Micro-Mesoscopic Modeling of Heterogeneous Chemically Reacting Flows (MMMHCRF) over Catalytic/Solid Surfaces

Presented by

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The team

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Goal

Develop a multiphysics and multiscale mathematics framework for accurate modeling of heterogeneous reacting flows over catalytic surfaces

Flow over a catalyst surface

- Chemically reactive flow over a surface is a basic building block that is central to many energy-related applications
- Illustrative benchmark to demonstrate the capability to integrate scales of several orders of magnitude

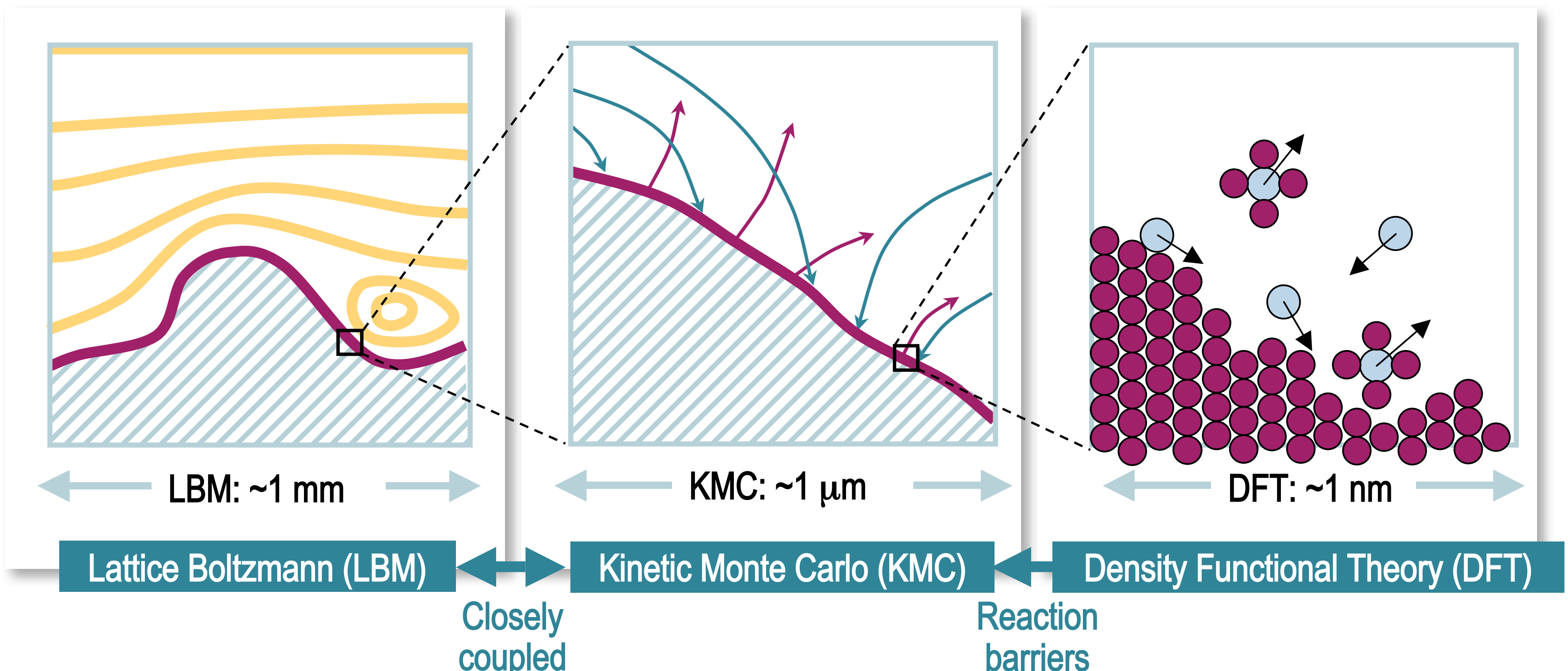
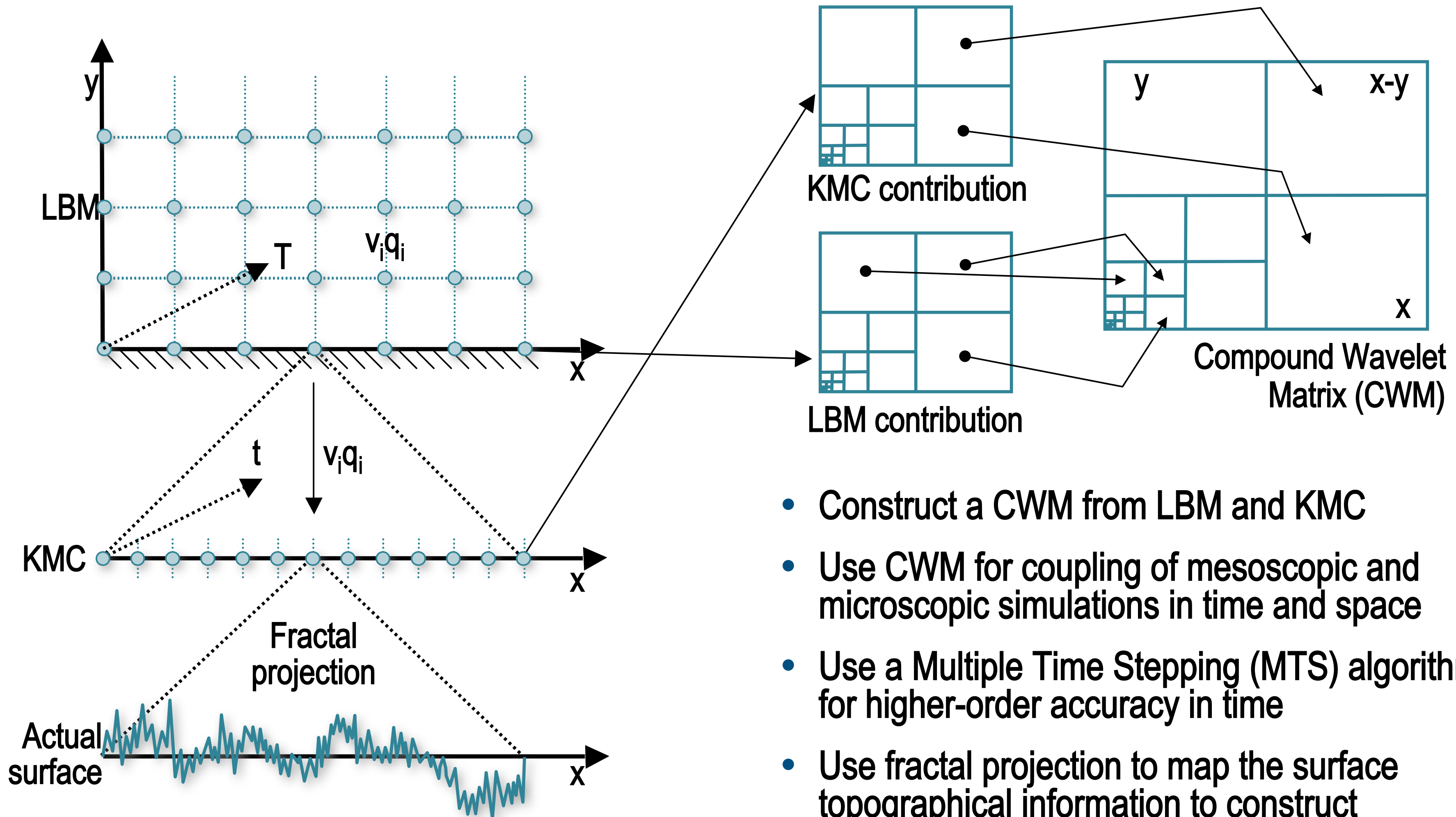


