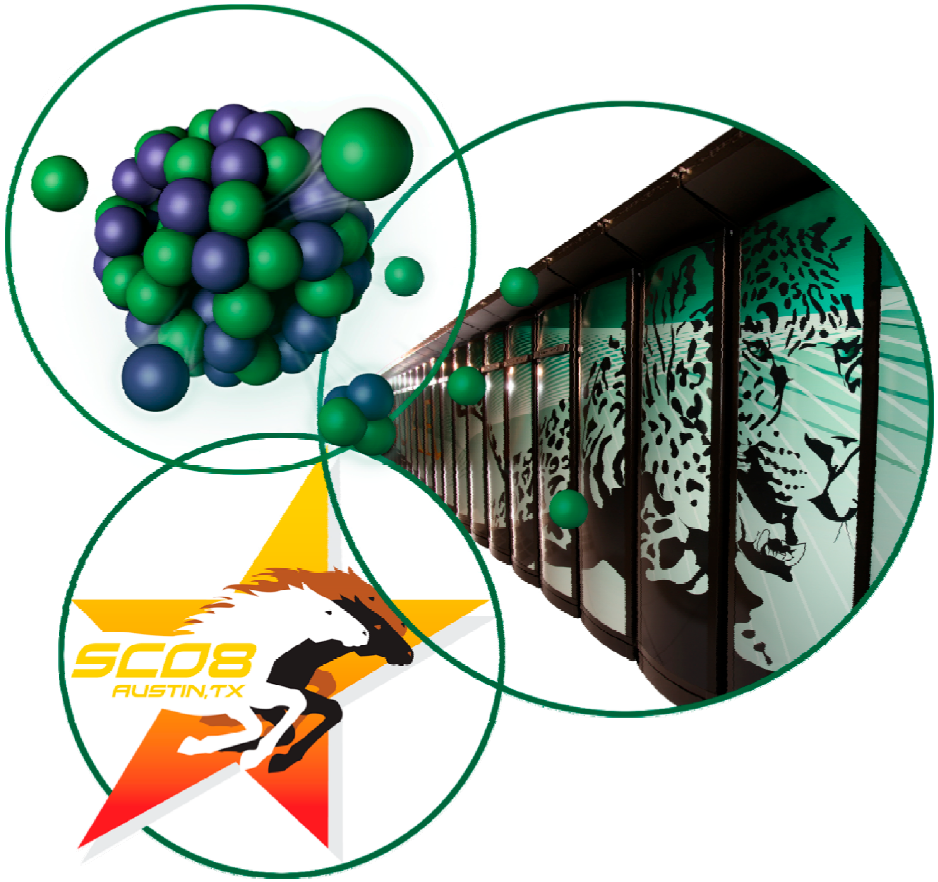
Computational Mathematics at the Oak Ridge National Laboratory



Presented by

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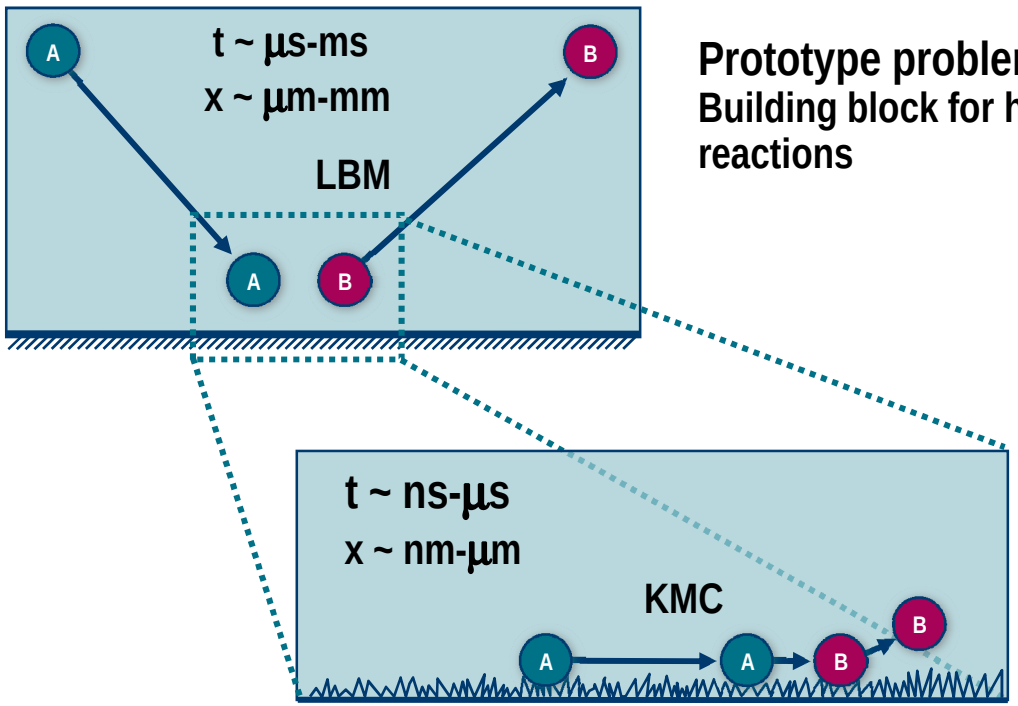
Computational Mathematics
Computer Science and Mathematics Division

