Multiscale/Multiphysics (MSMP) Simulations of Heterogeneous Chemically Reacting Flows (HCRF): Role in Energy Security and Sustainability

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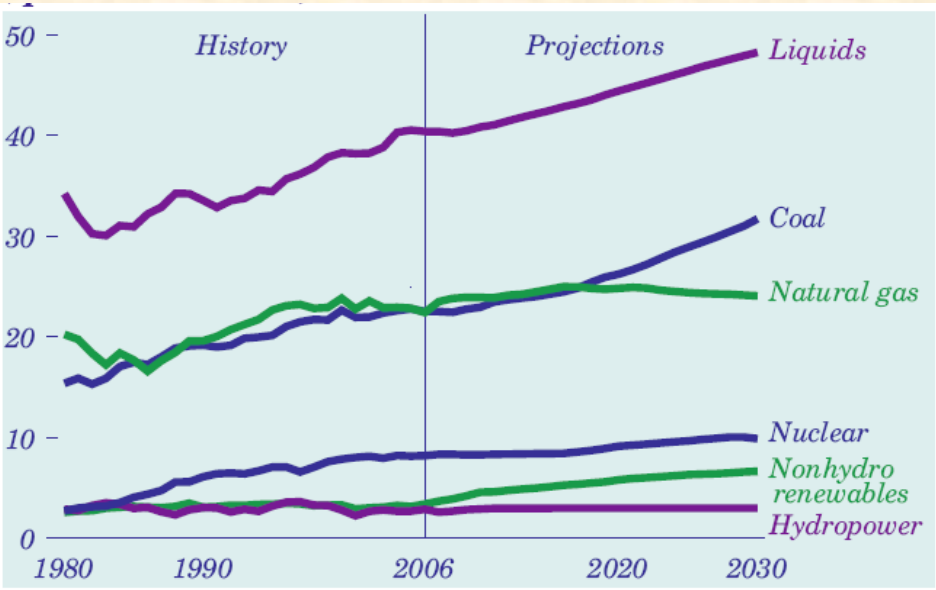
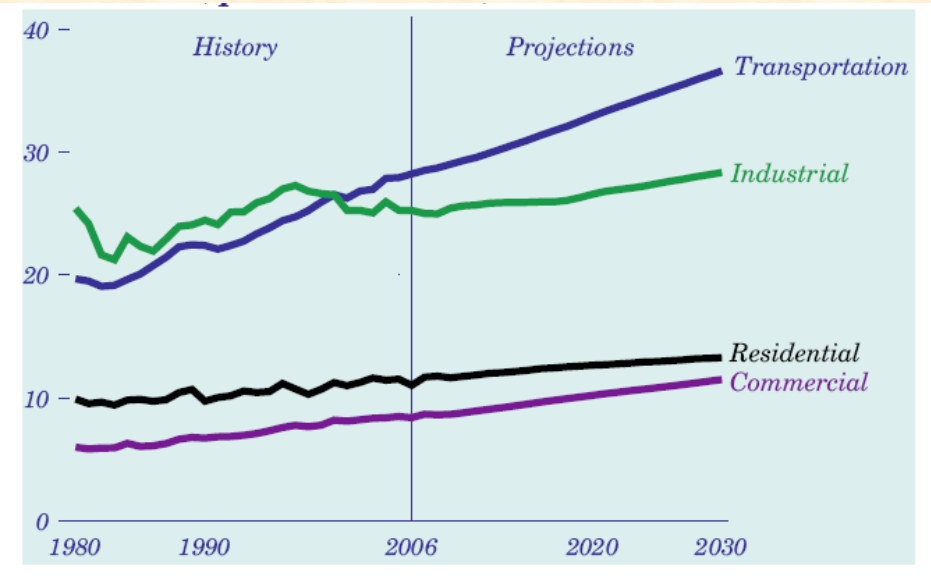
Sponsors: DOE OASCR, FE, NE and EERE

