Multiscale Systems Engineering (MSSE) Research Group

Current Members

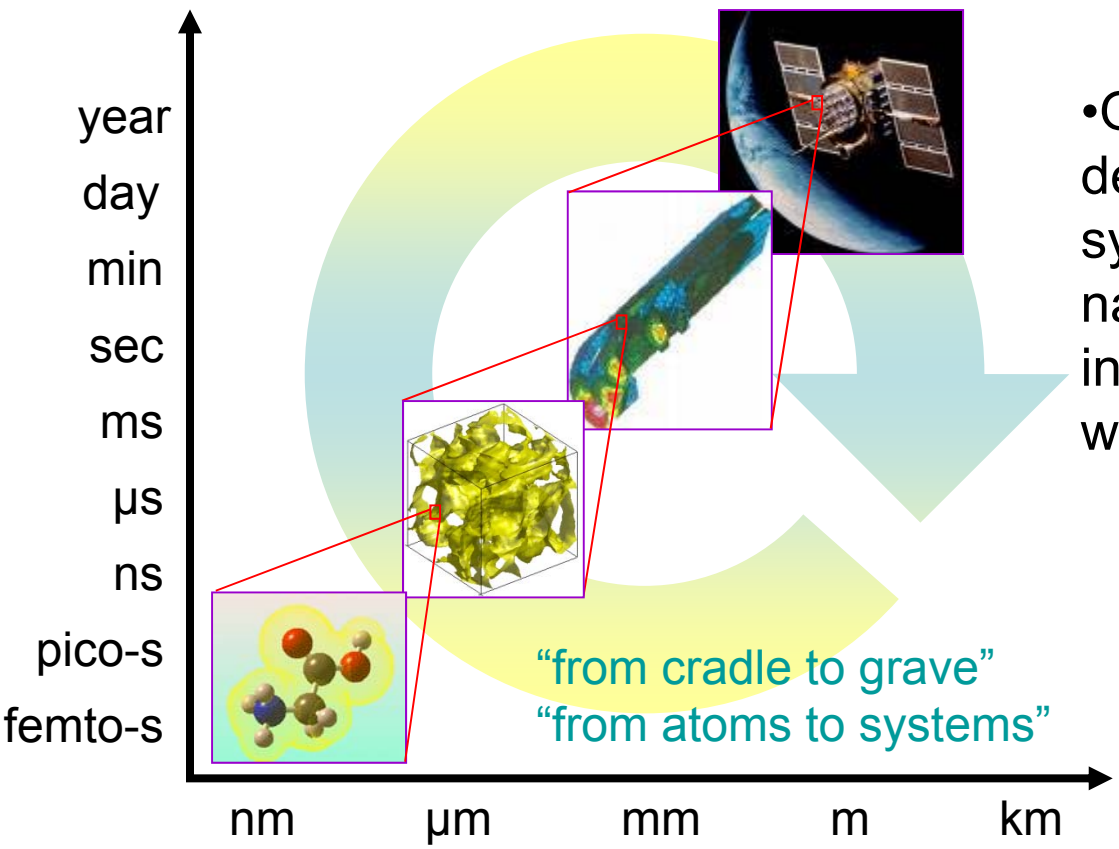
Dr. Yan Wang (faculty member)
Dehao Liu (Ph.D. student)
Jesse Sestito (Ph.D. student)
Yanglong Lu (Ph.D. student)
Michael Kempner (Ph.D. student)
Luka Malashkhia (Ph.D. student)

Recent Project Collaborators

Dr. Chaitanya Deo
Dr. Tequila Harris
Dr. Ling Liu
Dr. David McDowell
Dr. David Rosen
Dr. Wei Sun
Dr. Hongyuan Zha
Dr. Ting Zhu
Dr. Fadi Abdeljawad (Clemson)
Dr. Sung-Hoon Ahn (SNU)
Dr. Ji-Hyeon Song (NTU)
Dr. Anh Tran (Sandia)
Dr. Laura Swiler (Sandia)

Vision

- *Multiscale Systems* are systems consisting of hierarchical structures with different sizes that recursively exhibit patterns of behaviors as the diagnostics of interactions among subsystems at lower levels.



•Our ***vision*** is that computational design tools for multiscale systems with sizes ranging from nanometers to kilometers will be indispensable for engineers' daily work in the near future.

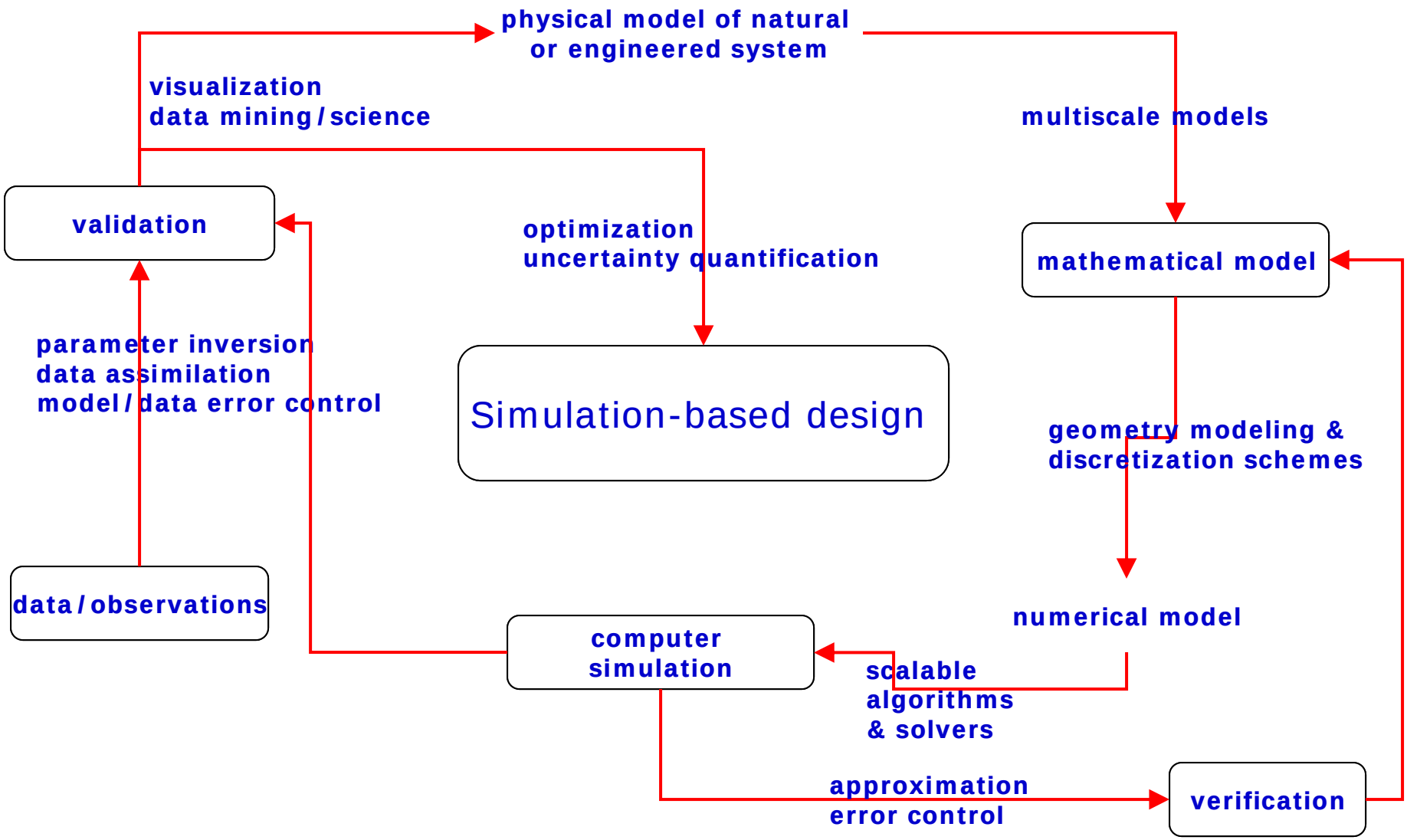
Research & Education Missions

- To create new modeling and simulation mechanisms and tools with underlying scientific rigor that are suitable for multiscale systems engineering for better and faster product innovation
- Train engineers of the future to gain necessary knowledge and skills for future work in a collaborative environment as knowledge creators and integrators

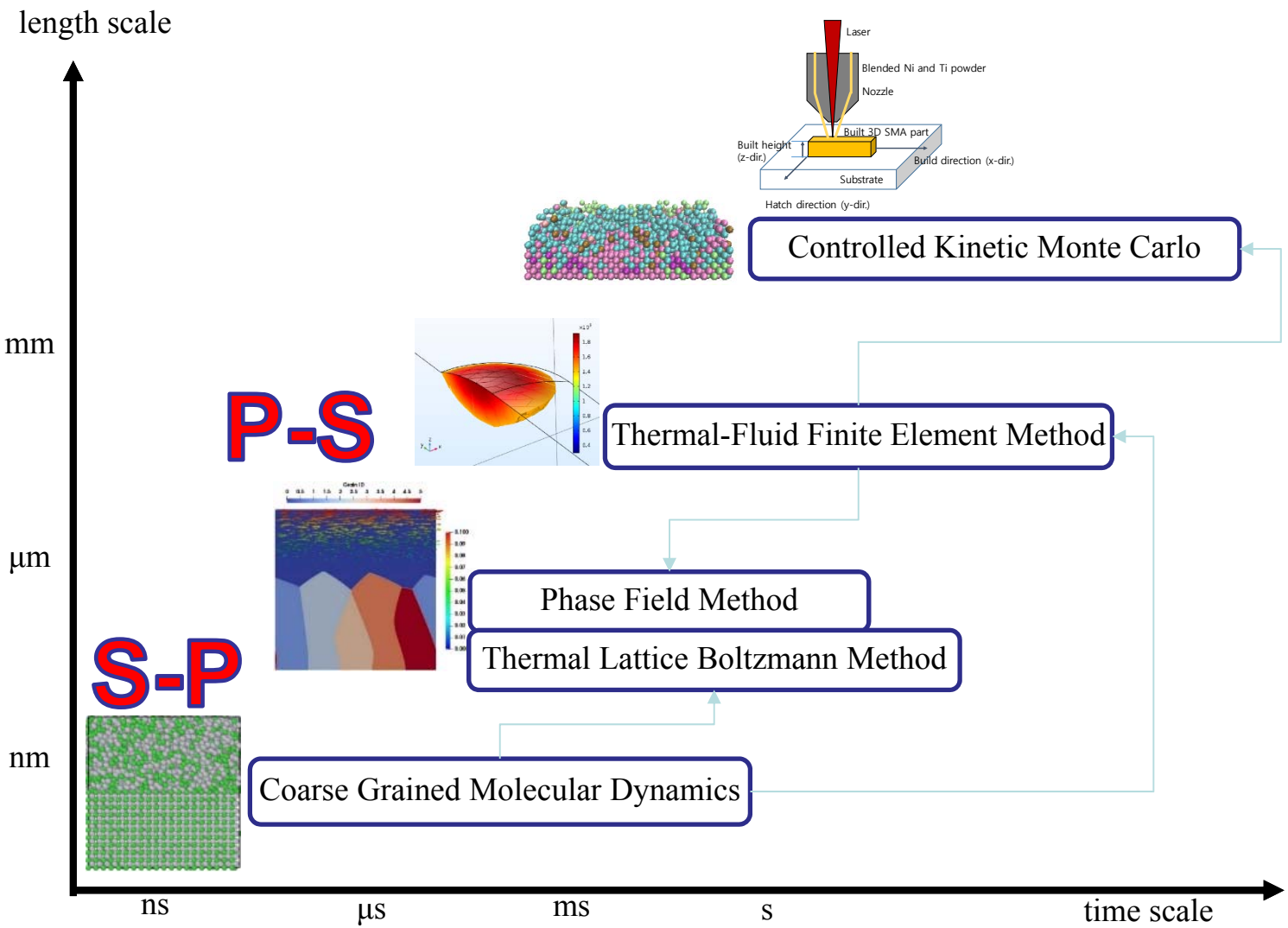
Research Thrust Areas @ MSSE

- The overarching goal of our research is to tackle the *curse-of-dimensionality* design challenge by developing new physics-based data-driven methods to enable engineers to establish comprehensive and robust process-structure-property relationships for systematic product, materials, and process design.
  - Multiscale CAD/CAM/CAE
    - Multiscale simulations (DFT, MD, KMC, PF, FEA, LBM, CFD)
    - Process-structure-property relationship for additive manufacturing process design
    - Design space exploration and global optimization
  - Uncertainty Quantification
    - Reliable multiscale simulation under uncertainty
    - Probabilistic design of systems of cyber-physical-social systems
    - Quantum scientific computing
    - Risk perception and risk-informed decision making
  - Product Lifecycle Informatics
    - Physics-based data-driven process monitoring
    - Data analytics for diagnostics & prognostics
    - Geometric modeling & processing, interoperability