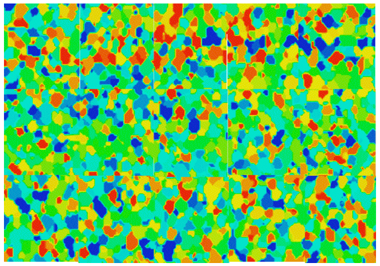
Figure adapted from Succi et al., *Computing in Science and Engineering*, **3(6)**, 26, 2001

Approach: KMC–LBM coupling through Compound Wavelet Matrix

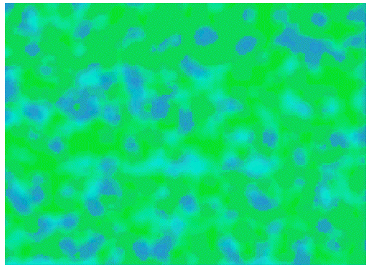


- Construct a CWM from LBM and KMC
- Use CWM for coupling of mesoscopic and microscopic simulations in time and space
- Use a Multiple Time Stepping (MTS) algorithm for higher-order accuracy in time
- Use fractal projection to map the surface topographical information to construct the KMC in one less dimension

CWM methodology in work:
Transferring information from KMC to LBM



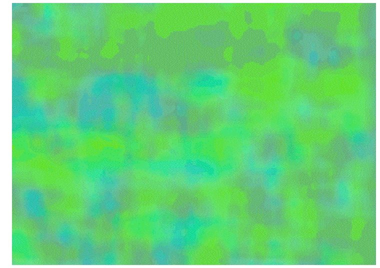
Micro-information KMC



Homogenized properties at next scale

Wavelet transformation

• • •



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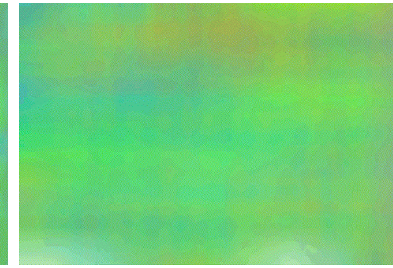

Homogenization at the level corresponding to LBM, feeding from KMC to LBM

Increasing spatial or temporal scales

Objective: Develop algorithms to construct projection operators and time integration methods to connect the microscale (e.g., KMC) and the mesoscale (e.g., LBM)	The interactions between various physical processes at different scales are encapsulated by CWM and can be employed in control and design of reacting surfaces
	Time separation between methods and scales simplifies the problem
	The method recovers the mean field behavior in the macroscopic limit

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Recent results*

- 1-D reaction/diffusion simulation performed at two different length and time scales:
  - Fine (KMC and diffusion equation using finite difference at fine scale)
  - Coarse (analytical species solution and diffusion equation using finite difference at coarse scale)
- Pseudo-2-D reaction diffusion multiscale simulations with error analysis
- A dynamic CWM implementation for non-stationary processes
- Reconstructed the fine simulation results to reasonable accuracy using CWM at fraction of cost
- Method allows for bi-directional transfer of information, i.e., upscaling and downscaling

*Frantziskonis et al., *International Journal for Multiscale Computational Engineering*, **5-6**, 755, 2006
Mishra et al. (*SIAM J. of Sci. Comp.* – under review), Muralidharan et al. (*Phy. Rev. E* – under review)

