Wavelet-based Spatiotemporal Multiscaling in Diffusion Problems with Chemically Reactive Boundary

Oak Ridge National Laboratory

Sreekanth Pannala
Srdjan Simunovic
Stuart Daw
Phani Nukala

University of Arizona

George Frantziskonis
Sudib Mishra
Pierre Deymier
Aditi Mallik
Krishna Muralidharan

Ames Laboratory Iowa State University

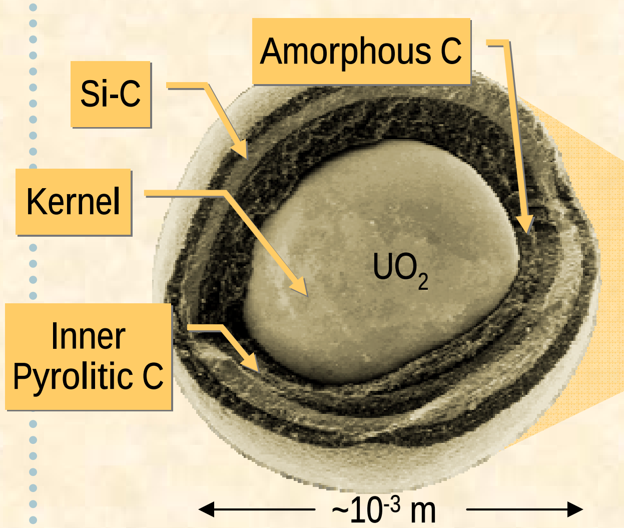
Rodney Fox
Zhaoseng Gao

National Energy Technology Laboratory

Thomas O'Brien
Dominic Alfonso
Madhava Syamlal

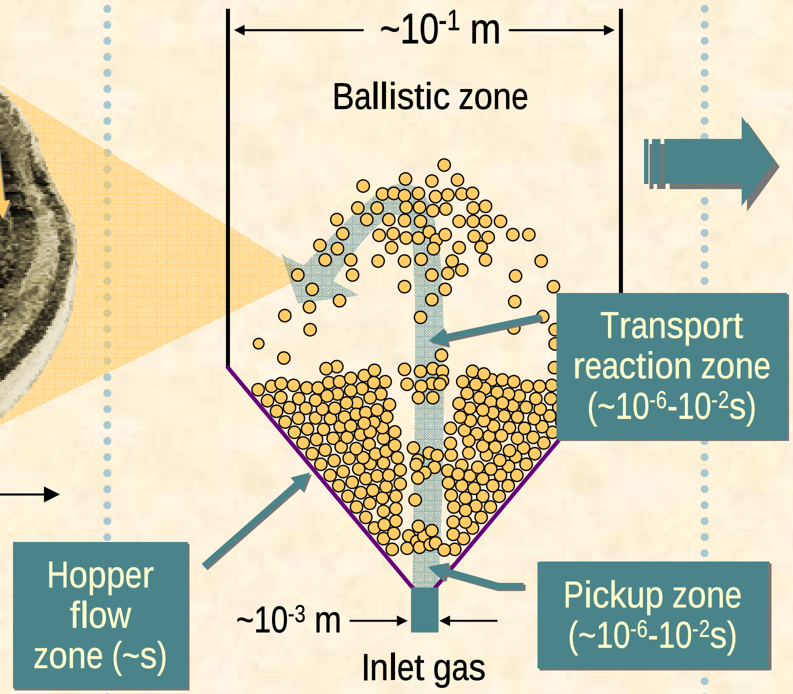
Background 1: Nuclear fuel coating process – a specific example of gas-solid contacting device

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)



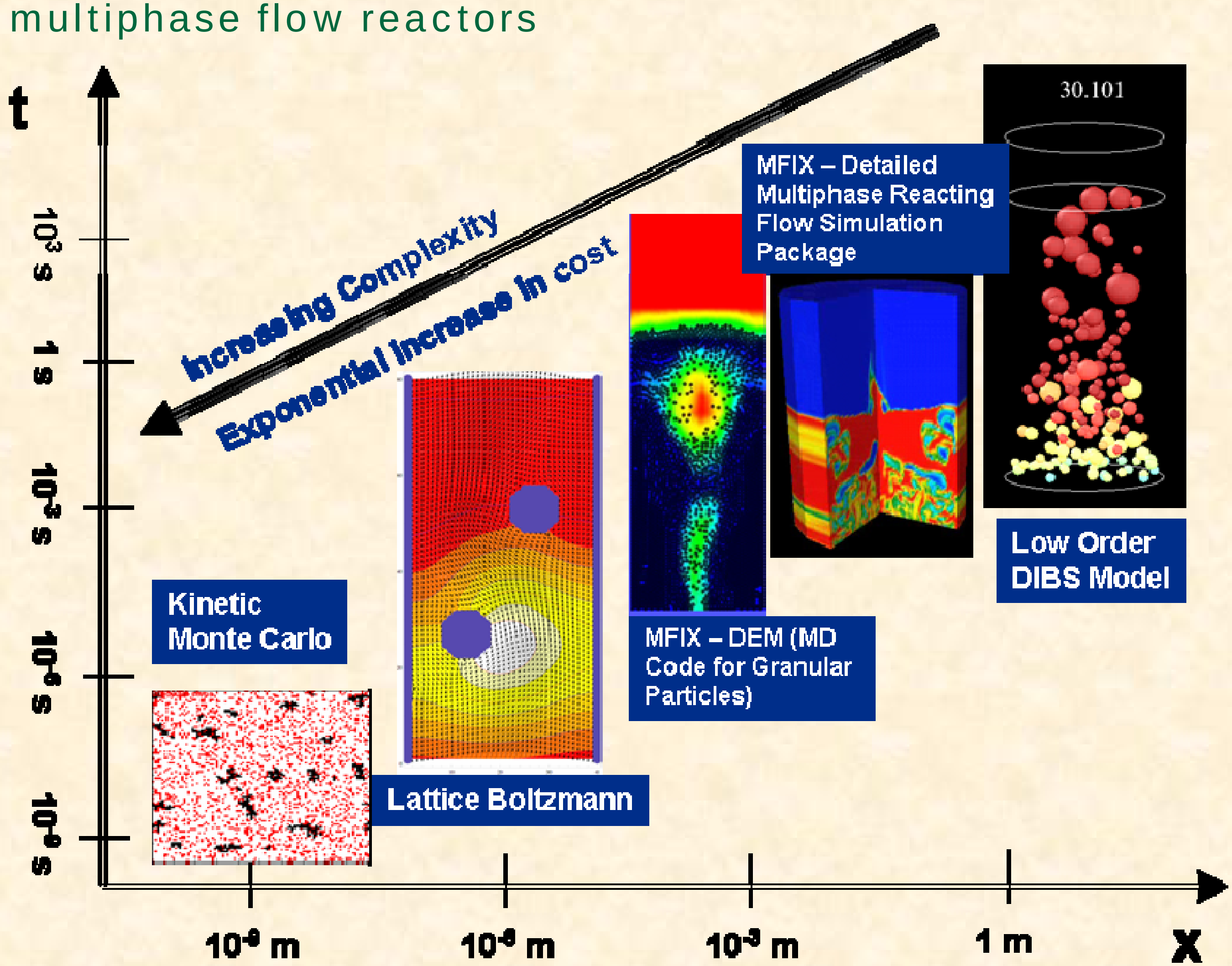
- Coating at high temperature (1300–1500°C) in batch spouted bed reactor for ~10^4 s
- Particles cycle thru deposition and annealing zones where complex chemistry occurs

- 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

Background 2: Multiphysics heterogeneous chemically reacting flows for energy systems

