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

Presented by

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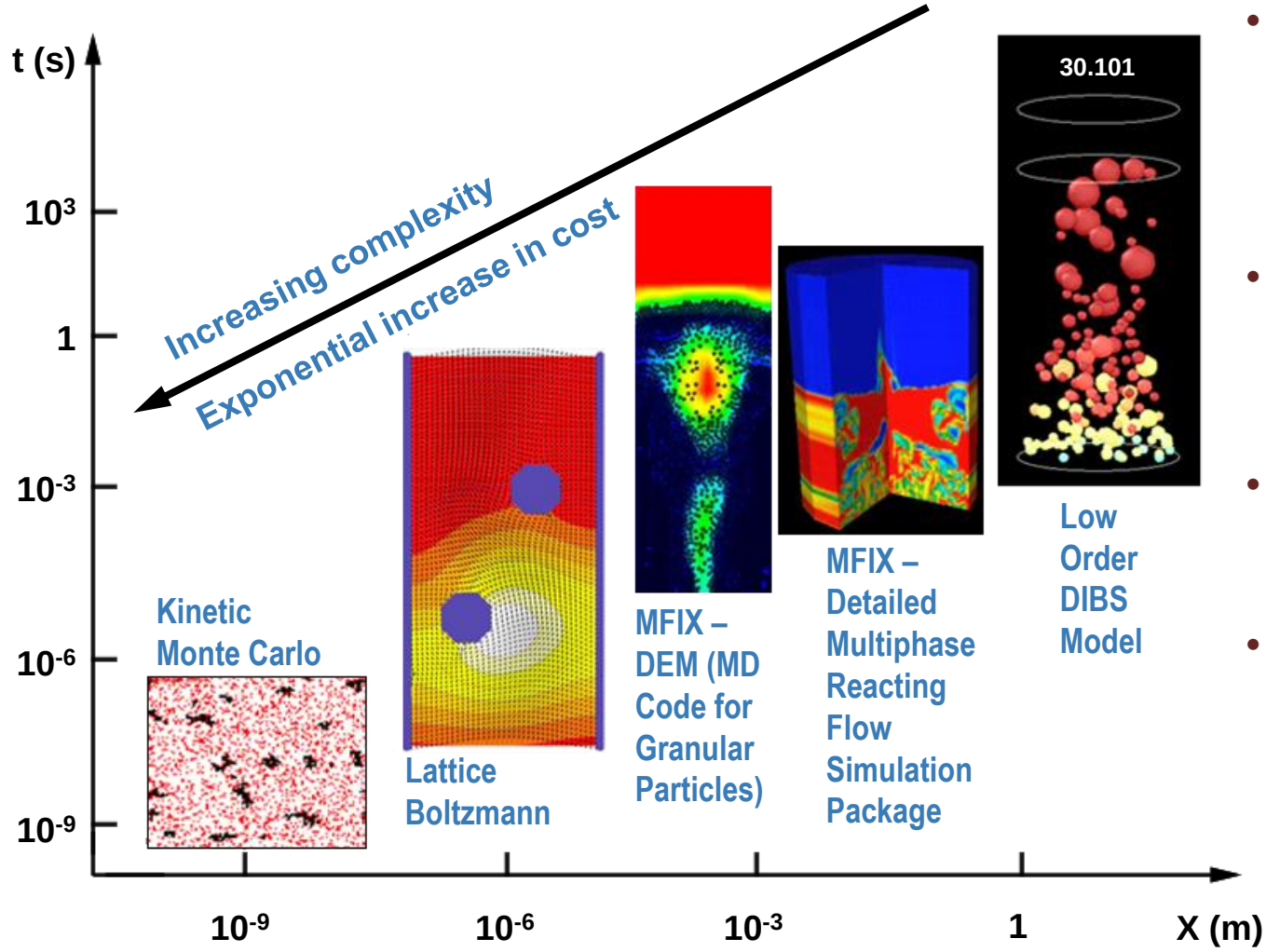
Goal

Develop a computationally scalable mathematics framework for accurate modeling of multiphysics, multiscale problems with heterogeneous chemically reactive flow over catalytic surfaces as the prototype problem