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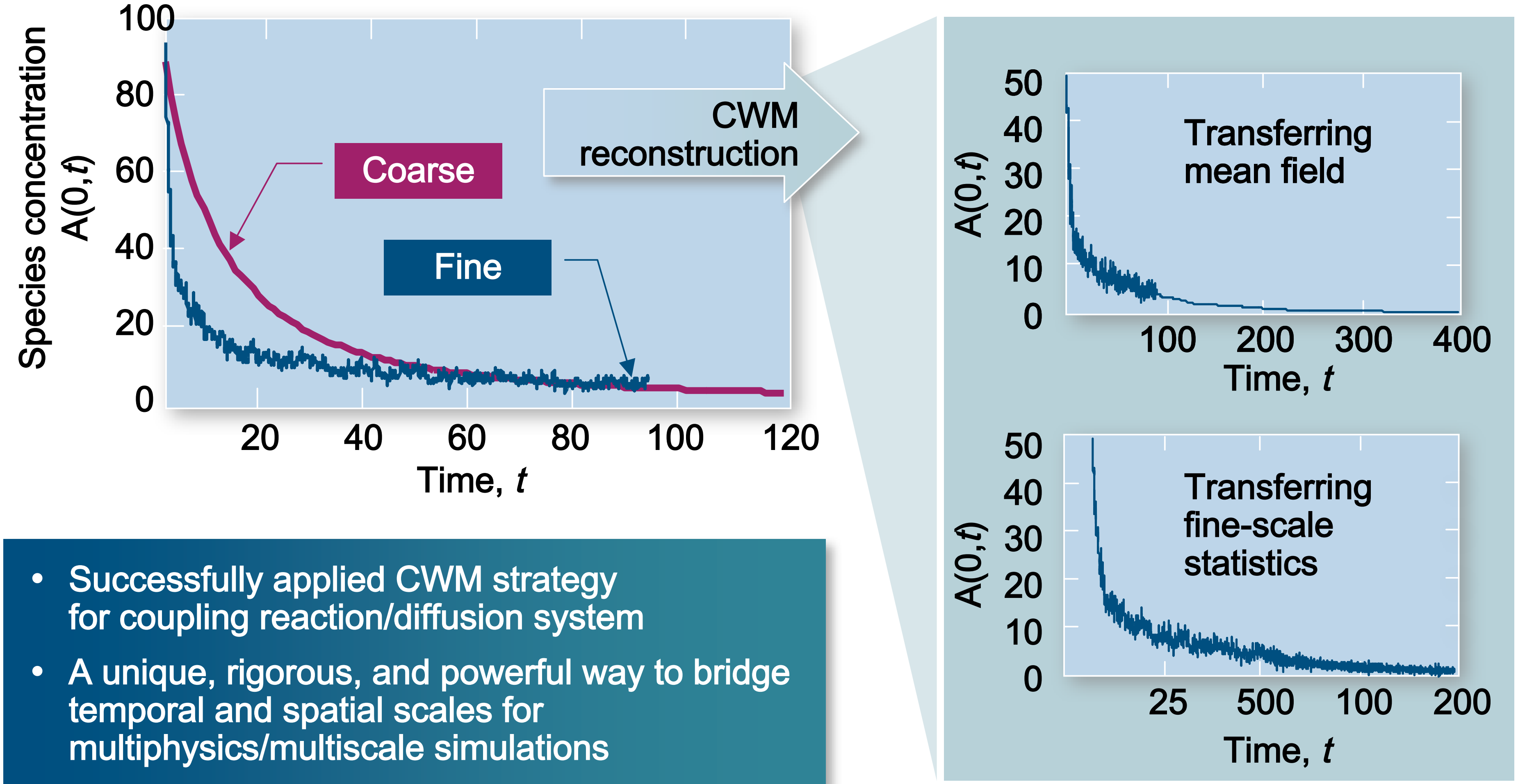
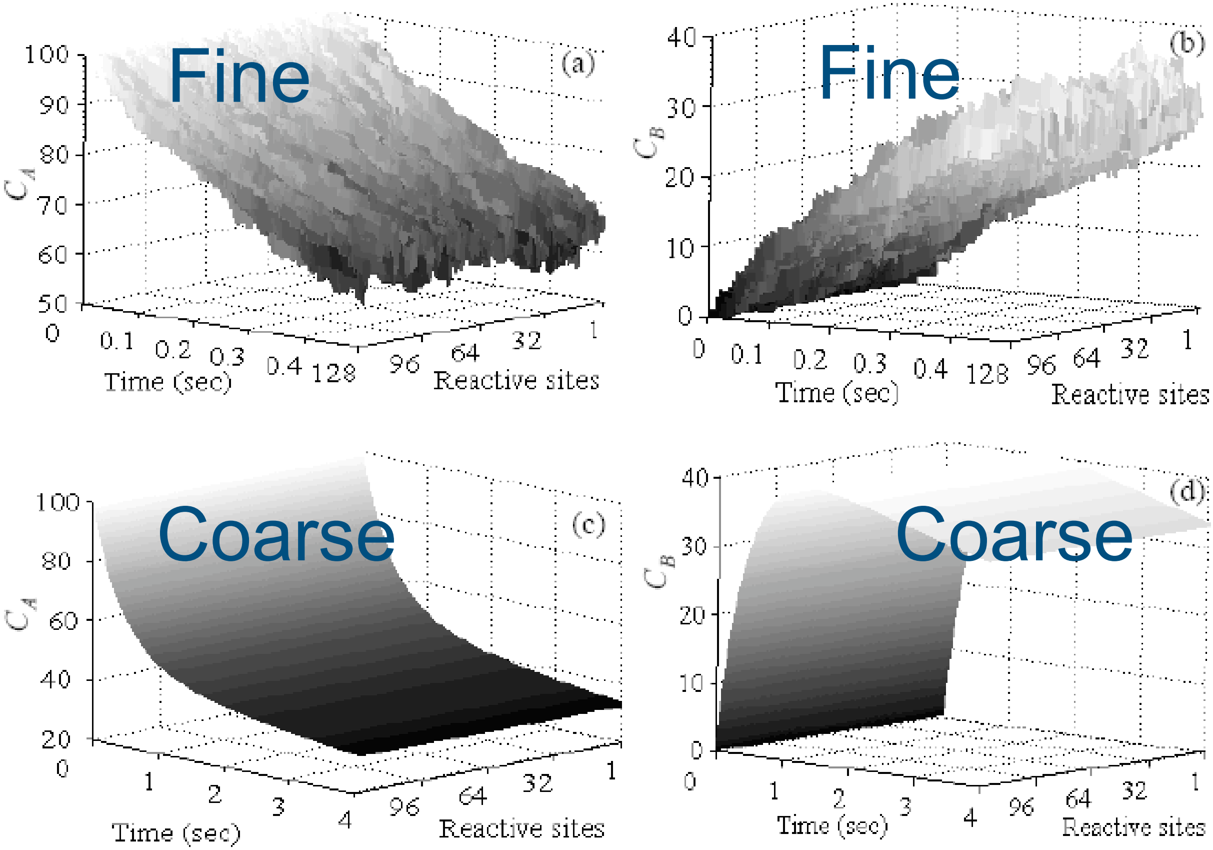
Example 1: 1-D reaction diffusion system*



