

# Pervasive Multiscale Modeling, Analysis, and Solvers

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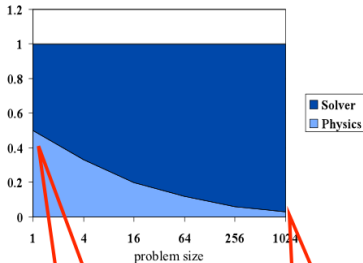
# Motivation

- ▶ Nature has many spatial and temporal scales
  - ▶ Porous media, turbulence, kinetics, fracture
- ▶ Robust discretizations and implicit solvers are needed to cope
- ▶ Computer architecture is increasingly hierarchical
  - ▶ algorithms should conform to this structure
- ▶ Solver scalability is a crucial bottleneck at scale
- ▶ “black box” solvers are not sustainable
  - ▶ optimal solvers must accurately handle all scales
  - ▶ optimality is crucial for large-scale problems
  - ▶ hardware puts up a spirited fight to abstraction

# It's *all* about algorithms (at the petascale)

- **Given, for example:**
  - a “physics” phase that scales as  $O(N)$
  - a “solver” phase that scales as  $O(N^{3/2})$
  - computation is almost all solver after several doublings
- **Most applications groups have not yet “felt” this curve in their gut**
  - as users actually get into queues with more than 4K processors, this will change

Weak scaling limit, assuming efficiency of 100% in both physics and solver phases



Solver takes 50% time on 128 procs

Solver takes 97% time on 128K procs

(c/o David Keyes)

# Phenomenological Models

*With four parameters I can fit an elephant, and with five I can make him wiggle his trunk. — John von Neumann*

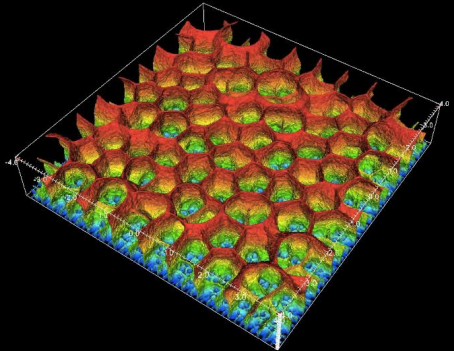
- ▶ Over-fitting is a pathology
- ▶ *Good* subgrid models do not require re-tuning parameters
- ▶ Fracture
- ▶ Turbulence modeling

*A professional problem exists [...] there is a need for higher standards on the control of numerical accuracy. [...] it was impossible to evaluate and compare the accuracy of different turbulence models, since one could not distinguish physical modeling errors from numerical errors related to the algorithm and grid. [...] The Journal of Fluids Engineering **will not accept for publication any paper [...] that fails to address the task of systematic truncation error testing and accuracy estimation.** — 1986*

# Diffusive cooling



- ▶ Pentagonal structures occur only for narrow band of thermal conditions and composition
- ▶ Variational (phase-field) approach reproduces thresholds without tuning [Bourdin, Francfort, Marigo]



# Numerical Homogenization/Upscaling

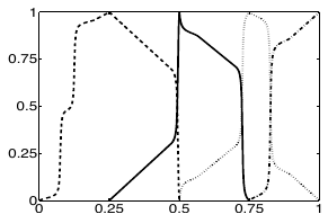
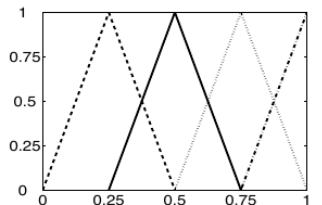
## 1. Multiscale basis functions

- ▶ integrate against microscale coefficients
- ▶ robust theory for linear elliptic equations
- ▶ popular in porous media and composite materials
- ▶ practically computable using multigrid ideas, partition of unity method
- ▶ no support for stochastic microscale

## 2. Coefficient/equation upscaling

- ▶ a good method reproduces statistics
  - ▶ cannot recover fine grid solution
  - ▶ suitable for nonlinear coarse problems
  - ▶ can derive coarse Hamiltonian
- 
- ▶ can exploit repetitive structure in fine grid
  - ▶ coarse space is *sufficient* if compatible relaxation/Monte-Carlo converges fast
  - ▶ procedure can be global or local

# Why I like subdomain problems



[Arbogast 2011]

- ▶ subassembly avoids explicit matrix triple product  $A_{\text{coarse}} \leftarrow P^T A_{\text{fine}} P$
- ▶ can update the coarse operator locally (e.g. local nonlinearity)
- ▶ need not assemble entire fine grid operator
- ▶ if repetitive structure, need not store entire fine grid state
- ▶ can coarsen very rapidly (especially in smooth regions)
- ▶ lower communication setup phase