Multiphysics heterogeneous chemically reacting flows for energy systems

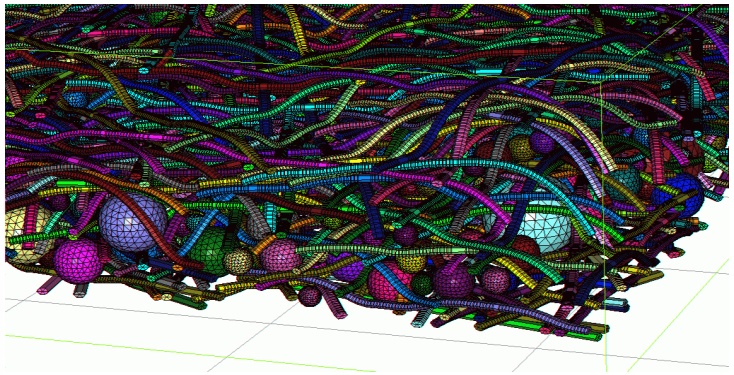
Goal: building a suite of models for multiscale (space, time) capability to simulate multiphase flow reactors



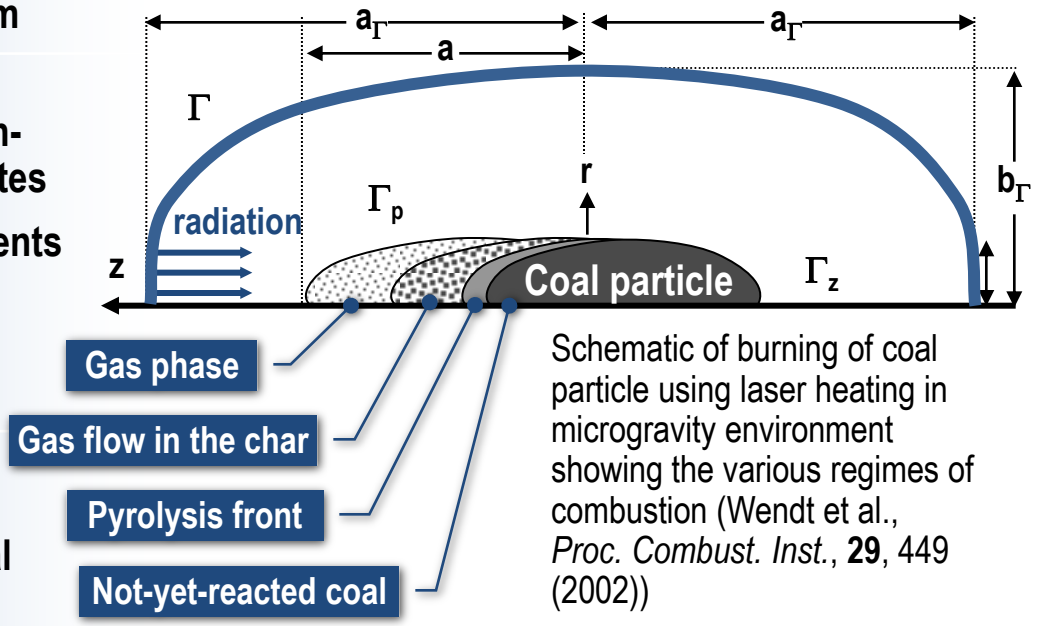
- A set of models is used to simulate heterogeneous chemically reacting flows
- Interfacing the models requires rigorous methods for upscaling and downscaling
- Hybrid methods to couple two physical models (e.g., MFIX DEM)
- Uncertainty quantification to probe only quantities of interest at smaller scales

Applications

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



- Fibrous substrate for discontinuous fiber substrate
- The caging volume found by probing the substrate with a fixed-size sphere is 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))