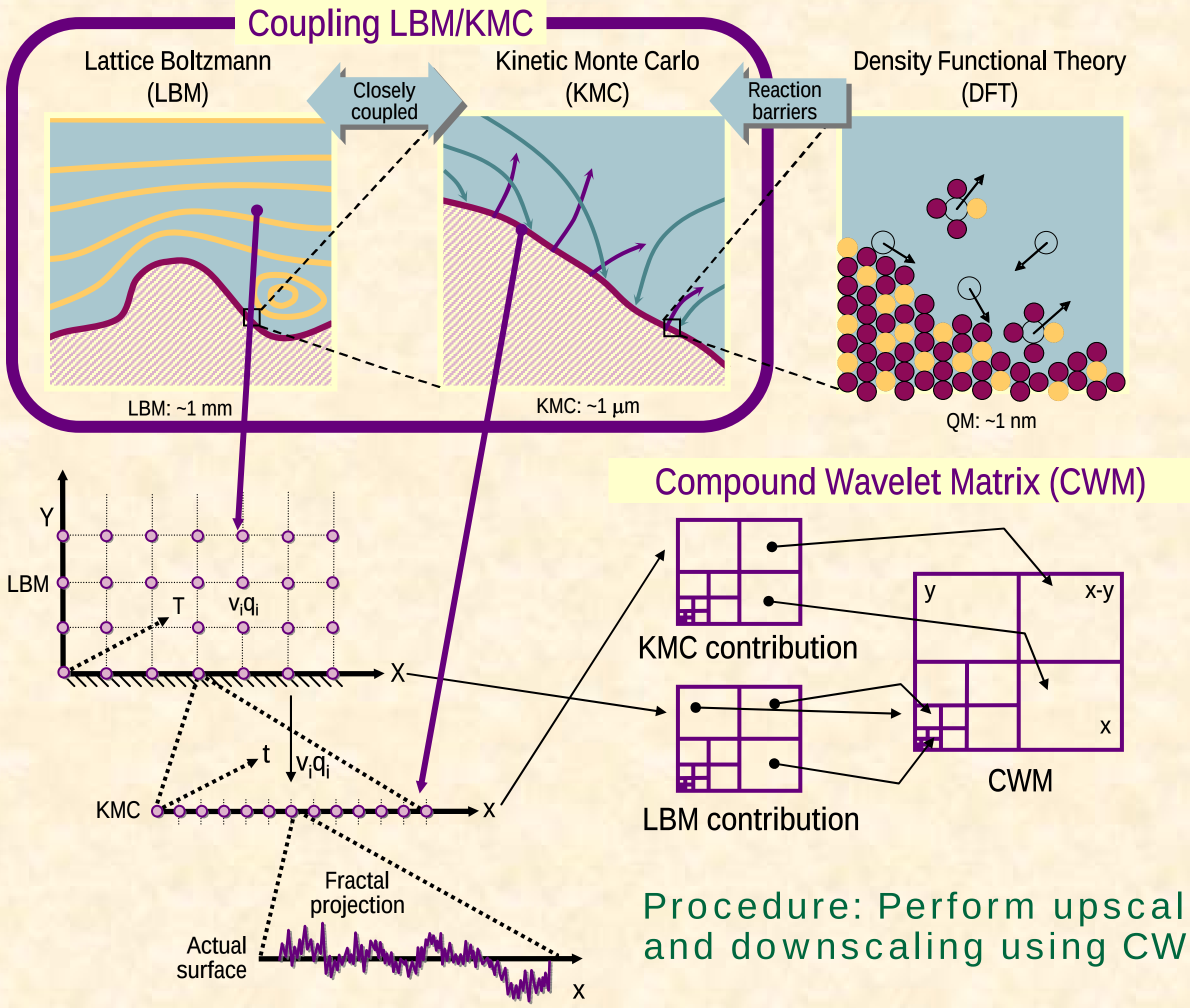
Goal: Building a suite of models for unprecedented capability to simulate multiphase flow reactors



- 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

Background 3: 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

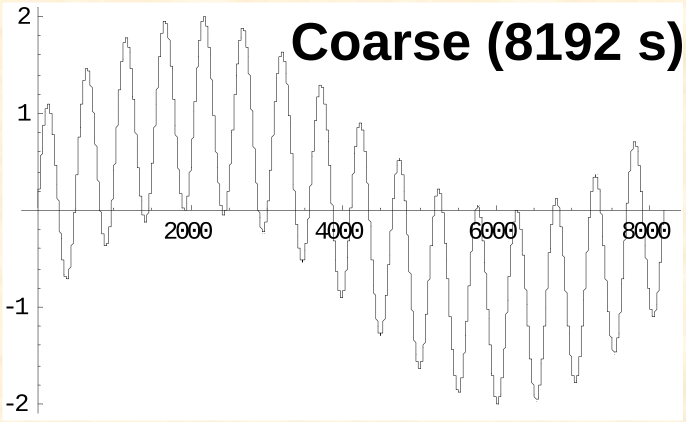


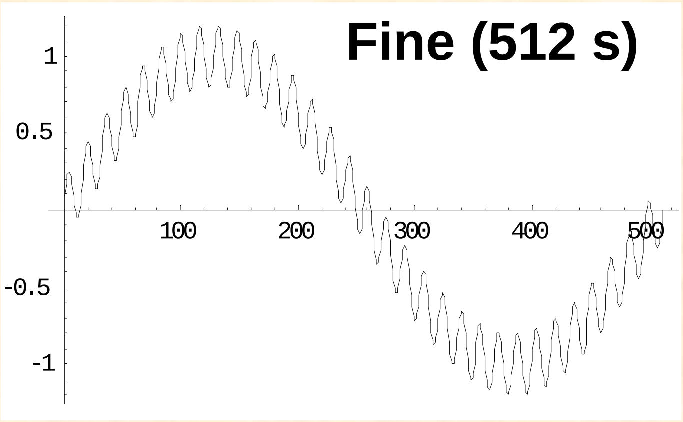
Procedure: Perform upscaling and downscaling using CWM

Compound Wavelet Matrix (CWM) for Multiscaling

- **CWM is a wavelet based spatio-temporal operator which has different functions depending on the context**
  - **Compounding operation (combine information from multiple scales)**
  - **Projection or transfer operations**
    - **Up-scaling fine scale information to coarse scale fields**
    - **Down-scaling coarse information to reconstruct fine scale fields**
    - **Fits within the general HMM framework**

Simple illustration of the compounding process – Coarse and Fine Signal



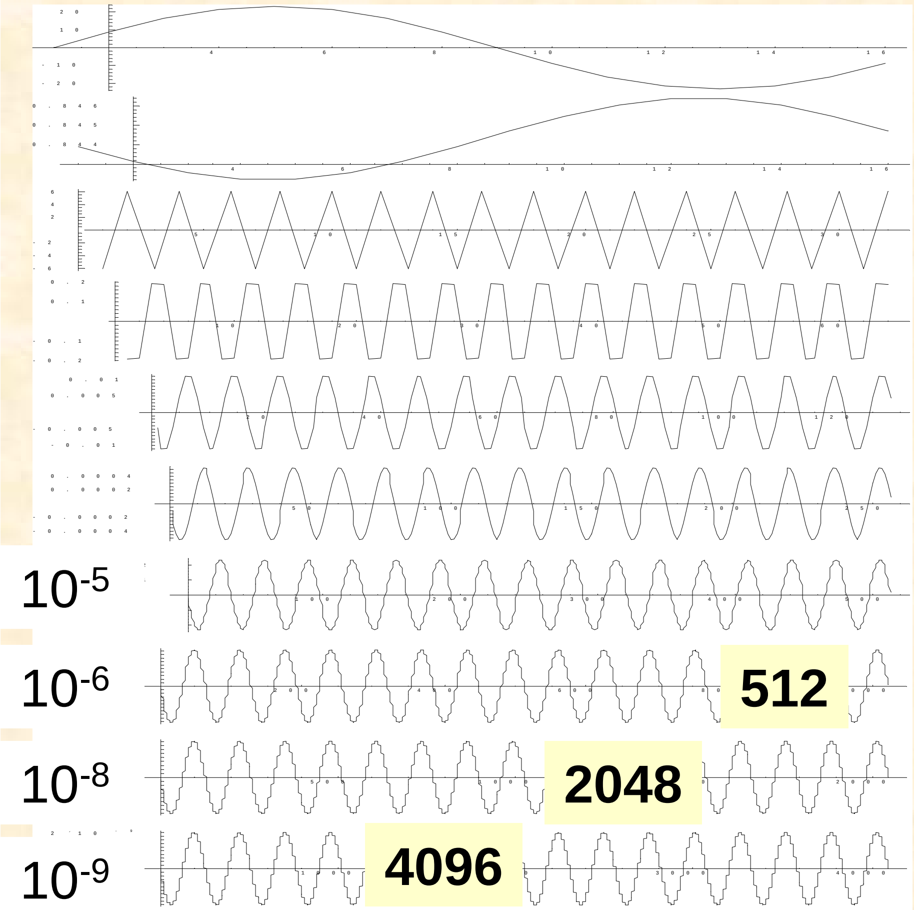


Resolves the slow and intermediate frequency over a long duration

Resolves the intermediate and fast frequency over a short duration

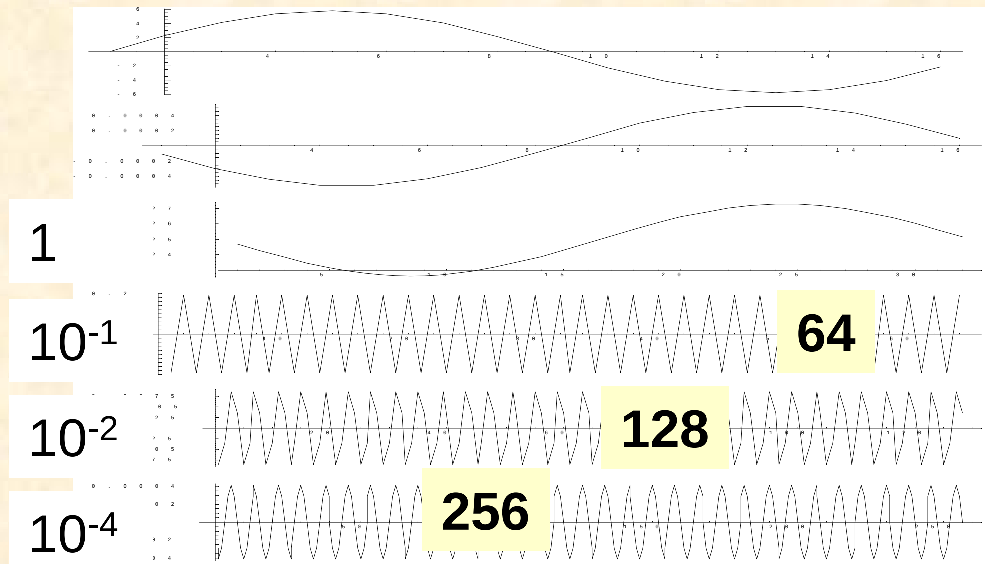
Simple illustration of the compounding process – Decomposition

