Creating Coarse-Scale Models with Robust Multigrid Methods

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  - Rob Falgout in CASC at LLNL.

Multiscale Simulation

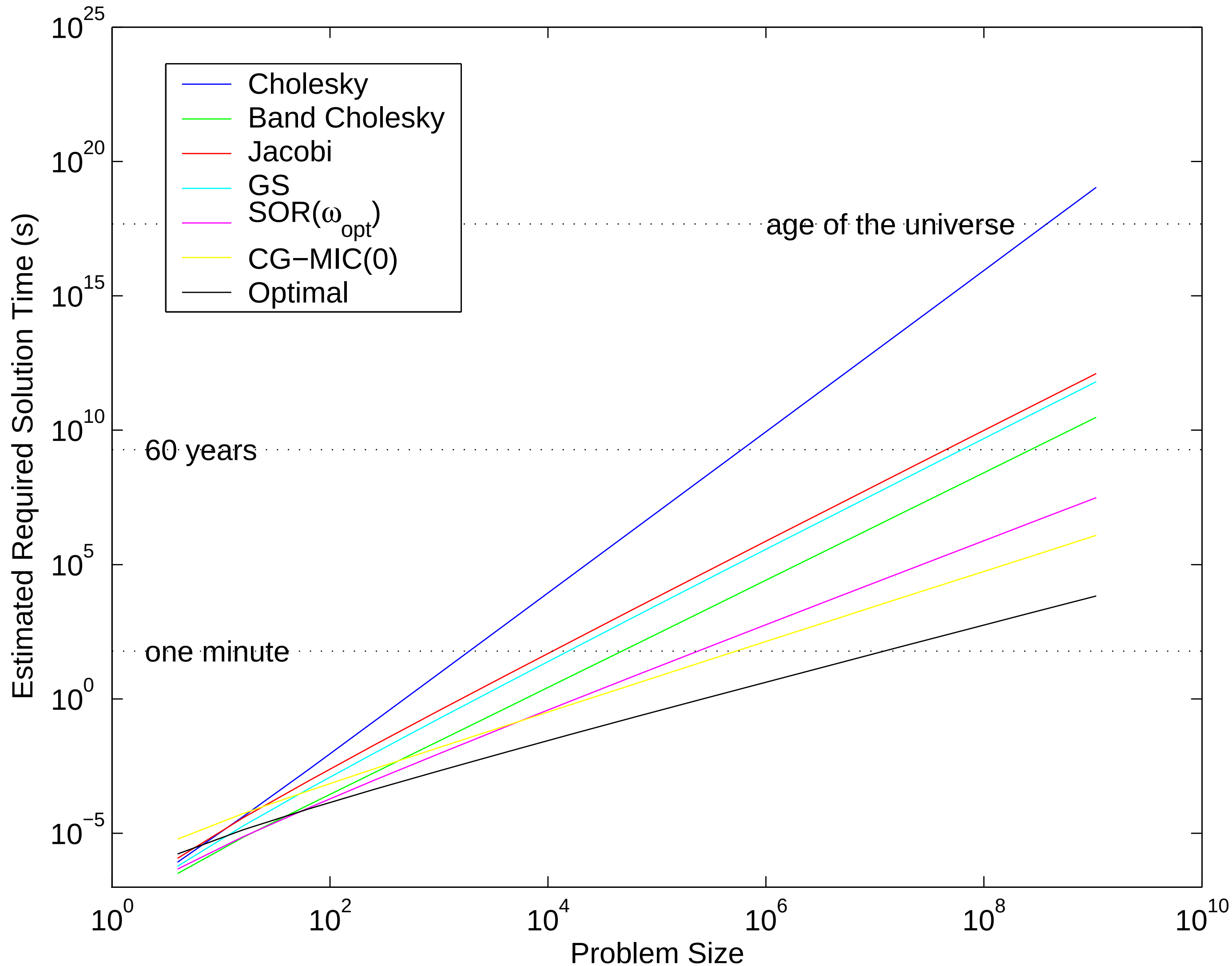
Efficient simulation of multiscale phenomena requires multiscale approaches

- Multigrid is a *rich multiscale technology* for solving a large class of linear (and nonlinear) systems
- New developments in *fundamental multigrid theory* are expanding the range of applicability
- *Useful multiscale information* is encoded in the coarse-scale operators of a robust variational multigrid method

Algorithmic goal: maximize accuracy per computational cost

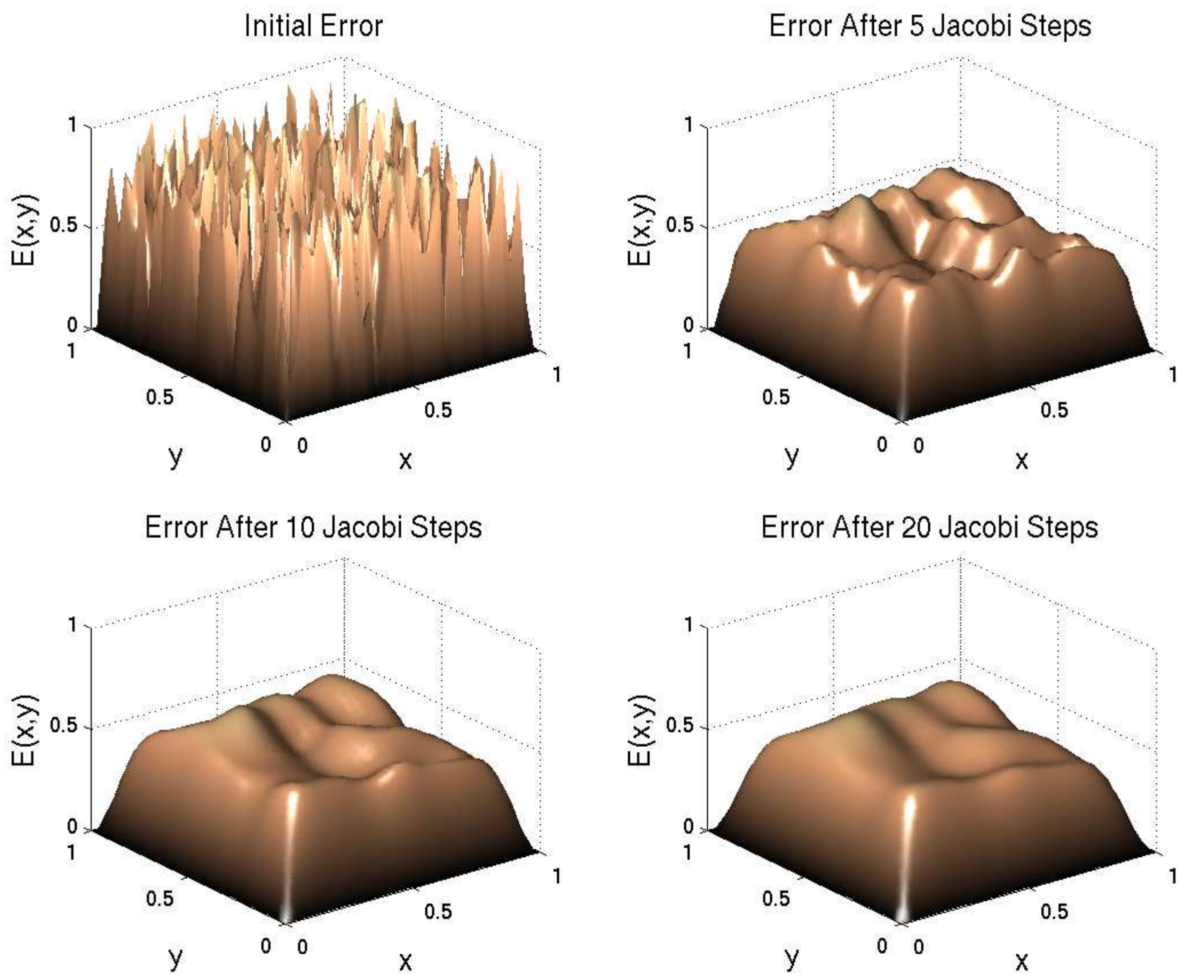
$\Rightarrow$ *Previously intractable simulations become feasible*

