Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security

Town Hall Meeting: Industrial Processes and Manufacturing Breakout

May 17, 2007
Oak Ridge National Laboratory

Moderators: S. Simunovic, B. Radakrishnan, J. More

Room: SNS L382
http://computing.ornl.gov/workshops/town_hall/index.shtml

Participants

- Sharon Robinson, ORNL
- Ray Bair, ANL
- David Kiefer, Cray Inc.
- Boyana Norris, ANL
- Richard Graham, ORNL
- Richard Murphy, SNL
- Olaf O. Storaasli, ORNL
- Sreekanth Pannala, ORNL
- Paul Wang, Mississippi State University
- Gorti Sarma, ORNL
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- Jorge More, ANL
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Agenda

- Industrial Processes and Manufacturing: Sharon Robinson, ORNL Industrial Technologies Program Manager
- Simulations in Chemical Processing, Sreekanth Pannala, ORNL
- The Optimization Viewpoint, Jorge More, ANL
- Discussion, exascale requirements, planning

Motivation for Supercomputing for Industrial Processing and Manufacturing

- Development and adaptation of next-generation technologies that can revolutionize U.S. industrial processes
- Integrate and optimize existing processing routes to build up industrial competitiveness
- Develop entirely new processing routes and supply chains
- Enable mass production of nano-scale materials, structures, devices

Impact

- Enable significant reductions in energy consumption and emissions through advanced simulations
  - Advance utilization of renewable energy sources
  - Minimize energy consumption in energy-intensive industrial processes
- Advance competitiveness of the U.S. industry
  - New processing routes, energy savings, new products

Exa-scale Computational Targets

- Energy
  - Device optimization & manufacturing for efficient coal conversion with CO_2 sequestration (clean coal combustion)
- Competitiveness
  - Mass production of nano-structured materials for energy applications (optimal nano-scale manufacturing)
  - Intelligent and integrated manufacturing
- Sustainable Ecology
  - Processes for cellulose bio-fuel (efficient bio-fuel production)
- Security
  - Nano-scale sensor design and manufacturing
- Manufacturing overlap for nuclear energy initiative
  - *Fabrication of new nuclear fuel pellets (safe and clear fuel)*
  - *Catalysts for separations of nuclear waste for closing fuel cycle (securing nuclear waste)*

Actions

- Establish clear connection to DOE applied programs and industry
  - EERE, OIT, Interagency Groups, Industry consortia
- Leverage existing OS investments in multi-scale

Questions

- What are current simulation limitations in industrial processing?
  - Software, performance, efficiency and scaling
- How would manufacturing benefit from exaFLOPS computing?
  - What can be achieved if exaFLOPS computing is available that cannot be achieved now?

Technical Barriers

- Length scales O(5-11) in 3D
- Time scales O(6-12)
- Exa-scale algorithms
  - Scalable nonlinear solvers, transport algorithms
  - Coupled, physics-based, multi-scale, multi-physics models
  - Process optimization for multi-* problems
- Efficient implementation
  - Computational algorithm implementation on hierarchical supercomputing architectures
- Clear benefit tradeoff, uncertainty and error estimates
  - Limitation of current models, areas of unacceptable uncertainty
  - Do new methods reduce uncertainty to acceptable levels?

Presentations Summary

Industrial Processes and Manufacturing

Presented by:
Sharon Robinson
ORNL Industrial Technologies Program Manager

Presented at:
Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security Town Hall Meeting: Manufacturing Breakout Session

