Multiscale Systems Engineering (MSSE) Research Group

Current Members
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Jesse Sestito (Ph.D. student)  
Yanglong Lu (Ph.D. student)  
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Recent Project Collaborators
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Dr. Bin He (SHU)  
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- **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.

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"from cradle to grave"
"from atoms to systems"
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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

- **Multiscale CAD/CAM/CAE**
  - Multiscale simulations (DFT, MD, KMC, PF, FEA, LBM, CFD)
  - Simulation based additive manufacturing process planning
  - Design space exploration and global optimization

- **Uncertainty Quantification**
  - Reliable multiscale simulation under uncertainty
  - Probabilistic design of systems of cyber-physical systems
  - 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
Multiscale System Analysis & Synthesis
Interactive Multiscale Product-Materials Modeling
Modeling & Simulation (M&S) at Multiple Scales

- Various methods used to simulate at different length and time scales
- Engineering solutions need multiscale information integration

Length Scales

- nm
- μm
- mm
- m

Time Scales

- s
- ms
- μs
- ns
- pico-s
- femto-s

Methods:
- Molecular Dynamics / Force Field
- Tight Binding
- Kinetic Monte Carlo
- Finite Element Analysis
- Dislocation Dynamics
- Quantum Monte Carlo
- Density Functional Theory
- Self-Consistent Field (Hartree-Fock)
Physics-Based Data-Driven Additive Manufacturing Process Prediction

- Solidification
  - Process simulation

- Sintering
  - Process simulation
  - Property prediction
In-situ Health Monitoring & Prognostics of 3D Printing

- Non-intrusive on-line machine state detection
- Time-frequency analysis of sensor data
- Support vector machine for prediction
- Compressive sensing
Manufacturing Cost Estimation with Data Analytics

1. **Feature vector**
   - Geometric
   - Non-geometric

2. **Old jobs**

3. **Costs of similar jobs**

4. **Final prediction**

5. **Prediction by simulation**
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
Multiscale Uncertainty Quantification

- **Generalized Hidden Markov Model (GHMM)**
  
- **Generalized Interval Bayes’ Rule (GIBR)**

\[
p(E_i | A) = \frac{p(A | E_i) p(E_i)}{\sum_{j=1}^{n} \text{dual } p(A | E_j) \text{dual } p(E_j)}
\]

- 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**

  major contributors of epistemic uncertainty in multiscale analysis:
  - lack of data
  - inconsistent observations
  - measurement errors

- \( x \): resistivity of single CNT
- \( y_1 \): conductivity of composite (1\%CNT) 
  (\( Y_1 \): observable)
- \( y_2 \): conductivity of composite (2\%CNT) 
  (\( Y_2 \): observable)
- \( z \): bending strain rate of actuator 
  (\( Z \): observable)
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

- Validate unobservable nanoscale model parameters $\theta$ with observable macro-scale measurements ($\Delta \rho/n$: resistivity change)

- Bayesian calibration and validation

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

$$p(\theta|\Delta \rho/n) = \frac{p(\theta) \int \int [p(\Delta \rho/n|T_m)p(T_m|T_d)p(T_d|\theta)]dT_ddT_m}{\text{dual} \int \int \int [p(\Delta \rho/n|T_m)p(T_m|T_d)p(T_d|\theta)p(\theta)]dT_ddT_md\theta}$$
**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

\[ \alpha\% = 0.1\%, \text{ classical intervals} \]