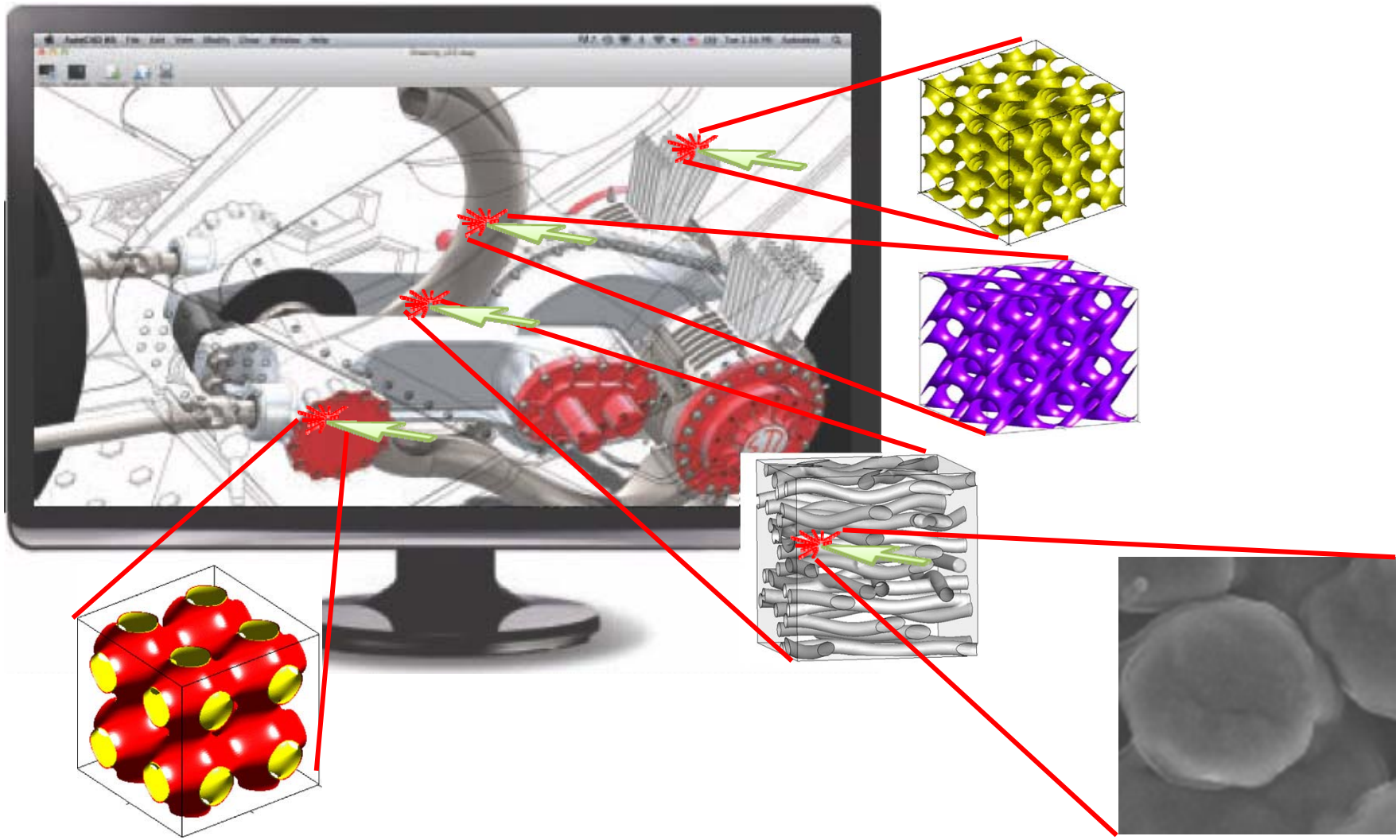
Simulation-Based Product, Materials, & Process Design



Multiscale Multiphysics Modeling & Simulation for Materials Design and Process Design



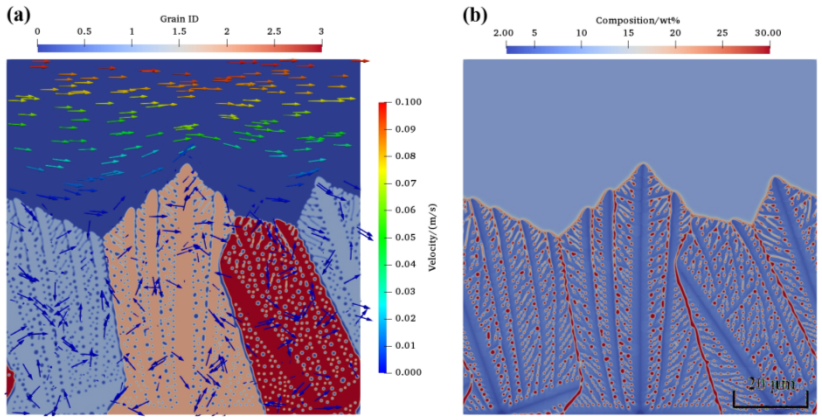
Interactive Multiscale Product-Materials Modeling



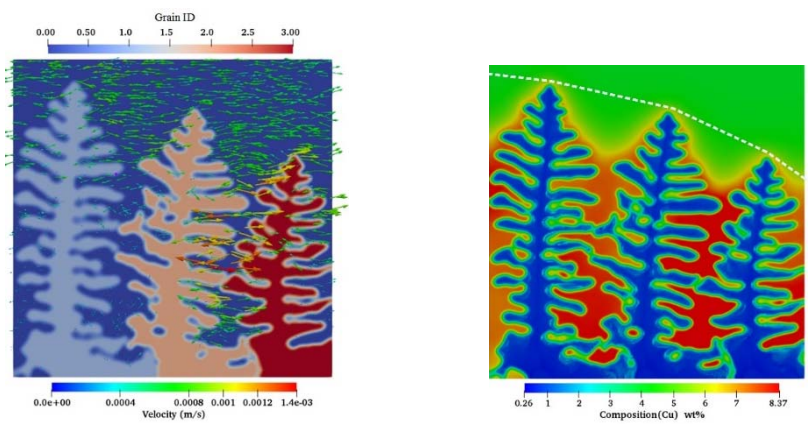
Wang Y. (2007) Periodic surface modeling for computer aided nano design. *Computer-Aided Design*, **39**(3): 179-189.

Additive Manufacturing (AM) Process-Structure Relationship

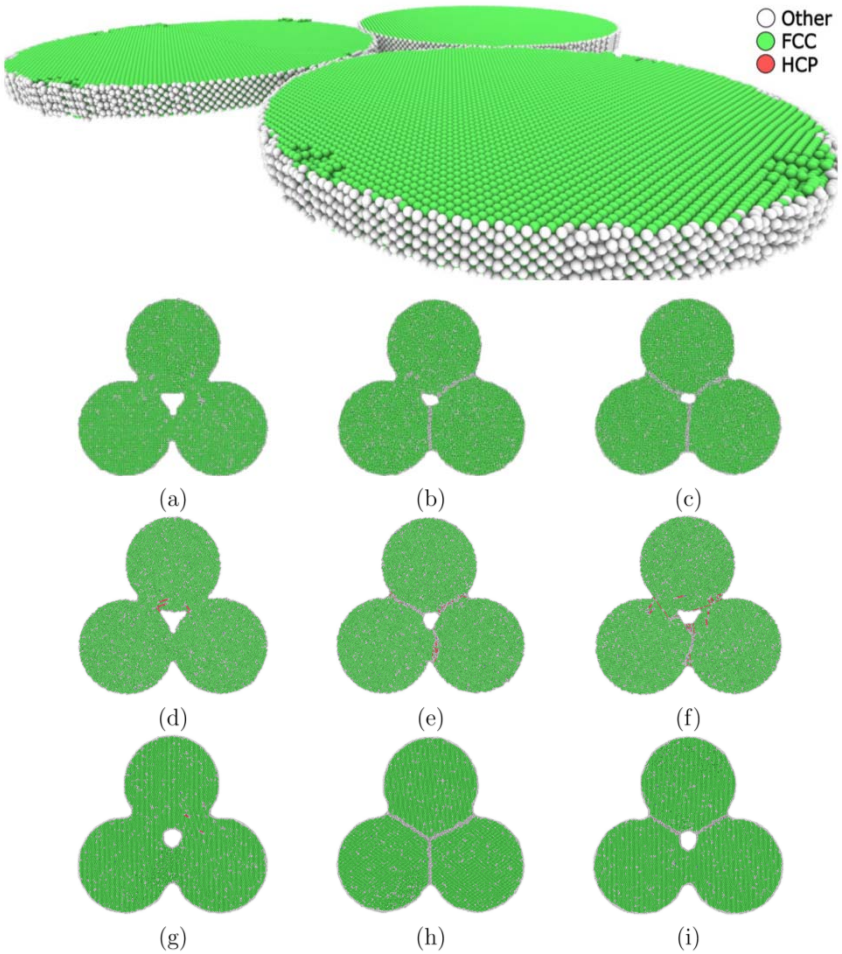
- Solidification
  - Phase field and thermal lattice Boltzmann methods



  - Phase field, magnetic field, and lattice Boltzmann methods

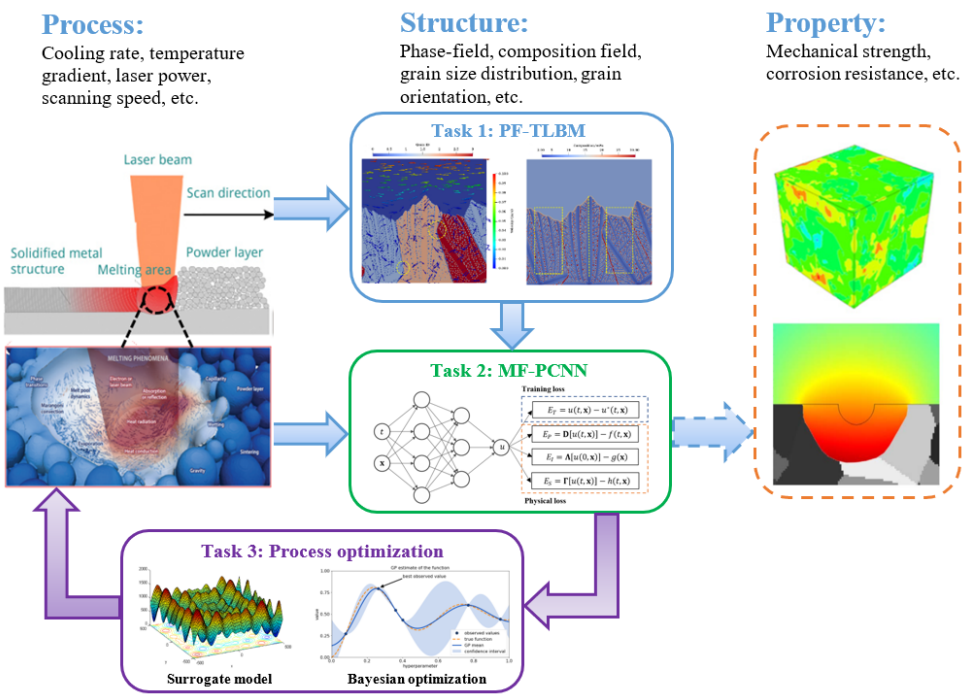


- Sintering
  - Process simulation

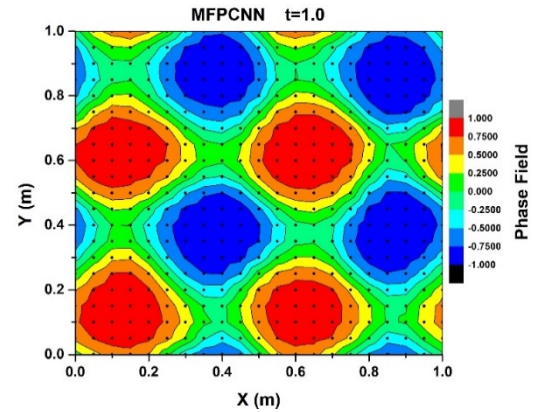


Physics-Constrained Machine Learning for P-S-P Relationship

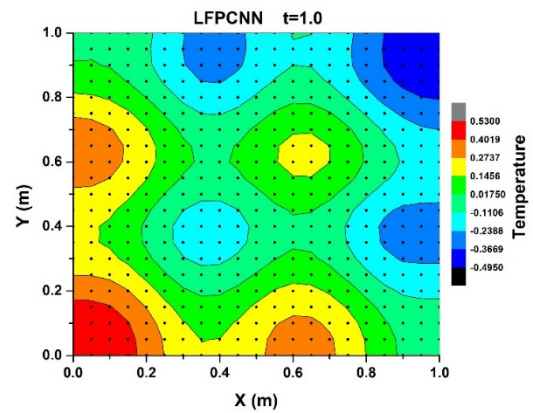
- Multi-Fidelity Physics-Constrained Neural Network (MF-PCNN)
  - Efficient training with ***less data***