- Successfully applied CWM strategy for coupling reaction/diffusion system
- A unique, rigorous, and powerful way to bridge temporal and spatial scales for multiphysics/multiscale simulations

*Frantziskonis et al., *International Journal for Multiscale Computational Engineering*, **5-6**, 755, 2006

Example 2: 2-D diffusion with reacting boundary plane



Evolution of reactants A and B

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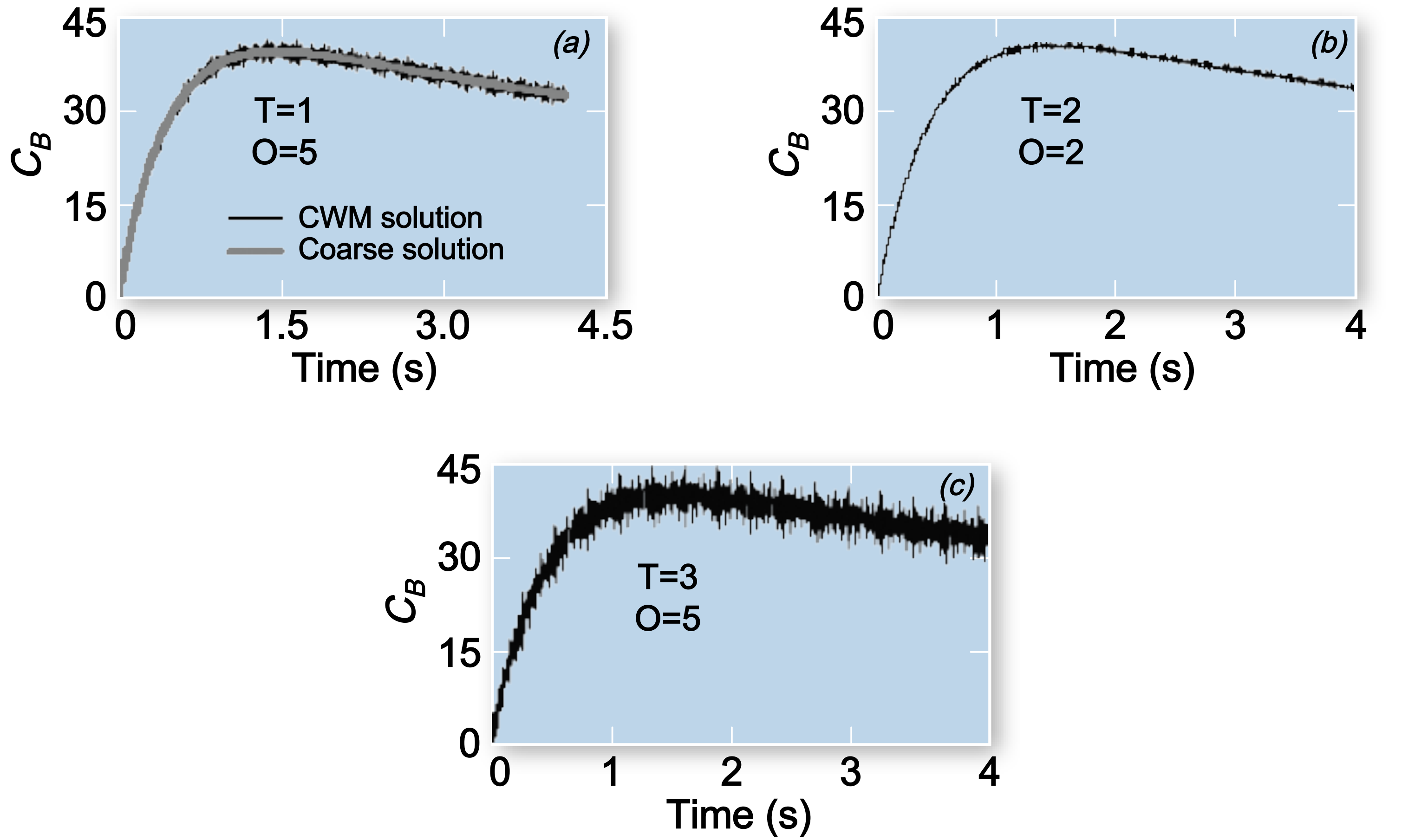
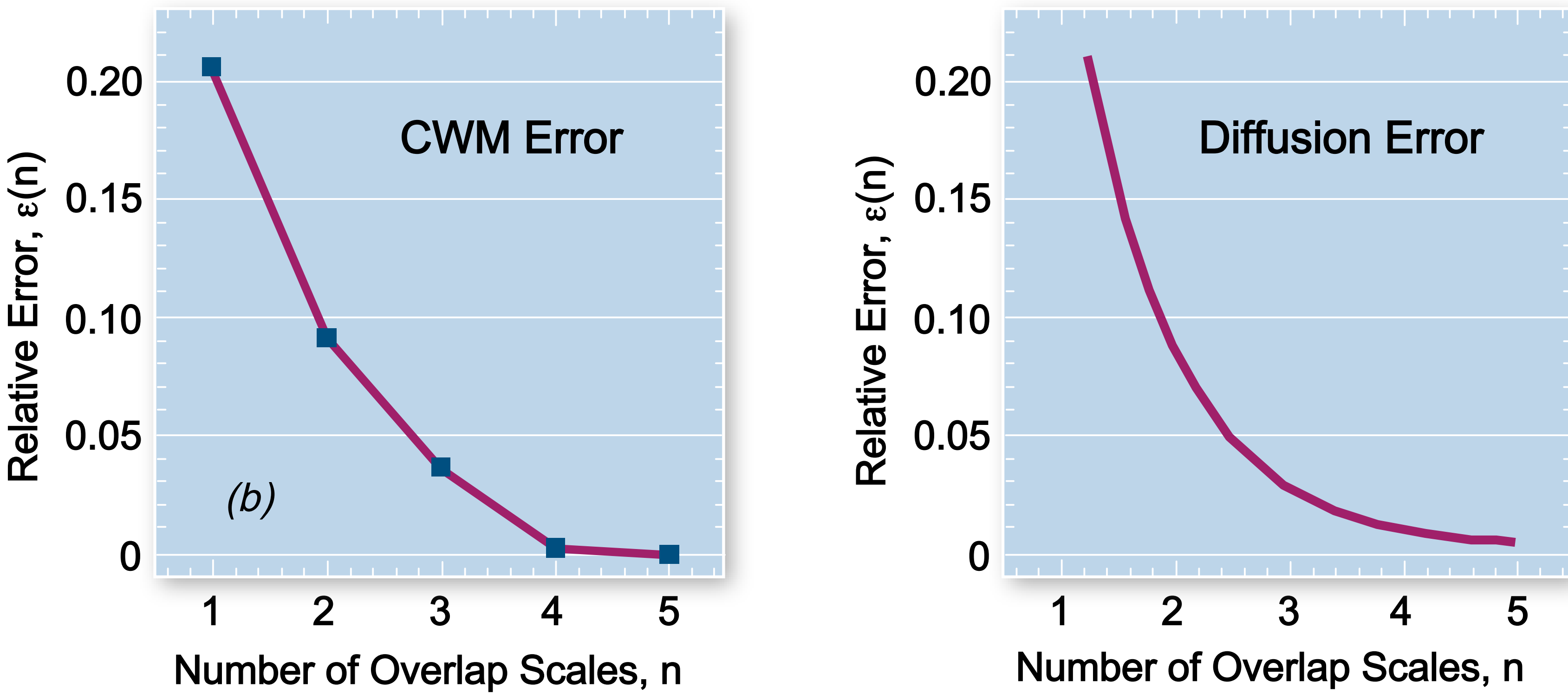
Example 2: 2-D diffusion with reacting boundary plane