Classical Methods do not Suffice



Stationary Iterative Methods

- The Jacobi and Gauss-Seidel iterations are not scalable solvers for elliptic operators



Fine-Scale View: Multigrid

Multigrid Methods achieve optimality through complementarity

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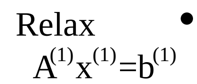
Multigrid Methods achieve optimality through complementarity

Multigrid Components

- Relaxation



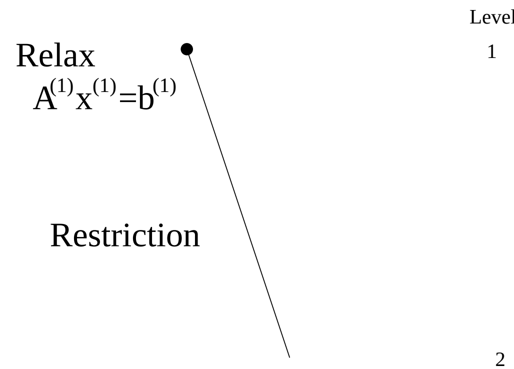
- Use a smoothing process (such as Gauss-Seidel) to eliminate oscillatory errors
- Remaining error satisfies $Ae = r \equiv b - Ax$

Fine-Scale View: Multigrid

Multigrid Methods achieve optimality through complementarity

Multigrid Components

- Relaxation
- Restriction



- Transfer residual to coarse grid

Fine-Scale View: Multigrid

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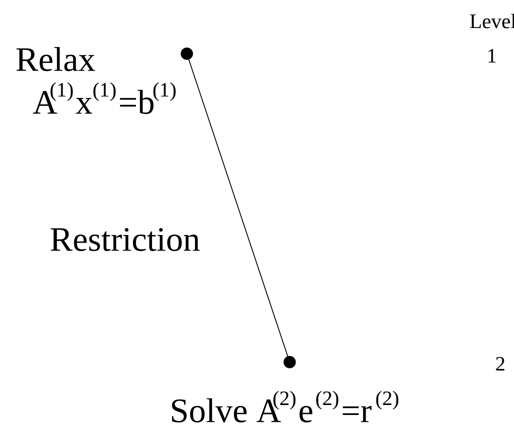
Multigrid Components

- Relaxation
- Restriction
- Coarse-Grid Correction



- Use coarse-grid correction to eliminate smooth errors
- To solve for error on coarse grid, use residual equation

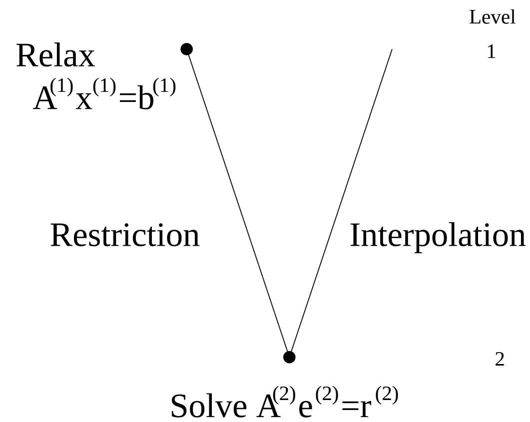
$$A^{(2)}e^{(2)} = r^{(2)}$$

Fine-Scale View: Multigrid

Multigrid Methods achieve optimality through complementarity

Multigrid Components

- Relaxation
- Restriction
- Coarse-Grid Correction
- Interpolation



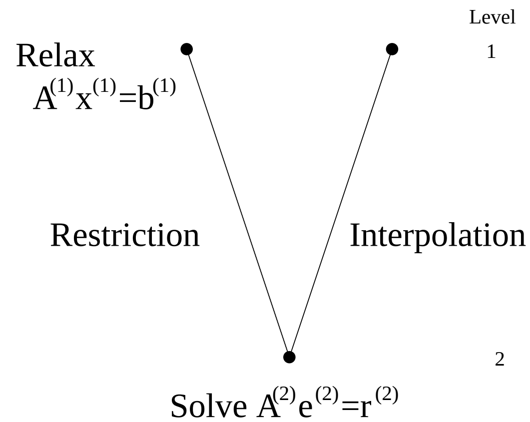
- Transfer correction to fine grid

Fine-Scale View: Multigrid

Multigrid Methods achieve optimality through complementarity

Multigrid Components

- Relaxation
- Restriction
- Coarse-Grid Correction
- Interpolation
- Relaxation



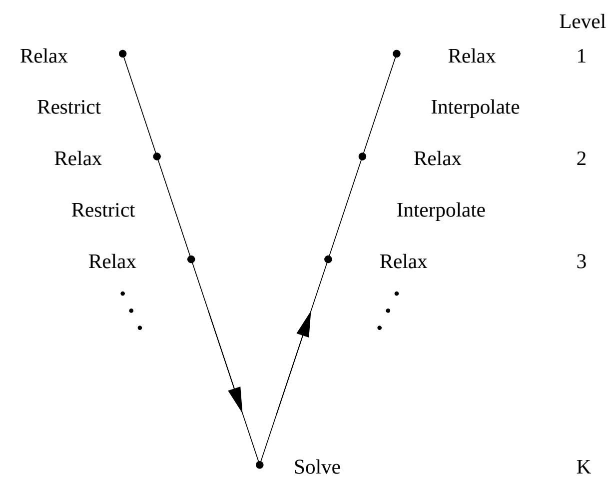
- Relax once again to remove oscillatory error introduced in coarse-grid correction

Fine-Scale View: Multigrid

Multigrid Methods achieve optimality through complementarity

Multigrid Components

- Relaxation
- Restriction
- Coarse-Grid Correction
- Interpolation
- Relaxation



Obtain optimal efficiency through recursion

Variational Multigrid

- Multigrid with $R = P^T$ and $A_c = RAP$ is called a *variational formulation*
- Terminology comes from minimization form of $Ax = b$:

$$F(v) = \frac{1}{2}\langle Av, v\rangle - \langle b, v\rangle$$

$$x = \arg\min_{v \in \mathcal{H}} F(v)$$

- Given an approximation, v, to the fine-level solution, the optimal coarse-grid correction, Pw, solves

$$(P^T AP)w = P^T(b - Av)$$

Coarse-Scale Models

- Multigrid methods reduce error through *relaxation* and *coarse-grid correction*
- Error that is not efficiently reduced by relaxation is called *algebraically smooth* and must be reduced by coarse-grid correction
- Many relaxation schemes leave algebraically smooth error that is also low energy:

$$\mathbf{e}^T A \mathbf{e} \ll \|A\| \mathbf{e}^T \mathbf{e}$$

- Variational coarsening encodes multiscale information in the coarse-grid operators through scale-transfer (interpolation) operators
- Coarse-scale operators must reflect information about the *low-energy modes* of the fine-scale operator

Adaptive Algebraic Multigrid

- If we don’t know what algebraically smooth error looks like, can we still develop an effective multigrid method?