Coarse (8192 s)



$$W_f(a,b) = \int_{-\infty}^{\infty} f(x)\psi_{a,b}(x)dx$$

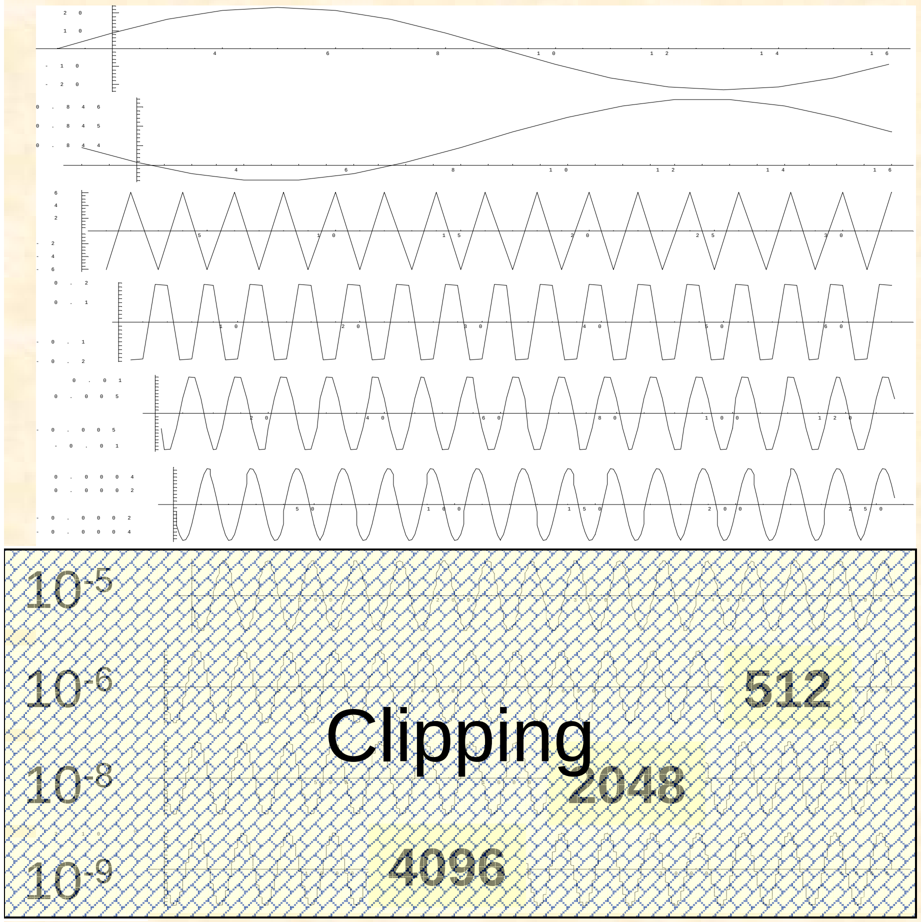
Fine (512 s)



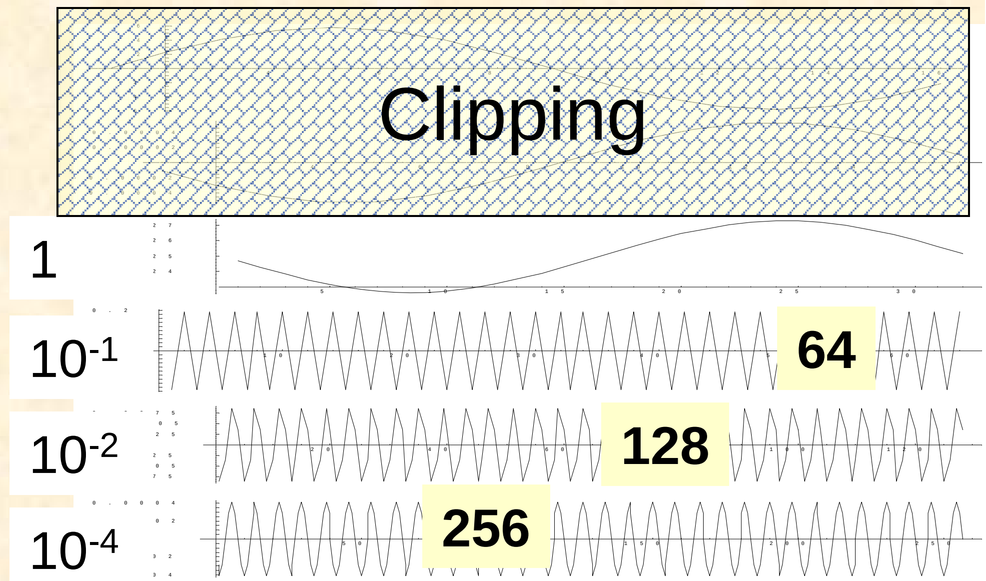
Simple illustration of the compounding process – Clipping

Coarse (8192 s)

$$f_{s_1 s_2}(x) = \frac{1}{c_\psi} \int_{s_1}^{s_2} \int_{-\infty}^{\infty} W_f(a,b)\psi_{a,b}(x)\,db\,\frac{da}{a^2}$$

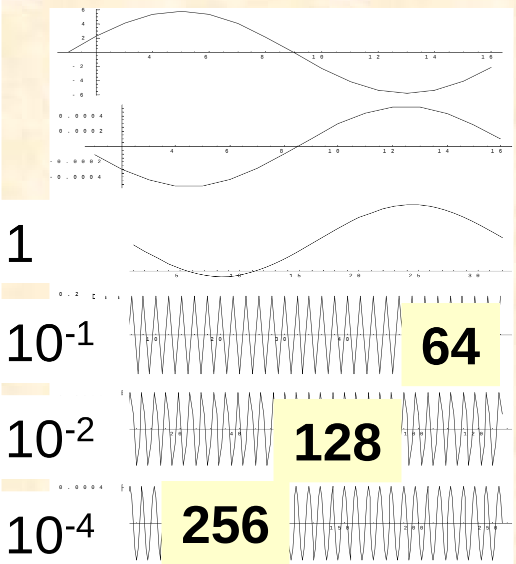


Fine (512 s)



Simple illustration of the compounding process – Prolongation

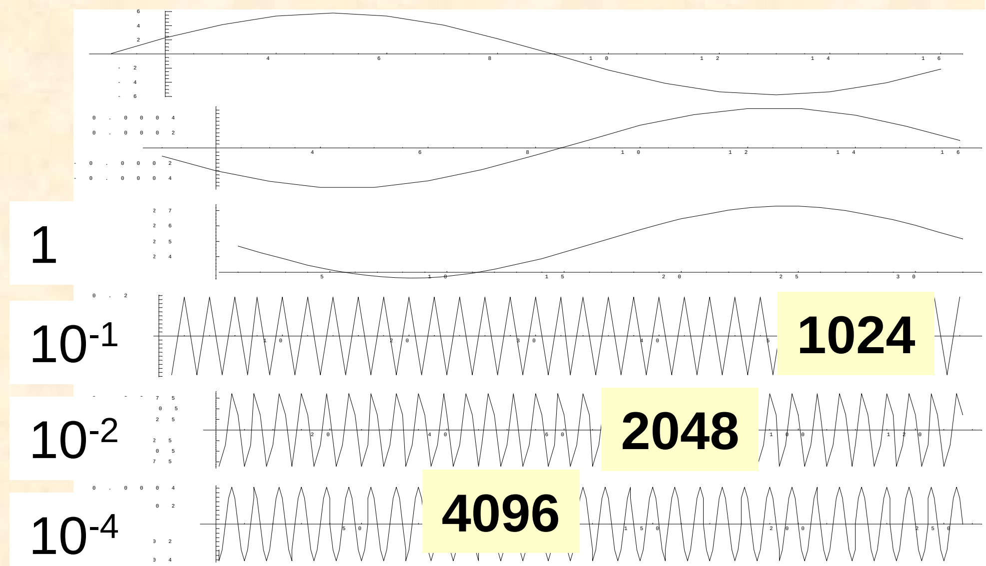
Fine (512 s)