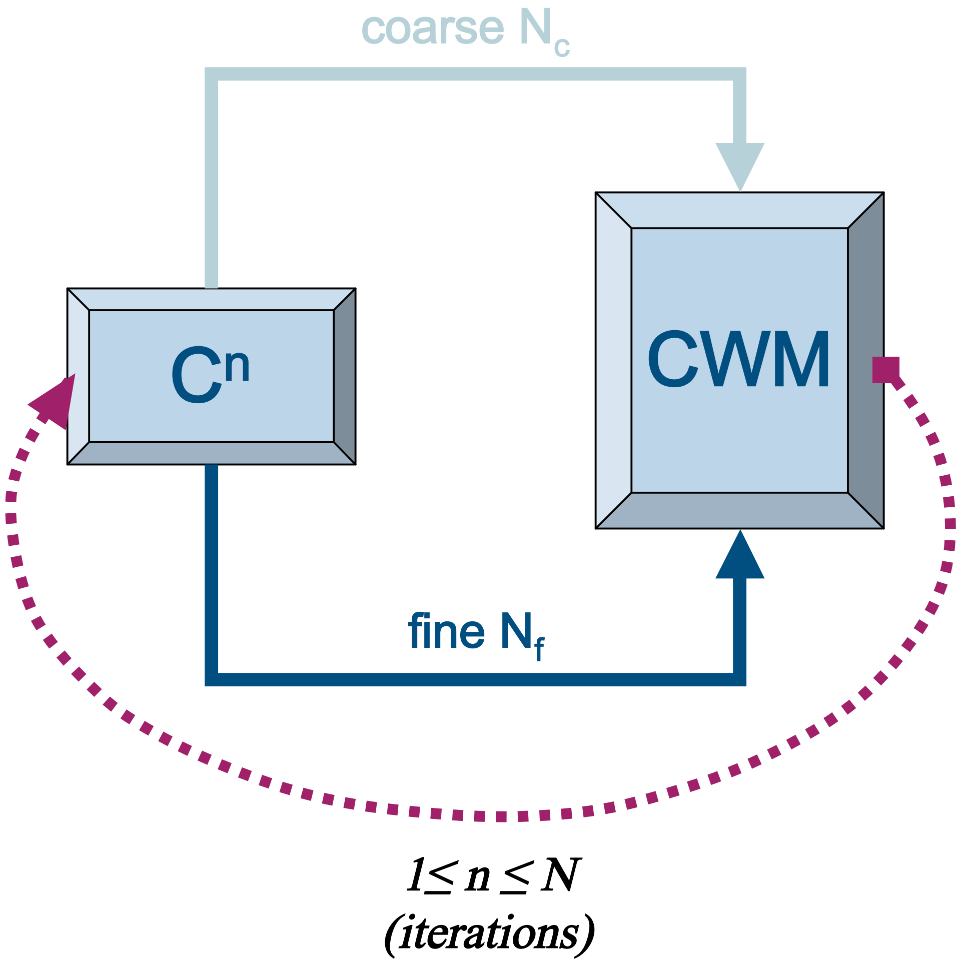
Reconstructed species profile
(effect of overlap and thresholding)