- multi-physics predictions
  - Phase transition



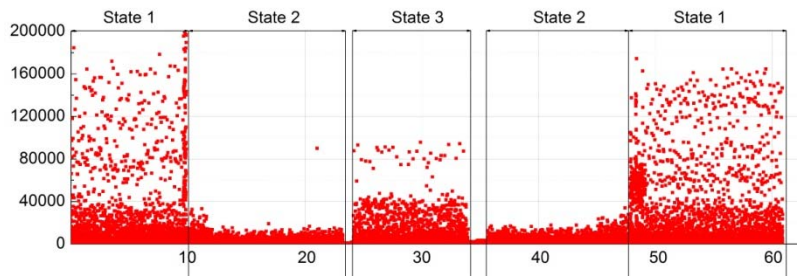
  - Temperature

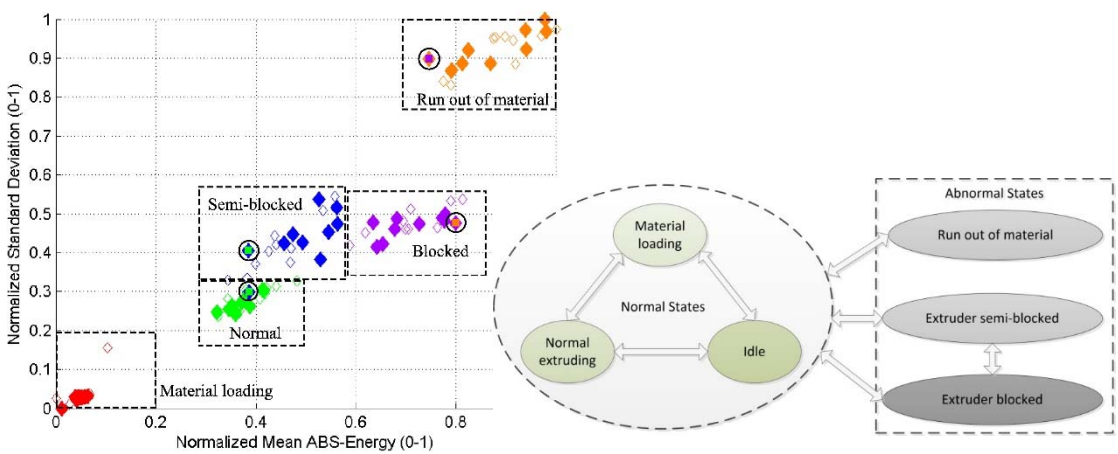


In-situ Process and Machine Health Monitoring

Data-Driven

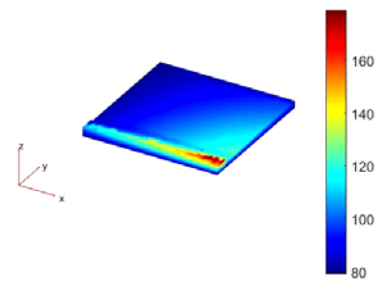
- Statistical machine learning
  - Machine health diagnostics and prognostics



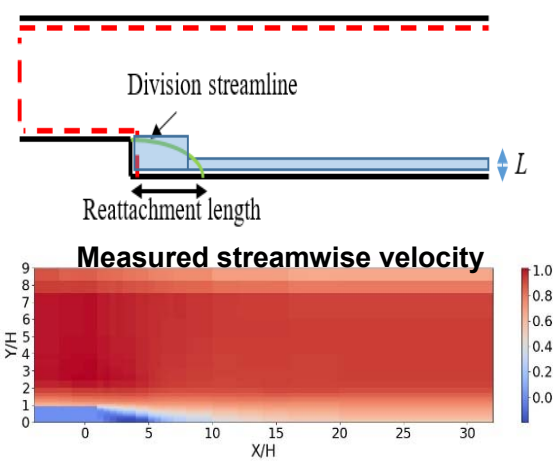


Physics-Based Data-Driven

- Physics-Based Compressive Sensing
  - Monitor temperature

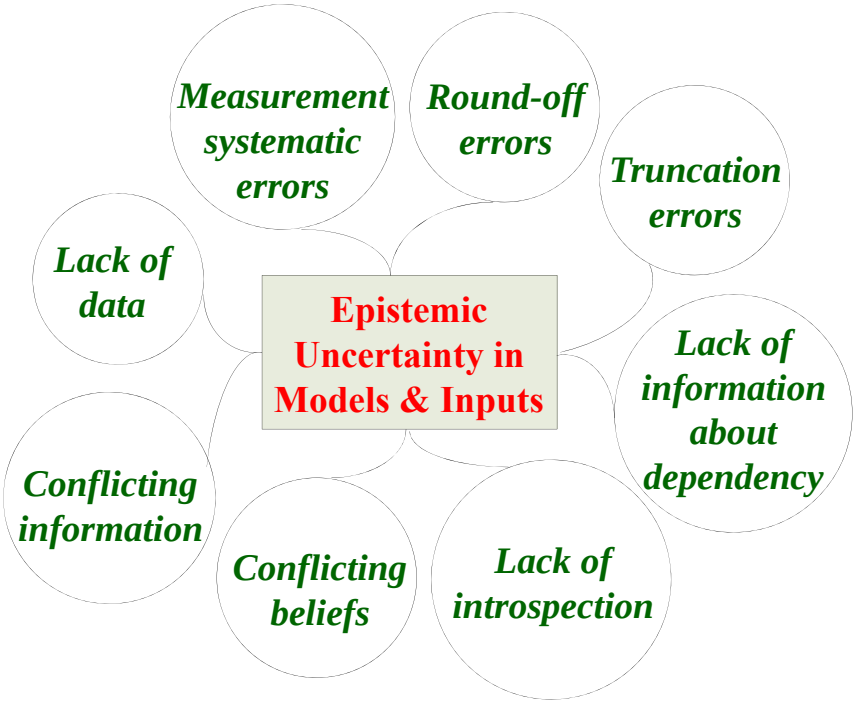


  - Monitor fluid flow

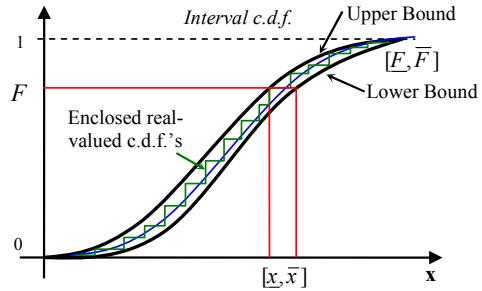


Uncertainty Quantification in M&S

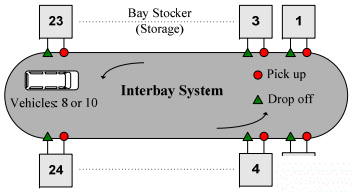
- ***Aleatory Uncertainty:***
  - *inherent randomness*
- ***Epistemic Uncertainty:***
  - *lack of perfect knowledge*



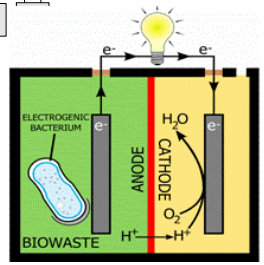
- Interval-based stochastic simulations

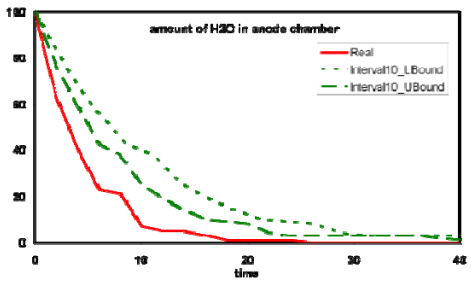


- Queueing Systems:

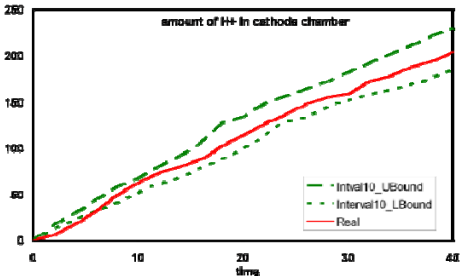


- Microbial Fuel Cell:





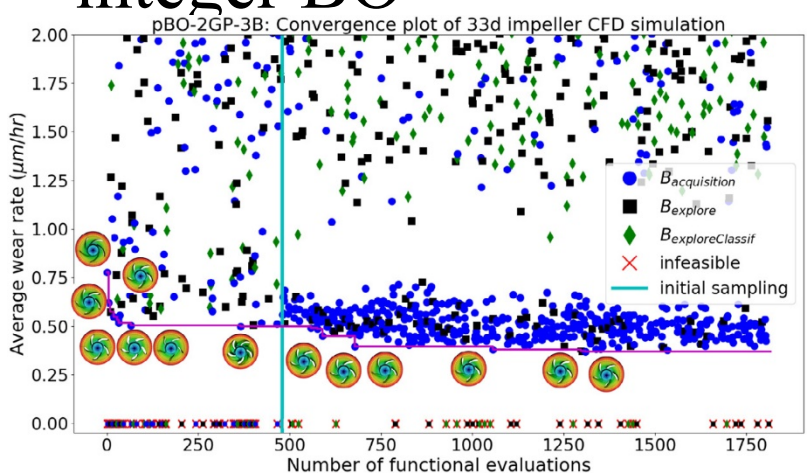
(a) H_2O in anode chamber



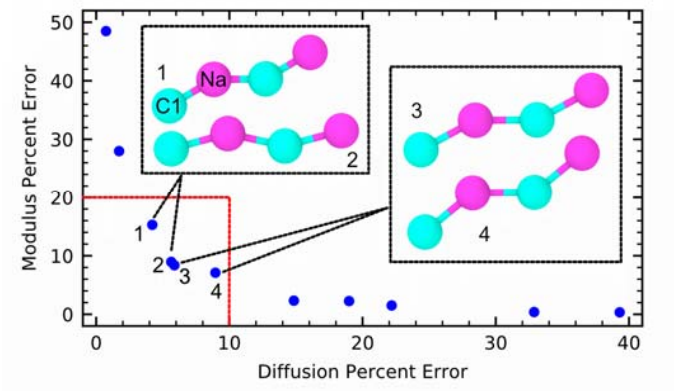
(b) H+ in cathode chamber

Bayesian Optimization

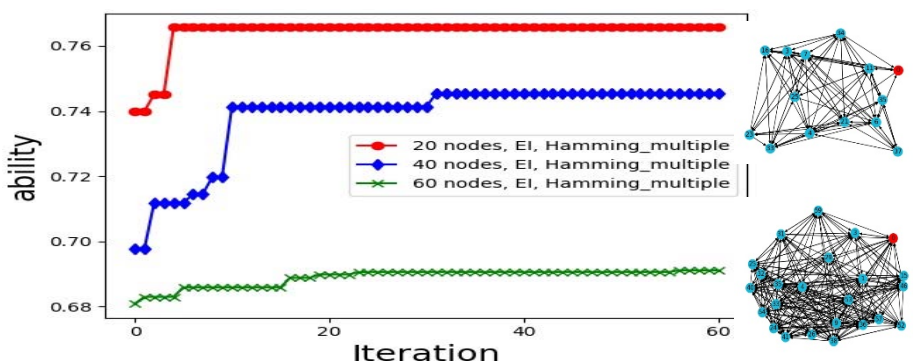
- Constrained and mixed-integer BO



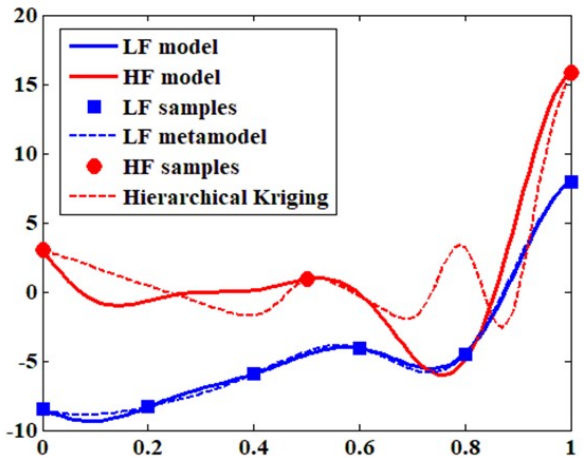
- Multi-objective BO



- Discrete BO

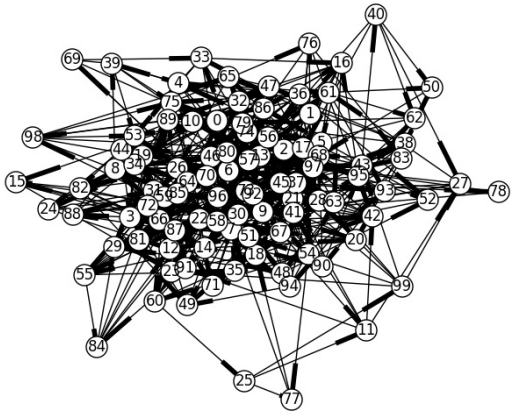


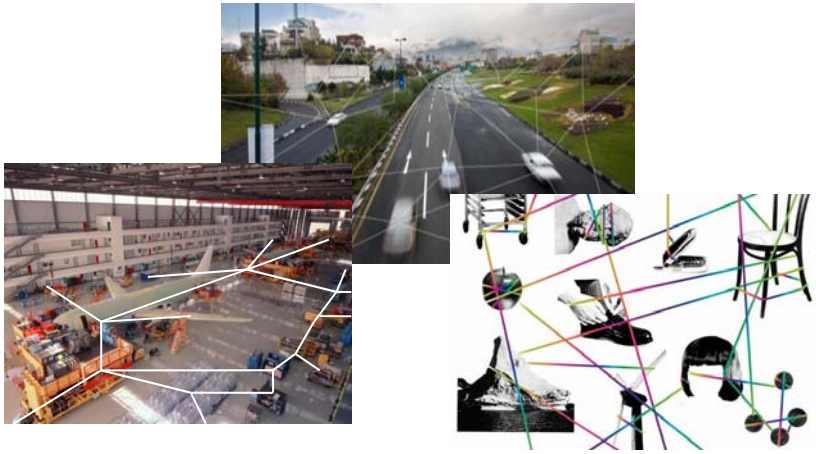
- Multi-fidelity BO



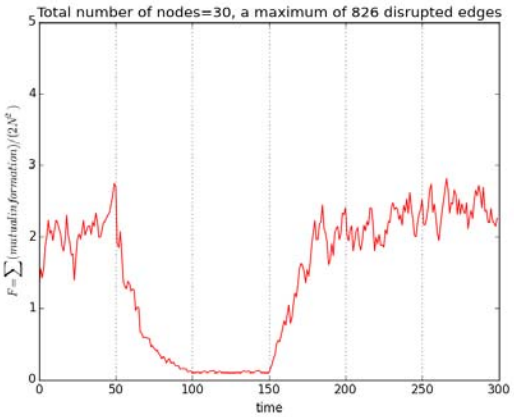
Probabilistic Design of Systems of Cyber-Physical-Social Systems

- Internet of Things (IoT)

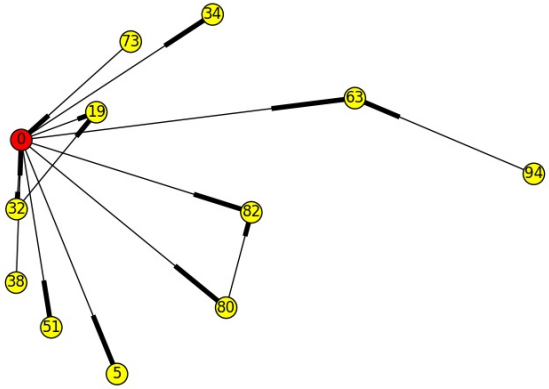




- Resilience

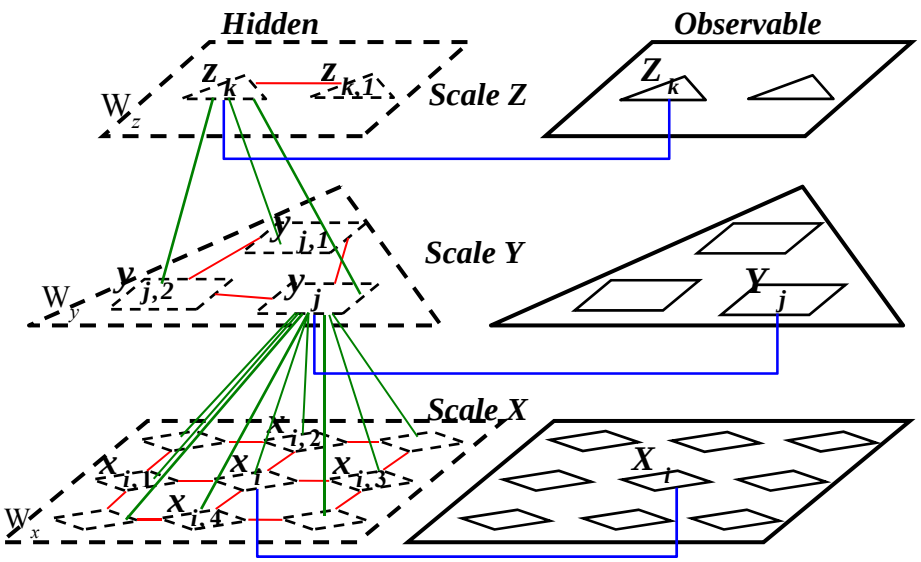


- Trust based network design



Multiscale Uncertainty Quantification

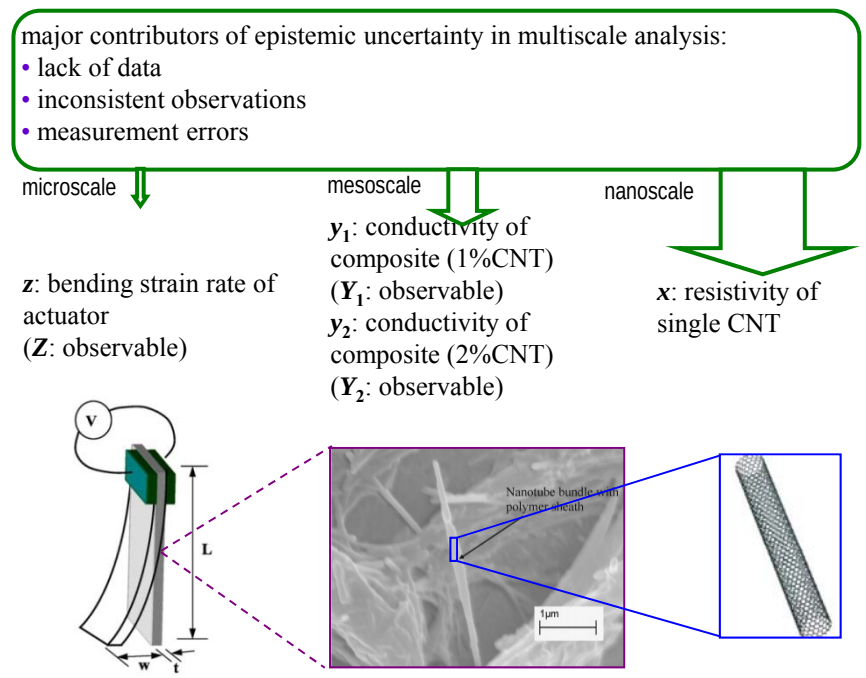
- ***Generalized Hidden Markov Model* (GHMM)**



- ***Generalized Interval Bayes' Rule* (GIBR)**

$$\mathbf{p}\left(E_i \mid A\right) = \frac{\mathbf{p}\left(A \mid E_i\right)\mathbf{p}\left(E_i\right)}{\sum_{j=1}^{n} \mathrm{dual}\,\mathbf{p}\left(A \mid E_j\right)\mathrm{dual}\,\mathbf{p}\left(E_j\right)}$$

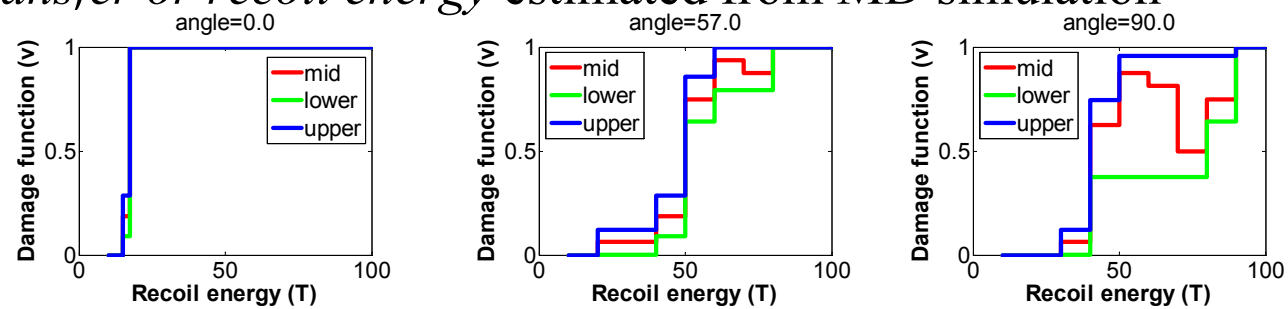
- Multiscale information assimilation
  - Single-Scale Single-Point observation
  - Single-Scale Multi-Point observation
  - Multi-Scale Multi-Point observation
- Carbon nano-tube (CNT) composite actuator design example



Cross-Scale Model Validation Example

molecular dynamics model of material defects

- Imprecise *damage function* from irradiation
  - Imprecise probability that a stable Frenkel pair is generated at certain level of *transfer or recoil energy* estimated from MD simulation



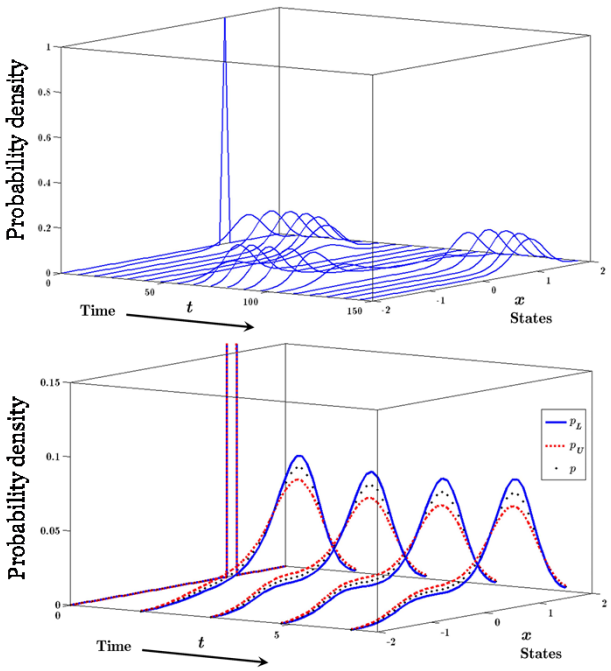
$$f(A,B,C|X,Y) \propto f(X,Y|A,B,C)f(A|B,C)f(B|C)f(C)$$