Adaptive Algebraic Multigrid

- If we don't know what algebraically smooth error looks like, can we still develop an effective multigrid method? Yes!
- Use relaxation on $Ax = 0$ to expose algebraic smoothness
- Fine-grid relaxation quickly exposes *local character* of algebraic smoothness
- Use this representation to determine interpolation
- Interpolation weights are chosen through a *local collapsing* of the operator done to fit the *prototypical* algebraically smooth error
- Apply these ideas recursively, using relaxation to expose appropriate components of the error on each level of the multigrid hierarchy

Test Problems

- $-\nabla \cdot \mathcal{K}(\mathbf{x})\nabla p(\mathbf{x}) = 0$ on $[0,1]^2$
- Problem 1:
  - $\mathcal{K}(\mathbf{x}) = 1$ (Laplace), Full Dirichlet BCs
- Problem 2:
  - $\mathcal{K}(\mathbf{x}) = 10^{-8}$ on 20% of elements chosen randomly, $\mathcal{K}(\mathbf{x}) = 1$ otherwise
  - Dirichlet BCs on left and right, Neumann on top and bottom
- Bilinear FE stiffness matrix diagonally scaled (scaled nodally by 10^{5r}, where r is chosen uniformly between 0 and 1)
- Report asympototic convergence factor of V(1,1) cycles
- Geometric choice of coarse grids

Convergence Factors

Asymptotic convergence factors of resulting V(1,1) cycles

	Problem 1		Problem 2	
h	Standard AMG	Adaptive AMG	Standard AMG	Adaptive AMG
$1/64$	0.991	0.069	0.996	0.187
$1/128$	0.997	0.078	0.996	0.212
$1/256$	0.996	0.077	0.996	0.235
$1/512$	0.996	0.078	0.996	0.292
$1/1024$	0.996	0.079	0.995	0.383

Multiscale View: Upscaling

- Multigrid incorporates useful fine-scale information in coarse-scale operators
- Solutions of coarse-scale models are relevant to features of the fine-scale
- In a variational setting, multiscale information is recursively encoded through the operator-dependence of interpolation
- Robust multigrid methods naturally create effective multiscale basis functions
- Can select relevant accuracy from operators in multigrid hierarchy

Interpretation of Multigrid CGOs

- Fine-scale, finite-element discretization of porous-media problem:

$$A_{ij} = \mathbf{e}_j^T A \mathbf{e}_i = \int_\Omega \langle \mathcal{K}(\mathbf{x}) \nabla \phi_i, \nabla \phi_j \rangle d\Omega$$

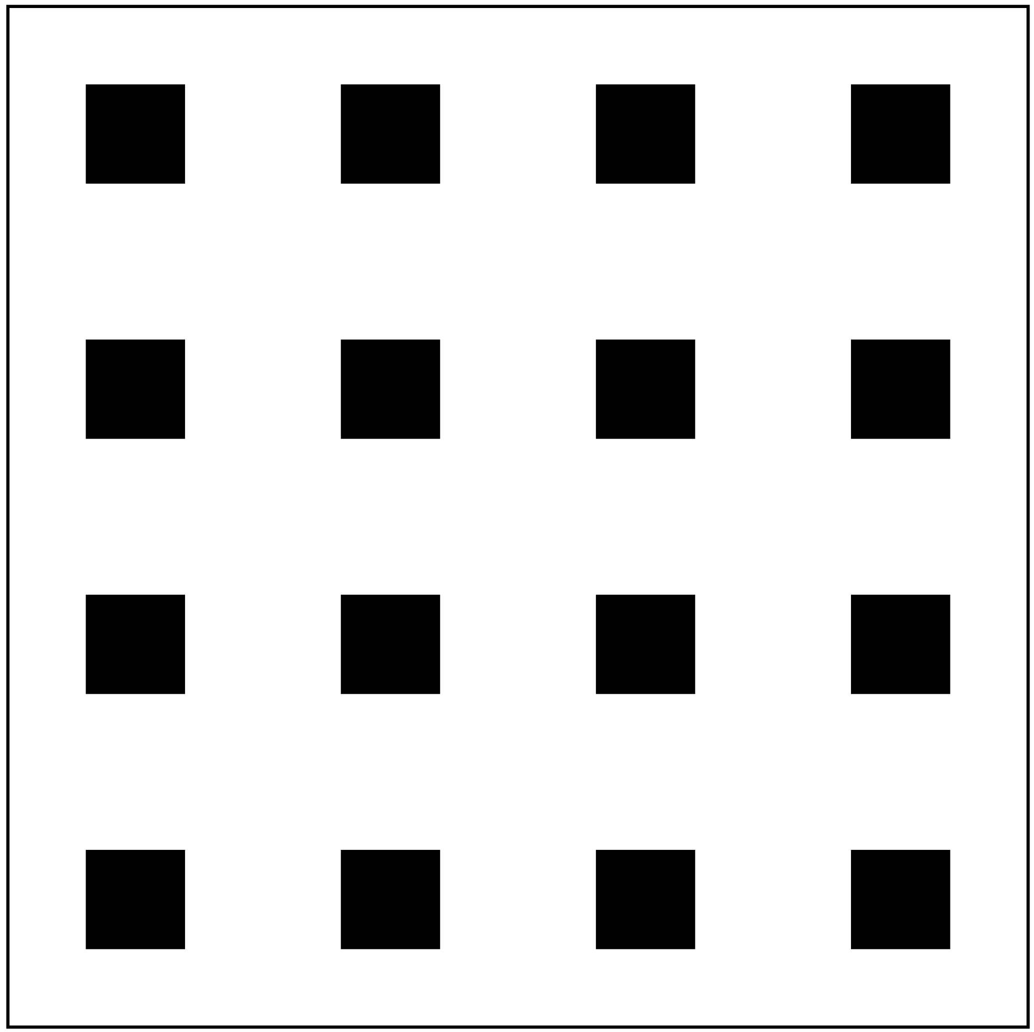
- Variational coarsening gives finite-element discretizations on coarse grids:

$$\begin{aligned}
(A_c)_{ij} = (P^T A P)_{ij} &= (P\hat{\mathbf{e}}_j)^T A (P\hat{\mathbf{e}}_i) \\
&= \int_\Omega \left\langle \mathcal{K}(\mathbf{x}) \nabla \left(\sum_l p_{li} \phi_l \right), \nabla \left(\sum_k p_{kj} \phi_k \right) \right\rangle d\Omega \\
&= \int_\Omega \langle \mathcal{K}(\mathbf{x}) \nabla \hat{\phi}_i, \nabla \hat{\phi}_j \rangle d\Omega
\end{aligned}$$

- Coarse-grid basis functions are linear combinations of fine-grid basis functions (weighted by the interpolation operators)

