# Pervasive Multiscale Modeling, Analysis, and Solvers

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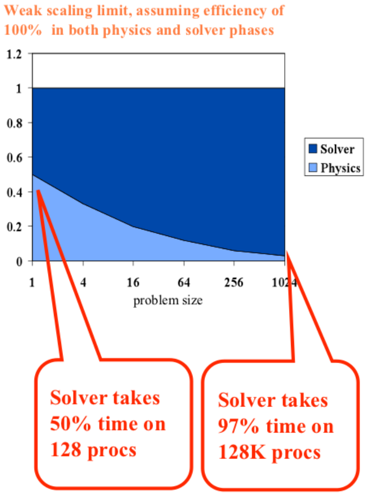
# Motivation

- 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




(c/o David Keyes)

# Phenomenological Models

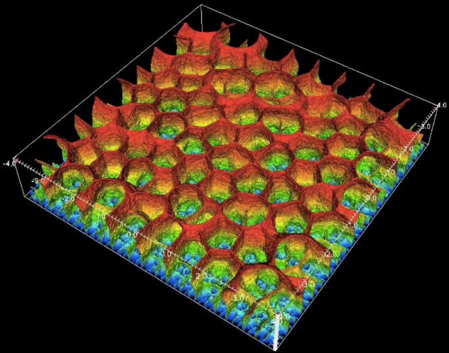
*With four parameters I can fit an elephant, and with five I can make him wiggle his trunk. — John von Neumann*

- 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]

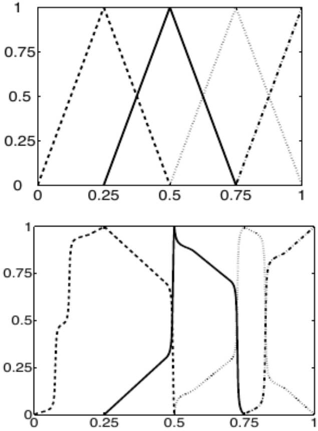


# Numerical Homogenization/Upscaling

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

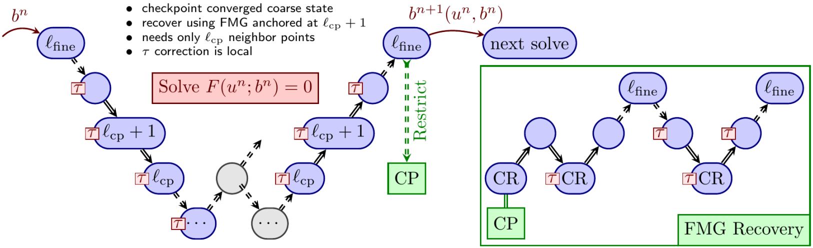
# $\tau$ formulation of Full Approximation Scheme (FAS)

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

$$
\begin{aligned}
\text{pre-smooth} \quad & \tilde{u}^h \leftarrow S^h_{\text{pre}}(u^h_0, f^h) \\
\text{solve coarse problem for } u^H \quad & N^H u^H = f^H + \underbrace{N^H \hat{I}^H_h \tilde{u}^h - I^H_h N^h \tilde{u}^h}_{\tau^H_h} \\
\text{correction and post-smooth} \quad & u^h \leftarrow S^h_{\text{post}}\left(\tilde{u}^h + I^h_H (u^H - \hat{I}^H_h \tilde{u}^h), f^h\right)
\end{aligned}
$$

| | |
|---|---|
| $I^H_h$ | residual restriction |
| $\hat{I}^H_h$ | solution restriction |
| $I^h_H$ | solution interpolation |
| $f^H = I^H_h f^h$ | restriction of forcing term |
| $\{S^h_{\text{pre}}, S^h_{\text{post}}\}$ | smoothing operations on the fine grid |

# Multiscale compression and recovery using $\tau$

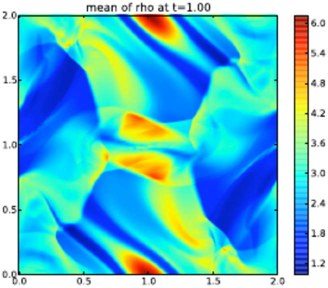


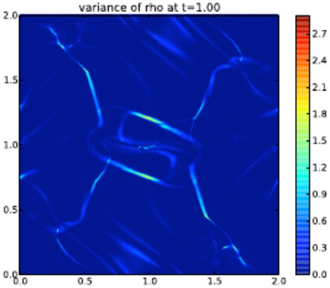

- Compress transient simulation with local decompression
- Remove communication from all but coarse grid
  - Convergence speed not affected, modest redundant computation
- In-situ visualization and reanalysis with very few full checkpoints
- Checkpointing for discrete adjoints
- Resiliency to hardware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

# Cool Topics in Multiscale Computation

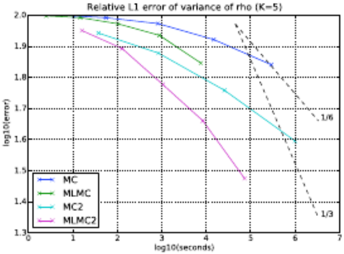
- Solve PDE in fewer flops than evaluating an analytic solution
- Solve PDE in $\mathcal{O}(|\log n|\,|\log \varepsilon|^d)$ memory
- Compute $k$ eigenvalues in $\mathcal{O}(n \log k)$
- Project vector onto eigenbasis in $\mathcal{O}(n \log k)$
- Optimal-order graph partitioning and clustering
- Continuation 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




[Mishra, Schwab, Šukys, 2012]

# 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