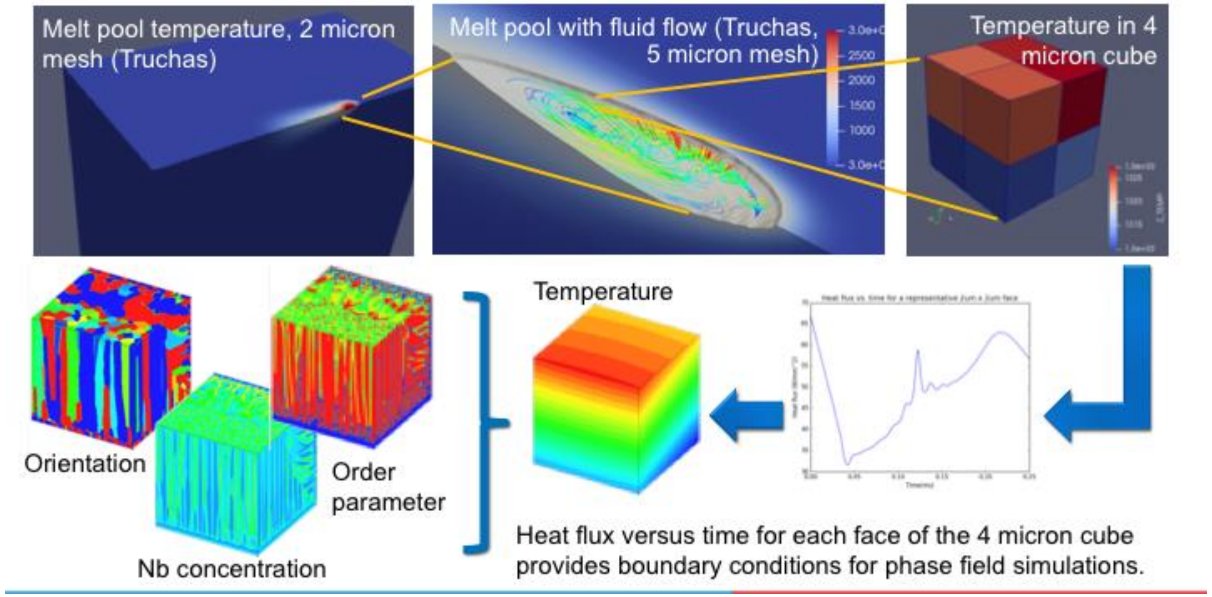
Advances in Experimental Design, Optimization and Learning for Uncertain Complex Systems

ACCOMPLISHMENT HIGHLIGHT: Reduced modeling, process control, and uncertainty quantification for additive manufacturing (AM)

- **Two-scale solidification model** couples thermo-mechanics (continuum) & microstructure evolution (phase-field model)
- Testbed optimization problem for **AM process control**, accounting for **random coefficients** and **microstructure evolution** via grain growth, solid-state phase transformations, multicomponent alloys, & fluid flows at the microscale, combined with thermo-mechanical continuum models at the macroscale



Initial process – structure linkage (melt pool – microstructure)



- **"Lift & Learn" reduced models**: identify variable transformations that expose structure in the governing equations; learn the low-dimensional representation directly from simulation snapshot data
- Reduced-order models show **100x speedups** in 1D

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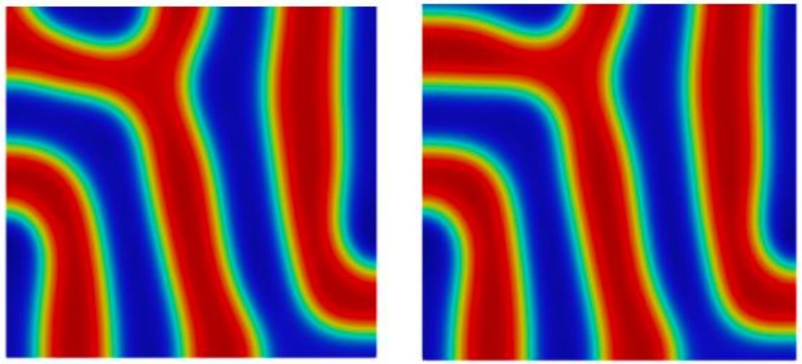
Advances in Experimental Design, Optimization and Learning for Uncertain Complex Systems