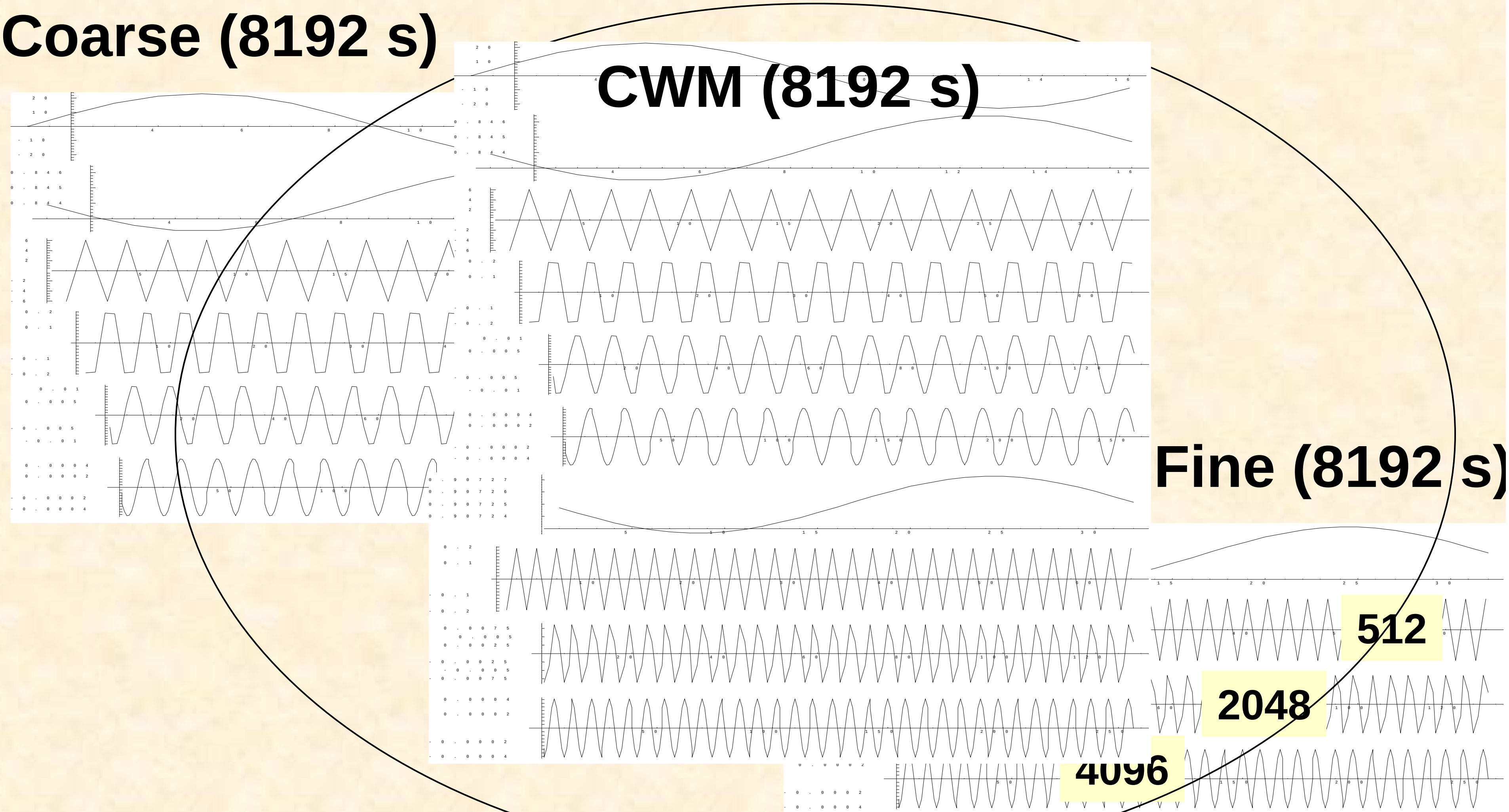
Replicate

16 times

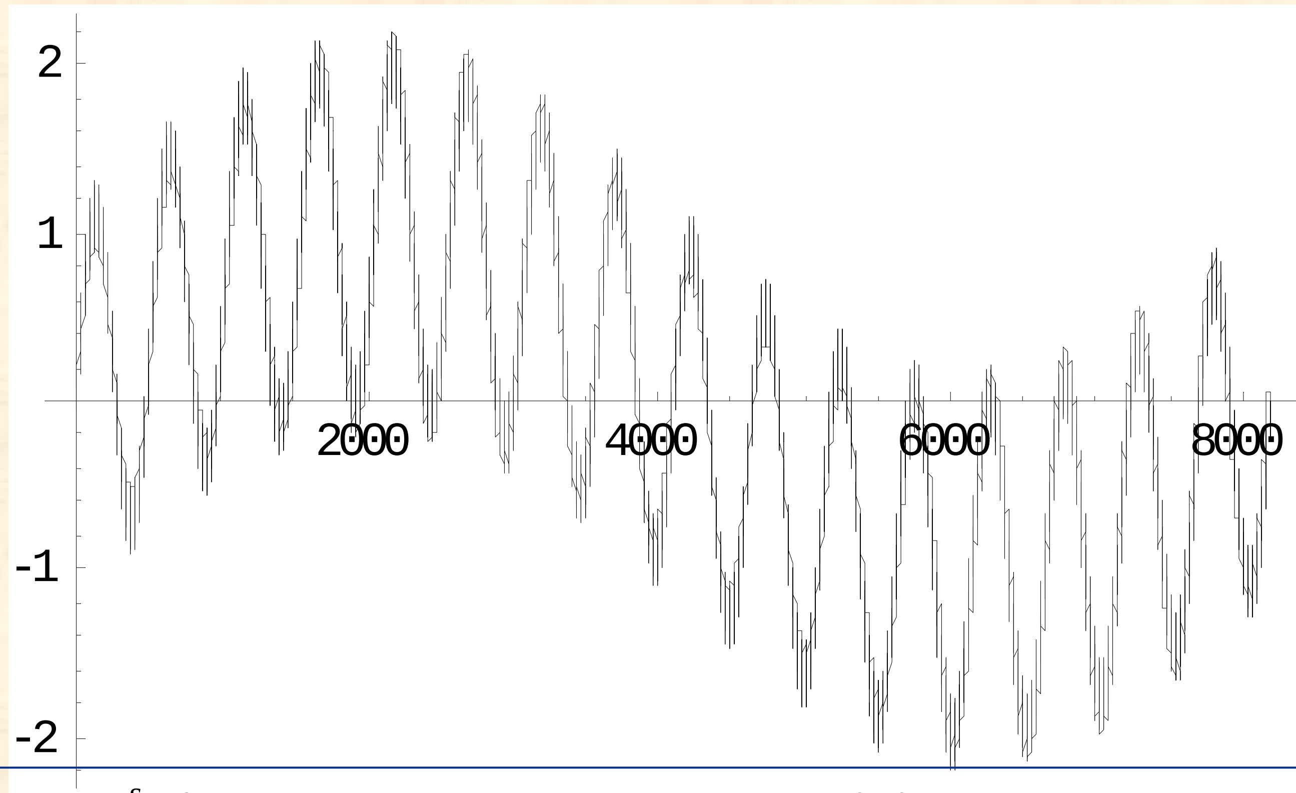
Fine (8192 s)



Simple illustration of the compounding process – Compounding

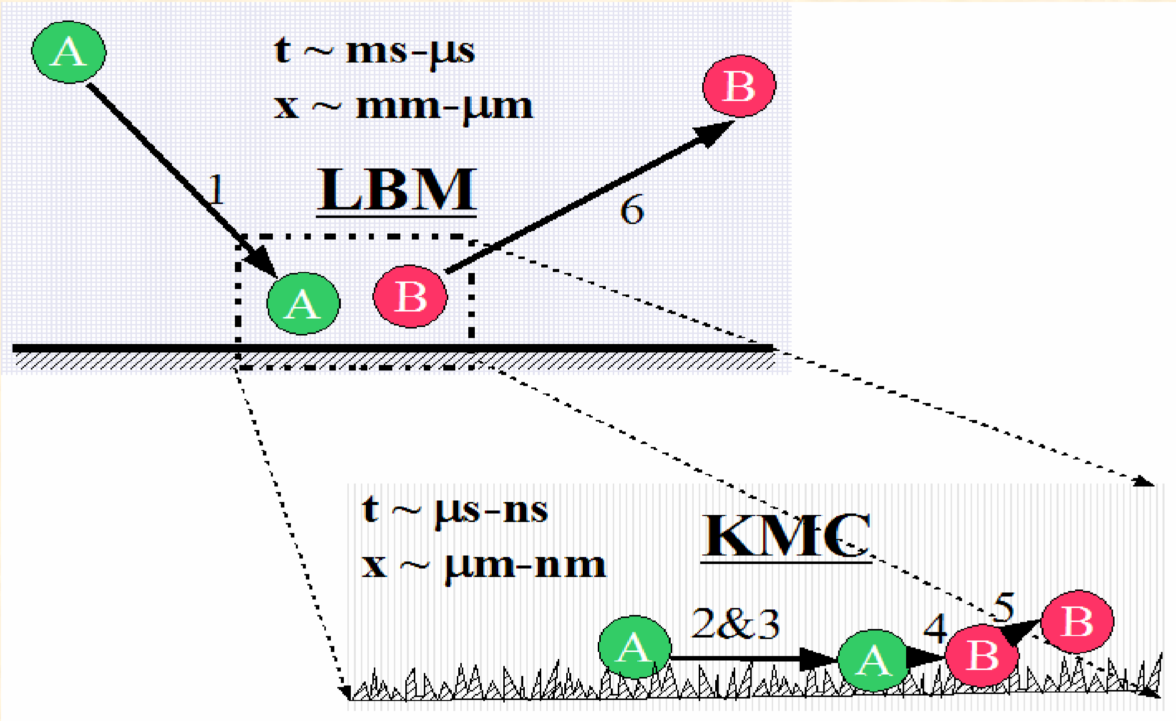


Simple illustration of the compounding process – Reconstruction



$$f_{0,\infty} = \frac{1}{c_\psi} \int_0^{s_1} \int_{-\infty}^{\infty} W_f^{P_1}(a,b)\psi_{a,b}(x)\,db\,\frac{da}{a^2} + \frac{1}{c_\psi} \int_{s_1}^{\infty} \int_{-\infty}^{\infty} W_f^{P_2}(a,b)\psi_{a,b}(x)\,db\,\frac{da}{a^2}$$