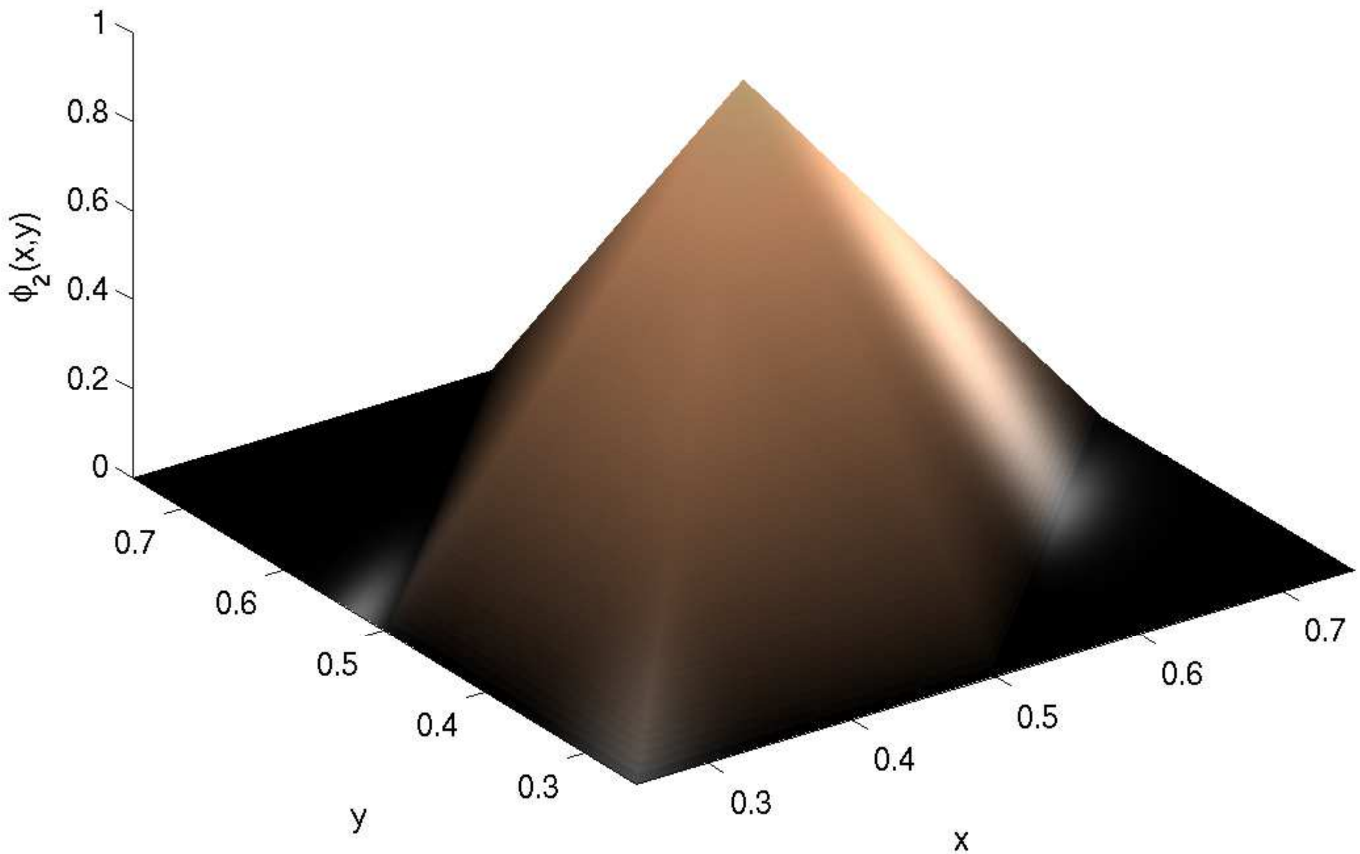
Sample Basis Functions

Periodic permeability field, $\mathcal{K}(\mathbf{x})$, with jump of 10^3



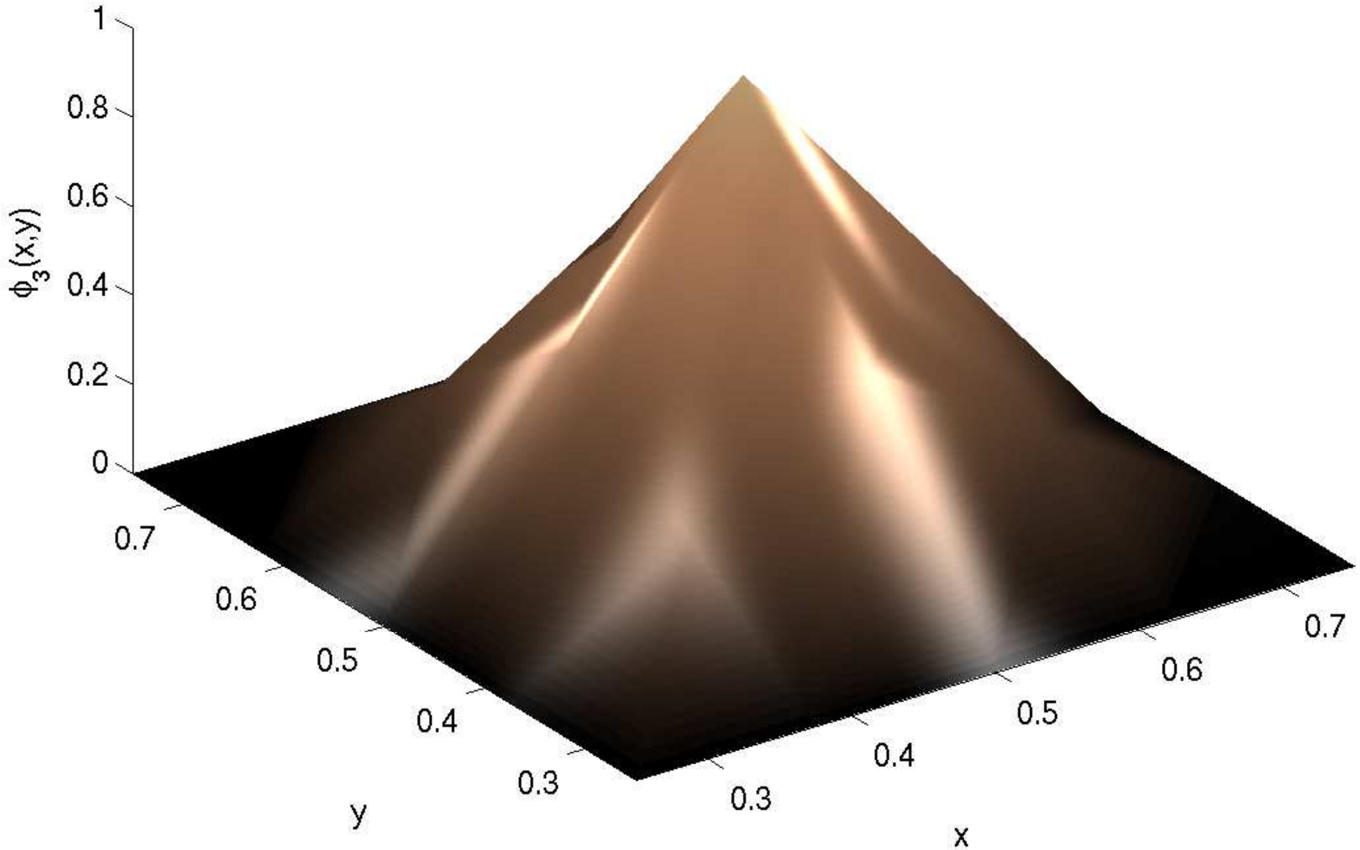
Sample Basis Functions

Bilinear basis function on 4×4 grid



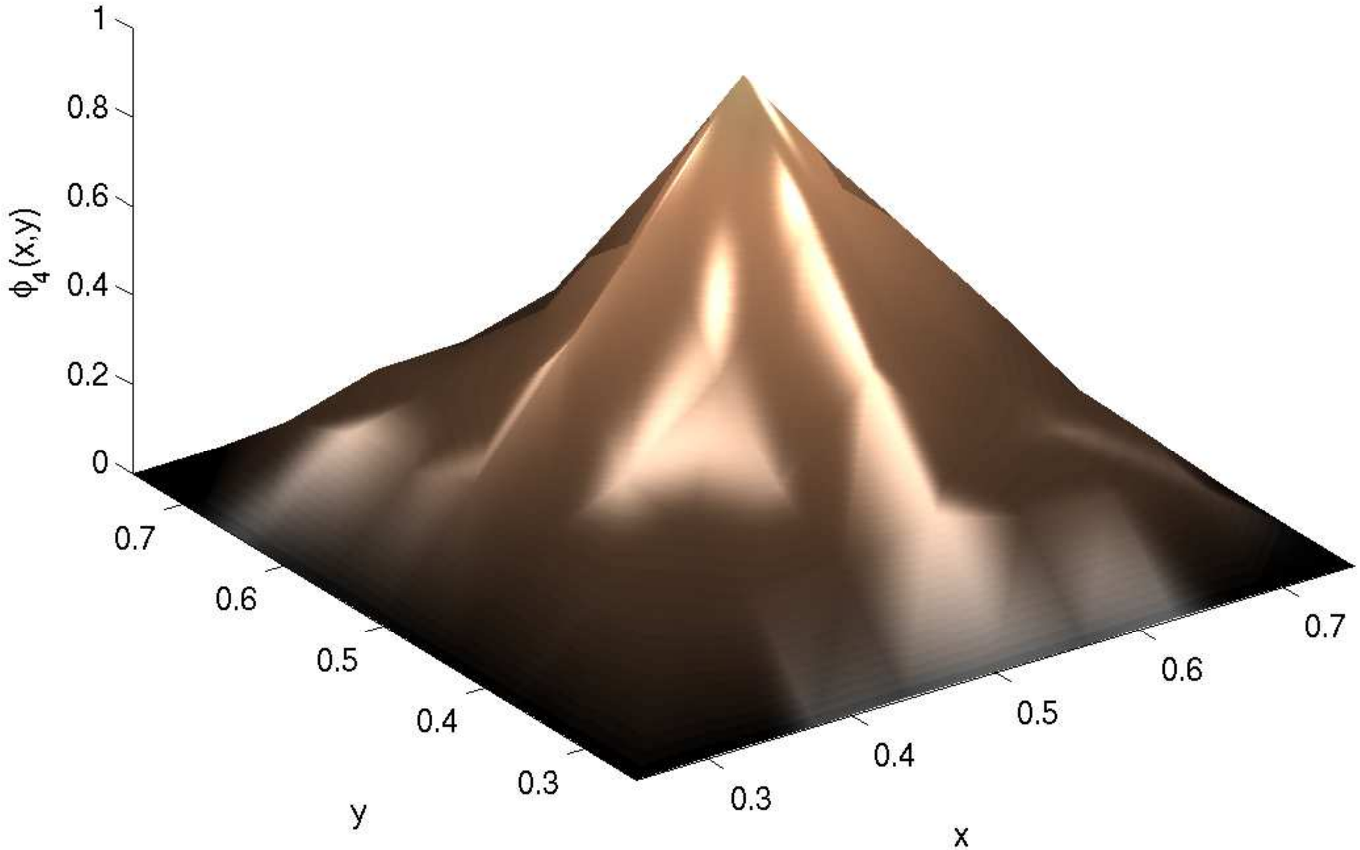
Sample Basis Functions