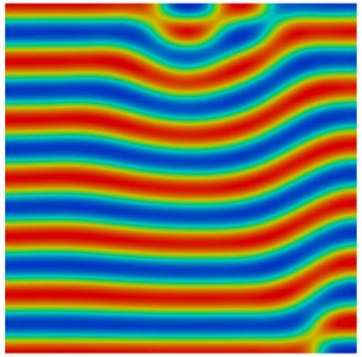
ACCOMPLISHMENT HIGHLIGHT: Models of block copolymers (BCPs) for Bayesian inversion and optimal design



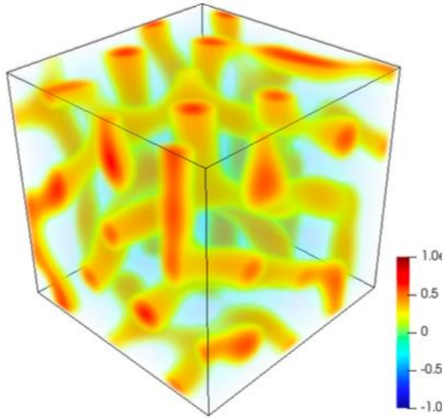
We developed **a new PDE-constrained optimization formulation for direct energy minimization** of non-local CH model to find equilibrium states (left). A Newton solver, globalized for non-convexity, is **40X faster** and as accurate as integrating the time-dependent gradient flow equation to equilibrium (right).

Forward modeling and Bayesian inversion for BCP models

- Controlling material parameters, quench temperatures, & initial and boundary conditions of **block copolymers** results in spontaneous phase separation, with structures as small as 5nm. These patterns guide lithography processes for nanoscale devices, critical for advanced semiconductors and nanotechnology.
- We have developed mathematical formulations/analysis, FE discretization, and fast solvers for **nonlocal Cahn-Hilliard phase-field models** of BCPs (with a fractional Laplacian for long-range interactions and material phase a via double well potential).
- The equilibrium solver is **ideally suited for inversion and optimal design of BCPs,** since it avoids time-dependent adjoint Cahn-Hilliard equations.
- Parameters in nonlocal CH model can be estimated under uncertainty via Bayesian inversion from BNL experimental imaging data (slide 1, lower left) and from **training data synthesized from higher fidelity** (or "DNS") models.



We developed a **Self Consistent Field Theory** (SCFT) high fidelity model to generate training data in 2D (top) and 3D (bottom) to calibrate CH model.



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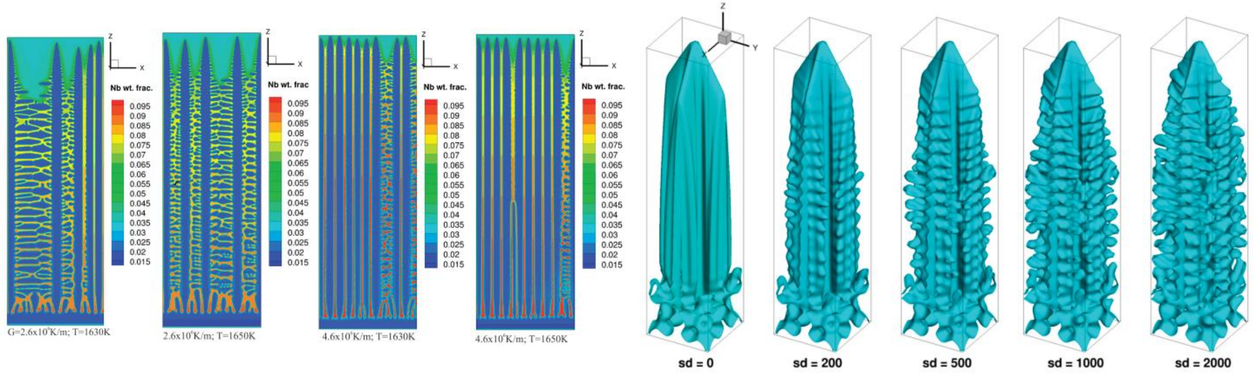
FUTURE WORK