Prototype Problem: Building Block for Heterogeneous Surface Reactions



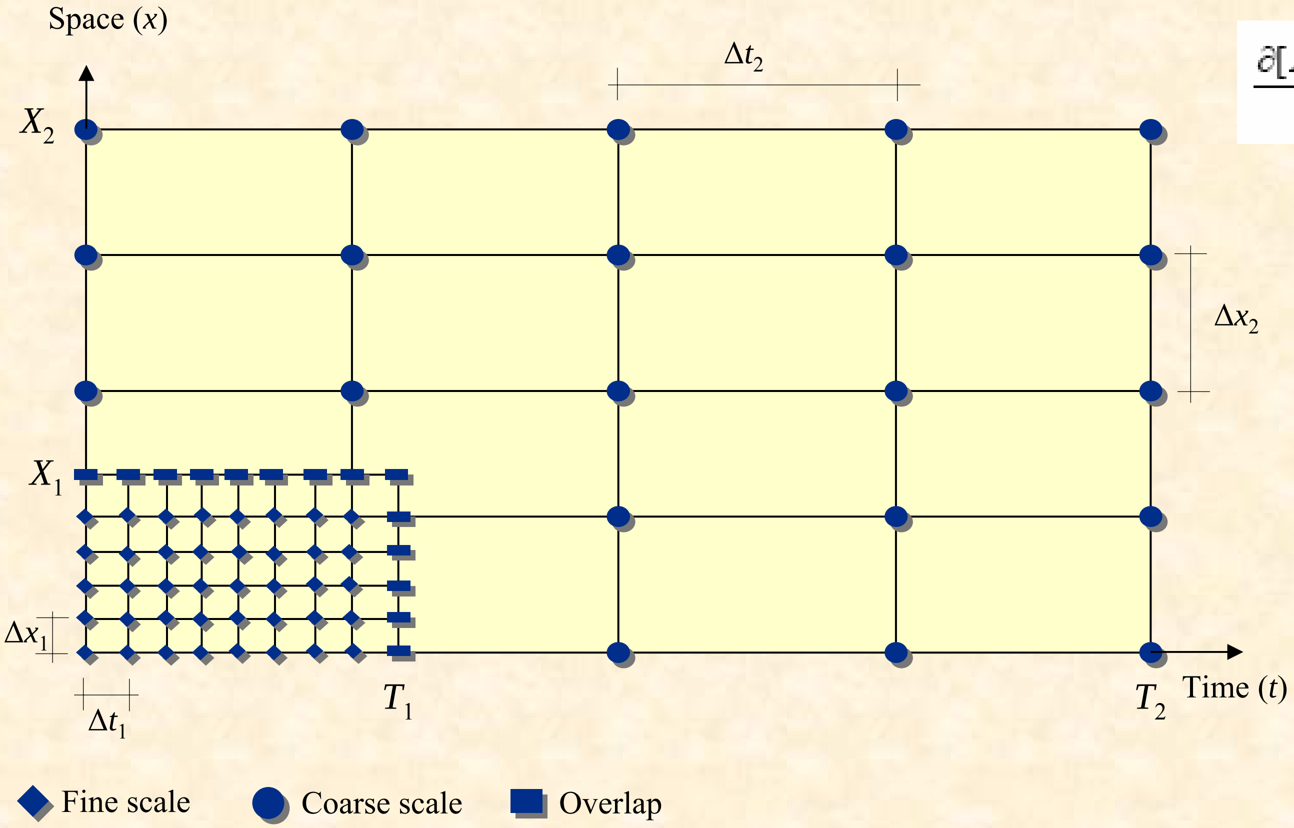
1. Transport (LBM)
2. Diffusion on surface (KMC)
3. Absorption (KMC)
4. Production of B (KMC)
5. Desorption of B (KMC)
6. Transport (LBM)

Ni system for Chemical Looping

$2Ni + O_2$ => 2 O-(Ni), Fast
O-(Ni) => (NiO), Slow

Schematic of a simple A → B heterogeneous chemical reaction with various elementary steps modeled using Kinetic Monte Carlo (KMC) and Lattice Boltzmann Method (LBM).

Example 1: 1D diffusion with reacting boundary point



Fine scales results are obtained from the *fine* solution method while coarse ones are obtained from the *coarse* method.

Diffusion

$$\frac{\partial[A(x)]}{\partial t} = \left(D_{Ax} \frac{\partial^2[A(x)]}{\partial x^2} + D_{Ay} \frac{\partial^2[A(x)]}{\partial y^2} \right)$$

Reactions

$$A \xrightarrow{k_{AB}} B$$

$$B \xrightarrow{k_{BA}} A$$

Deterministic

$$\frac{d[A]}{dt} = -k_{AB}[A] + k_{BA}[B]$$

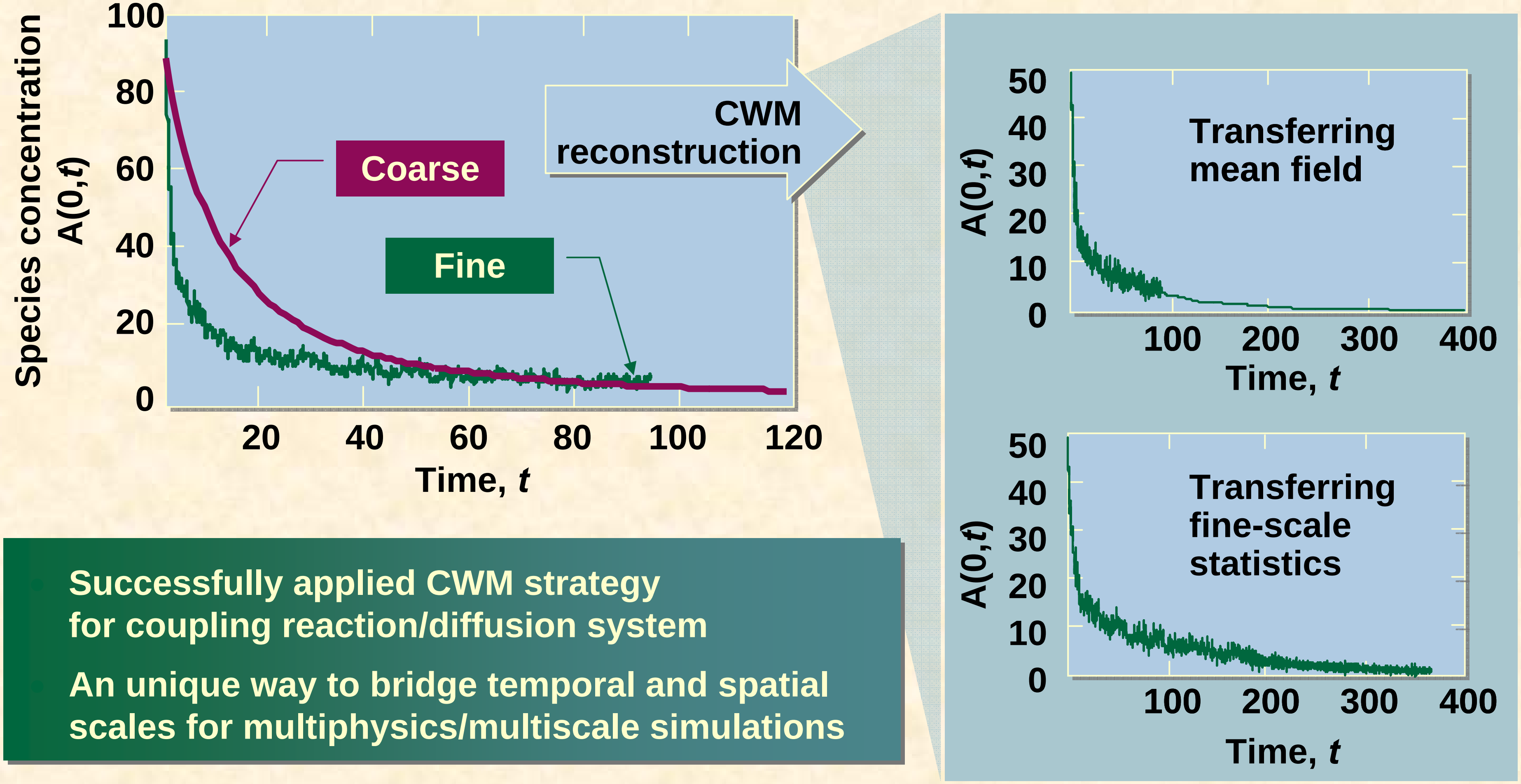
$$\frac{d[B]}{dt} = -k_{BA}[B] + k_{AB}[A]$$