**Sensitivity Analysis results ±2%**

**Kaucher intervals**

**Interval-valued position**
### Reliable Kinetic Monte Carlo

<table>
<thead>
<tr>
<th>Event type</th>
<th>Species and reactions</th>
<th>Rate constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1: water dissociation</td>
<td>$\text{H}_2\text{O} \leftrightarrow \text{OH}^- + \text{H}^+$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R2: carbonic acid dissociation</td>
<td>$\text{CO}_2 + \text{H}_2\text{O} \leftrightarrow \text{HCO}_3^- + \text{H}^+$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R3: acetic acid dissociation</td>
<td>$\text{AcH} \leftrightarrow \text{Ac}^- + \text{H}^+$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R4: reduced thionine first dissociation</td>
<td>$\text{MH}_3^+ \leftrightarrow \text{MH}_2 + \text{H}^+$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R5: reduced thionine second dissociation</td>
<td>$\text{MH}_4^{2+} \leftrightarrow \text{MH}_3^+ + \text{H}^+$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R6: acetate with oxidized mediator</td>
<td>$\text{Ac}^- + \text{MH}^+ + \text{NH}_4^+ + \text{H}<em>2\text{O} \rightarrow X</em>{\text{Ac}} + \text{MH}_3^+ + \text{HCO}_3^- + \text{H}^+$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R7: oxidation double protonated mediator</td>
<td>$\text{MH}_4^{2+} \rightarrow \text{MH}^+ + 3\text{H}^+ + 2\text{e}^-$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R8: oxidation single protonated mediator</td>
<td>$\text{MH}_3^+ \rightarrow \text{MH}^+ + 2\text{H}^+ + 2\text{e}^-$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R9: oxidation neutral mediator</td>
<td>$\text{MH}_2 \rightarrow \text{MH}^+ + \text{H}^+ + 2\text{e}^-$</td>
<td>$10^1$</td>
</tr>
<tr>
<td>R10: proton diffusion through PEM</td>
<td>$\text{H}^+ \rightarrow \text{H}_+^+$</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>R11: electron transport from anode to cathode</td>
<td>$\text{e}^- \rightarrow \text{e}_-$</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>R12: reduction of oxygen with current generated</td>
<td>$2\text{H}^+ + 1/2\text{O}_2^- + 2\text{e}^- \rightarrow \text{H}<em>2\text{O}</em> -$</td>
<td>$10^5$</td>
</tr>
<tr>
<td>R13: reduction of oxygen with current generated</td>
<td>$\text{O}<em>2^- + 4\text{e}^- + 2\text{H}<em>2\text{O}</em>- \rightarrow 4\text{OH}</em>-$</td>
<td>$10^3$</td>
</tr>
</tbody>
</table>
Probabilistic Design of Systems of Cyber-Physical Systems

- Internet of Things (IoT)
- Resilience
- Trust based network design
Reliable Simulation of Stochastic Dynamics

- Simultaneous evolution of aleatory and epistemic uncertainties
- Bi-stable stochastic resonance
- Van der Pol oscillator

![Graphs showing probability density evolution over time for different states and times.](image)
Quantum Walks for Stochastic Dynamics Simulation and Global Optimization

- drift-diffusion simulation with quantum acceleration
  - drift
  - bi-stable oscillation

- global optimization

Graphs and diagrams illustrating drift-diffusion simulations and bi-stable oscillations, as well as optimization results.
Earlier Projects
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.

\[ \psi(\mathbf{r}) = \sum_{l=1}^{L} \sum_{m=1}^{M} \mu_{lm} \cos \left( 2\pi \kappa_{l} (\mathbf{p}_{m} \cdot \mathbf{r}) \right) \]

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**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.

**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.

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**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).

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**Mathematical models of Bravais Lattice**

- Cubic
- Tetragonal
- Trigonal
- Hexagonal

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**Computer-Aided Nano-Design**

- Reverse engineering
- Model construction
- Mathematical models of Bravais Lattice

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**Multiscale Systems Engineering Research Group**

**Georgia Tech**

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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)

Geometry-guided pathway search for $H_2$ storage material FeTi
Concurrent Saddle Point Search

- Saddle points on potential energy surfaces are used to estimate activation energies in phase transitions and chemical reactions.

Objective
- Search both local minimums and saddle point at the same time.
- Search multiple transition paths to provide a global view of energy landscape.
Computer-Aided Nano-Manufacturing

**Scanning Probe Lithography**
- absorbent species
- controlled diffusion events
- vaporized workpiece species
- workpiece species

**Focus Ion Beam Lithography**
- absorbent
- Ga_src
- Ga+
- workpiece species

**Ionized PVD**
- absorbent
- target
- deposited metal
- substrate

**Nanoimprint Lithography**
- mold2
- path2
- mold1
- mobilized_resist
- path1_activex
- path1
- resist
- 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
Objective: To investigate and develop an integrated representation, dual-Rep, of geometry and materials that support seamless zoom operations in a multiscale CAD environment.