Energy Trends



Energy consumption by Fuel



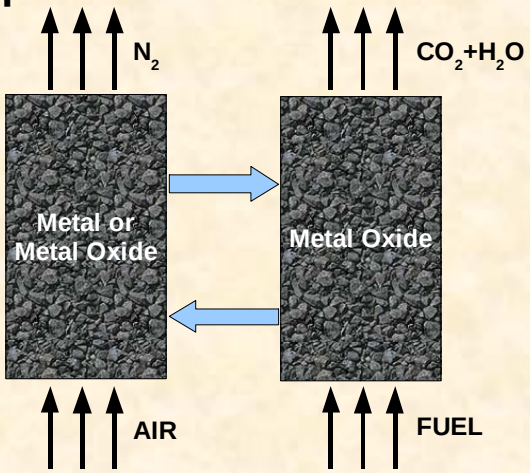
Energy consumption by Sector

If we want to change these trends, it is critical to make key investments today

Source: Annual Energy Outlook 2008, Early Release

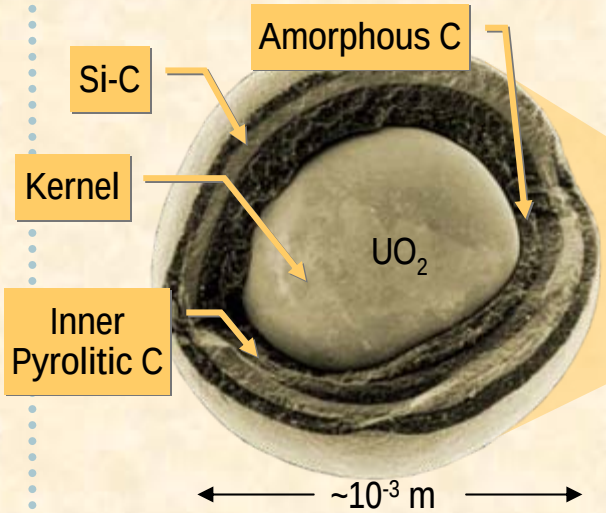
Role of HCRF in Energy Security and Sustainibility

- **Fuel Production and Processing**
  - **Refineries: catalytic crackers, H_2 production, S removal, …**
  - **Coal gasification, clean-up (SOx, NOx, Hg, CO_2)**
  - **Biomass (cellulosic) pyrolysis and gasification**
  - **Nuclear fuel production**
- **Energy Production**
  - **Fuel cells**
  - **Coal and biomass combustion**
  - **Nuclear reactors, separation etc.**
  - **Silicon production and coating for photovoltaic applications**
  - **Novel combustion technologies:**
    - **Oxycombustion**
    - **Chemical looping combustion**
      - **Higher efficiency with lower entropy losses**
      - **No thermal NOx**
      - **Separated CO_2 stream for sequestration**
      - **Potential carbon-negative technology**
- **Energy Utilization and Efficiency**
  - **Polymerization reactors**
  - **Catalytic Reactors**
  - **Multiphase flows occur in most energy intensive industrial processes**



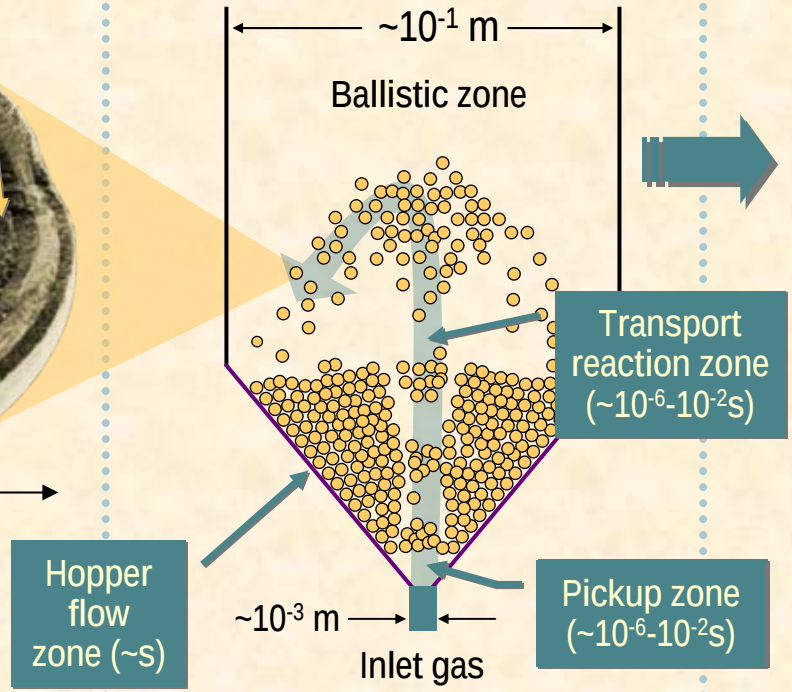
Nuclear fuel coating process – a specific example of gas-solid contacting device

Coated fuel particle (small scale)



- 0.5- to 1-mm particles
- Coating encapsulates fission products
- Failure rate < 1 in 10^5
- Quality depends on surface processes at nm length scale and ns time scales