KMC

$$t_{AB} = -\frac{1}{k_{AB}[A]}\ln(1-R_1)$$

$$t_{BA} = -\frac{1}{k_{BA}[B]}\ln(1-R_2)$$

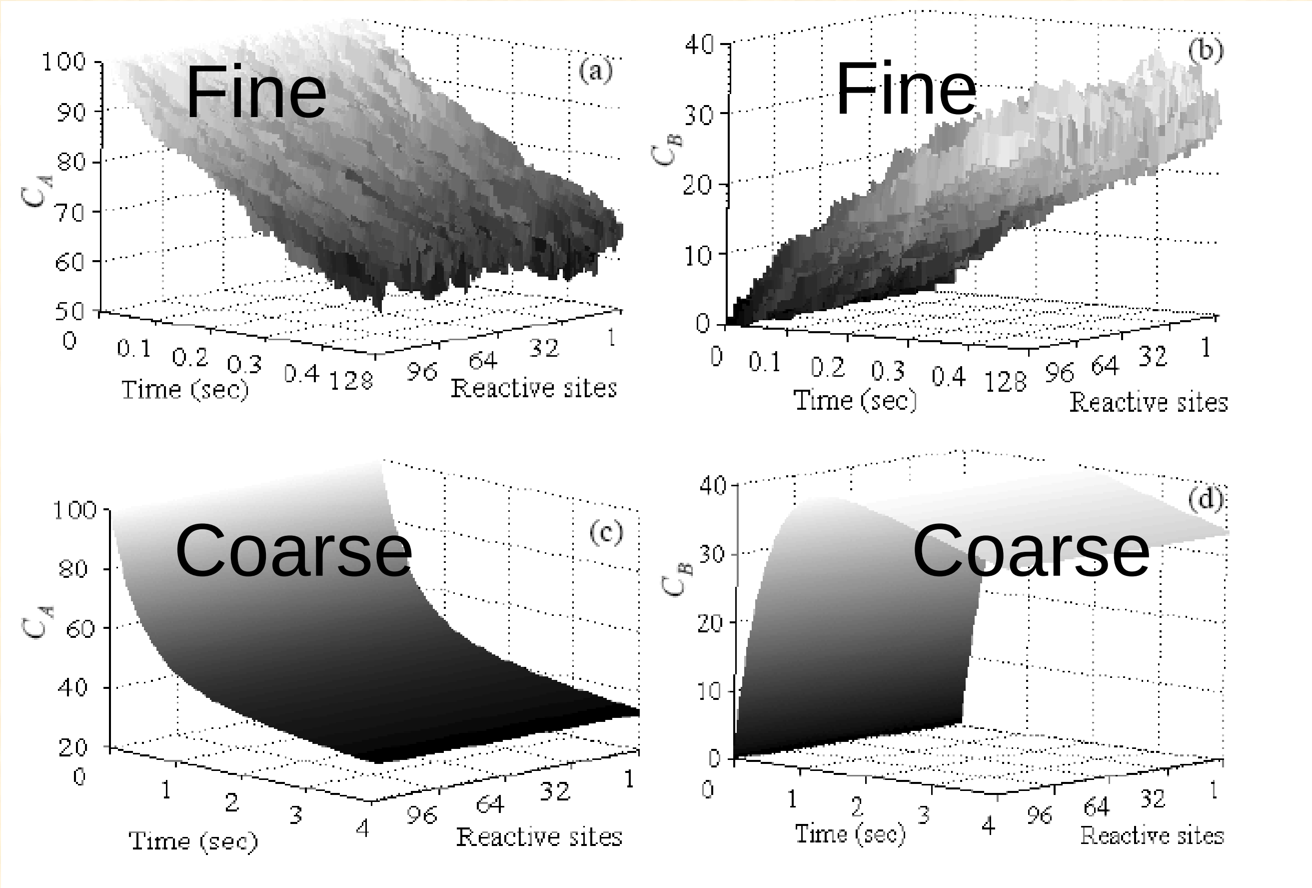
Results for Example 1*



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

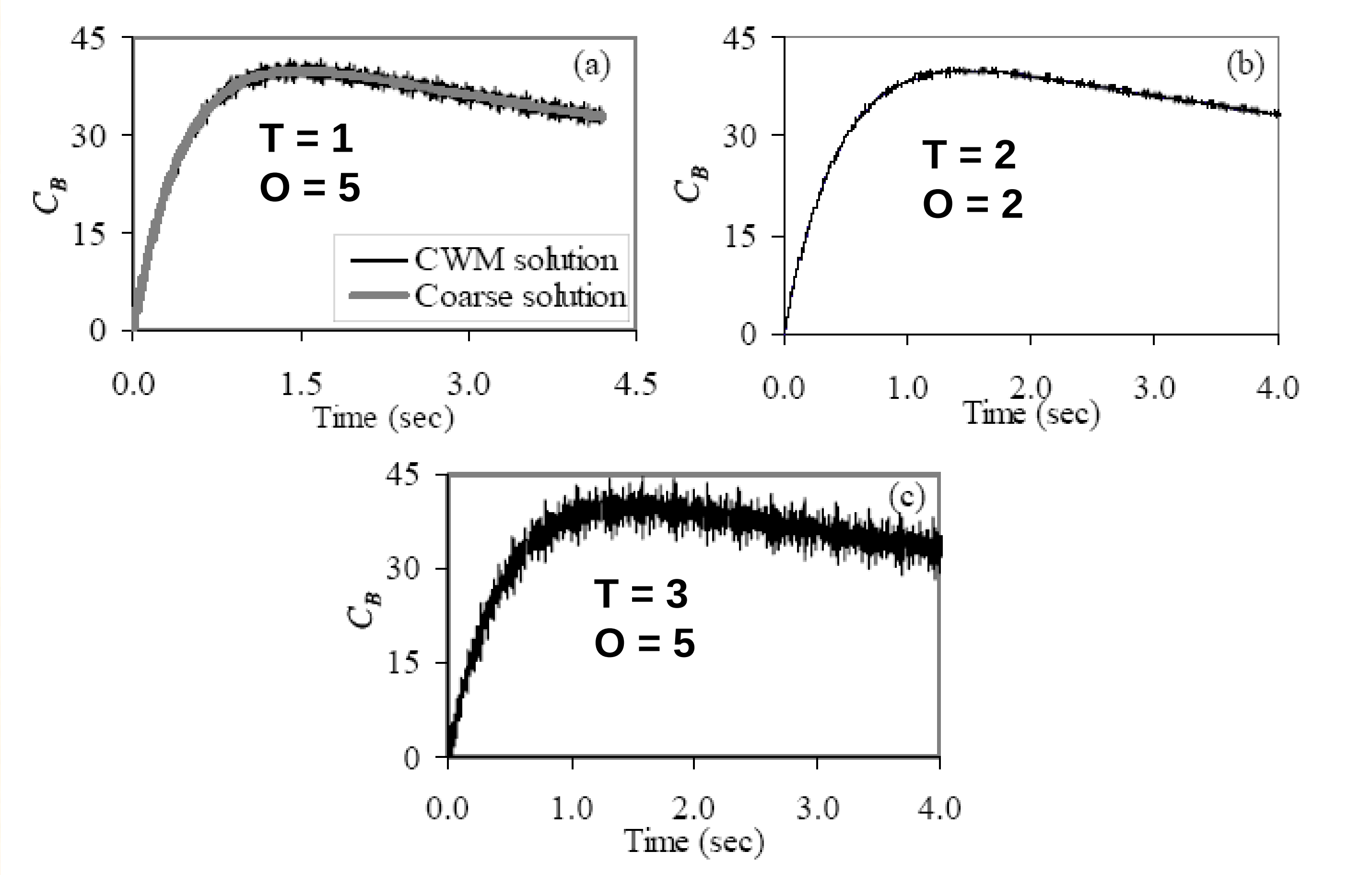
*Frantziskonis, Mishra, Pannala, Simunovic, Daw, Nukala, Fox, Deymier (IJMCE, 2006).