8×8 grid multiscale basis function



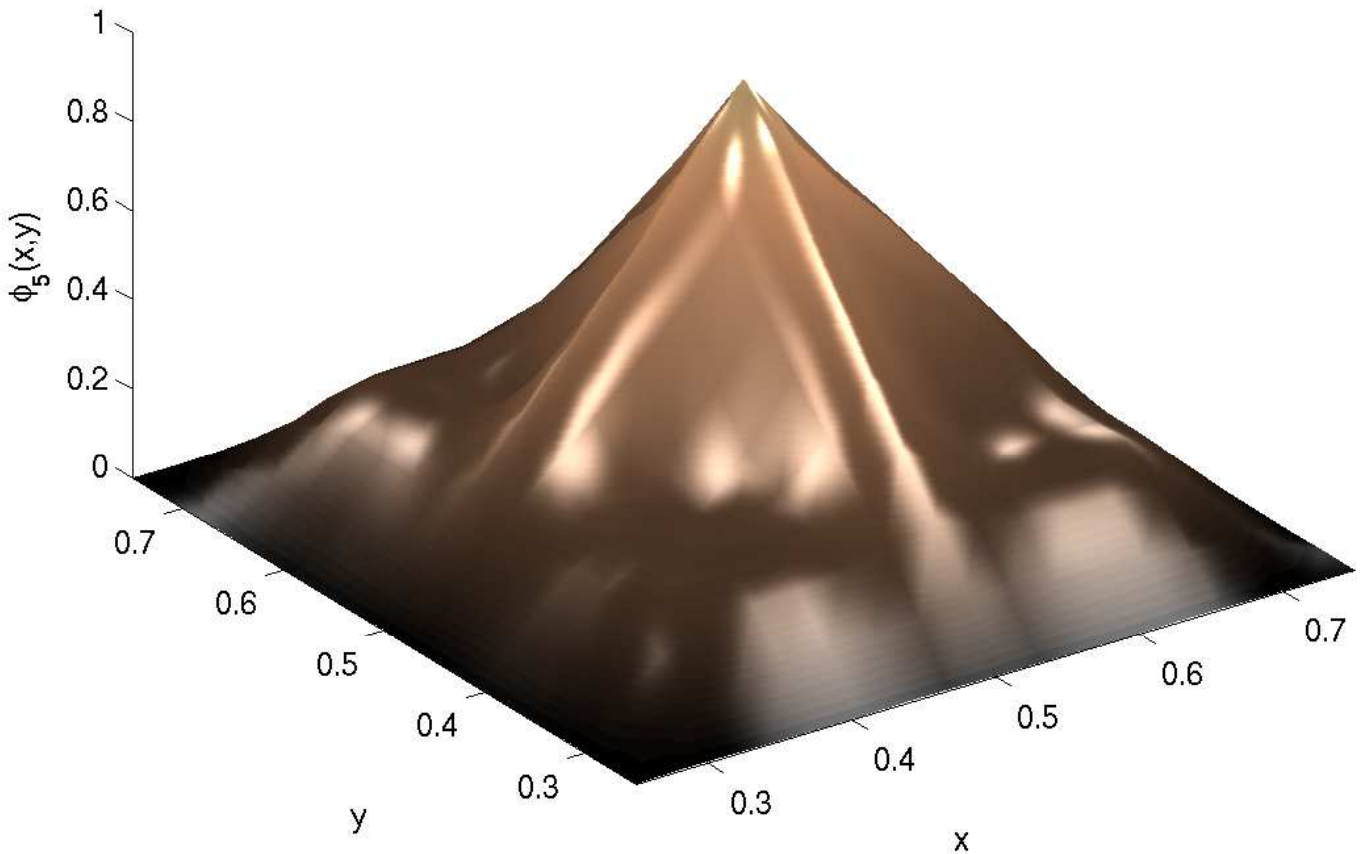
Sample Basis Functions

16×16 grid multiscale basis function



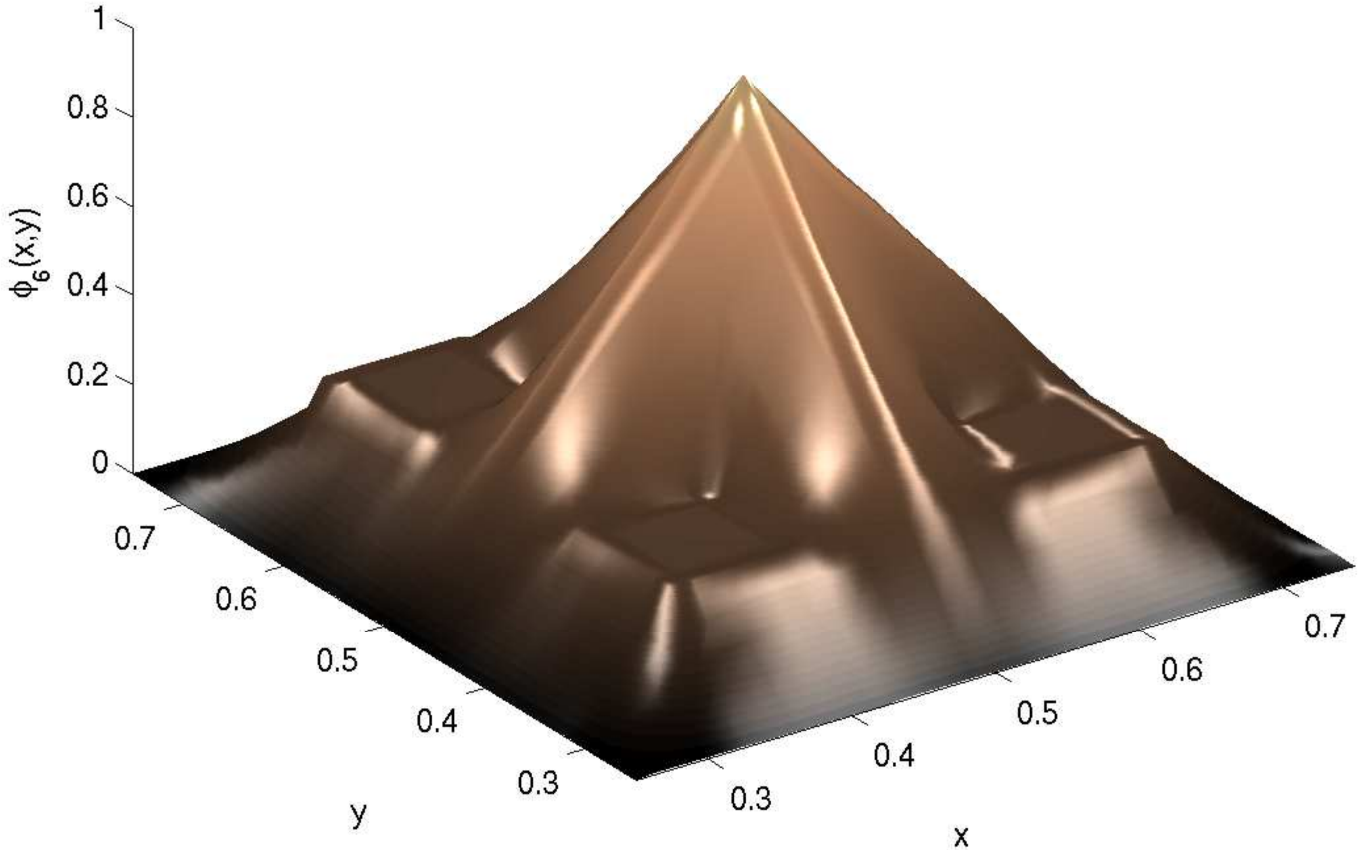
Sample Basis Functions

32×32 grid multiscale basis function



Sample Basis Functions

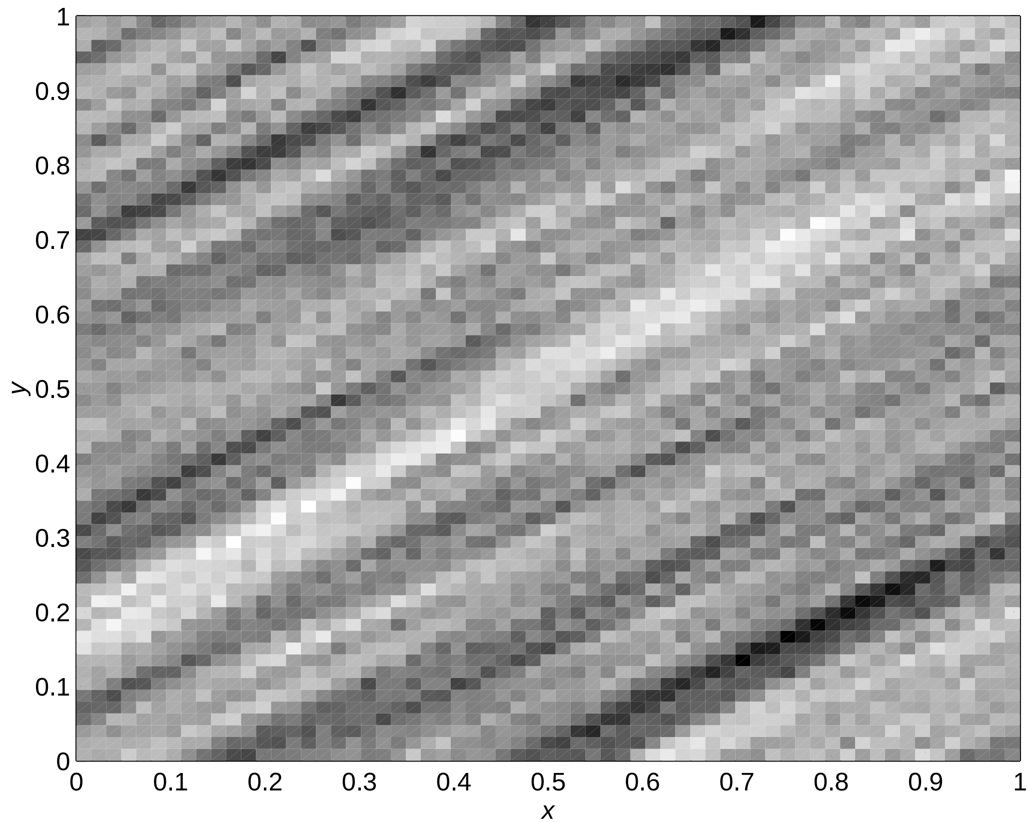