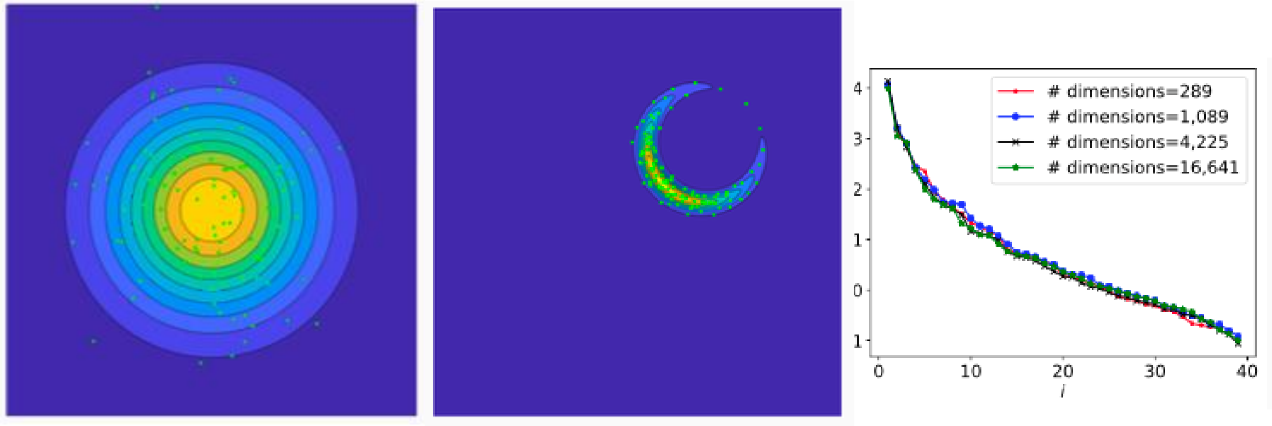


Process control under uncertainty for additive manufacturing

- Develop **fast solver** for macroscale and microscale problems
- Incorporate **hydrodynamics** due to fluid flow, and **phase-field models** for alloys, mixture; extend to **multiple phase-field models**
- Develop **reduced models for microscale** model and for the input-output map that couples the micro to the macroscale
- Incorporate **uncertainty** into multiscale modeling and optimization, e.g. stochastic forces at the level of phase-field models
- Apply reduced modeling methods to **ExaAM** models

Fast & scalable algorithms for Bayesian inversion for BCPs

- New **transport theory** algorithms for Bayesian inversion of complex models**.** Rather than directly sample the posterior distribution, we seek a mapping from prior (bottom, left) to posterior (bottom, right) via large-scale optimization, avoiding slow Monte Carlo convergence.
- Preliminary results on PDE inverse problems show **scalability independent of parameter dimension** (right, bottom), rapid Newton-like convergence, and high accuracy.
- These transport theory-based algorithms will be applied to **Bayesian inversion of BCP models**, capitalizing on the fast nonlocal CH equilibrium solvers.



PhILMs

PhILMs: Collaboratory on Mathematics and Physics-Informed Learning Machines For Multiscale and Multiphysics Problems (PI: Karniadakis)

Motivation

- Complex systems are governed by **hidden physics of interfaces and cascades-of-scales**, e.g., multifunctional materials, subsurface transport, reactive transport, ….

- Cascades-of-scales (*inhomogeneous*) involve **long-range** spatio-temporal interactions and often lack proper closure relations to form complete and mathematically **well-posed** systems of governing equations.

Pacific Northwest NATIONAL LABORATORY · Sandia National Laboratories · BROWN

Goals

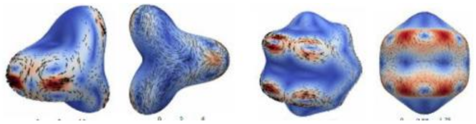
- To develop a synthesis of physics-based and data-driven **tools and approaches**, including non-local operators, multifidelity data and information fusion, deep neural networks (DNN), meshless methods, uncertainty propagation, and stochasticity.

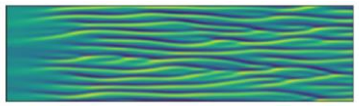
- Establish **PhILMs** as a new DOE center at the **interface** of mathematics, physics, data science, and deep learning.

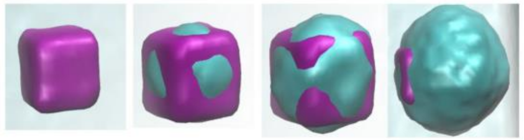
PhILMs: Summary of First-Year Accomplishments-I

<u>Research Area I. PDE-based Modeling of Macroscales</u>*: Develop a new generation of PDE-based simulation methods that remove the tyranny of grids, provide controlled accuracy, are suitable for nonlocal interactions, and allow flexibility in moving across s cales.*

- Physics-informed neural networks (PINNs) that learn from multi-fidelity data for forward & Inverse problems
- Unified nonlocal vector calculus, theory, and computation of nonlocal models: nonlocal PINNs (nPINNs)
- Inference of constitutive laws of complex hard materials and of polymers from synthetic data using PINNs
- Learning the hidden fluid mechanics and hidden fractional dynamics in seismology using PINNs
- Machine learning methods / Regression on scattered data sets and manifolds (GMLS and Neural Networks)
- Nonlinear functional and operator regression using GMLS parametrization and trunk-branch networks