- Validate unobservable nanoscale model parameters θ with observable macro-scale measurements ($\Delta\rho/n$: *resistivity change*)
- Bayesian calibration and validation

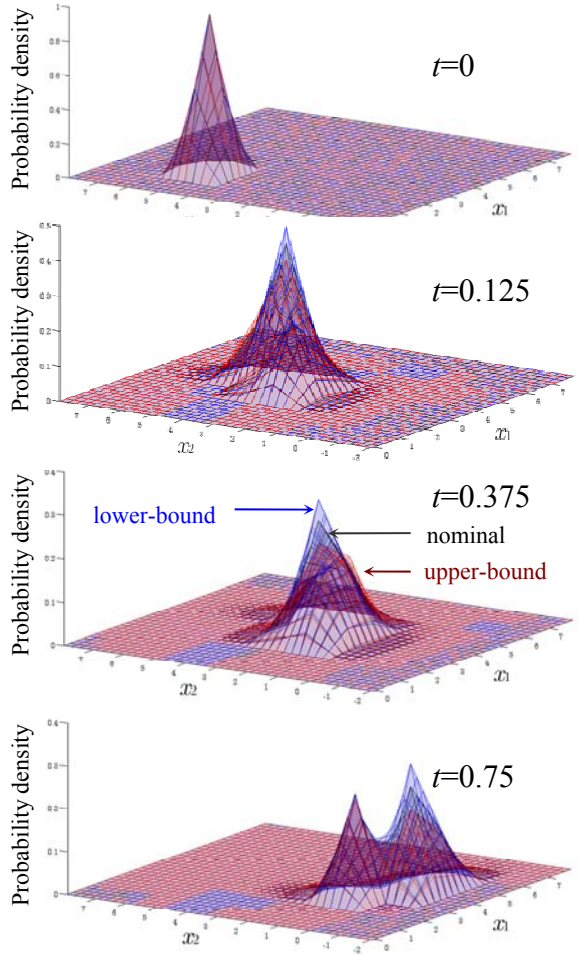
$$\mathbf{p}(\theta \mid \Delta\rho / n) = \frac{\mathbf{p}(\theta)\int\int\left[\mathbf{p}(\Delta\rho / n \mid T_m)\mathbf{p}(T_m \mid T_d)\mathbf{p}(T_d \mid \theta)\right]dT_d dT_m}{\text{dual}\int\int\int\left[\mathbf{p}(\Delta\rho / n \mid T_m)\mathbf{p}(T_m \mid T_d)\mathbf{p}(T_d \mid \theta)\mathbf{p}(\theta)\right]dT_d dT_m d\theta}$$

Reliable Simulation of Stochastic Dynamics

- Simultaneous evolution of aleatory and epistemic uncertainties
- Bi-stable stochastic resonance

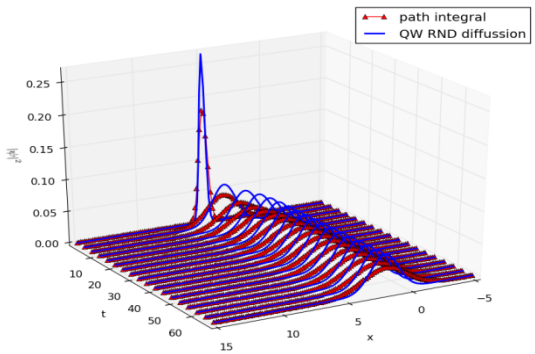


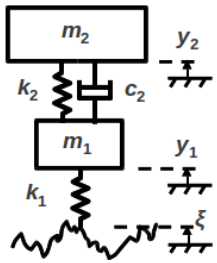
- Van der Pol oscillator



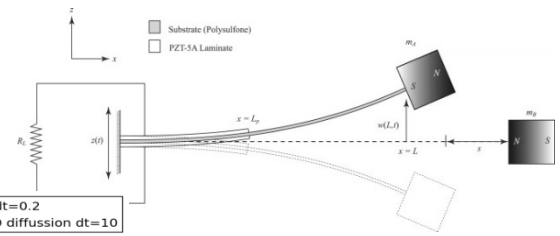
Quantum Scientific Computing

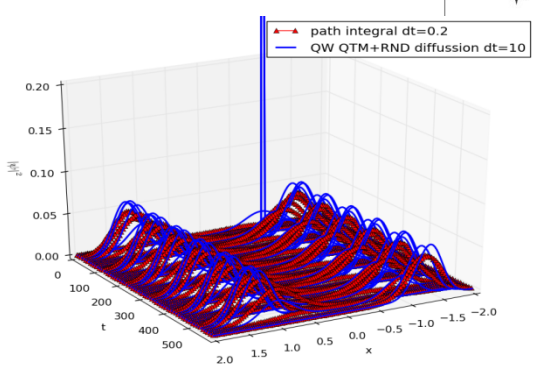
- Quantum walk accelerated drift-diffusion simulations
  - drift



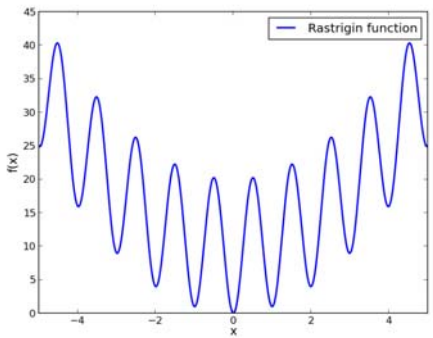


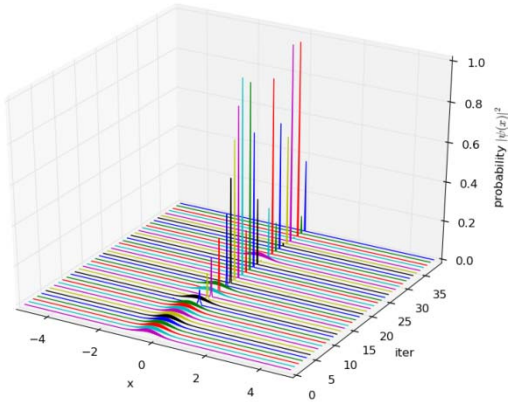
  - bi-stable oscillation

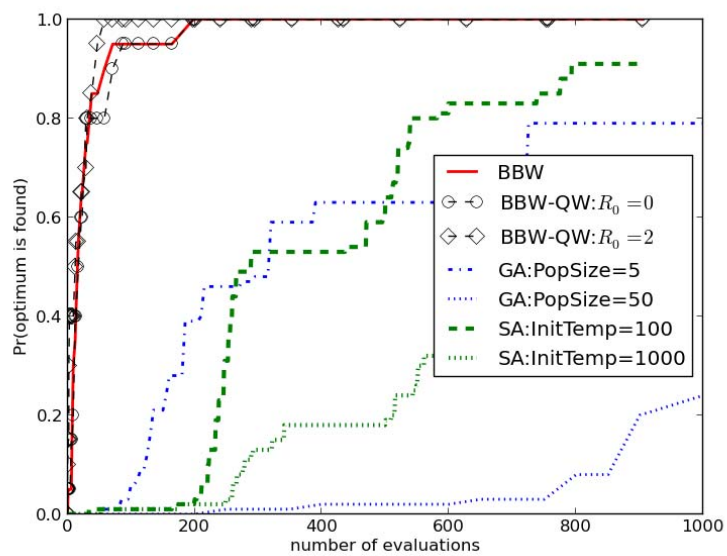




- Grover algorithm for global optimization





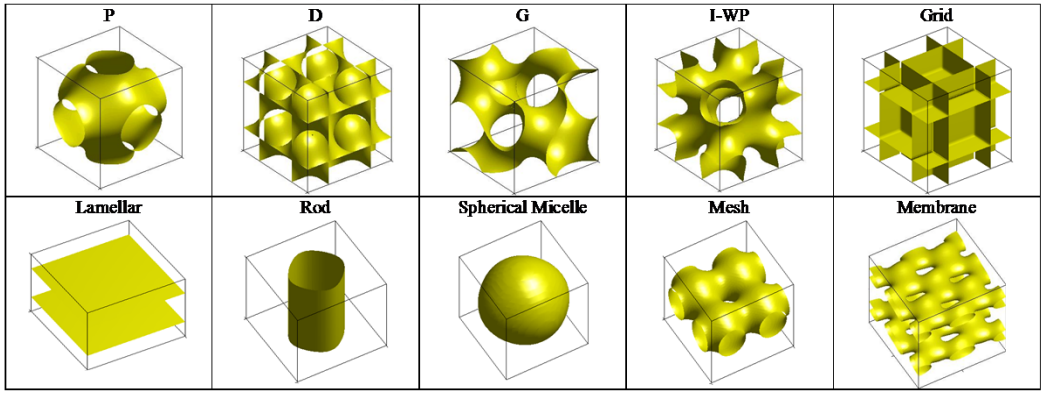


Earlier Projects

Computer-Aided Nano-Design

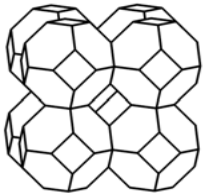
- *Objective*: To investigate the feasibility of modeling and simulating nano structures based on a proposed *periodic surface* model from atomic to meso scales and to expand the horizon of available shapes for design engineers.

$$\psi(\mathbf{r}) = \sum_{l=1}^{L}\sum_{m=1}^{M} \mu_{lm} \cos\left(2\pi\kappa_l(\mathbf{p}_m^T \cdot \mathbf{r})\right)$$

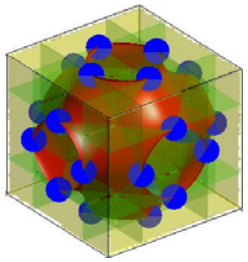


Model construction

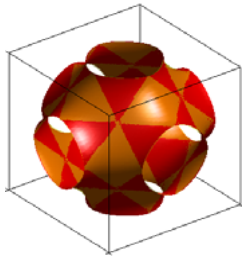
(1a) **Sodalite cages**. Vertices are Si (Al). Edges represent Si-O-Si (Si-O-Al) bonds.