## $\tau$ formulation of Full Approximation Scheme (FAS)

- ▶ classical formulation: “coarse grid *accelerates* fine grid solution”
- ▶  $\tau$  formulation: “fine grid improves accuracy of coarse grid”
- ▶ To solve  $Nu = f$ , recursively apply

$$\begin{array}{ll} \text{pre-smooth} & \tilde{u}^h \leftarrow S_{\text{pre}}^h(u_0^h, f^h) \\ \text{solve coarse problem for } u^H & N^H u^H = f^H + \underbrace{N^H \hat{I}_h^H \tilde{u}^h - I_h^H N^h \tilde{u}^h}_{\tau_h^H} \\ \text{correction and post-smooth} & u^h \leftarrow S_{\text{post}}^h \left( \tilde{u}^h + I_H^h (u^H - \hat{I}_h^H \tilde{u}^h), f^h \right) \end{array}$$

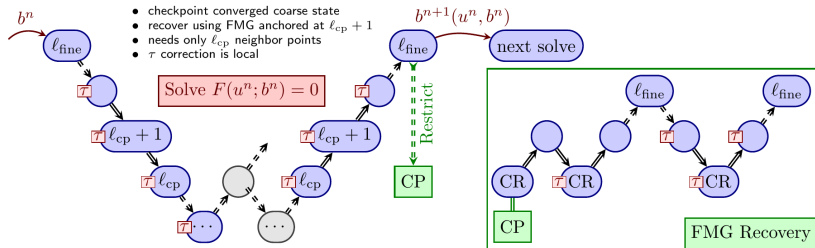
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$I_h^H$	residual restriction
$\hat{I}_h^H$	solution restriction
$I_H^h$	solution interpolation
$f^H = I_h^H f^h$	restriction of forcing term
$\{S_{\text{pre}}^h, S_{\text{post}}^h\}$	smoothing operations on the fine grid

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# Multiscale compression and recovery using $\tau$

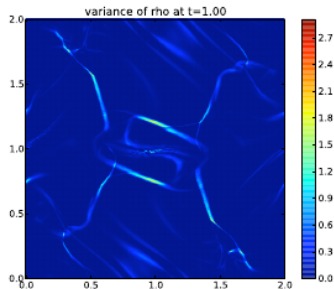
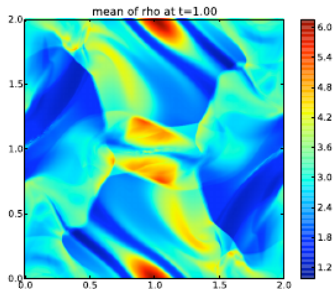


- ▶ Compress transient simulation with local decompression
- ▶ Remove communication from all but coarse grid
  - ▶ Convergence speed not affected, modest redundant computation
- ▶ In-situ visualization and reanalysis with very few full checkpoints
- ▶ Checkpointing for discrete adjoints
- ▶ Resiliency to hardware failure

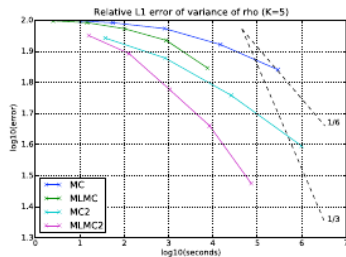
# Cool Topics in Multiscale Computation

- ▶ Solve PDE in fewer flops than evaluating an analytic solution
- ▶ Solve PDE in  $\mathcal{O}(|\log n| |\log \varepsilon|^d)$  memory
- ▶ Compute  $k$  eigenvalues in  $\mathcal{O}(n \log k)$
- ▶ Project vector onto eigenbasis in  $\mathcal{O}(n \log k)$
- ▶ Optimal-order graph partitioning and clustering
- ▶ Continuation and transient problems without revisiting fine grid
- ▶ Global optimization without sacrificing optimality, “multiscale annealing”
- ▶ Accelerate Monte-Carlo slowdown due to spuriously correlated sampling

# Multilevel structure for uncertainty quantification



- ▶ Geometric hierarchy of models
- ▶ More samples on coarse grids (much cheaper)
- ▶ Mean and variance in  $\sim 10\times$  cost of deterministic simulation
- ▶ Robust to dimension of stochastic space



# Outlook

- ▶ Multiscale processes are ubiquitous and important
- ▶ Multiscale computation necessary for modern simulation and analysis
- ▶ Embrace multiscale structure, make it work for you
- ▶ Raise level of abstraction at which we formulate problems
- ▶ Think in terms of robust functionals and statistics rather than pointwise solutions
- ▶ Multiscale computation often reveals modeling flaws, guides their rectification
- ▶ Good microscale models are important for deriving and correcting coarse models