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

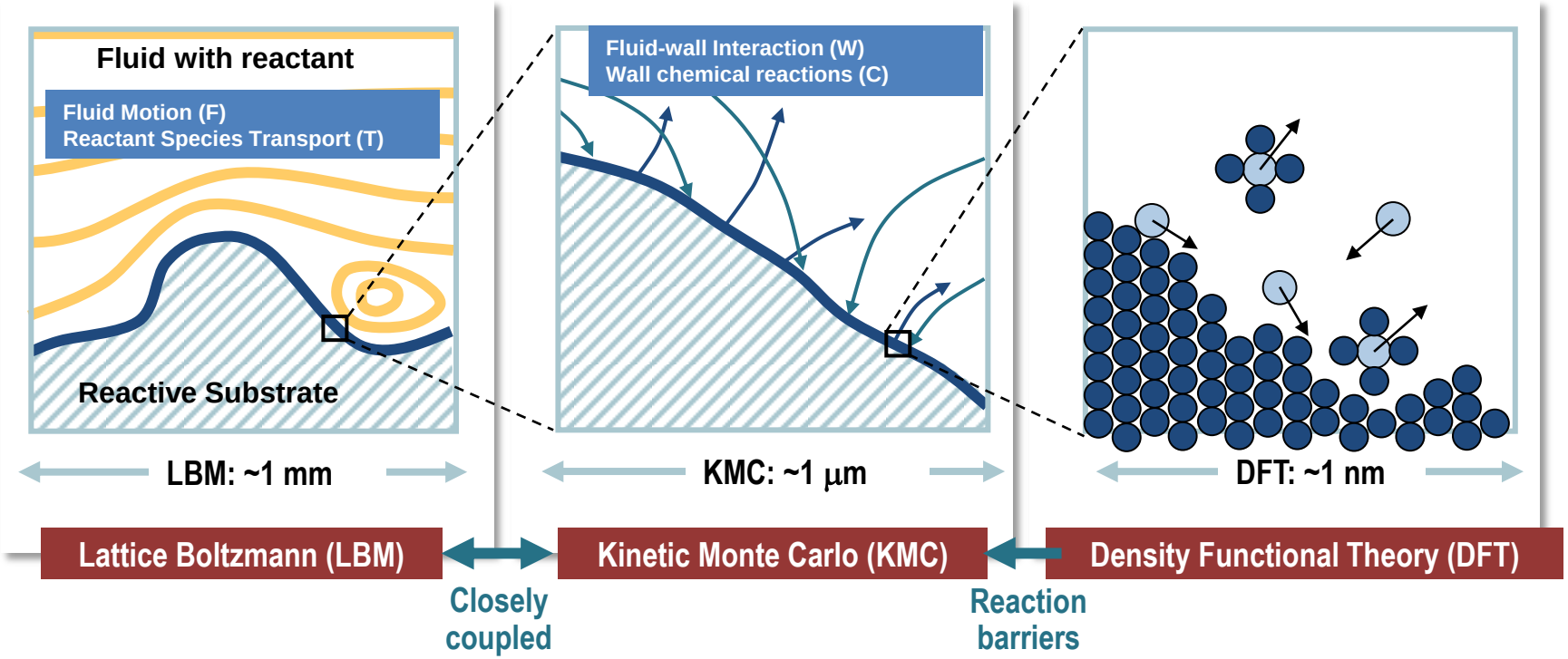
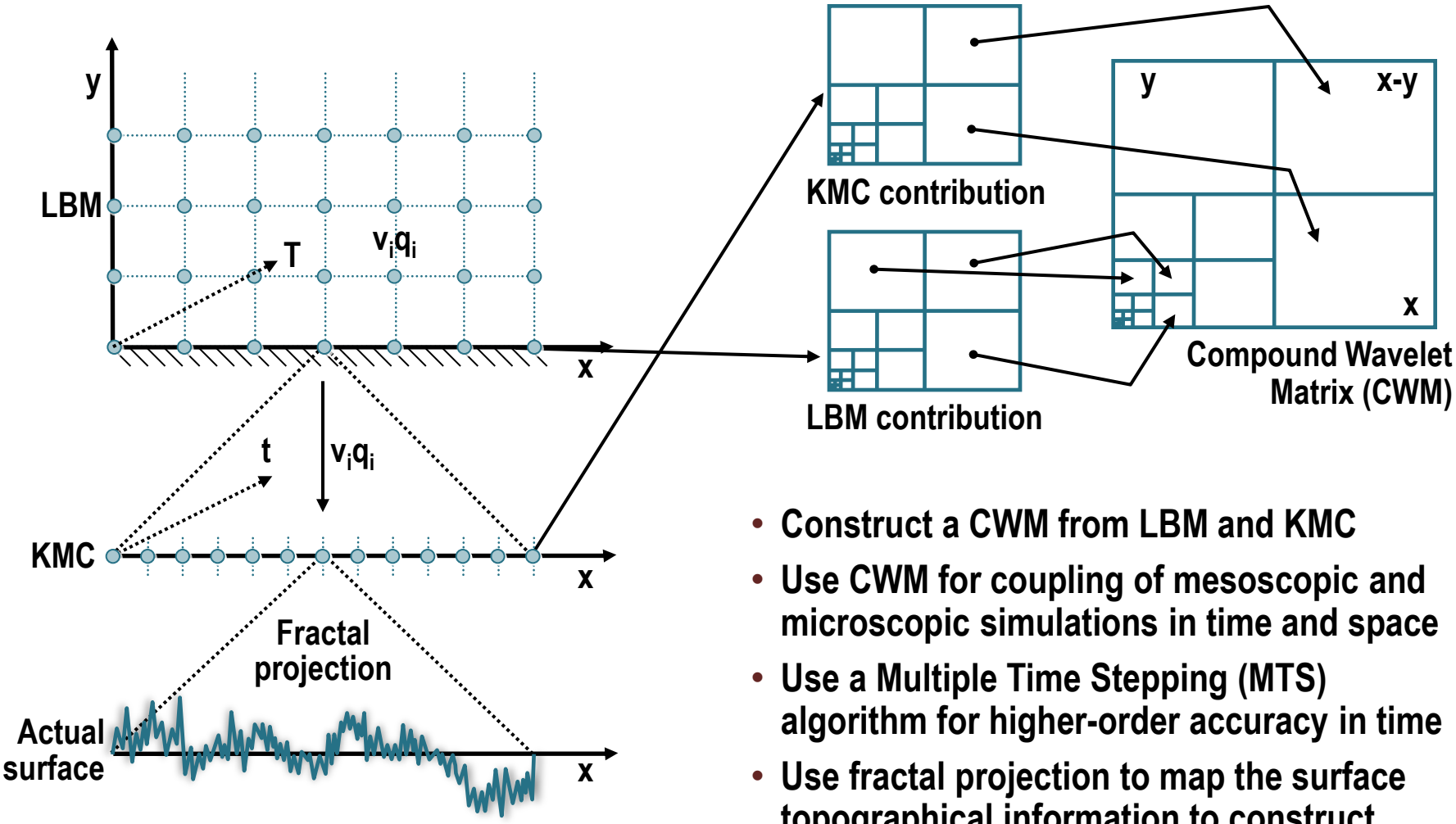