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

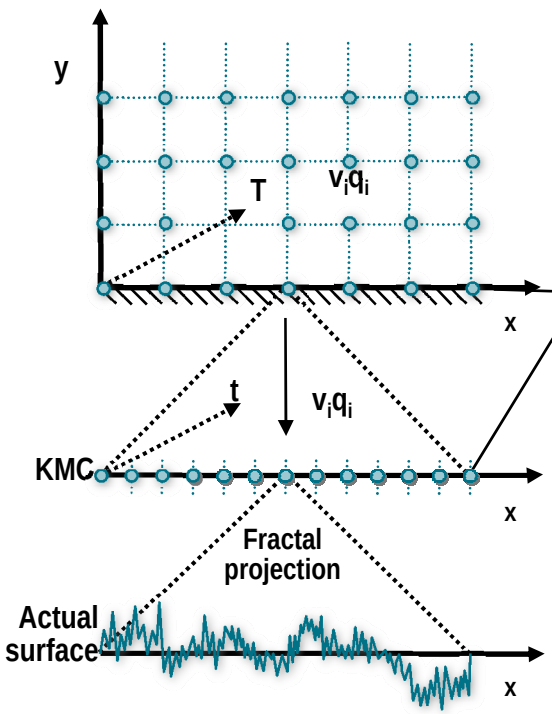


Prototype problem:
Building block for heterogeneous surface reactions

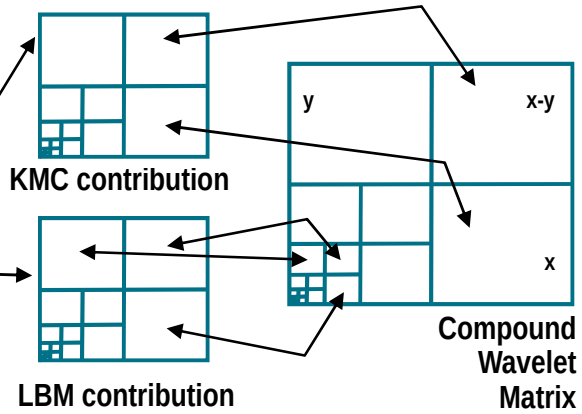
Simple A → B heterogeneous chemical reaction with various elementary steps modeled using kinetic Monte Carlo (KMC) and lattice Boltzmann method (LBM)

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 (cont.)