Spouted bed coater (device scale)



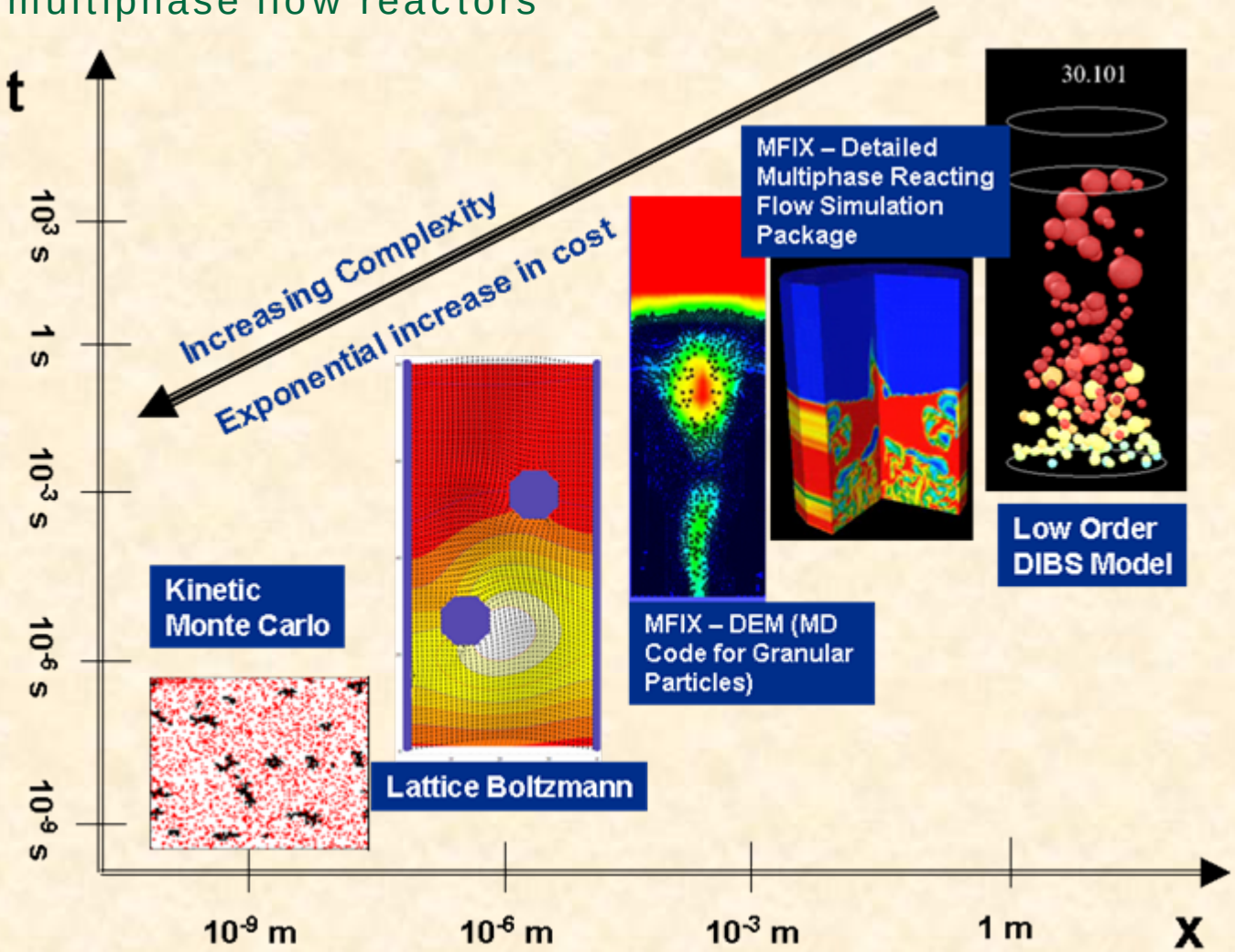
- Coating at high temperature (1300–1500°C) in batch spouted bed reactor for ~10^4 s
- Particles cycle thru deposition and annealing zones where complex chemistry occurs

- Design challenge: Maintain optimal temperatures, species, residence times in each zone to attain right microstructure of coating layers at nm scale
- Truly multiscale problem: ~O(13) time scales, ~O(8) length scales