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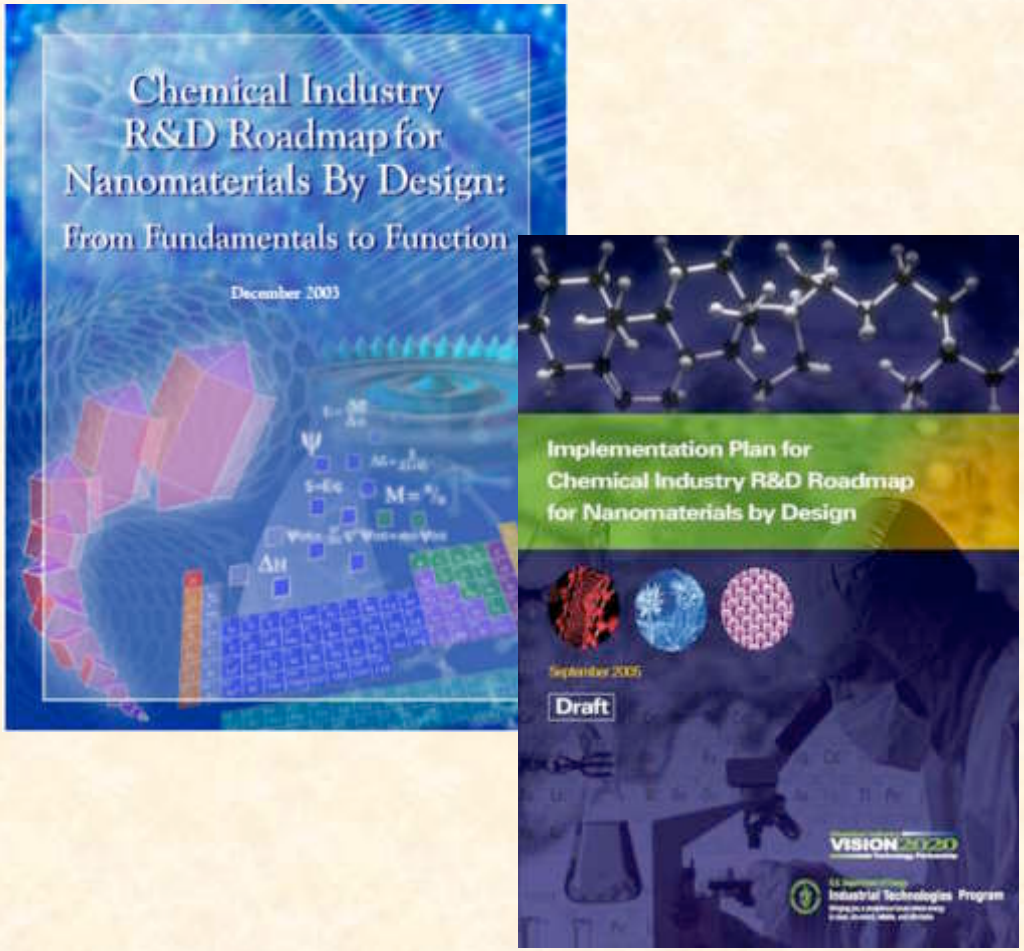
DOE Industrial Technologies Program New Programmatic Areas

- Energy Intensive Industrial Processes
  - Reactions and separations
  - High temperature processes
  - Energy conversion systems
  - Fabrication from basic materials
- Next Generation Manufacturing R&D
  - Manufacturing scale-up and innovation
  - Nanomanufacturing
  - Intelligent and integrated manufacturing
- Fuel and Feedstock Flexibility
  - Alternatives to oil and natural gas

Nanomanufacturing

Industrial R&D Needs Defined for Nanomaterials by Design

- Report identified over 30 priorities in 9 categories
- Ultimate goal:
  - *"accelerated commercialization of innovative technology based on nanomaterials"*



www.chemicalvision2020.org/nanotechnology.html

Modeling Needs: Infrastructure

- **Innovative algorithms to model over multiple length and timescales for realistic system sizes**
  - More foundational long term algorithm development is needed
- **Models experimentally validated**
- **Systematic experiments that develop fundamental understanding**
  - Metrology to characterize structure and properties
- **Increased access to high speed computing capabilities**
- **Improved portability of models on existing computing platforms**

Modeling Needs: Technical

- Designed Synthesis of Nanostructured Materials
- Nanomaterial Surface Chemical Reactivity
- Nanomechanical & Interface Properties
- Electronic Properties & Transport
- Self Assembled Material Properties
  - Mechanical, electronic, chemical reactivity, and magnetic

Fuel and Feedstock Flexibility

Vision2020's prioritized alternative fuel sources for chemical pathways

Red – Recommend pursuing

PRELIMINARY

Alternative Chemical Pathways	Alternative Fuel Sources		
	Coal	Biomass	Petcoke & Residual Gas
Olefins	Gasification - High	Gasification –Med Fermentation – High for ethanol dehydration	Gasification – High for Residual Gas
Aromatics	Gasification – High	Extraction - High from lignin	
Oxygenated Hydro-carbons		Fermentation - Med	
Halogen Hydro-carbons		Fermentation - Med	
Paraffinic	Fermentation - Med		

Computational R&D Needs to Support Alternative Fuel/Feedstocks

- Understanding chemical reactions
- Understanding kinetics
- Design of selective catalysts
- Prediction of physical properties