Example 2: 2-D diffusion with reacting boundary plane



The error is dominated by the discretization errors in solving the diffusion equation

Dynamic CWM (dCWM): Dynamic coupling of coarse and fine methods



- Coupling of the dynamics of both coarse and fine methods for non-stationary problems (similar to gap-tooth method)
- Better exploration of phase-space due to inclusion of stochasticity from fast scales
- Long-term behavior feedback to fast scales from coarse representation

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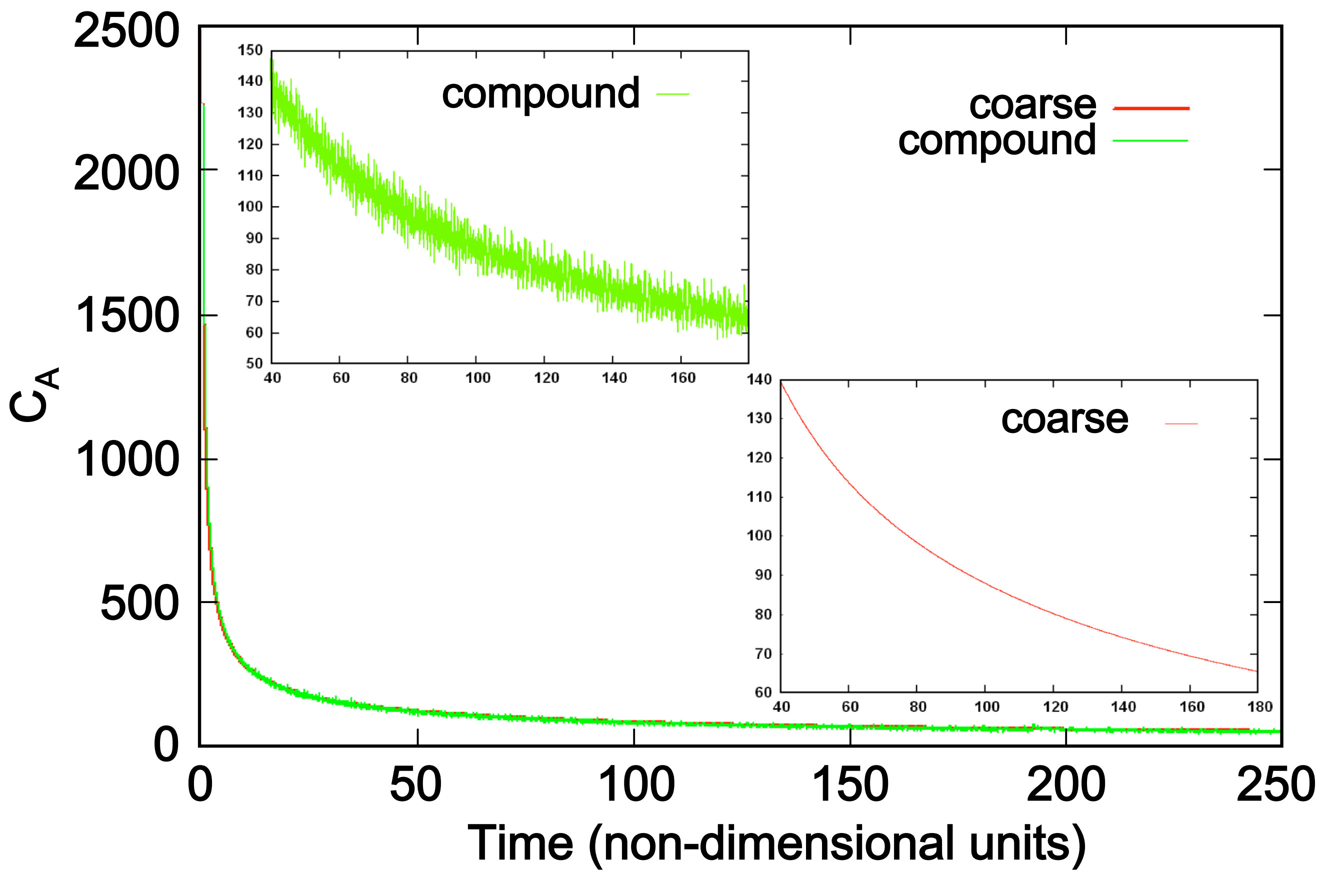
Example 3: 1-D diffusion with reacting boundary plane with dCWM