Links multiscale mathematics with petascale computing and NE

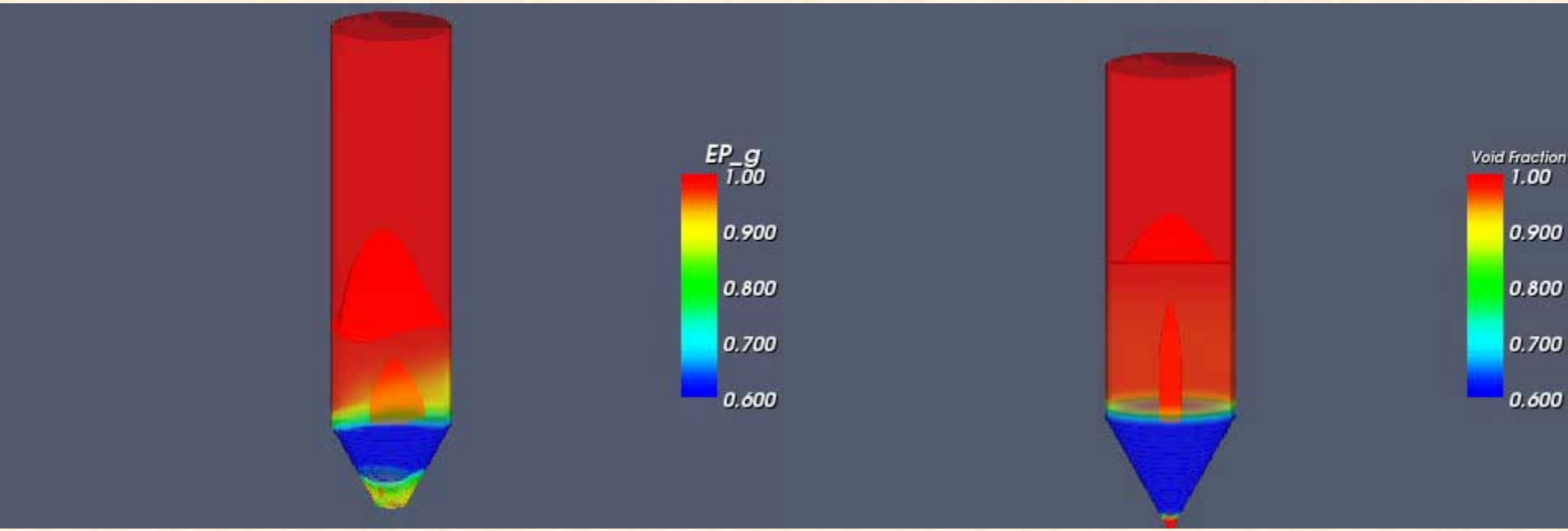
Multiphysics heterogeneous chemically reacting flows for energy systems

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

Nuclear Fuel Coating Simulations: Injector design very critical to overall spouting behavior



3D Multi-port (6 holes: 1 + 5)