Simulations in Chemical Processing

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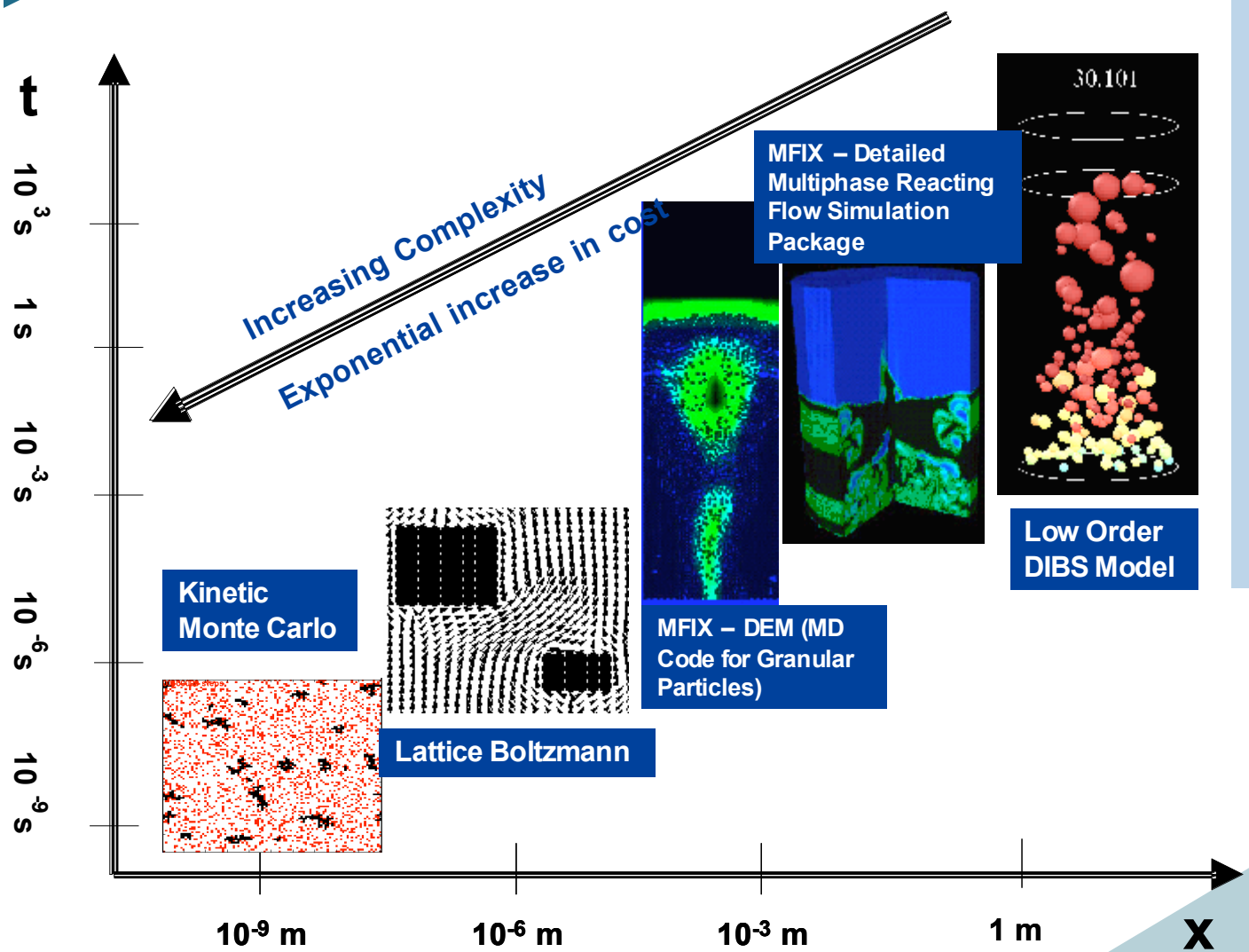
Multiphysics heterogeneous chemically reacting flows for energy systems

Goal: Building a suite of models for unprecedented capability to simulate multiphase flow reactors



- Through support from various DOE offices (FE, EERE, and NE) we have developed suite of models for unprecedented capability to simulate heterogeneous chemically reacting flows
- Hybrid methods to couple two physical models (e.g. MFIX DEM)
- Uncertainty quantification to probe only quantities of interest at smaller scales