$N_c = 16384; N_f = 2048; N = 8$



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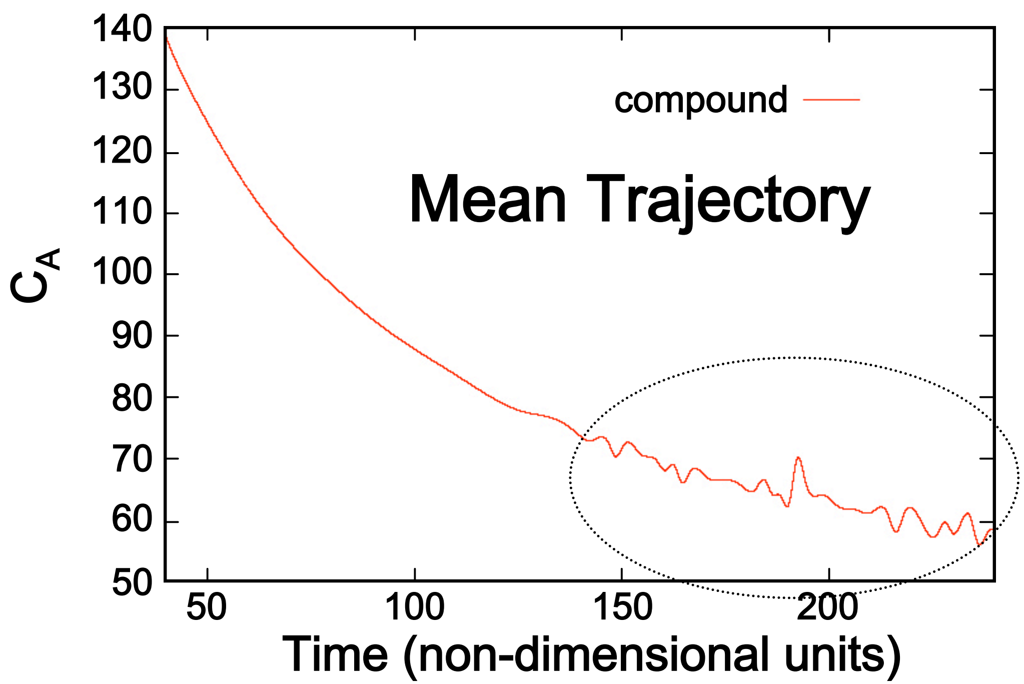
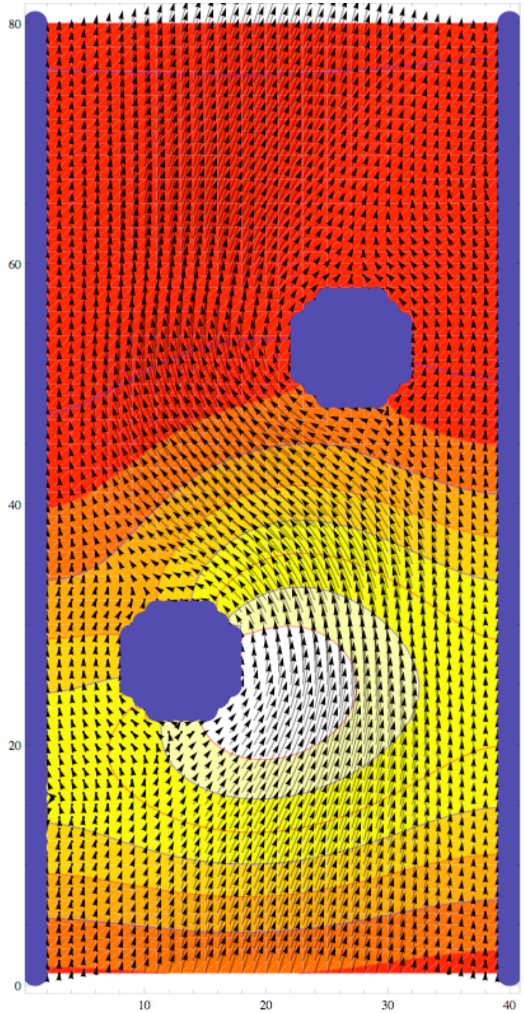


dCWM is able to capture the later-time fluctuations in the mean trajectory when there is competition between diffusion and reaction processes

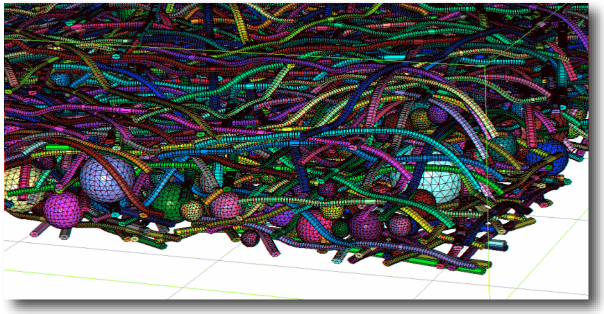
Work in progress: Reactive boundary with LBM

- Chemical reactions in the flow are represented by mass source on RHS
- Development of new boundary conditions for reactive boundary:
  - Transport from bulk fluid to boundary (flux/Neumann)
  - Reaction (concentration/Dirichlet)
  - Transport from boundary to bulk fluid (flux/Neumann)
  - Reactive term must reproduce correct density change rates for reactants, and total heat/release absorption per surface area
- Development of new combined flow-species transport with non-reflecting boundary conditions (absorbing layer, extrapolation method)