64×64 grid multiscale basis function



Sample Basis Functions

Geostatistical permeability field, $\mathcal{K}(\mathbf{x})$, with range of $[10^{-2}, 10^{2}]$

(Black pixels correspond to $\mathcal{K} = 10^{-2}$)



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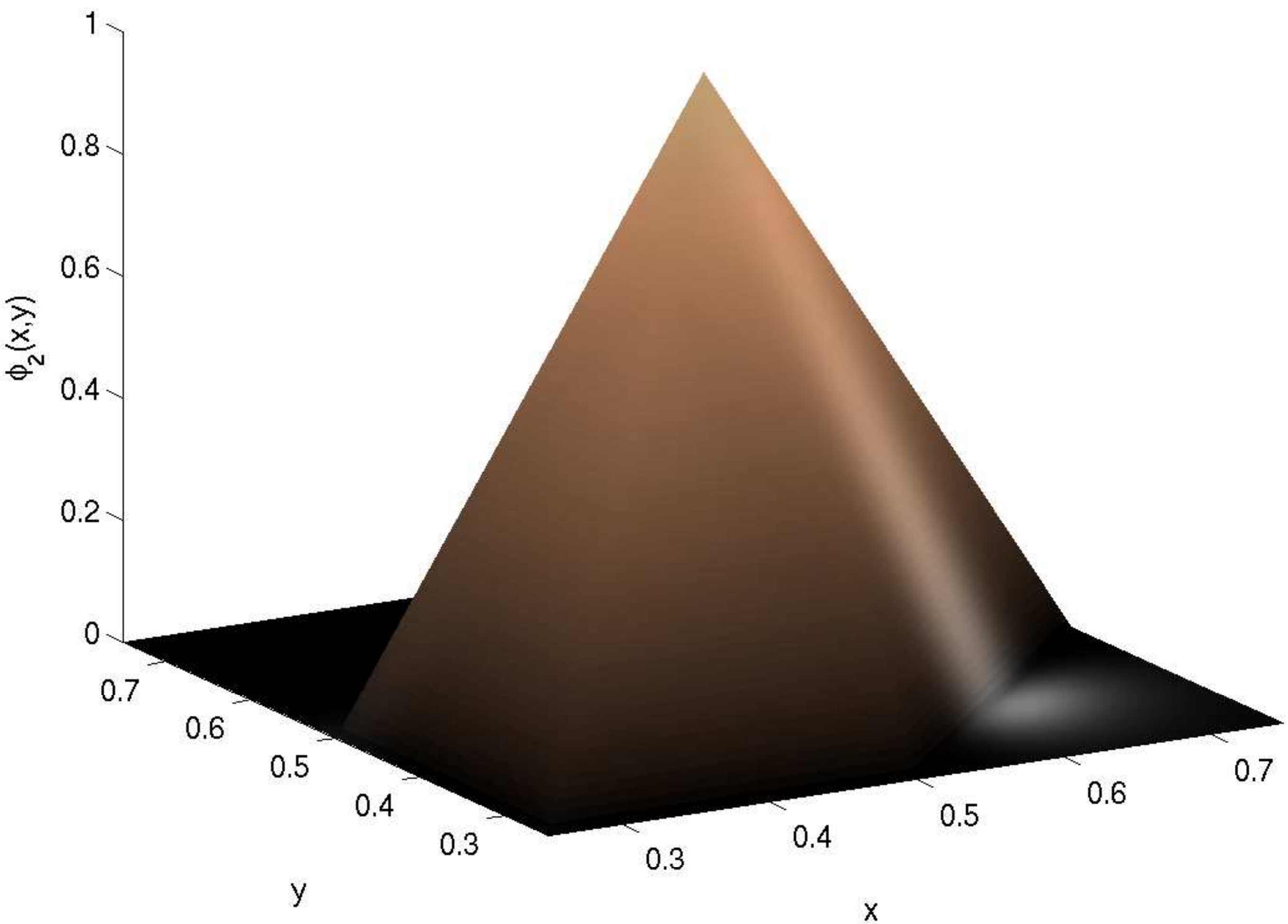