Multiscale/Multiphysics modeling is a recurring theme across heterogeneous reaction processes

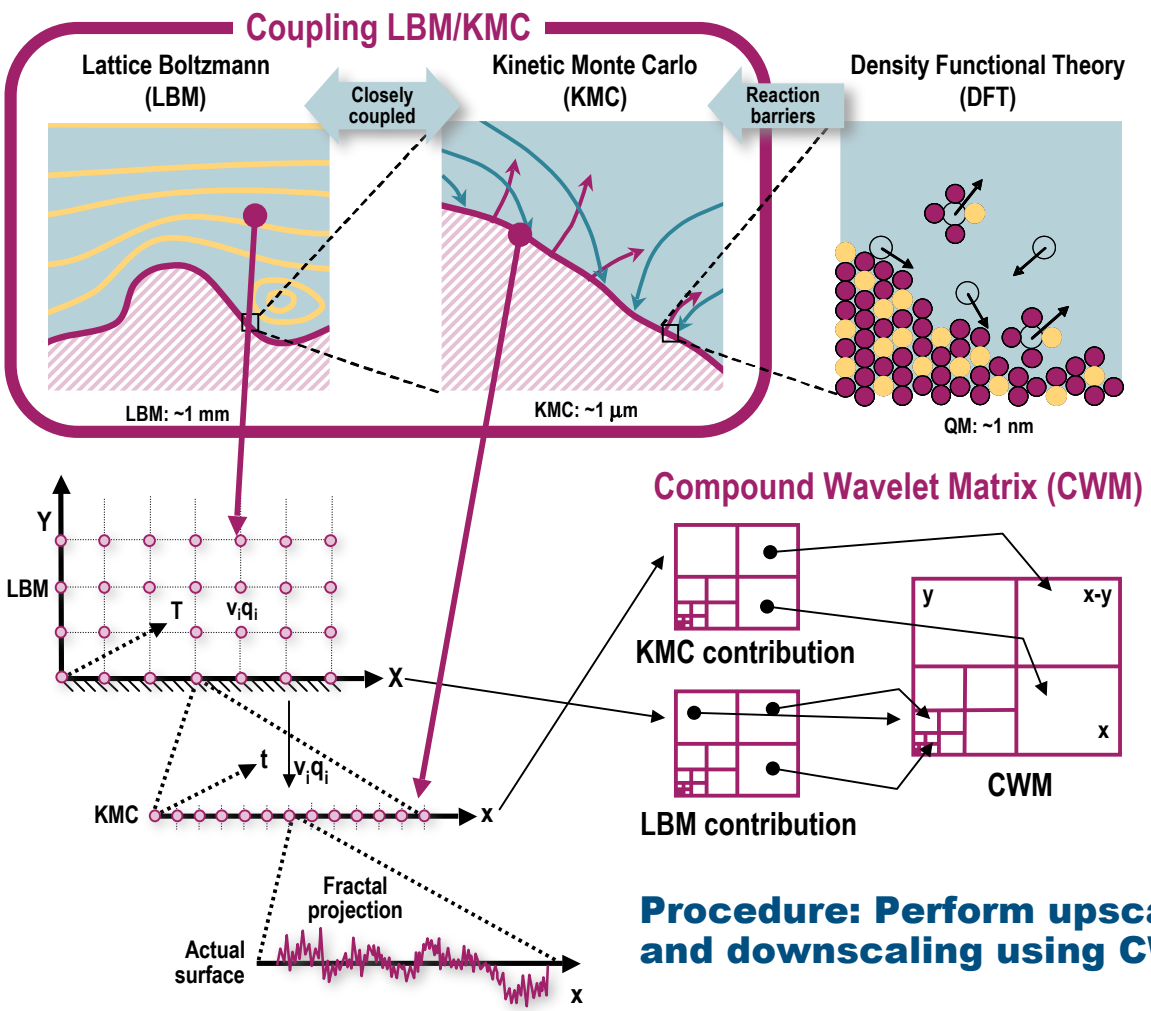
- Are multiscale and multiphysics coupling the same?
  - They are in a way……
  - The different physics modules typically operate at different length- and time-scales
    - Care should be taken when the different modules are coupled
    - Simple software plug-in offered by CCA or CORBA is not sufficient
  - Multiscale mathematics, computational scalable algorithms and corresponding software modules are necessary to simulate the various chemical processes

So what needs to be done?