Reference NUCO IPyC condition

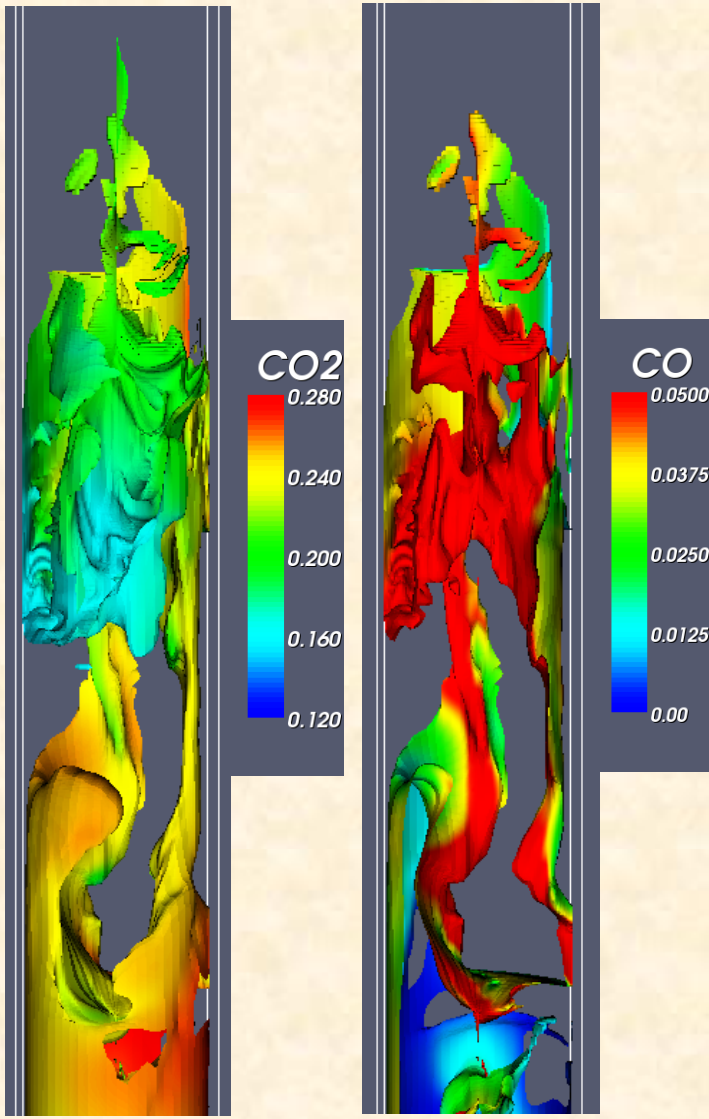
3D Single-port

First time a detailed CFD model is being used for scale-up of fuel coater

SP et al. (CVD, 2007)

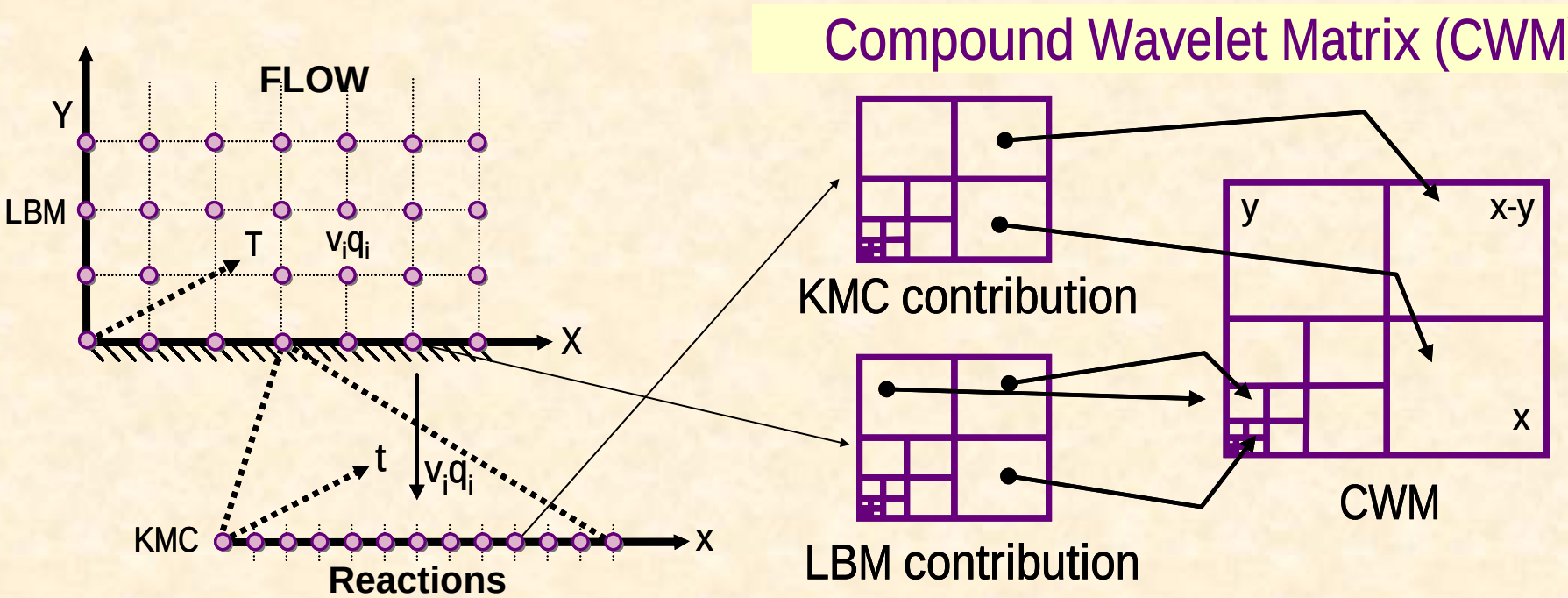
Hi-resolution Coal Gasifier Simulations on the OLCF machines

- **NETL researchers are conducting high resolution gasifier simulations**
  - **2 week run using 2048 processors for a 10M grid**
- **Earlier simulations led to design modifications**
- **Coal gasifiers are integral part of current clean coal technologies**
  - **the same set of tools can be applied to biomass gasification/combustion**