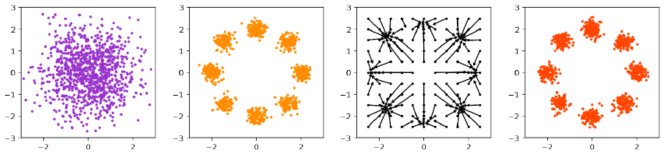
<u>Research Area II. Stochastic Modeling of Mesoscales</u>*: Extend the fundamental work started in CM4 on coarse-graining and model reduction using the Mori-Zwanzig formalism, a nd enhance it greatly using deep learning techniques.*

- Learning the nucleation of nano-bubbles using many-body Dissipative Particle Dynamics (mDPD)
- Self-cleansing of hydrophobic rough surfaces by coalescence-induced wettiing transition using mDPD
- Physics-informed Gaussian process regression (GPR) Bayesian methods for incorporating physical information data sets on manifolds
- Connections between machine learning and model reduction with applications to unsupervised (GANS) and reinforcement learning

PhILMs: Summary of First-Year Accomplishments-II

<u>Research Area III. Bridging Methods to Connect the Scales</u>*: Develop general forms of coupling by active learning of the microstructure in the subdomains and the hidden physics of interfaces in adjacent multiscale domains with no scale separation.*

- Active learning of constitutive laws via GPR for multiscale modeling of non-Newtonian fluids using DPD data
- SPH-SPH interface for viscoelastic media using the Multiscale Universal Interface (MUI)
- Domain decomposition for PINNs for porous media with largely disparate conductivities
- Learning coarse grained potentials for multiphase fluids (water-hexane system)
- Learning the kernel in nonlocal models for surface tension based on MD data
- Learning surrogate models for turbulent mixing and ignition (DSMC, DPD, MD)
- Learning (via GPR of fractional PDEs) of nonlocal flocking dynamics from particle trajectories (agent models)



<u>Research Area IV. Bayesian Deep Learning</u>*: Study uncertainty, high-dimensionality, r obustness, efficiency and learnability of general neural networks*.

- Generalized existing techniques for estimating learnability of the best classifier in a specified class in the data regime in which there is insufficient data to learn even an approximation of such a classifier
- Explored approaches for integrating certain classes of invariances within a convolutional DNN architecture
- Developed Generative Adversarial Networks for the optimal transport problem and for solving high-dimensional stochastic PDEs (e.g., 10,000 dimensions in a porous media model for the Hanford site)
- Designed stable optimization methods (‘optimistic’ gradient descent) for Generative Adversarial Networks

PhILMs: Outline of Future Work

- Develop total error theory for PINNs: approximation, optimization and generalization errors
- Endow PINNs with Uncertainty Quantification: neural network, parameters, models
- Enhance GANs with non-Gaussian PDF models (Generator & Discriminator)
- Investigate dying neural networks and develop new trainability requirements
- Functional regression of nonlinear operators using GMLS-Nets for unstructured data from high-fidelity simulations (molecular simulations, high-resolution DNS)
- Develop GMLS-Nets to incorporate physical invariances and operator/equation properties, such as div-free, curl-free, or related conservation laws or constraints
- Develop spectral-type decompositions with subdomain partitioning for PINNs
- Develop the library ADCME.jl to support more complex workflows, discretization schemes, and additional functional forms to represent solutions (e.g., NURBS)
- Develop physics-informed mixed Karhunen-Loeve and deep NN formulations
- Enforce physical constraints for reinforcement learning, continual and transfer learning
- Application of PhILMs to large multiscale/multiphysics problems such as the Hanford Site
- Integrate NN representation of partially known physics with physics-based codes
- Develop nonlocal PINNs (nPINNs) for the treatment of interfaces in multi-material simulations
- Use nPINNs in combination with the unified vector calculus to learn new diffusion, transport and flow processes (including turbulence)
- Use nPINNs for a PDE-based multi-fidelity framework and efficient nonlocal simulations
- Explore the potential for accurate prediction in settings with no assumptions on the underlying data sequence, i.e., predictions about unknown stochastic processes where the future may depend arbitrarily on the past, and other non time-homogeneous processes.

Upcoming Reviews

- **AEOLUS: Tuesday, October 8**
- **PhILMs: Monday, October 21**
- **MACSER: Tuesday, November 5**
- **Review questions:**
  - Mathematical accomplishments
  - Research plan and management
  - Integration of the multiple facets
  - Dissemination of research products
  - Program management
  - Workforce development
  - Digital infrastructure
  - Special features…