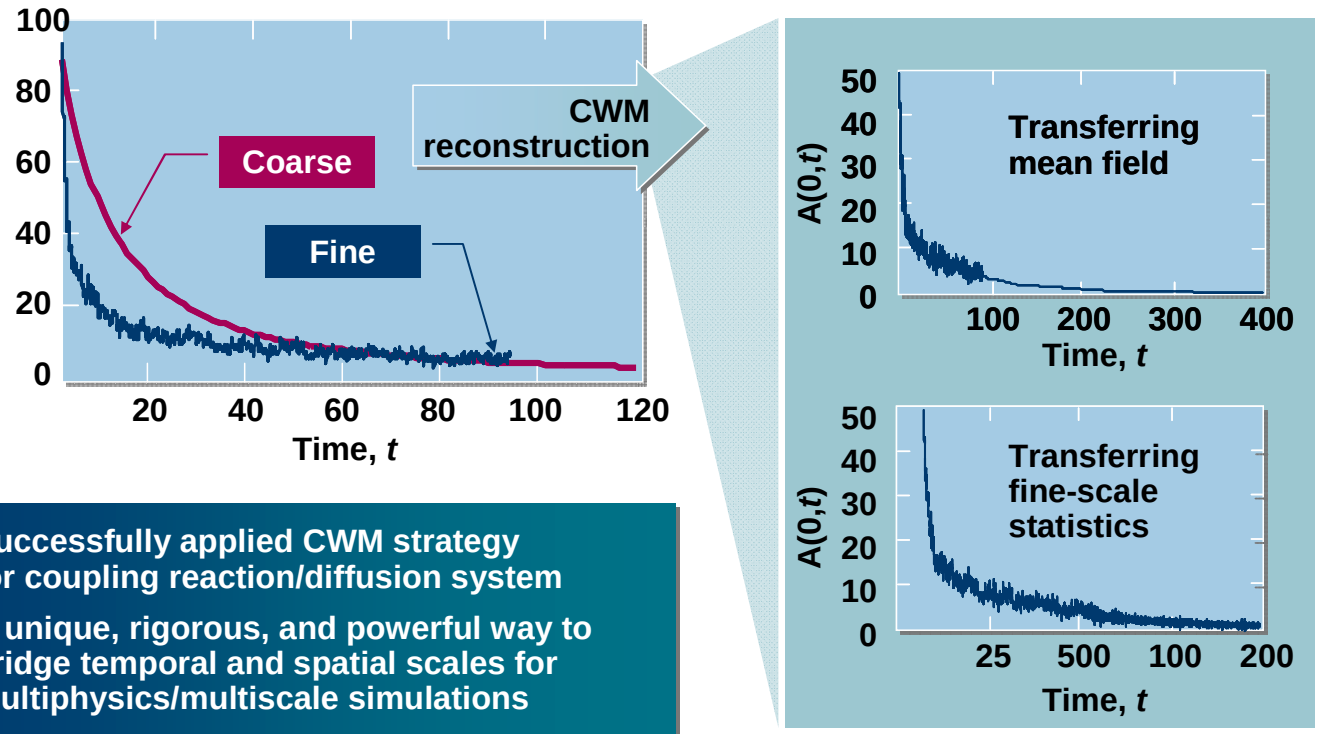
Compound Wavelet Matrix (CWM)



Procedure:
To perform upscaling and downscaling using CWM

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 (cont.)



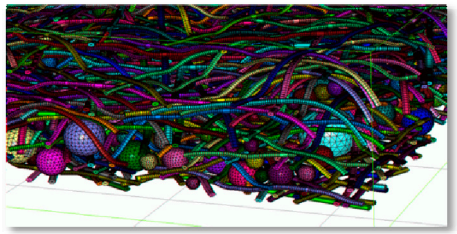
- Successfully applied CWM strategy for coupling reaction/diffusion system
- A unique, rigorous, and powerful way to bridge temporal and spatial scales for multiphysics/multiscale simulations

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

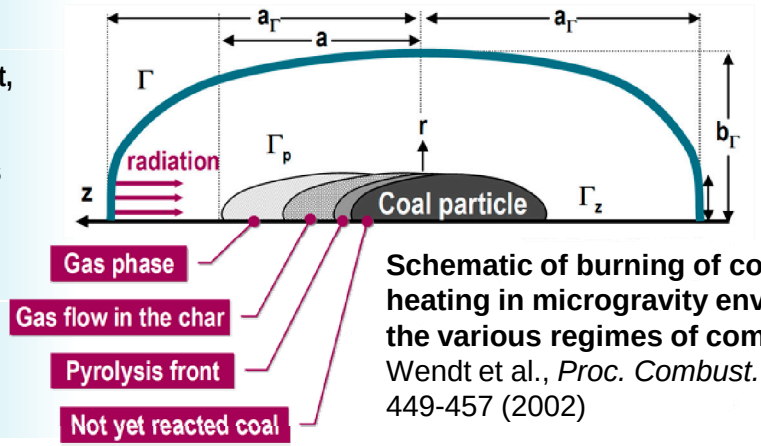
Goal: Develop a multiscale framework for accurate modeling of heterogeneous reacting flows over catalytic surfaces (cont.)