- How do we rewrite the equations or the solution methods so that only *relevant* information is propagated upward from fine- to coarse-scales (upscaling) and coarse- to fine-scales (downscaling) in a tightly coupled fashion?
  - New mathematics, theory and analysis
  - Unification of governing equations across several scales
    - Lattice based methods across all scales?
  - Long-term
- If that is not possible, can we take the information from different methods and perform this in a postpriori fashion with various degrees of coupling?
  - Widely practiced

Micro-mesoscopic modeling of heterogeneous chemically reacting flows over catalytic/solid surfaces

Goal: Develop a multiscale framework for accurate modeling of heterogeneous reacting flows over catalytic surfaces



Procedure: Perform upscaling and downscaling using CWM

Sample application:

Reactive flow through fiber substrate

AMES LABORATORY

IOWA STATE UNIVERSITY

NETL

OAK RIDGE National Laboratory

THE UNIVERSITY OF ARIZONA

General Multiphysics Framework Needs

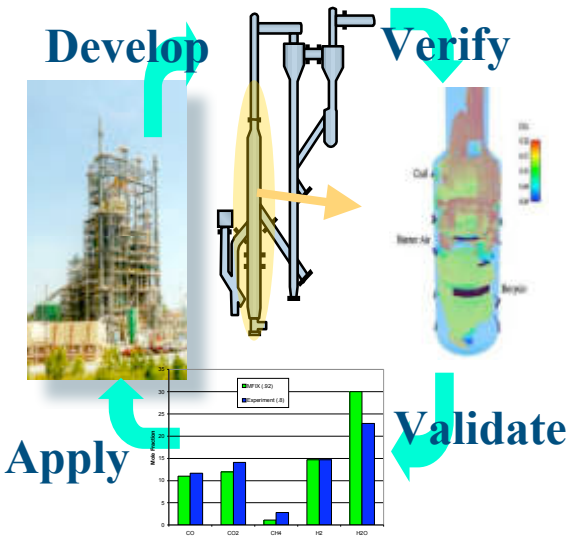
- Flexible and adaptive
  - To handle various multiphysics codes operating at various scales
- Scalable
- Can we solve the underlying components using multiresolution techniques so they can couple easily?
- Automatic optimization based on the architecture
  - Load balance, memory access, IO etc.
- Automated profiling options
- Automatically chose optimal physical models and numerical methods to give the required accuracy with given resources
  - Chosing scalable algorithms – these might not be the best algorithms on small set of processors
- Optimization of the code at run-time
- Ensure all conservation laws are valid at the coupling scales
  - e.g. conformance to second law of thermodynamics (entropy)

What can be achieved?

- Revolutionize the way simulation tools are used in the design process
  - Move away from the current edisonian approach
  - Design new industrial scale devices at a very short turn-around
    - Today depending on the system it can take 10-20 years from concept to lab-scale to pilot-scale to industrial-scale
- Develop new designs exploiting the efficient paths at the molecular scales
  - All reactions happen at the atomic and molecular scales
  - Today the design process is totally decoupled – data is handed over from a group working at one scale to the other group at another scale in a sequential iterative process
  - Some designs are 5-6 decades old
- Develop feedback control systems to run reactors in most optimal fashion

Challenges

- Bringing a broad set of researchers working on chemical processes together to get their buy-in
  - Academia, Research labs, Industry
  - Agree on common codes, interfaces, data standards etc.
- The future architectures (with millions of processors) are more conducive to locally coupled simulations
  - Most chemical processes are globally coupled
  - Running multiple codes would need large and fast data movements across the processors
- Validation and verification
  - Most validation is at steady state or subset of time-/space-trajectories
    - Very difficult to get all the data required to verify all the components of the simulations
    - Considerable investments need to be made in non-intrusive experimental techniques to obtain enough data
    - David Baider – integration of "Theory, Experiment and Simulation"



Coal Gasification

Courtesy: Chris Guenther, NETL

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The Optimization Viewpoint

Jorge J. Moré

Mathematics and Computer Science Division

Optimization Needs for Manufacturing

- Uncertainty quantification
- Application-specific modeling languages
- Stochastic components
- Sensitivity analysis
- Mixed integer-nonlinear optimization
- PDE-constrained optimization
- Combinatorial problems
- Inequalities
- Derivative-free optimization
- Global optimization?

Additional Issues

- Education
- Modeling
- Collaborations with application scientists
- Software development
- Software maintenance
- Verification and validation (of course!)