Dual-Rep represent both internal distribution and boundary information with a unified implicit form based on a new kind of basis functions, called surfacelets.

Zoom-in and zoom-out operations can be achieved.

**Surfacelet basis functions**

- **3D ridgelet**
- **Cylindrical surfacelet**
- **Ellipsoidal surfacelet**
Surfacelet Transform for Materials Knowledge Modeling and Data Compression

(a) SEM images of SiO2-MnO2 ceramics
(b) wedgelet surface integral
(c) surfacelet coefficients

(a) SEM images of polyacrylonitrile-based nanofibers
(b) cylindrical surface integrals
(c) surfacelet coefficients

Surface integral with ridgelet
1D wavelet transform with Haar
Centers of circular nanofibers

1D wavelet transform with Haar

Centers of circular nanofibers
Silicon Anisotropic Etching Simulation on GPUs

- Collaborative project with Dr. J. Li at East China University of Science & Technology (ECUST)

- Cellular Automata model on graphics processing units (GPUs)
  - Clustered cell parallelization
Machine State Recognition and Monitoring in Manufacturing Processes

- Collaborative project with Drs. Y. Hu and B. Wu at Huazhong University of Science & Technology (HUST)

- Recognition of cutting tool wear in machining by Generalized Hidden Markov Model (GHMM)
  - Incorporate uncertainty in measurements
  - Train GHMM with imperfect data
Searching Feasible Design Space 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**
  \[ \{ x \mid (\exists a \in [a, \bar{a}]) (\exists b \in [b, \bar{b}]) f(a, x) = b \} \]

- **tolerable solution set**
  \[ \{ x \mid (\forall a \in [a, \bar{a}]) (\exists b \in [b, \bar{b}]) f(a, x) = b \} \]

- **controllable solution set**
  \[ \{ x \mid (\forall b \in [b, \bar{b}]) (\exists a \in [a, \bar{a}]) f(a, x) = b \} \]

Vehicle chassis design example

Vehicle chassis design example

Vehicle level

Chassis design space searching problem
Performance parameters: $\omega_{s_f}$, $\omega_{s_r}$, $\omega_{t_f}$, $\omega_{t_r}$, $k_{us}$

System level

Suspension systems (Front and Rear)
Immediate Variables: $k_{sf}$, $k_{sr}$

Subsystem level

Tire systems (Front and Rear)
Immediate Variables: $k_{tf}$, $c_{af}$, $k_{tr}$, $c_{ar}$

Coil spring subsystems
Immediate Variables: $k_{lf}$, $k_{bf}$, $k_{lr}$, $k_{br}$

Design Variables: $d$, $D$, $p$

Layout parameters: $a$, $l_0$, $s$, $s_t$

Design Variables: $P_{lf}$, $P_{tr}$

united solution set
tolerable solution set
controllable solution set
Interoperable Data Sharing in Product Lifecycle Management (PLM)

**Current issues include:**
- Requires access to reliable translators
- Translations can cause significant delays
- Requires data rework when conversions are not 100% successful
- Broad bandwidth required for neutral model file transfer
- Loss of construction history, features, parameters

**Collaborative design requires:**
- Building a multi-disciplinary repository of all product data
- Long-term data and knowledge retention and reuse
- Legacy data migration
- Partner/supplier integration
- Well-defined, structured and controlled design processes
Cybermanufacturing

Service-oriented information infrastructure for cybermanufacturing
Ontology-Based Feature Representation and Verification between CAD Systems

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

(a) static mapping
(b) dynamic mapping
Data Interoperability for Verifiable Additive Manufacturing

- Process-oriented AM features
- Data exchange for verifiable quality

(a)  (b)  (c)  (d)  (e)