

Multiscale simulation for accelerating advanced process systems design

Products & Catalysts



Units & Processes



Enterprise-wide

Angstroms
Femtoseconds



Space/Time
Parallelization



Meters
Days/hours



Quantum Mechanics

- Energetics
- Physicochemical properties

Molecular Dynamics

- Reaction kinetics
- Solvent or catalyst design

Fluid Dynamics

- Transport phenomena
- Reactor design study

Process Simulation

- Heat & mass balance
- Process design & opt.

Enterprise-wide

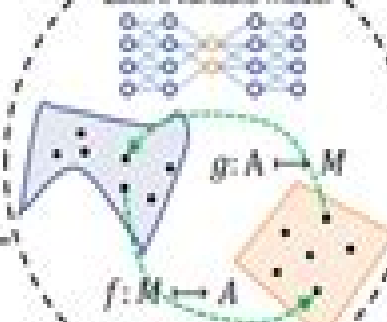
- Energy network systems
- Technoeconomic assessment

a



b

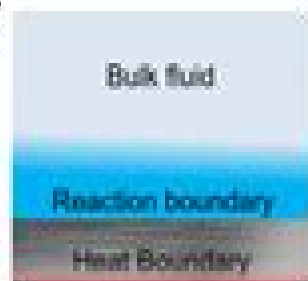
Latent variable model



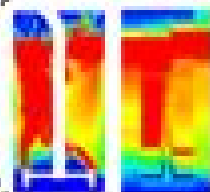
c



d



e



Particle Modeling Modeling And Simulation In Science Engineering And Technology

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Ameta, Tanmoy Chakraborty**

Particle Modeling Modeling And Simulation In Science Engineering And Technology:

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