Applications

Chemical looping combustion (CLC)	• Efficient, low emissions, and amenable to CO 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



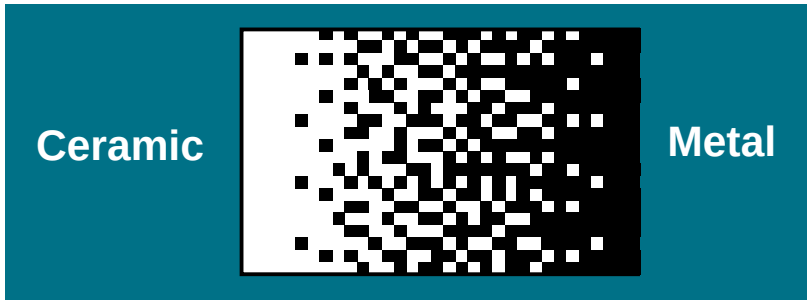
- Fibrous substrate for discontinuous fiber substrate
- The voids found by probing the substrate with a fixed-sized sphere are denoted by spheres



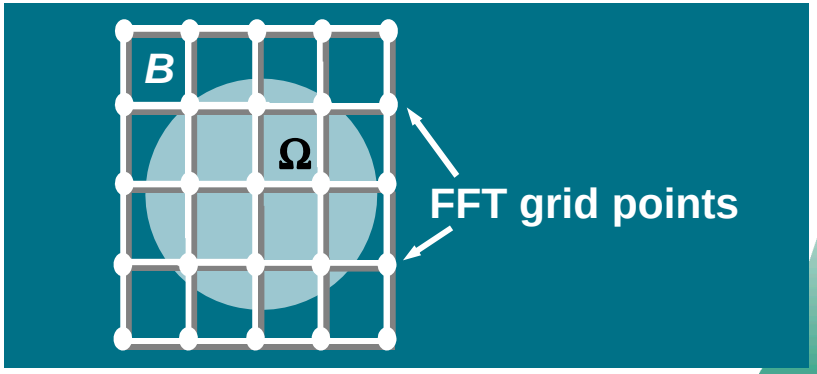
Schematic of burning of coal particle using laser heating in microgravity environment showing the various regimes of combustion
Wendt et al., *Proc. Combust. Inst.* **29**(1), 449-457 (2002)

Boundary integral modeling of functionally graded materials (FGMs)

- **FGM applications**
  - **Biomedical**
  - **Thermal barrier coatings**
  - **Sensors**
- **Recent results**
  - **Derived elasticity Green's Function for 2-demensional and 3-demensional exponentially graded materials**
  - **Implemented in Galerkin and collocation boundary integral codes in 3-D**
- **Fast solution of boundary integral equations**
  - **General framework using pre-corrected Fast Fourier Transform**
  - **Treatment of singular and hyper-singular equations**
  - **Applications in modeling electrospray process, crack propagation, and fiber composite materials**