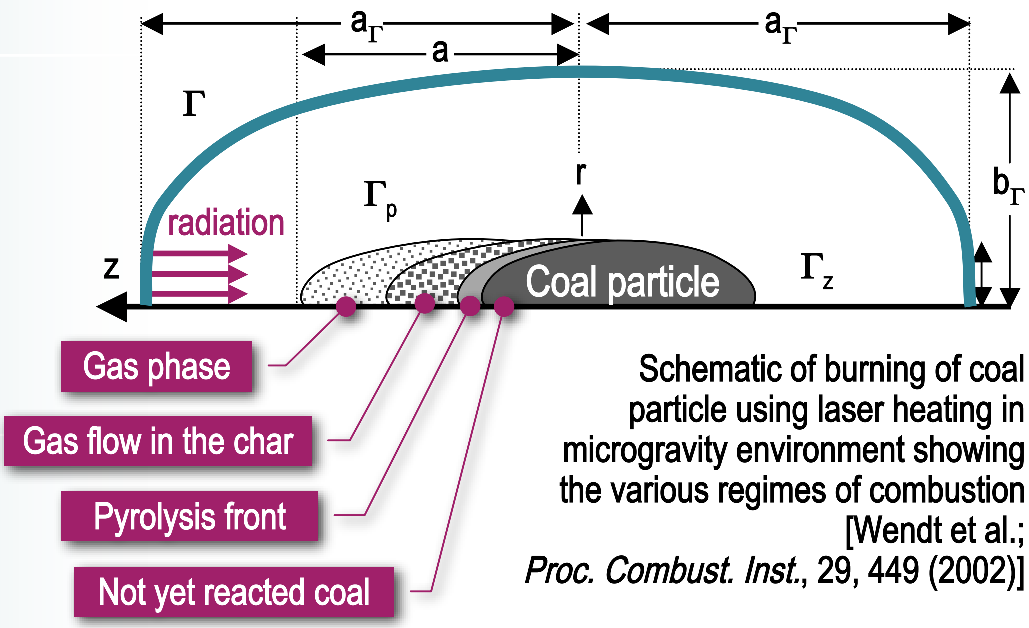


Applications

Chemical looping combustion (CLC)	• Efficient, low-emissions and amenable to CO_2 sequestration
SCOT (staged combustion with oxygen transfer)	• CLC adapted for transportation
Polyethylene production	• Important process that uses ~10% of crude petroleum
Reactive flows through fibrous media	• Light weight, low-cost and high-strength composites • Fuel cell components • Scaffolds for biomedical applications
Coal gasification and combustion	• New technologies for cleaner and efficient coal combustion



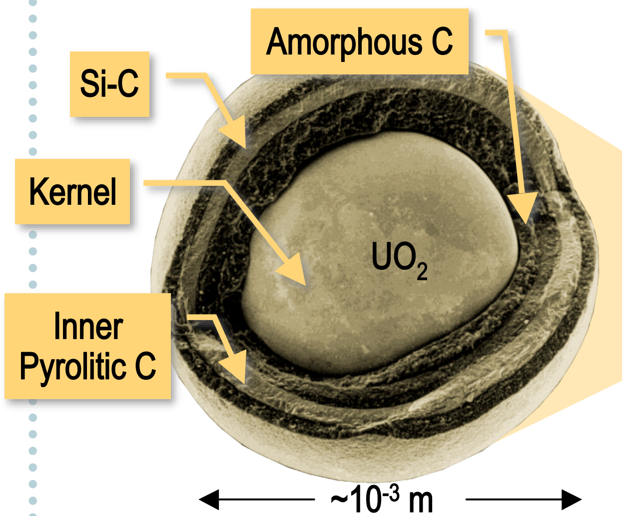
- Fibrous substrate for discontinuous fiber substrate
- The voids found by probing the substrate with a fixed-size sphere are denoted by spheres



Schematic of burning of coal particle using laser heating in microgravity environment showing the various regimes of combustion [Wendt et al.; *Proc. Combust. Inst.*, 29, 449 (2002)]

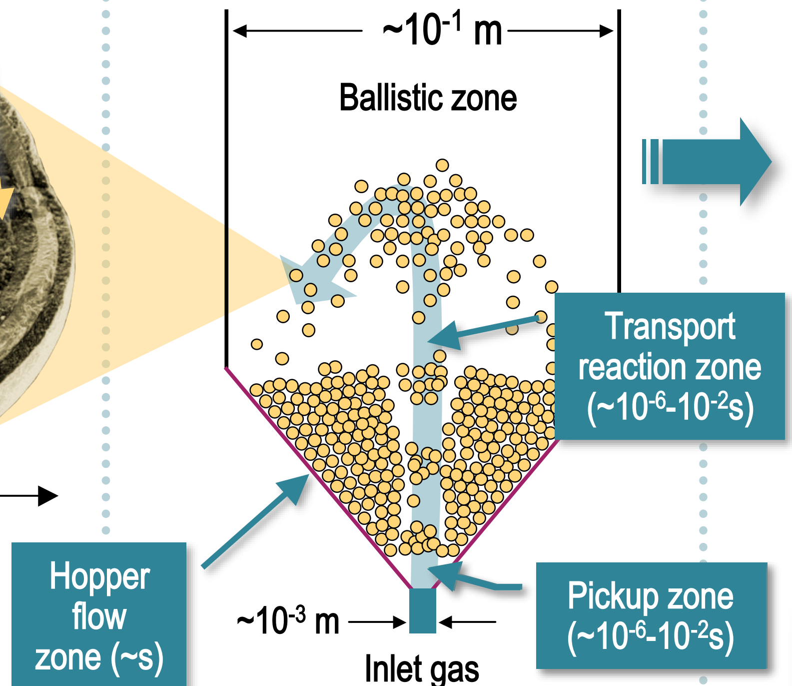
Additional applications:
Nuclear fuel coating process

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 GNEP

Going forward

- Generalize the process of constructing the CWM in the overlapping scales
- Energy matching
- Smooth variation of cross-correlation across the bridging scales
- Invoke conservation laws?
- Thermal LBM with chemistry
- LBM coupled with KMC and CWM
- Coarsening of KMC in space
- MTS comparison to dCWM for time coupling
- Application to NiO system and other realistic systems
- Parallel framework to couple multiphysics code
  - Will be released as open source on completion
  - Advertise to have other groups (applied math and computational scientists) involved to make additional improvements

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