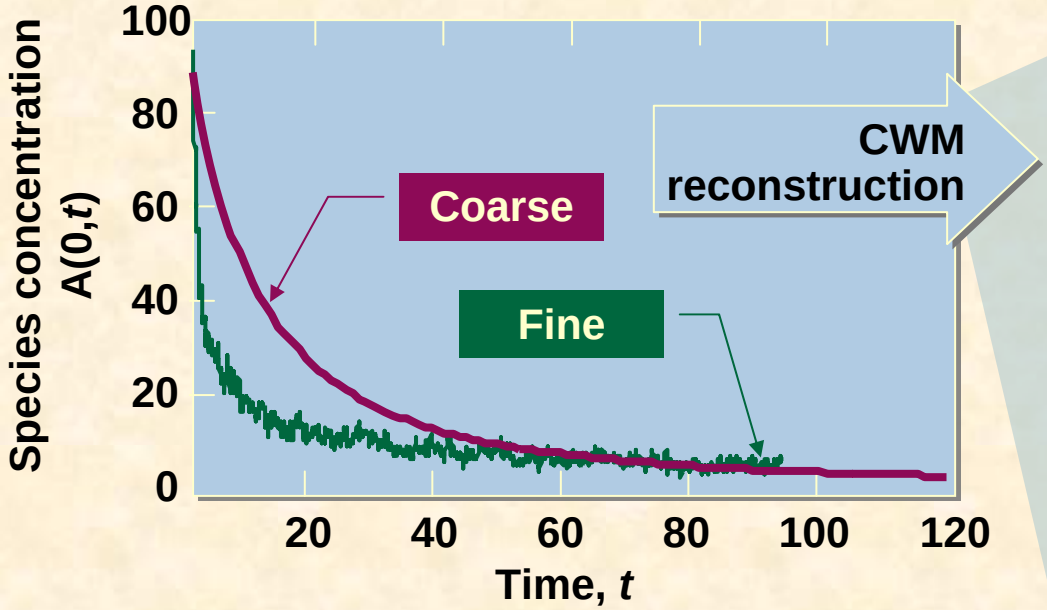
MSMP modeling of heterogeneous chemically reacting flows

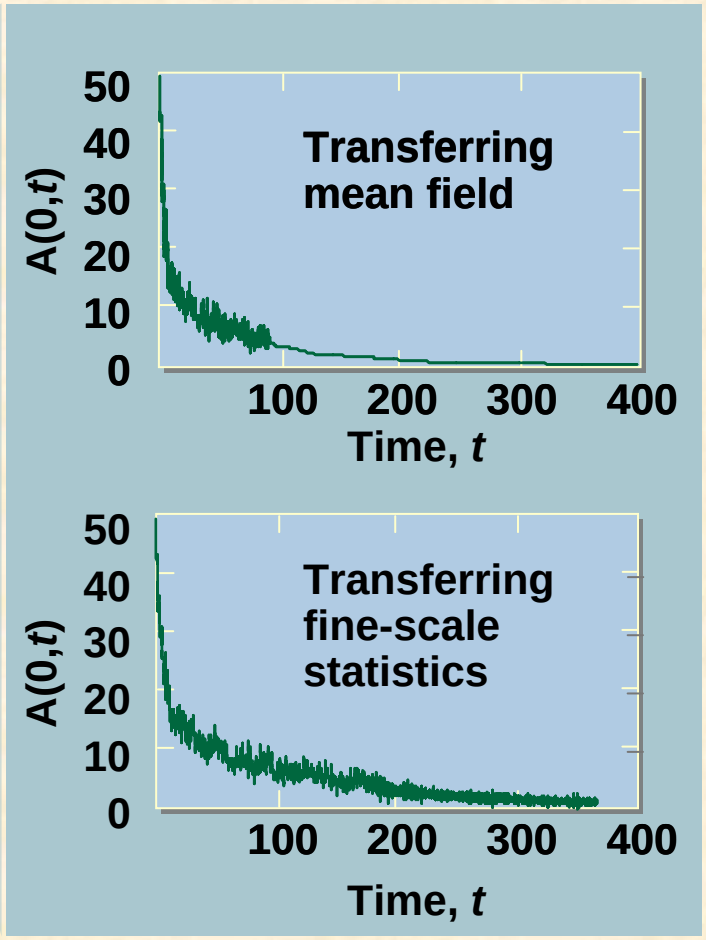
Goal: Develop a MSMP framework for accurate modeling of heterogeneous reacting flows over catalytic surfaces