Figure adapted from Succi et al., *Computing in Science and Engineering* **3**(6), 26, 2001

Compound Wavelet Matrix Method



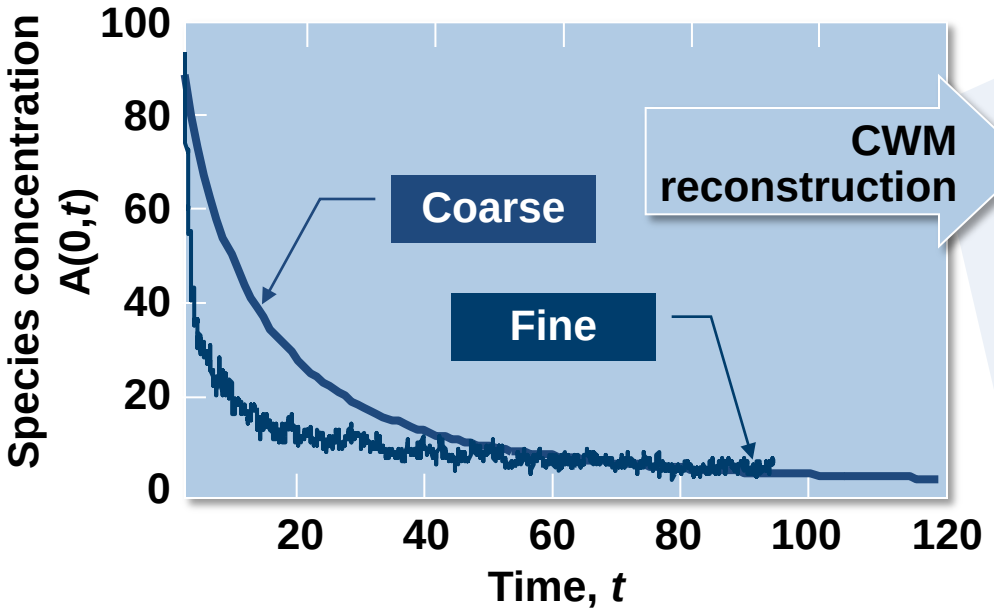
- Construct a CWM from LBM and KMC
- Use CWM for coupling of mesoscopic and microscopic simulations in time and space
- Use a Multiple Time Stepping (MTS) algorithm for higher-order accuracy in time
- Use fractal projection to map the surface topographical information to construct the KMC in one less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