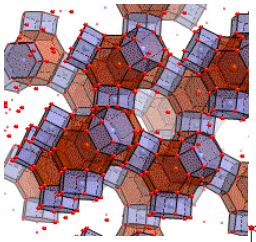
(1b) intersection of P surface and 2 Grid surfaces



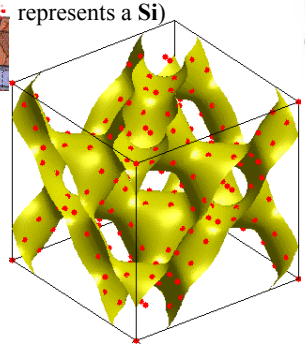
(1c) P surface and its modulation with a Grid surface

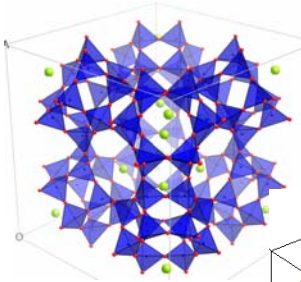


Reverse engineering

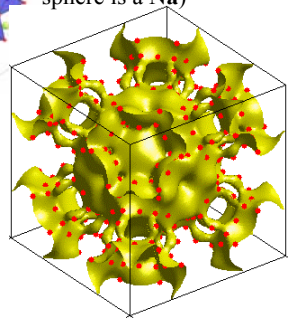


(2a) Reconstructed loci surface from a Faujasite crystal (Each tetradecahedron encloses a **Fe**, each hexagonal prism encloses an **Al**, and each vertex of the polygons represents a **Si**)

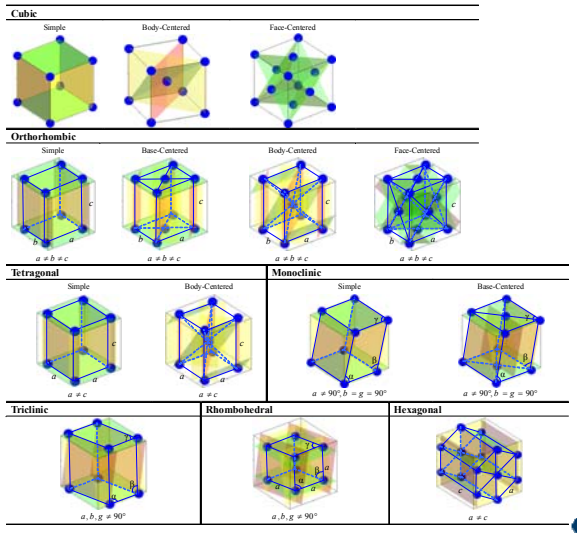




(2b) Reconstructed loci surface from a synthetic Zeolite crystal (Each tetrahedron encloses a **Si**, each vertex of the tetrahedral is a **O**, and each green sphere is a **Na**)



Mathematical models of Bravais Lattice

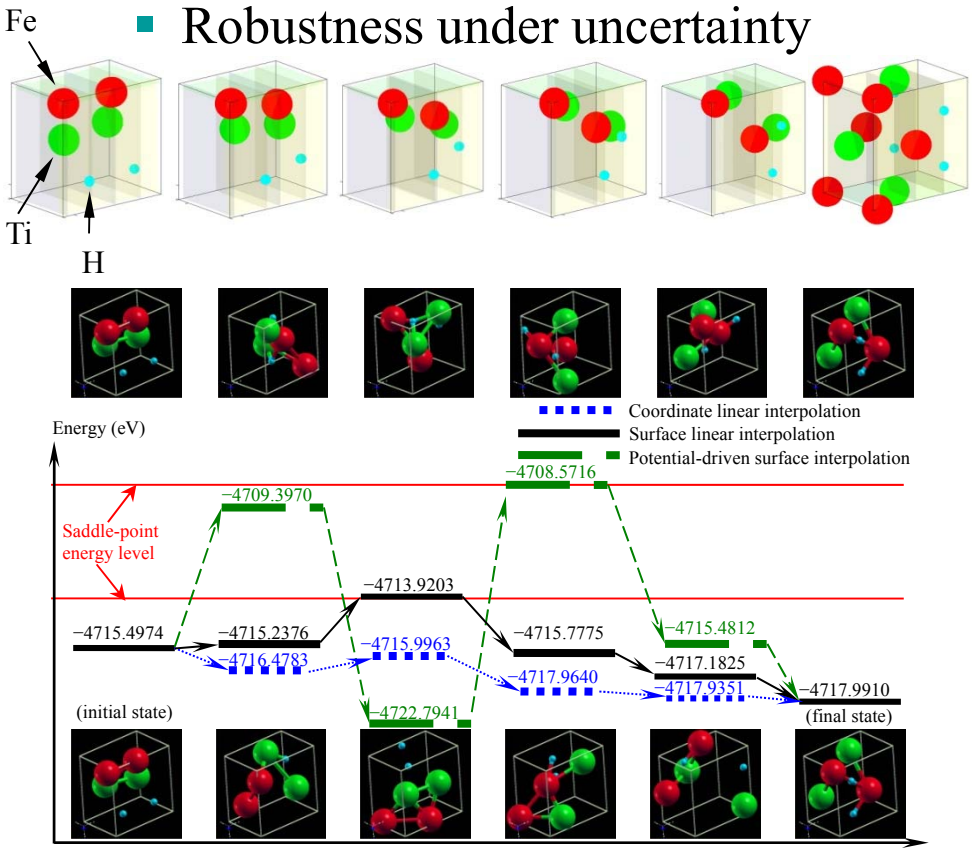


Computer-Aided Phase Transition Design

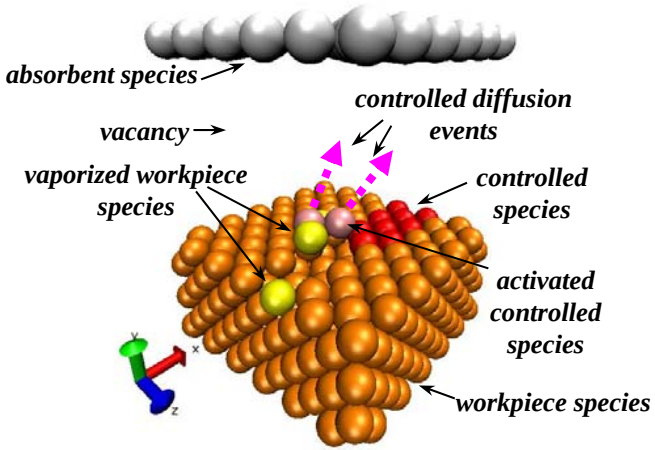
- A phase transition is a geometric and topological transformation process of materials from one phase to another, each of which has a unique and homogeneous physical property.
- Important to design various phase-change materials (e.g. for information storage and energy storage)



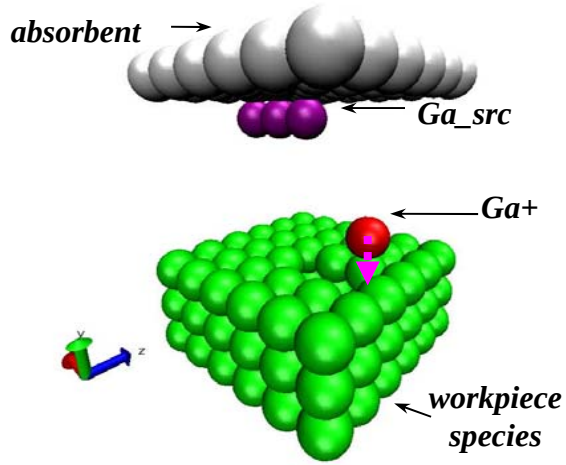

- Phase transition pathway search
  - Parallelization for efficency
  - Robustness under uncertainty



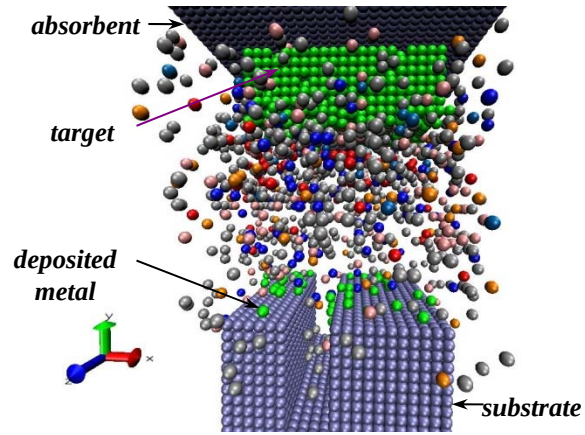
Computer-Aided Nano-Manufacturing



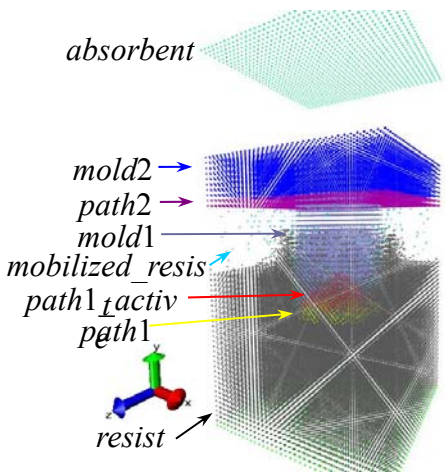
Scanning Probe Lithography



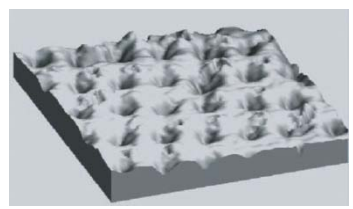
Focus Ion Beam Lithography



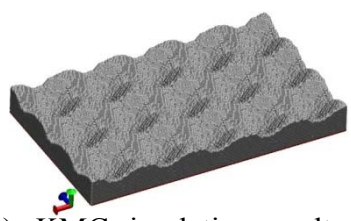
Ionized PVD



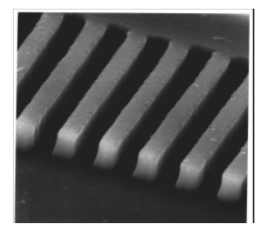
cKMC model of NIL process



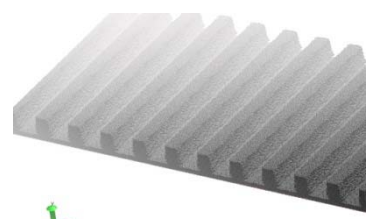
(a) SEM image [Zankovych 2001]



(b) cKMC simulation result



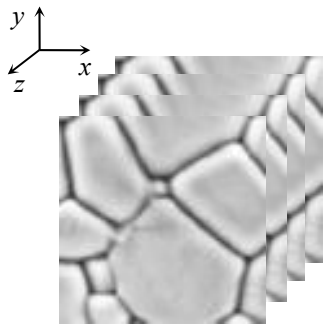
(a) SEM image [Chou et al. 1996]



(b) cKMC simulation result

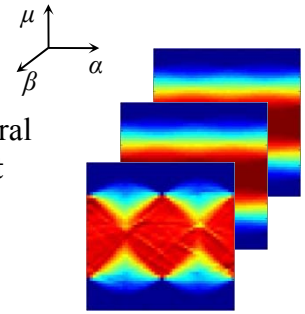
Nanoimprint Lithography

Surfacelets as Materials Descriptors



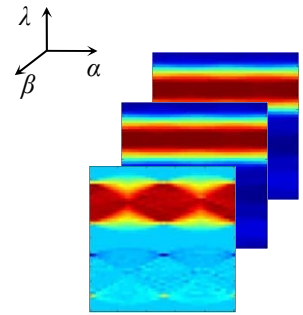
(a) SEM images of SiO2-MnO2 ceramics

surface integral with **ridgelet**

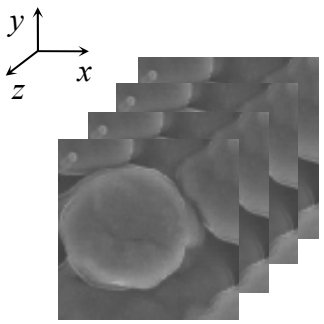


(b) wedgelet surface integral

1D wavelet transform with Haar

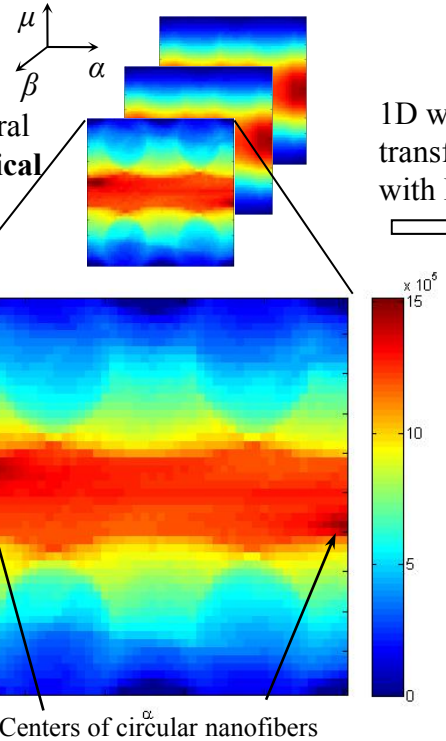


(c) surfacelet coefficients



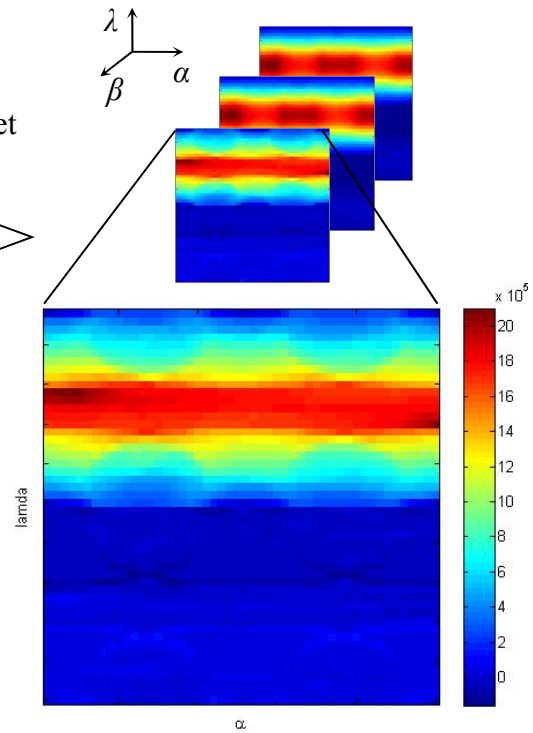
(a) SEM images of polyacrylonitrile-based nanofibers

surface integral with **cylindrical surfacelet**



(b) cylindrical surface integrals

1D wavelet transform with Haar



(c) surfacelet coefficients

Searching Feasible Design Space in Set Based Design
by Solving Quantified Constraint Satisfaction Problem (QCSP)