2D diffusion with reacting boundary plane



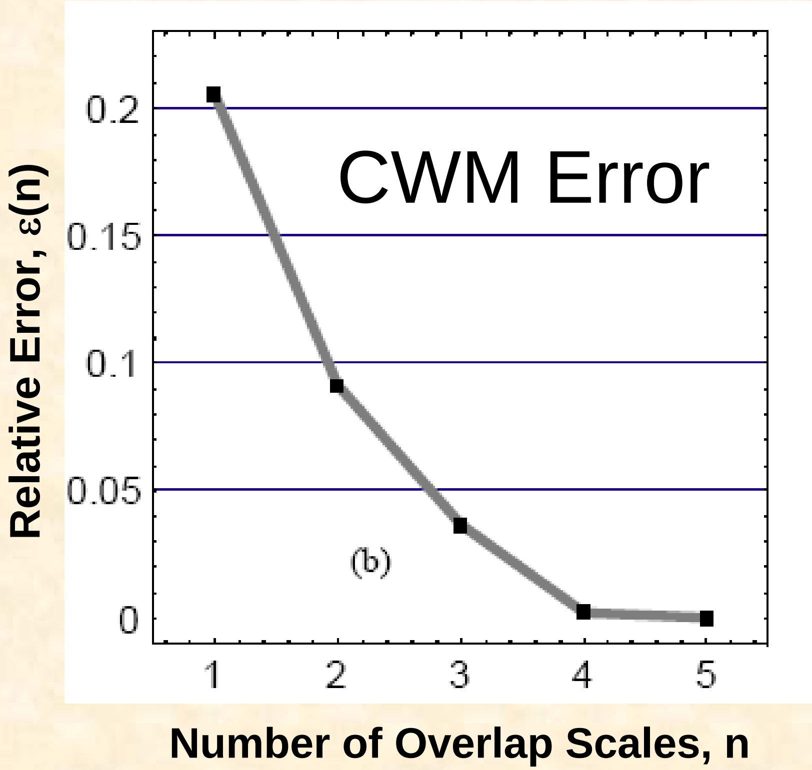
Evolution of reactants A and B

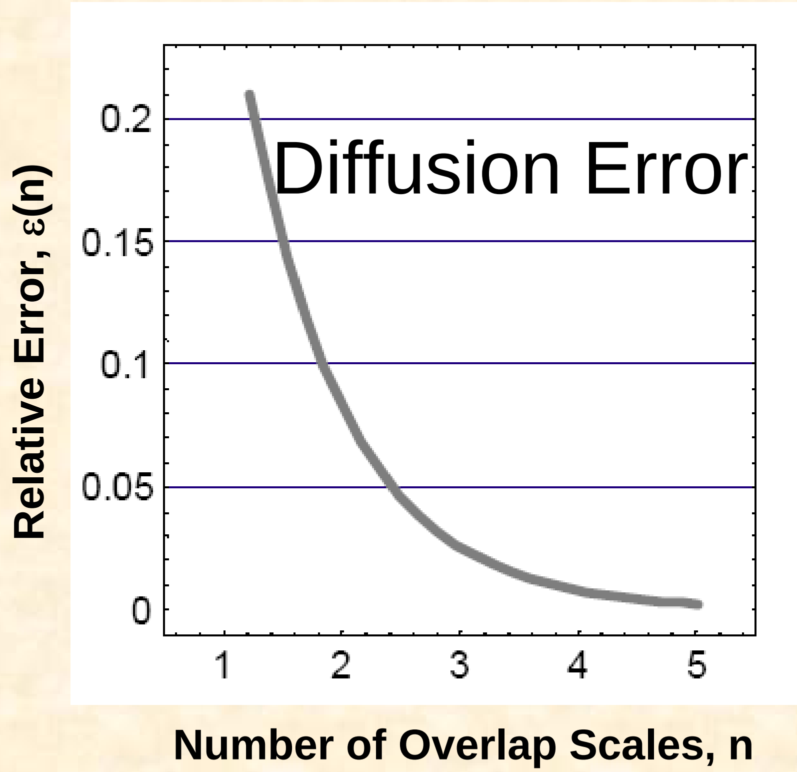
2D diffusion with reacting boundary plane



Reconstructed species profile (effect of overlap and thresholding)

2D diffusion with reacting boundary plane





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

2D diffusion with reacting boundary plane

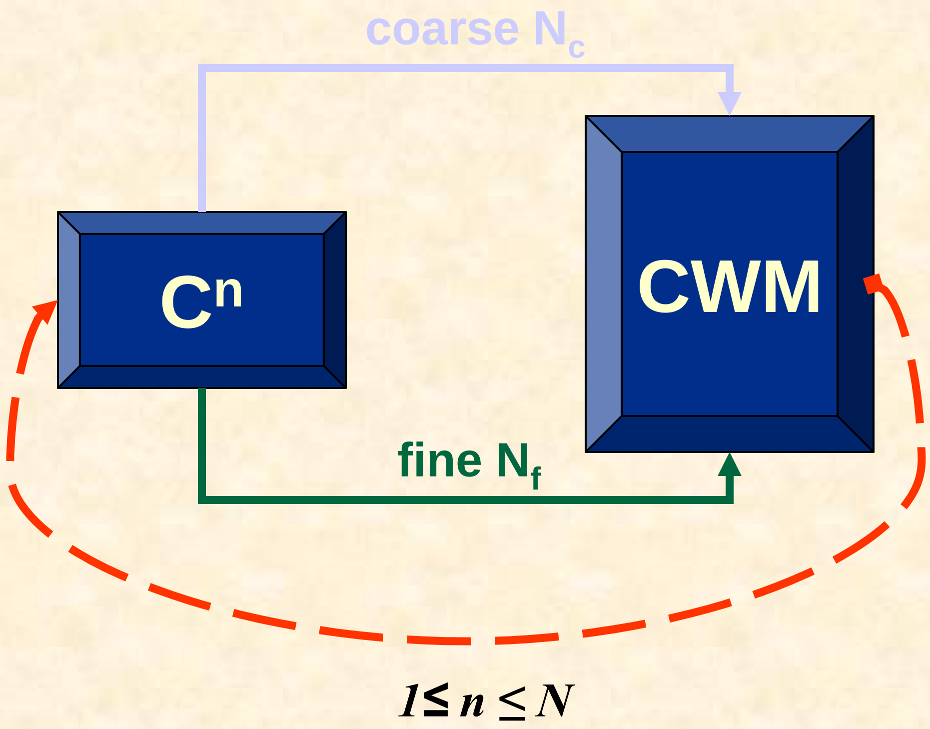
Comparison of computational expense

Model	nx (X -nodes)	ny (Y-nodes)	Kinetic evolution time of the model	computer processing time
Fine	512	128	0.22 sec (2048 steps)	459 sec
			0.41 sec (4096 steps)	948 sec
			3.5520 sec (35520 steps)	8579 sec
Coarse	512	128	3.5144 sec (4096 steps)	928 sec
			1.7572 sec (2048 steps)	515 sec
Wavelet transform				7 sec
CWM	512	128	0.22 sec fine model 3.5144 sec coarse model	7+459+928=1394 sec

A gain of six times

This is without any coarsening in space

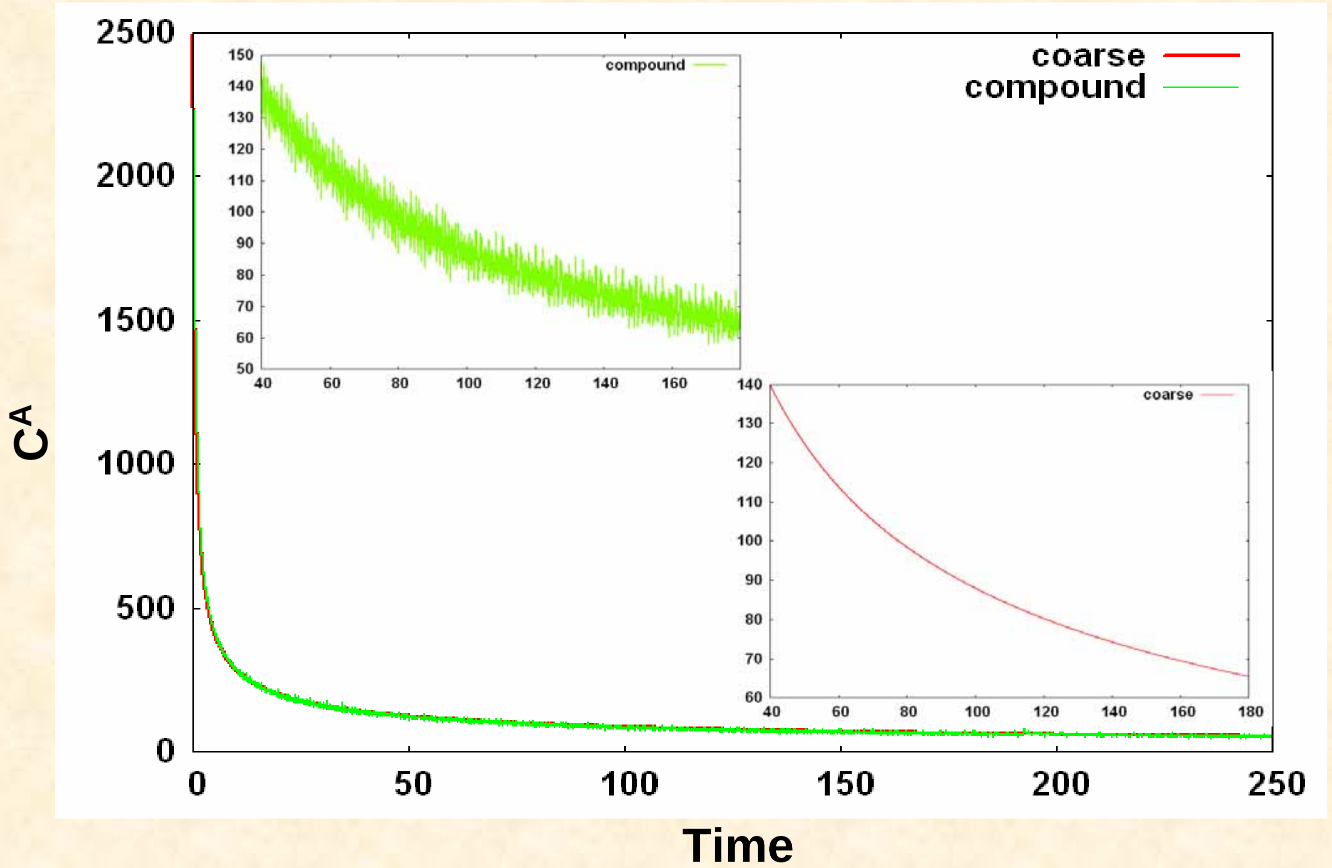
Dynamic CWM (dCWM): Dynamic coupling of coarse and fine methods