Procedure: Perform upscaling and downscaling using CWM

Results from a prototype reaction diffusion problem



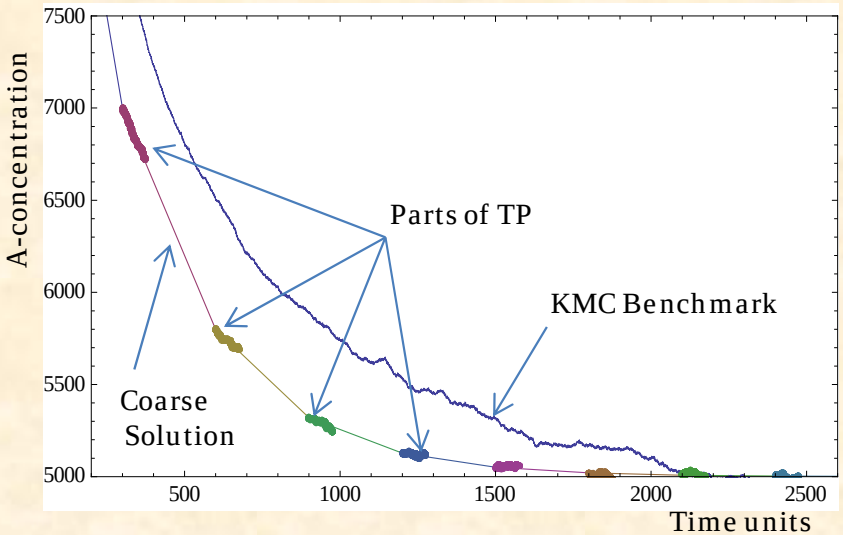


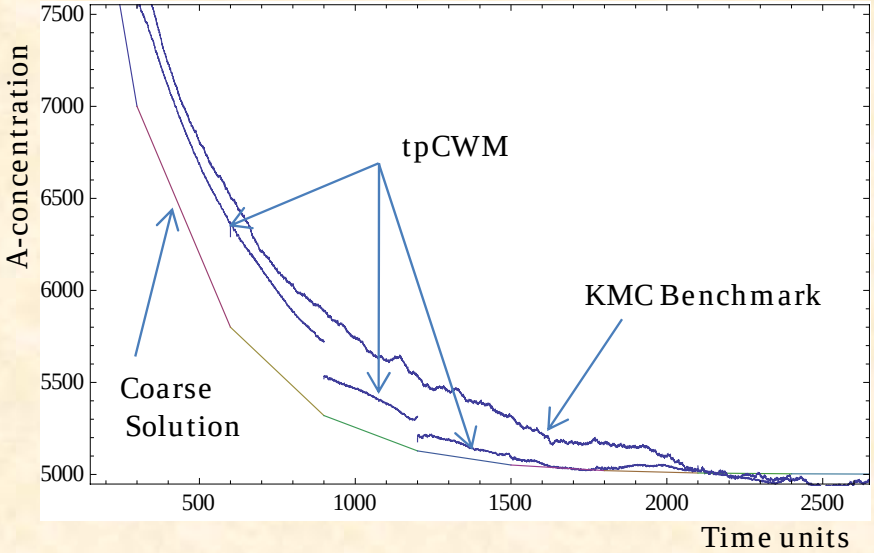
- Successfully applied CWM strategy for coupling reaction/diffusion system
- An unique way to bridge temporal and spatial scales for MSMP simulations

SP with Frantziskonis et al. (IJMCE, 2006)

Ongoing work (infrastructure)

- **Extensions to 2D space and time**
  - **Order of magnitude and more gain with each dimension**
- **Extensions to non-stationary dynamic processes (dCWM)**
- **Integration with experimental data**
- **Currently developing a time parallel CWM (tpCWM)**
  - **Gain proportional to number of instances in parallel**





SP with Mishra et al. (IJCRE, 2008, Under Review)
SP with Mishra et al. (To appear in LNCS, 2008)
SP with Muralidharan et al. (PRE, 2007, Under Review)