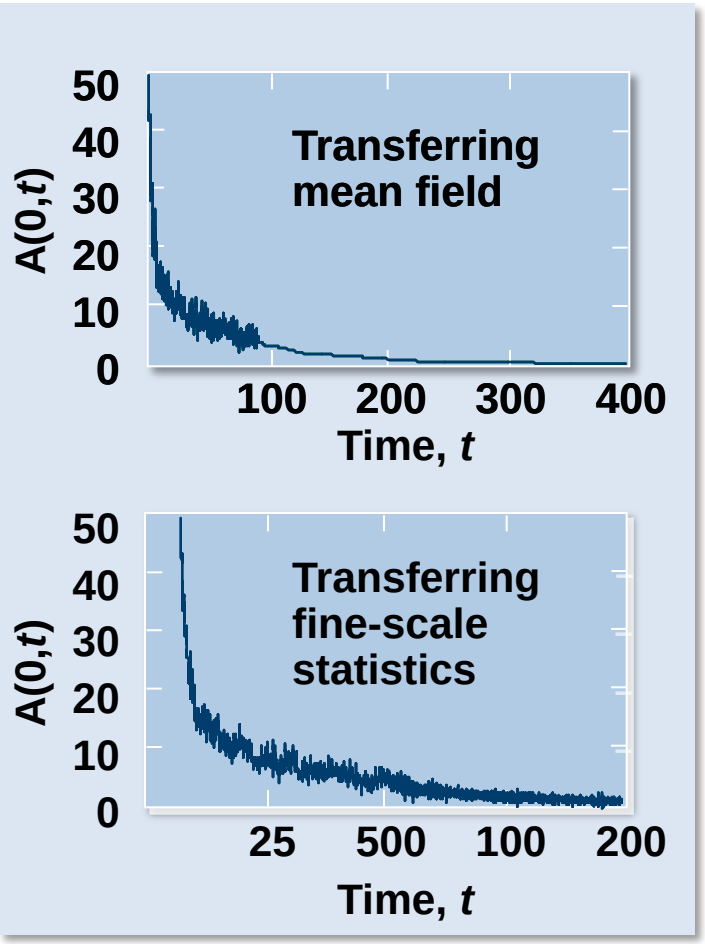
Recent results*

- 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
  - Wavelet-based spatial upscaling and downscaling
- A time parallel implementation of CWM for Lotka-Volterra predator-prey equations

*Frantziskonis et al., *International Journal for Multiscale Computational Engineering* **5-6**, 755, 2006 Muralidharan et al., *Phy. Rev. E* **77**, 2, 026714, 2008
Mishra et al., *International Journal for Chemical Reactor Engineering* **6**, A28, 2008
Mishra et al., *Proceedings of the 2008 ICCS Conference, Lecture Notes in Computer Science*, Springer
Frantziskonis et al., 3rd IC-SCCE Conference, Athens, 2008