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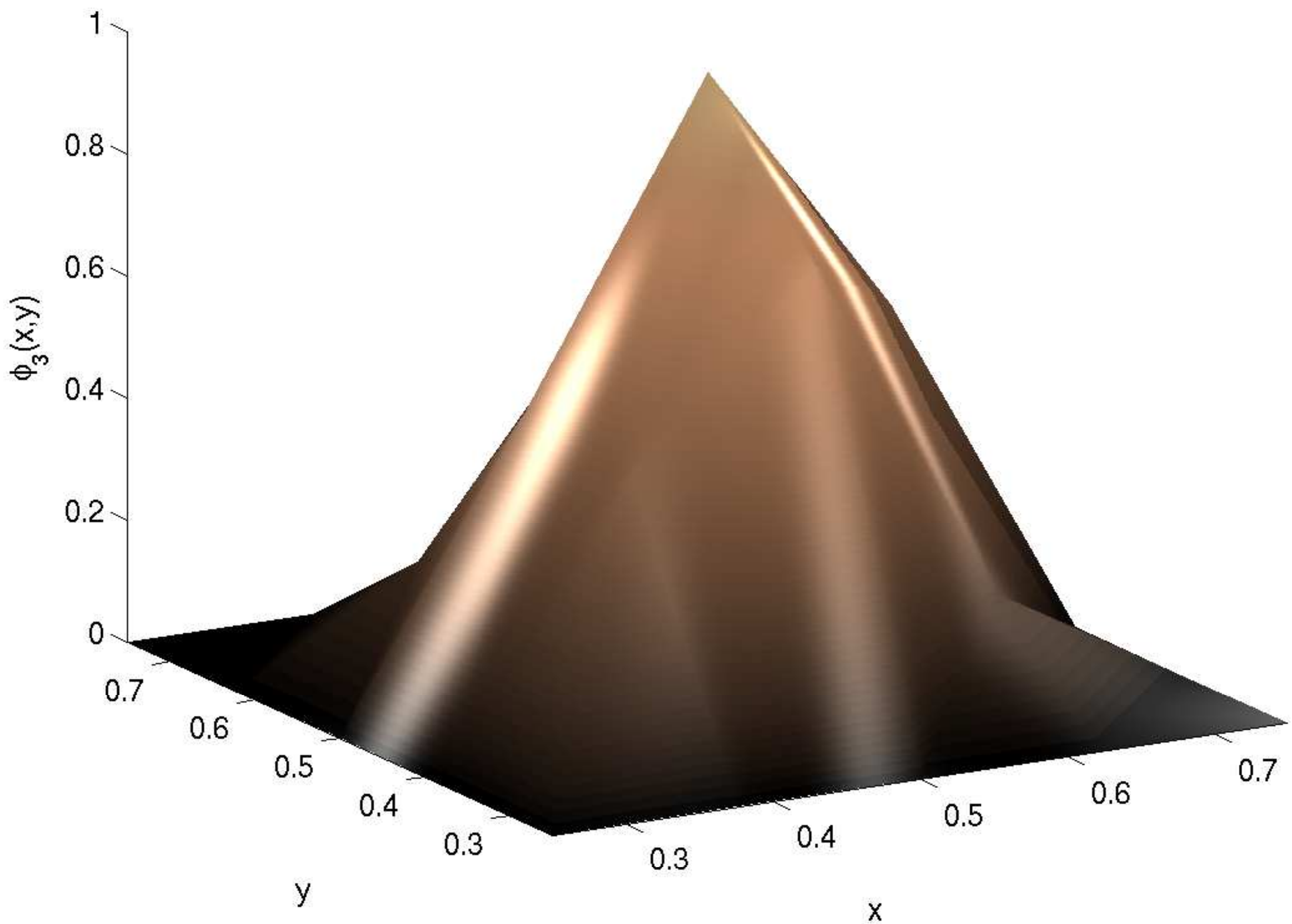
8×8 grid multiscale basis function



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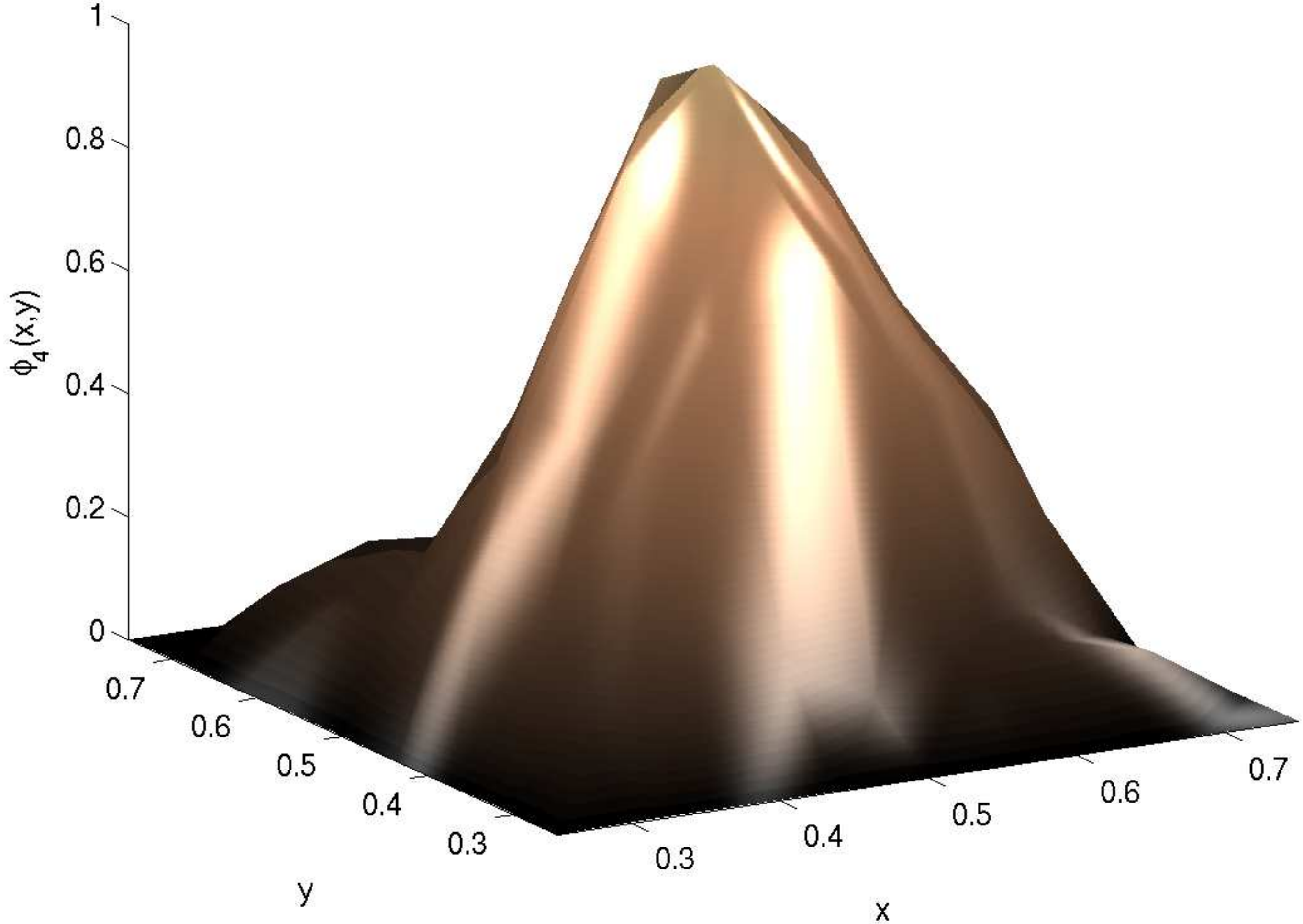