- For design constraint $f(a,x)=b$ with *input parameter* a, *design target* b, and *design variable* x, we can have
  - united solution set

$$\left\{x \middle| (\exists a \in [\![\underline{a},\overline{a}]\!])(\exists b \in [\![\underline{b},\overline{b}]\!]) f(a,x)=b\right\}$$

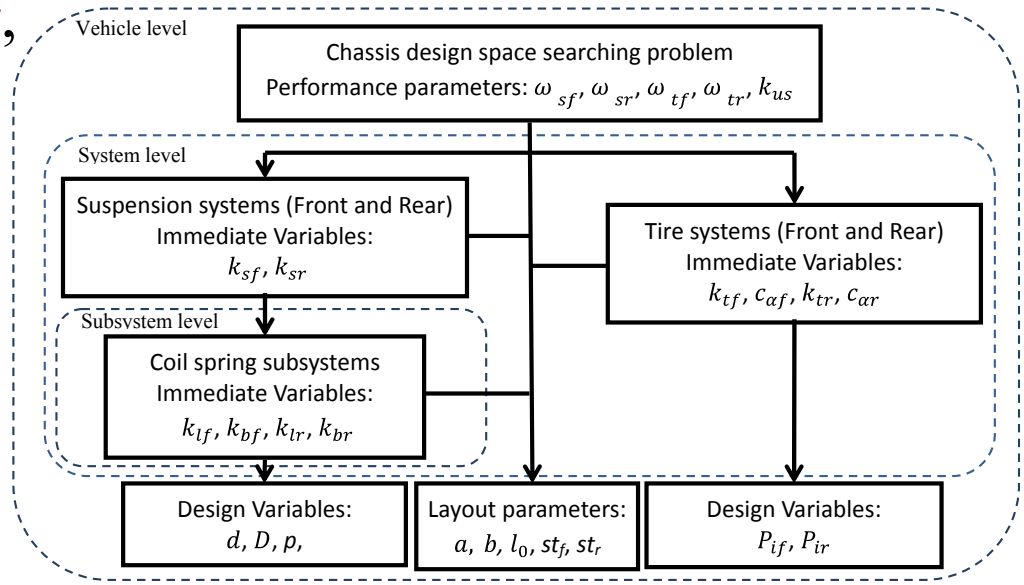
  - tolerable solution set

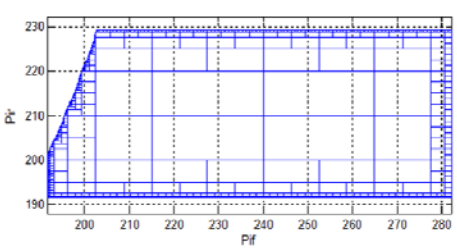
$$\left\{x \middle| (\forall a \in [\![\underline{a},\overline{a}]\!])(\exists b \in [\![\underline{b},\overline{b}]\!]) f(a,x)=b\right\}$$

  - controllable solution set

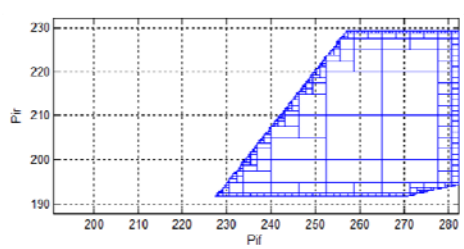
$$\left\{x \middle| (\forall b \in [\![\underline{b},\overline{b}]\!])(\exists a \in [\![\underline{a},\overline{a}]\!]) f(a,x)=b\right\}$$

- Vehicle chassis design example

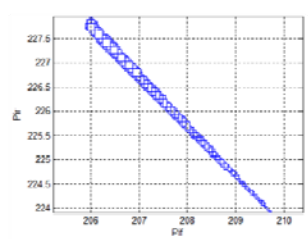




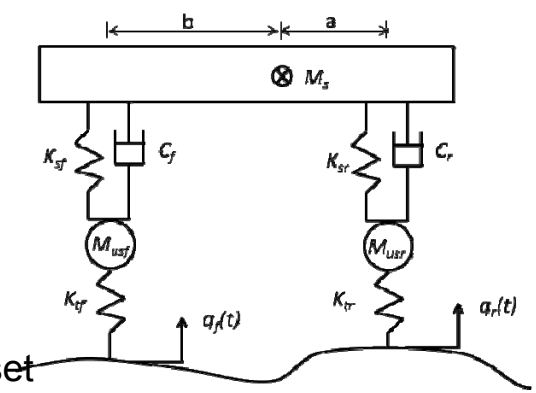
united solution set



tolerable solution set

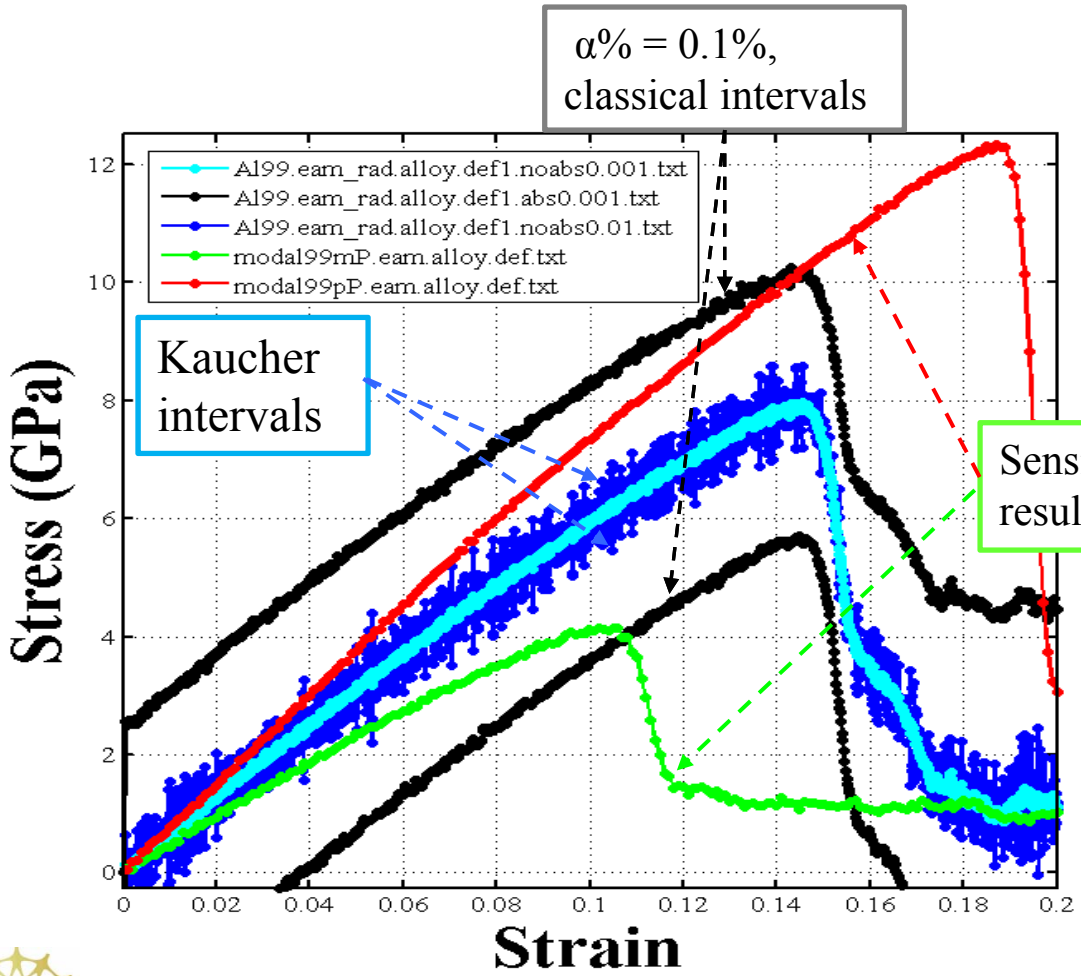


controllable solution set

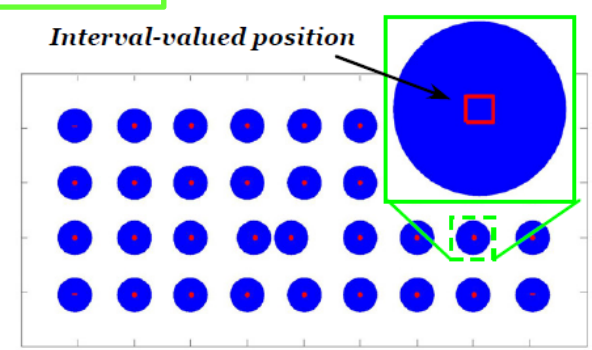


Reliable Molecular Dynamics

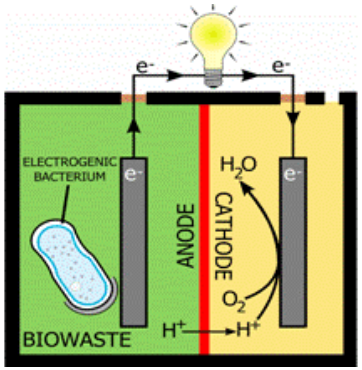
- *Objective*: To develop an efficient alternative to traditional sensitivity analysis for MD and KMC simulations under model form and input uncertainty.