Example 1: 1-D reaction diffusion system*

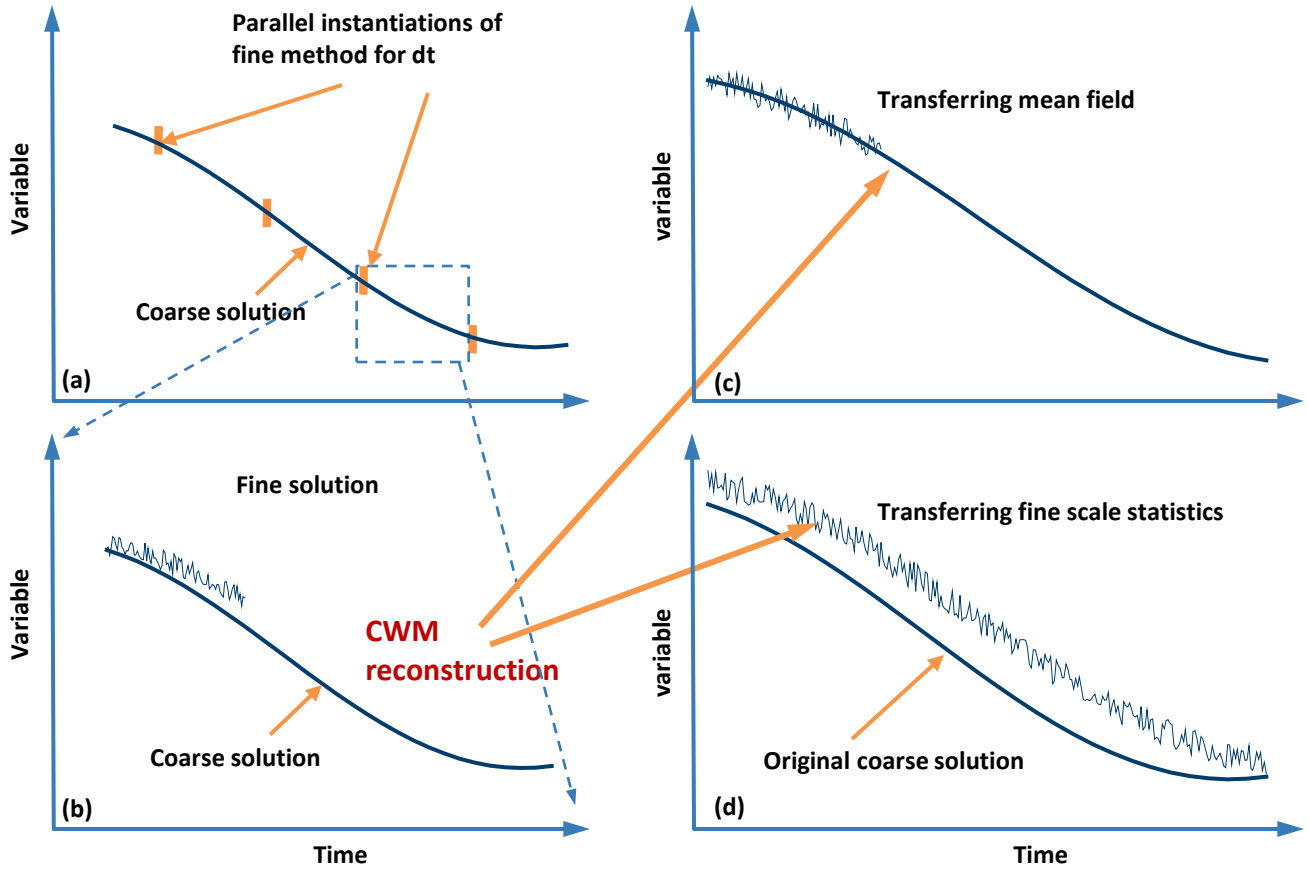




- Successfully applied CWM strategy for coupling reaction/diffusion system
- A unique, rigorous, and powerful way to bridge temporal and spatial scales for multiphysics/multiscale simulations

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

tpCWM (time parallel CWM)