- **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**

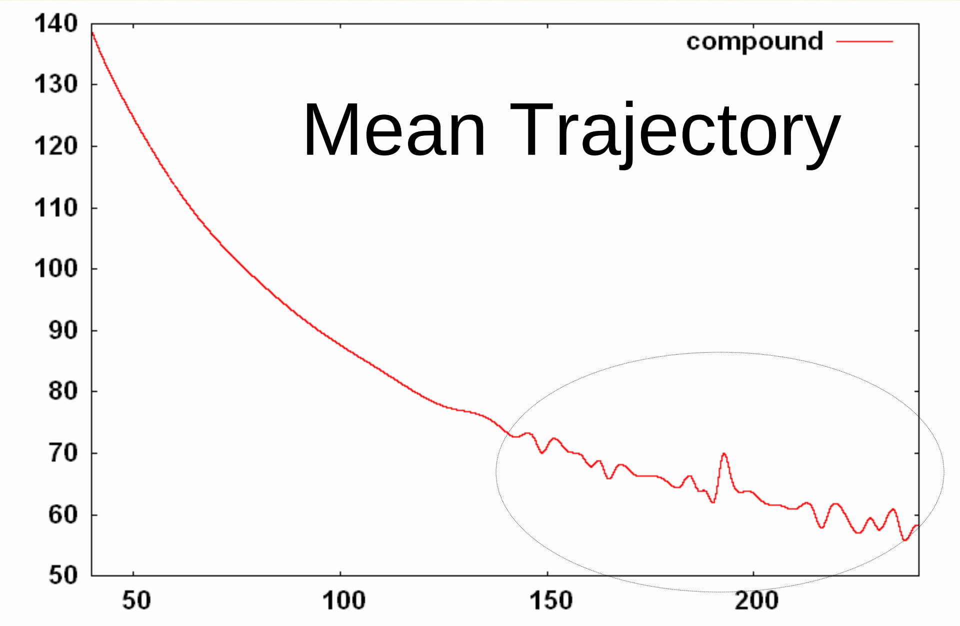
Example 3: 1D diffusion with reacting boundary plane with dCWM

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



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

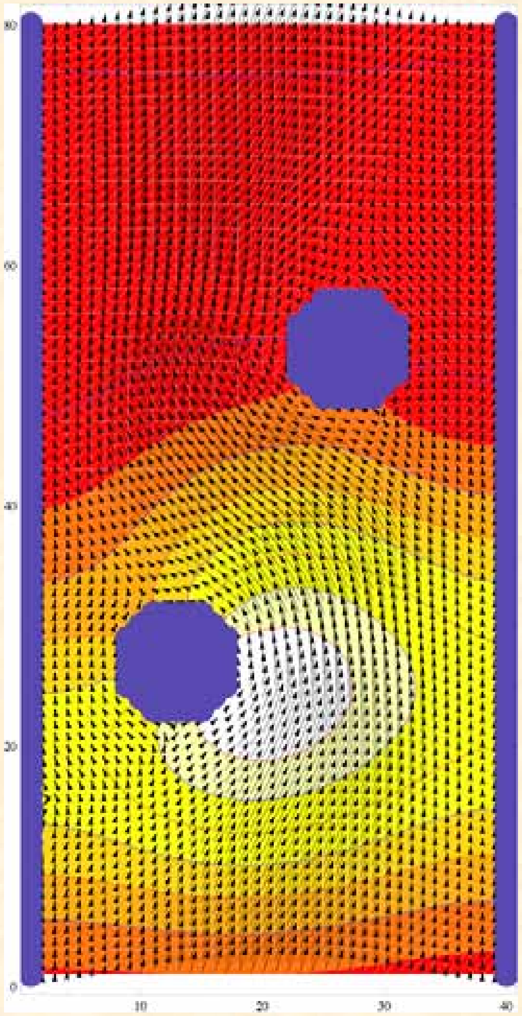
N_c = 16384; N_f = 2048; N = 8



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**
- **Implementation of 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)**



Work in Progress and Future Work

- **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**
  - **to be released as open source**
  - **solicit contributions from other applied math and computational science groups**

Thank you and any questions?

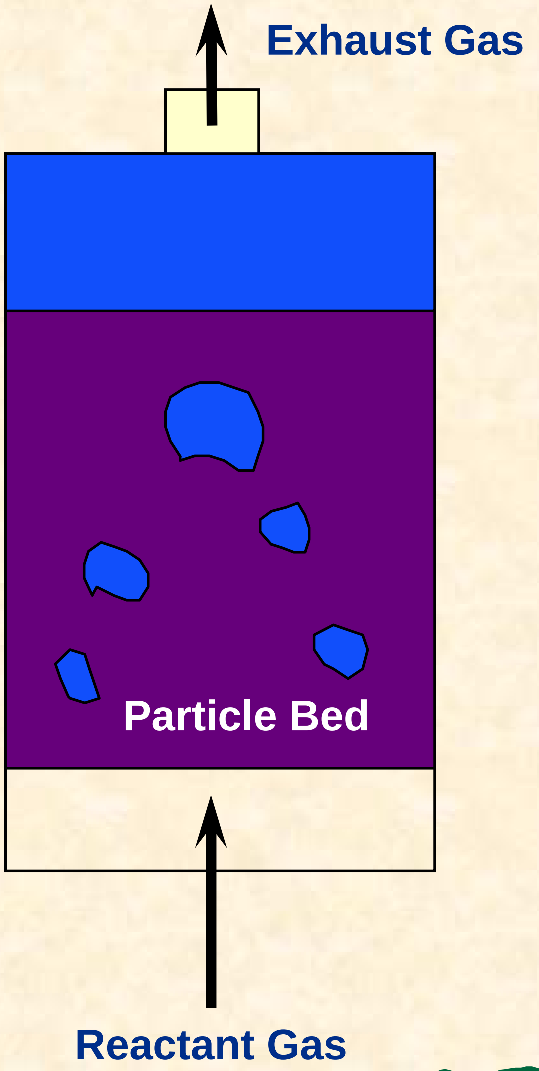
Backup Slides

Background 1: Fluidized beds are widely used for gas-particle contacting (one special case of multiphase flow reactors

- **Nonlinear gas-solid drag promotes turbulent mixing**
- **Good mixing produces high conversion, product quality**
- **Nonlinearities also cause density waves (e.g., bubbles) that interfere with good mixing, promote attrition**

Challenge:

- **Direct measurements are very difficult**
- **Need simulations to improve design and operating strategies**
- **Several orders of magnitude in both temporal and spatial scales**
  - **from the surface particle processes scales to the large scale mixing scales**



Background 5: Challenges in having predictive simulations for HCR Flows

- **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?**
  - **Possible when clear separation of scales between the multiphysics modules**
  - **New mathematics, theory and analysis**
  - **Unification of governing equations across several scales**
    - **Lattice based methods across all scales?**
- **If that is not possible, can we take the information from different methods and perform this in an online/offline fashion with various degrees of coupling?**
  - **Widely practiced**
  - **Can this be generalized?**

CWM limitations

- **Wavelets are linear operators**
  - **Compounding only buys linear superposition across scales**
  - **Not an issue with well-separated scales**
  - **For non-separated scales, this would imply that the CWM process has to be performed frequently to ensure local quasi-linear correlation across bridging scales**
- **The process developed in this project is general and down the line wavelets can be replaced with any other suitable nonlinear transforms**