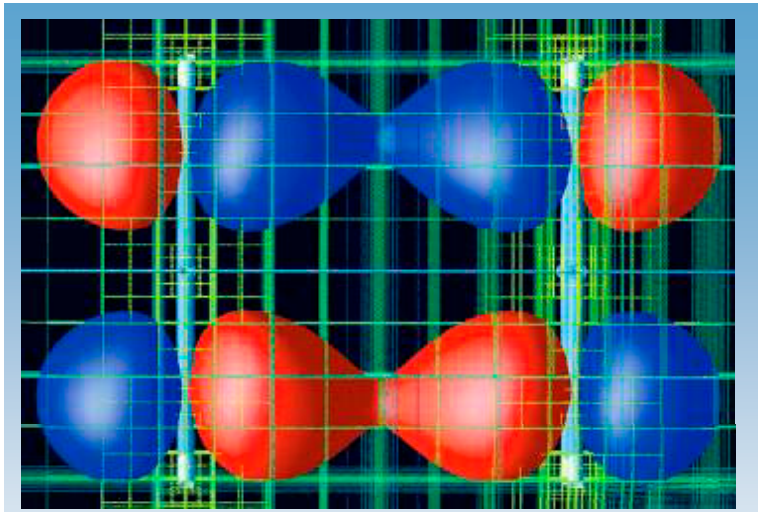


K. S. Ravichandran, *Materials Science and Engineering* **A201 (1995)** 269-276



MADNESS: multiresolution analysis for integro-differential equations and Ψ-PDE

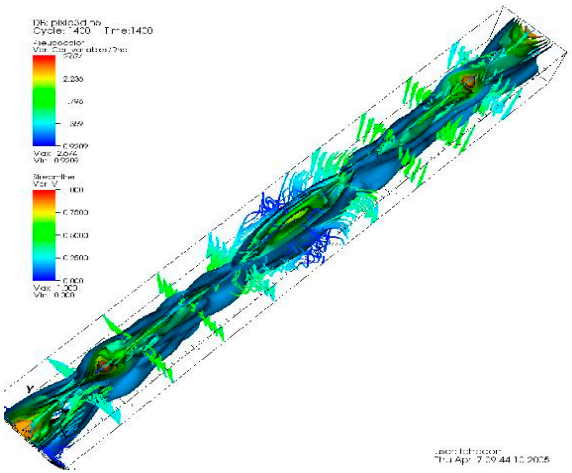
- Developed 3-D multiwavelet, low separation rank approximation, and high-order panel singular value approximations for static and time-dependent Schrodinger's equation (Hartree-Fock and density functional theory) in chemistry and nuclear physics
- Approximated d-D functions and operators using discontinuous basis with compact support and dictionaries that scales as log(d). Developing fast O(N) real analysis-based algorithms to approximate functions and operators to arbitrary but finite precision
- Computed some of the most accurate energies and energy levels for small molecules to date
- Obtained positive initial results for 6-D, 2-body Schrodinger's equations
- Scales to thousands of cores on Cray and IBM BG/L

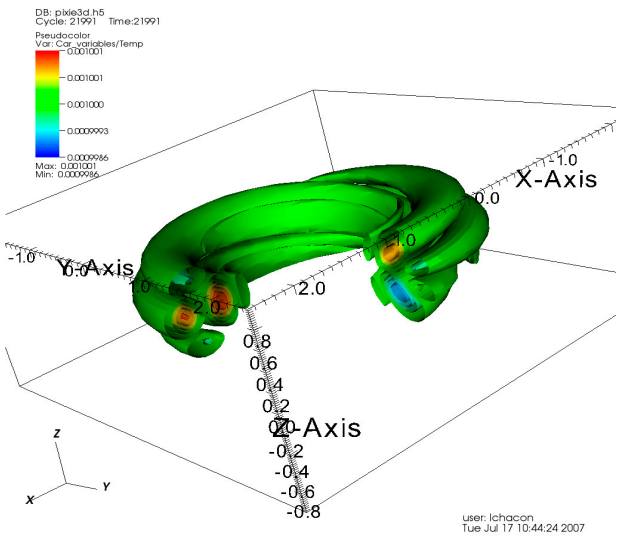


A molecular orbital of the benzene dimer computed using the multiresolution solver MADNESS in a multiwavelet basis and low separation rank approximation. Note the adaptive refinement, which automatically adjusts to guarantee precision

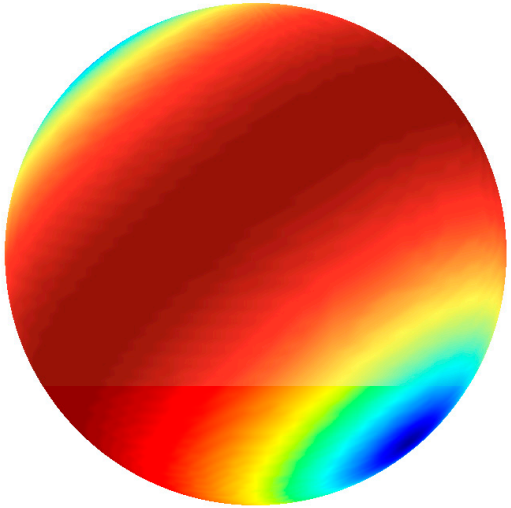
PIXIE3D: a 3-D extended MHD parallel, fully implicit code

- **Fully 3-D, general geometry, Newton-Krylov-based solver**
- **Spatial discretization: second-order, conservative, solenoidal finite volumes**
- **Temporal discretization: fully implicit, second-order (Crank-Nicolson, BDF2)**
- **Massively parallel: excellent scaling demonstrated up to 4096 processors**
- **Algorithmically scalable**
  - **Key: multigrid physics-based preconditioning**
  - **Optimal scaling up to np=1000 processors**