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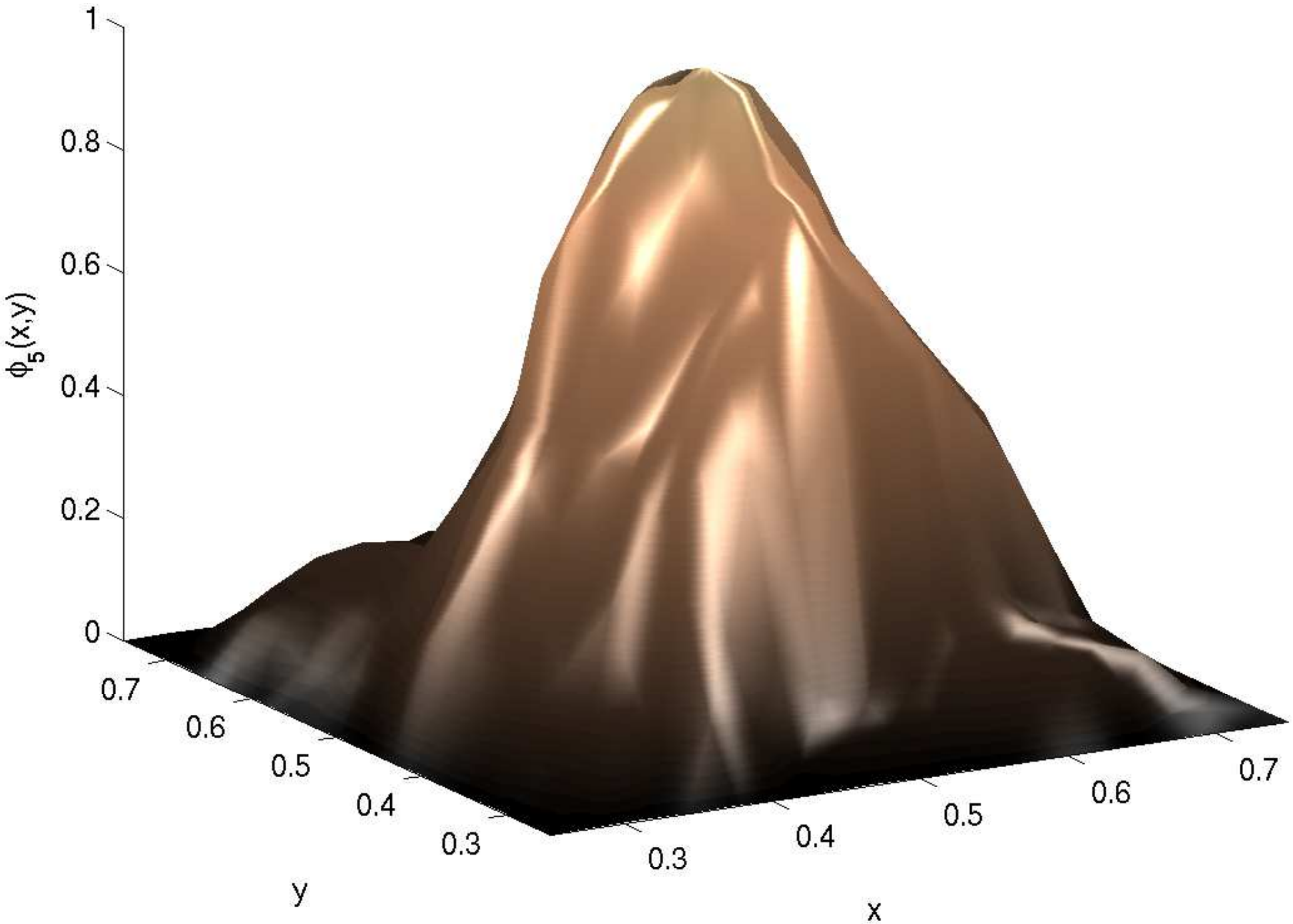

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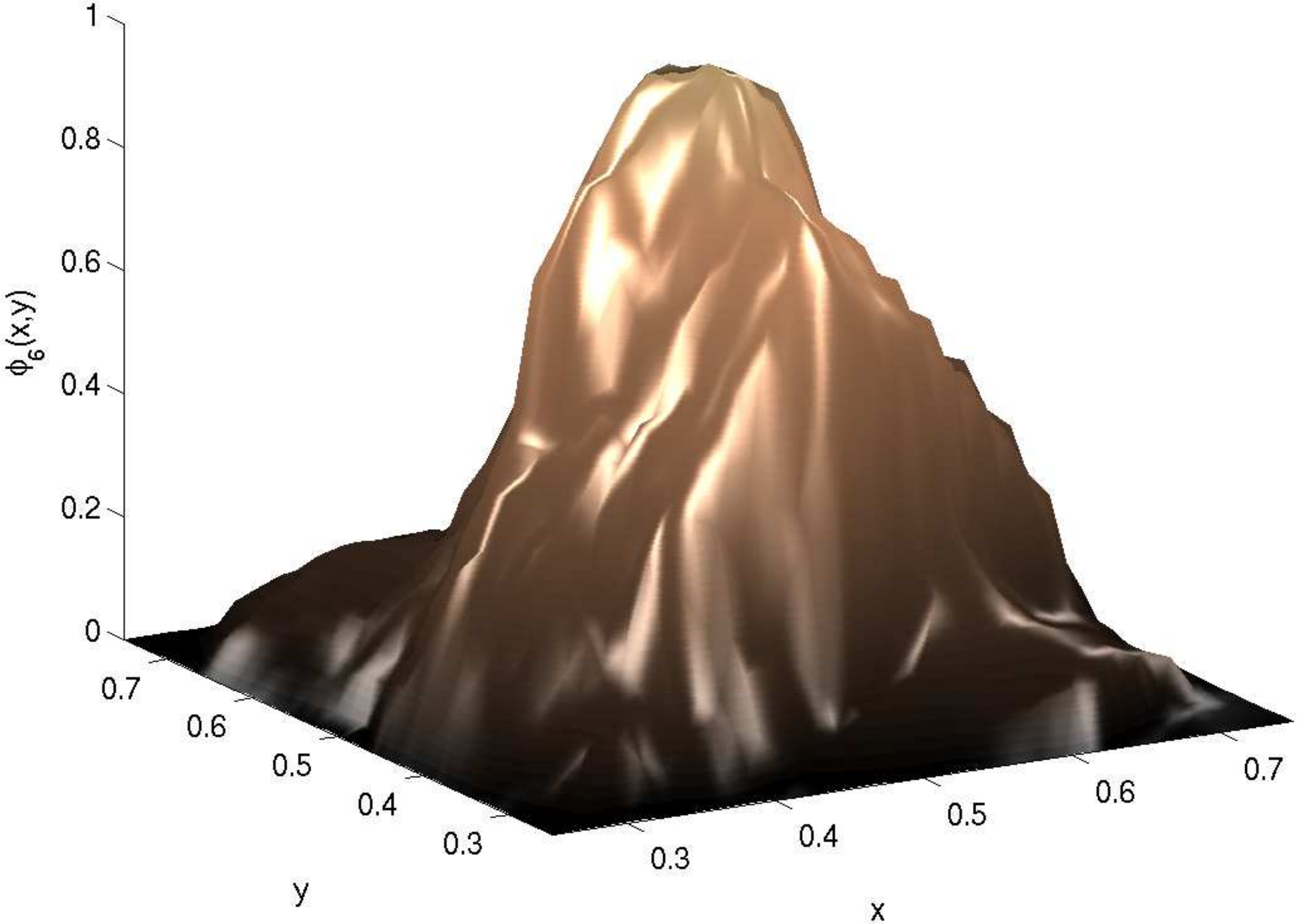

Summary

- Variational multigrid approach allows coarse-scale models to be viewed through multiscale basis functions
- Adaptive multigrid process creates accurate coarse-scale models through careful exposure of algebraically smooth error
- Solutions to variational coarse-scale problems accurately predict fine-scale behavior
- Multigrid methods are still evolving