Schematic of the TP and CWM methods: (a) the TP method – the fine method instantiates at several temporal "nodes" typically for a period δt that covers time until the next node; (b) the temporal CWM – the fine method is employed for a fraction of the coarse method; (c) the CWM reconstruction updates the mean field; and (d) the CWM reconstruction updates the temporal statistics

tpCWM applied to Lotka-Volterra predator-prey equations

$$X + Y_1 \xrightarrow{\alpha} 2Y_1$$

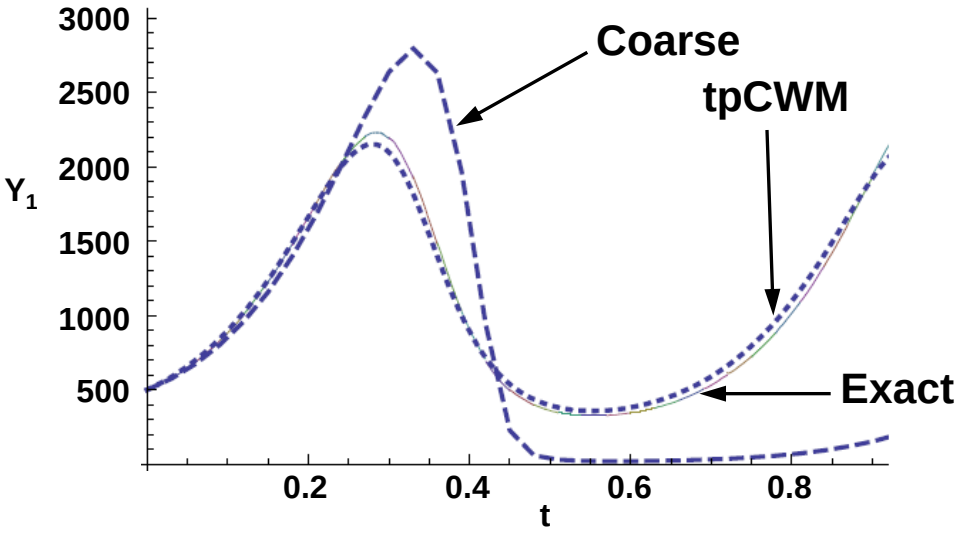
$$Y_1 + Y_2 \xrightarrow{\beta} 2Y_2$$

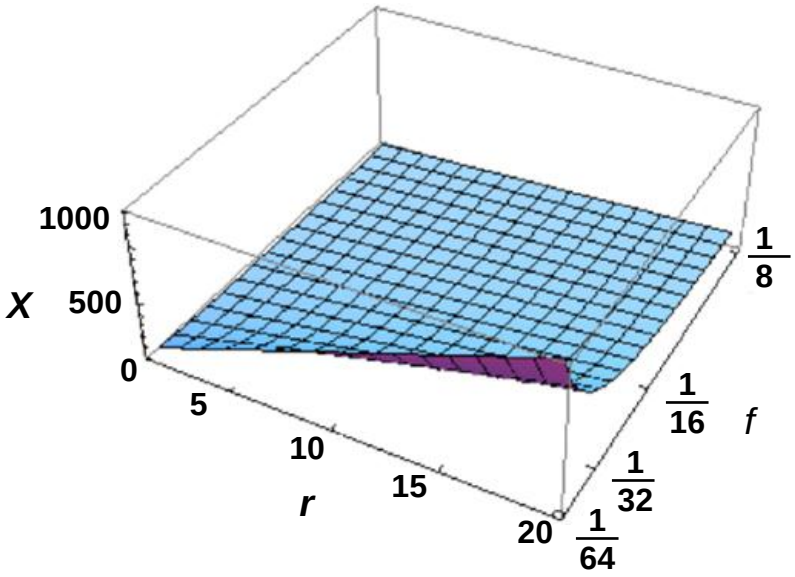
$$Y_2 \xrightarrow{\gamma} Z$$

$$\frac{dY_1}{dt} = \alpha X Y_1 - \beta Y_1 Y_2$$

$$\frac{dY_2}{dt} = \beta Y_1 Y_2 - \gamma Y_2$$

Lotka-Volterra system





Factor of computational savings, *X* as a function of the ratio *r* (number of processors/number of iterations) and the fraction *f* (fraction of KMC time used in each assigned time interval)

Three orders of magnitude savings can be achieved by *r* in the range of 20 and *f* in the order of 1/64.

Frantziskonis et al., J. Comp. Phy., 2009

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