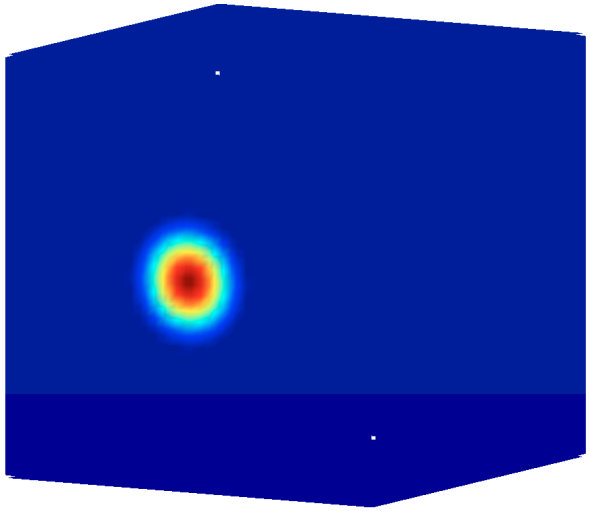




Shallow water equations on the sphere: Multiwavelet DG cube sphere method



Advecting wind magnitude



Wind pattern sends advected cosine bell through four corners and two cube edges

<u>Result</u>: Scaling and squaring time-stepping method provides a 64× speed-up; in combination with the 2× gained from Multiwavelet DG, the end result is a 128× speed-up in comparison to Runge-Kutta DG at the same accuracy levels

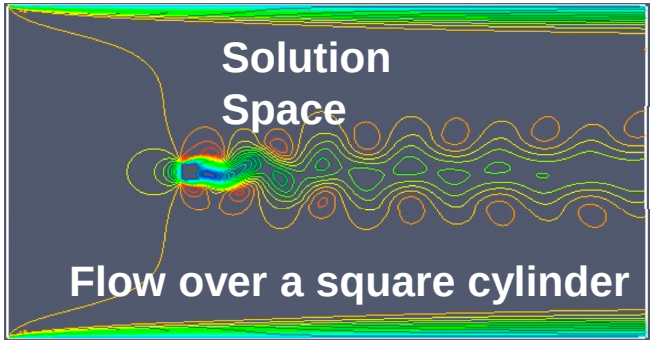
Adaptive discontinuous Galerkin methods in multiwavelets bases

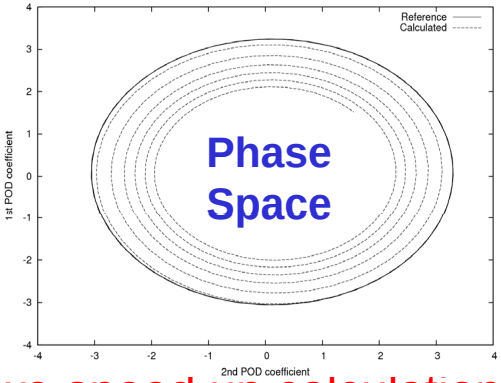
- **The DG method inherits a hierarchical structure from multiwavelets that produces a weak decoupling across different length scales**
- **The problems of when and how to perform hp-adaptivity in the DG method is answered by the scaling properties of multiwavelets**
- **The matrix of the multiwavelet DG operator and its inverse share the same sparse pattern, which provides nearly linear scaling of memory and computational performance with increasing degrees of freedom and dimensionality while providing a direct path for constructing preconditioners**
- **The above properties are strongly manifested for higher dimensional problems and for large degrees of freedom**

Phase-space-based reduced-order models (ROM) for flow problems

- **Most physical systems on which Proper-Orthogonal Decomposition (POD)–based ROMS are applied are nonlinear**
- **For highly nonlinear systems, this results in a large number of POD modes and associated accuracy and efficiency is**