- Uncertain positions and velocities as a result of imprecise interatomic potentials
- Uncertainty effect is assessed on-the-fly with single run of simulation



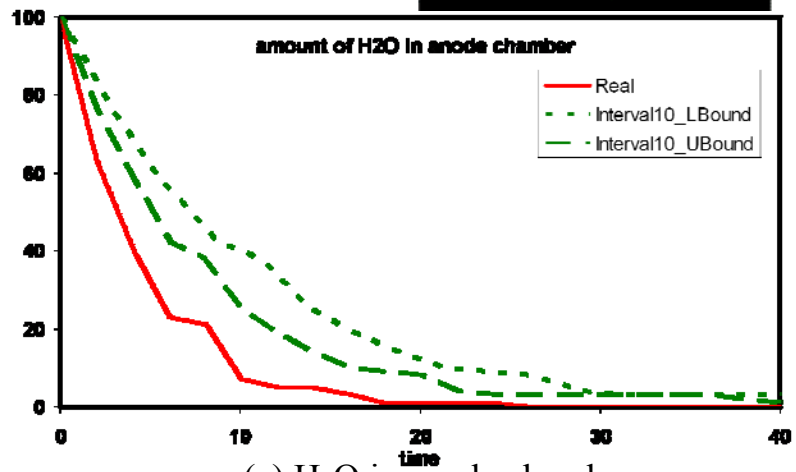
Reliable Kinetic Monte Carlo



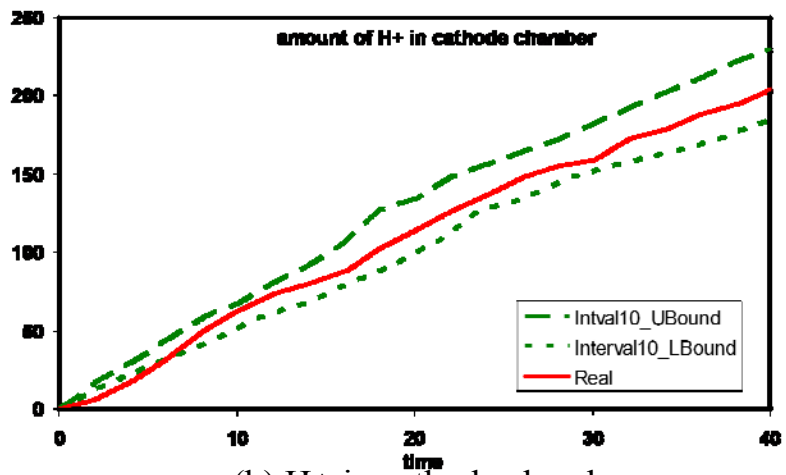
anode chamber

cathode chamber

Event type	Species and reactions	Rate constant
R1: water dissociation	$H_2O \leftrightarrow OH^- + H^+$	10^1
R2: carbonic acid dissociation	$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$	10^1
R3: acetic acid dissociation	$AcH \leftrightarrow Ac^- + H^+$	10^1
R4: reduced thionine first dissociation	$MH_3^+ \leftrightarrow MH_2 + H^+$	10^1
R5: reduced thionine second dissociation	$MH_4^{2+} \leftrightarrow MH_3^+ + H^+$	10^1
R6: acetate with oxidized mediator	$Ac^- + MH^+ + NH_4^+ + H_2O \rightarrow X_{Ac} + MH_3^+ + HCO_3^- + H^+$	10^1
R7: oxidation double protonated mediator	$MH_4^{2+} \rightarrow MH^+ + 3H^+ + 2e^-$	10^1
R8: oxidation single protonated mediator	$MH_3^+ \rightarrow MH^+ + 2H^+ + 2e^-$	10^1
R9: oxidation neutral mediator	$MH_2 \rightarrow MH^+ + H^+ + 2e^-$	10^1
R10: proton diffusion through PEM	$H^+ \rightarrow H\_^+$	10^{-2}
R11: electron transport from anode to cathode	$e^- \rightarrow e\_^-$	10^{-2}
R12: reduction of oxygen with current generated	$2H\_^+ + 1/2O_2\_ + 2e\_^- \rightarrow H_2O\_$	10^5
R13: reduction of oxygen with current generated	$O_2\_ + 4e\_^- + 2H_2O\_ \rightarrow 4OH\_^-$	10^3

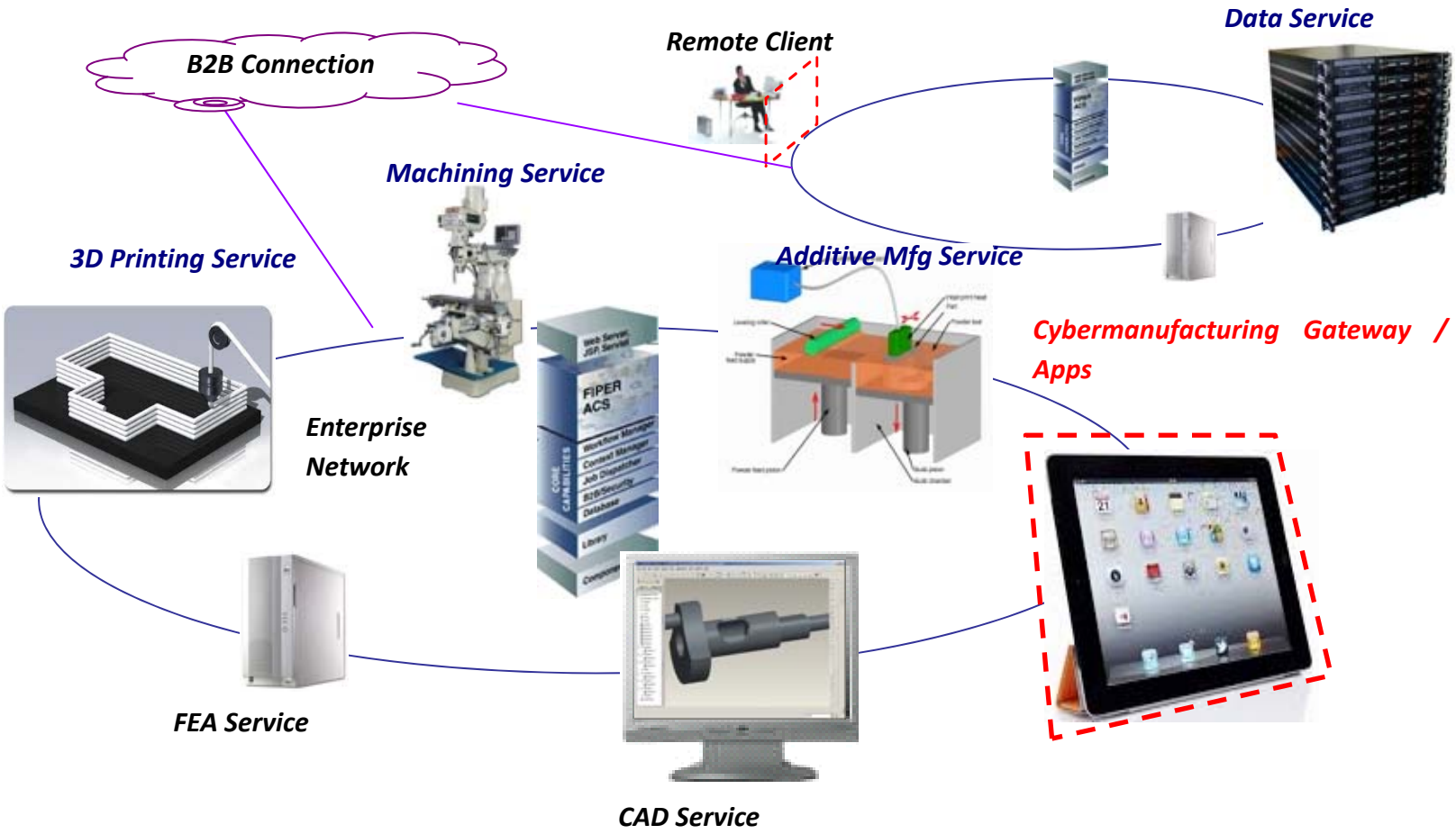


(a) H_2O in anode chamber



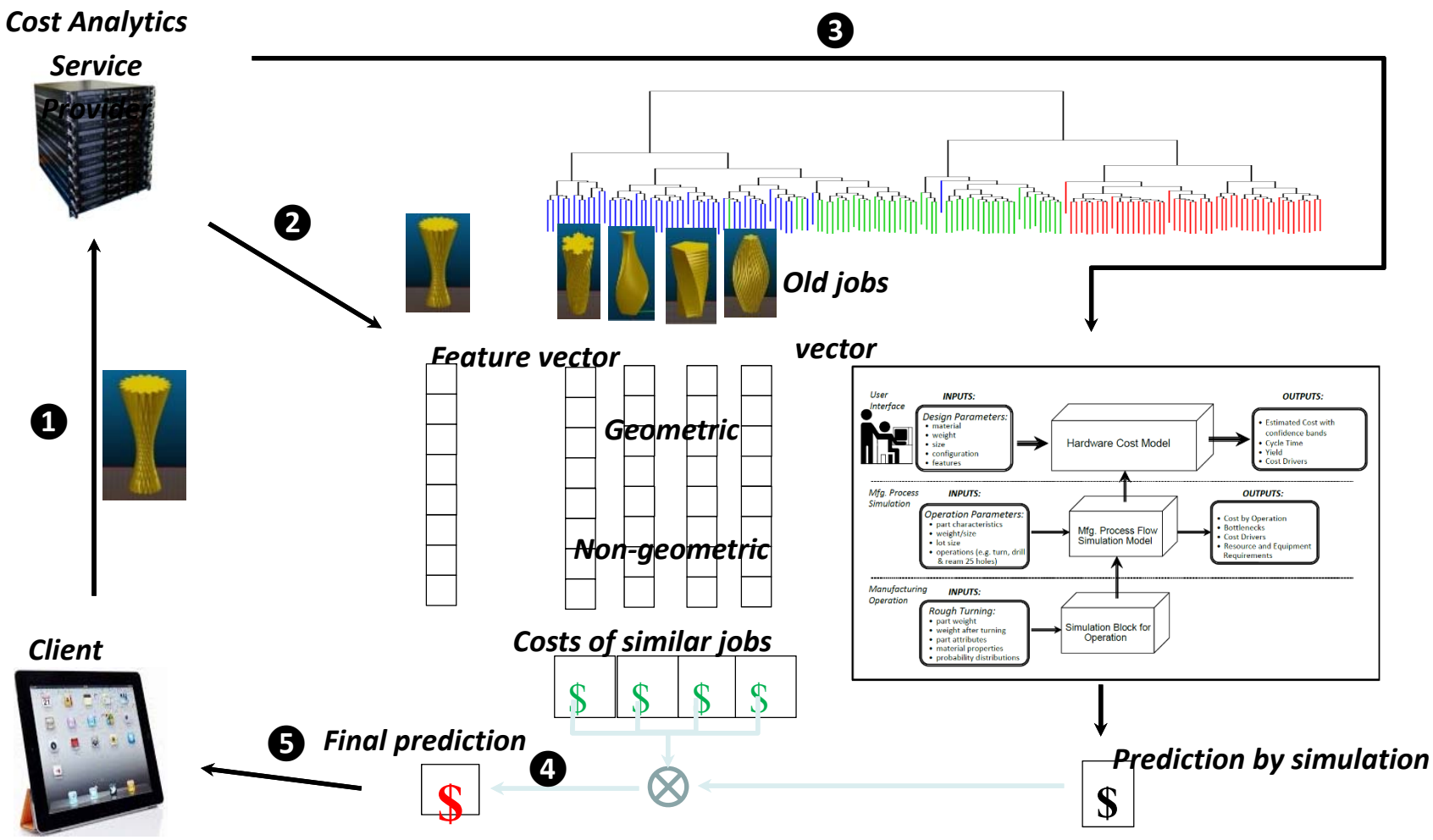
(b) H+ in cathode chamber

Cybermanufacturing

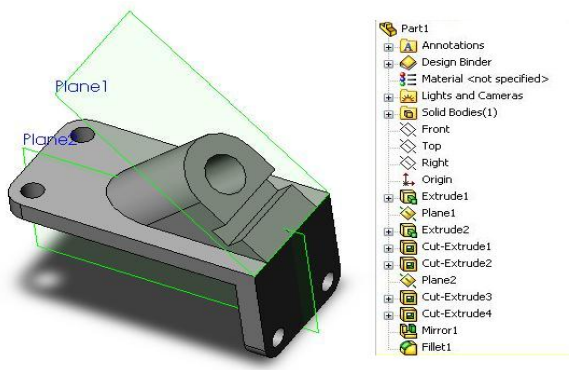


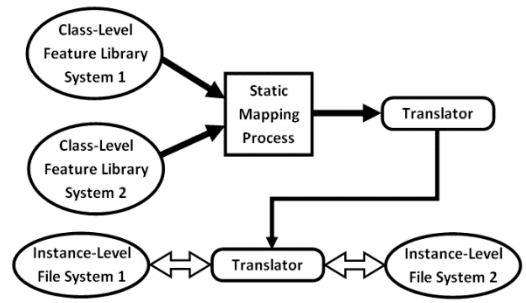
"Manufacturing as Service" based on service-oriented information infrastructure

Manufacturing Cost Estimation with Data Analytics

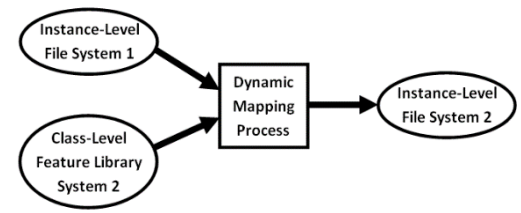


Ontology-Based CAD Interoperability and Verification





(a) static mapping



(b) dynamic mapping

- Promote an open environment with no restrictive single standard of features
- Protect CAD software companies' intellectual property