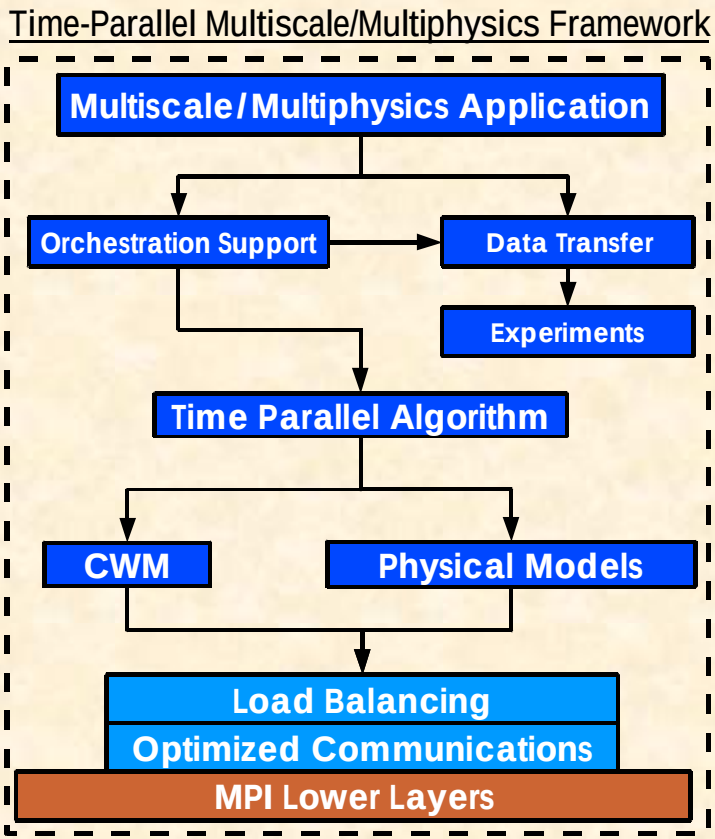
Ongoing work (coal gasification, 1-2 year time frame)

- **Scale-up to commercial scale gasifier**
- **Important design questions to be answered:**
  - **Effect of coal jet penetration on SynGas composition**
  - **Reactor length/diameter**
  - **Coal feed rate**
  - **Solids recirculation rate**
  - **Effect of recycled syngas**
- **Addresses some of the goals set by FE multiphase flow research roadmap (2006)**

Near-Term (by 2009)	Mid-Term (by 2012)	Long-Term (by 2015)
High-fidelity, transient, 3-D, two-phase with PSD (no density variations), hydrodynamics-only simulation of transport reactor at TRDU-scale (200 kg/h coal feed rate) to run on high performance computers of 2009 overnight.	High-fidelity, transient, 3-D, two-phase with PSD (no density variations), hydrodynamics with heat and mass transfer simulation of transport reactor at a scale of at least 12.5 MW (or 5,000 kg/h coal feed rate) to run on high performance computers of 2012 overnight.	High-fidelity, transient, 3-D, two-phase with particle size and density variations, hydrodynamics with chemical reactions simulation of transport reactor at a scale of at least 25 MW (or 10,000 kg/h coal feed rate) to run on high performance computers of 2015 overnight.

Critical investments for next 5 years: Multiphysics/Multiscale Framework

- **Flexible and adaptive**
  - **To handle various multiphysics codes operating at various scales in an hierarchical fashion**
- **Scalable**
- **Automatically chose optimal physical models and numerical methods**
  - **Choosing scalable algorithms**
- **Ensure all conservation laws are valid at the coupling scales**
- **Uncertainty propagation through various models and quantification**



Effort: 6-8 FTEs per year for 5 years

Critical investments for next 5 years: Applications

- **Primary application areas**
  - **Biomass gasification/combustion**
    - **Aid the design of novel biomass gasification processes**
  - **Chemical looping combustion for bio-ethanol**
    - **Determining the catalytic/material properties required for the process**
- **Experiments where needed to get all the required parameters (kinetics, transport properties etc.) to:**
  - **conduct large scale continuum simulations (3 year deliverable)**
  - **carry out detailed MS/MP simulations to determine the closures for continuum simulations**
- **Lab-scale experiments to validate the models**
- **Integrate the simulations at the lab-scale, pilot-scale and device-scale with those of the lab-scale experiments to arrive at new designs**

Effort: 6-8 FTEs per year for 5 years

Summary

- **Energy crisis is real and we need tomorrow's technology today**
- **Integrated experiments and simulations at scale can revolutionize the design of energy devices**
  - **Include all relevant scales so that molecular scale interactions are included when designing device scale**
  - **Cut down the current 20-30 year design cycle**
  - **Break cultural barriers**
- **Develop computations based feedback control systems to run devices in most optimal fashion**
  - **Adjust for feedstock etc. online rather than offline adjustments with huge safety margins**
- **Simulation science can and *has to* play a catalytic and important role in bringing innovation to the energy market place**
  - **Reinvigorate the economic machine**

Collaborators

Oak Ridge National Laboratory

- Srdjan Simunovic
- Stuart Daw
- Phani Nukala
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- Ed D'Azevedo
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