Transferring full solution to phase space can be inefficient



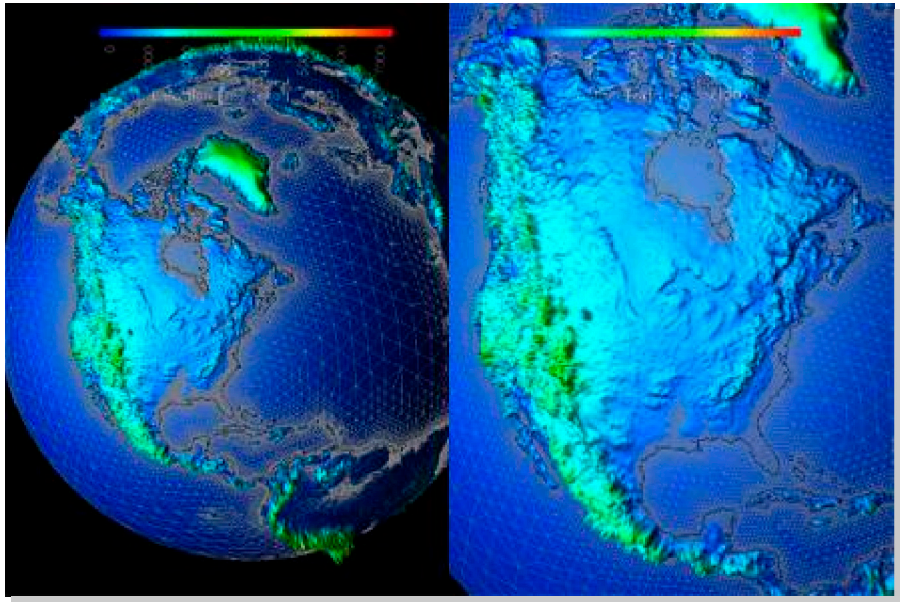


Knowing the phase-space structure, can we speed up calculations?

- **New approach**
  - **Create local linear maps from phase space to real space**
  - **Construct POD–based reduced models on the linear parts**
  - **Can employ isomap algorithm or locally linear embedding to find the linear subparts of a more complicated phase portrait**
- **Preliminary results suggest that few POD modes are required when the phase space is partitioned for the vortex shedding problem shown above**

Adaptive shallow atmosphere simulation

- Orography field plays a fundamental role in shallow-atmosphere fluid flow simulations
- The orography surface gradient is a dominant momentum driving force in climate modeling
- hp-adaptive meshing method is used to approximate high-resolution (rough) data fields
- h-adaptive meshes are refined in large gradient regions and coarse or small gradients
- p-adaptive method of high polynomial degree is used on regions where data are approximated satisfactorily

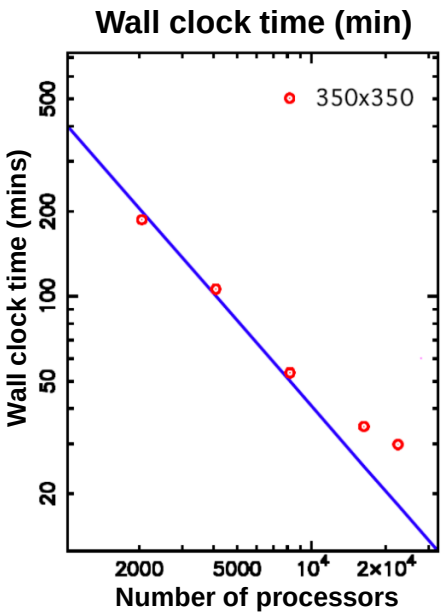


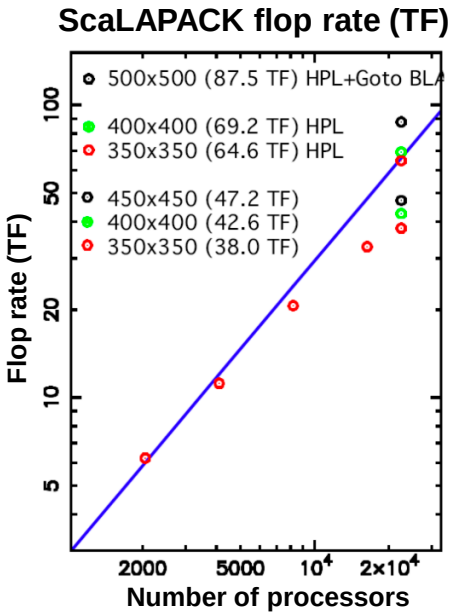
hp-adaptive elevation approximation of GLOBE data (zoom-in on North America)

- Solution singularities at the poles can be resolved via hp adaptivity
- The method provides an accurate representation of landscape data at much lower storage cost

HPL complex dense solver

- High Performance Linpack (HPL) is written in C and used in Top500 benchmark
- HPL performs parallel LU factorization in double but uses hybrid left/right-looking panel method and look-ahead algorithms
- Semi-automatic scripts to generate complex*16 version and interface to ScaLAPACK library
- Integrated to AORSA fusion INCITE application
- Developing version for reduced precision + iterative refinement





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