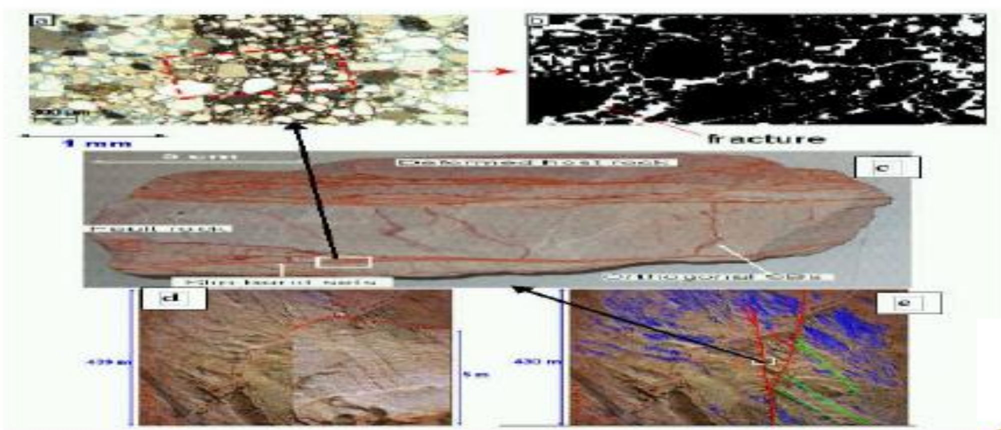
Multiscale model reduction for flows in heterogeneous porous media

Yalchin Efendiev
Texas A&M University
Collaborators: J. Galvis (TAMU), E. Gildin (TAMU), F. Thomines (ENPC), P. Vassilevski (LLNL), X.H. Wu (ExxonMobil)

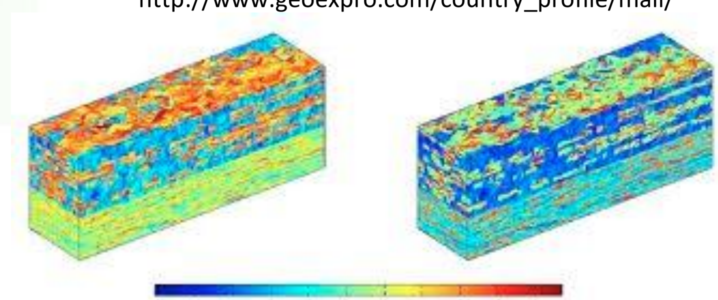
Introduction

- Natural porous formations have multiple length scales, complex heterogeneities, high contrast, and uncertainties



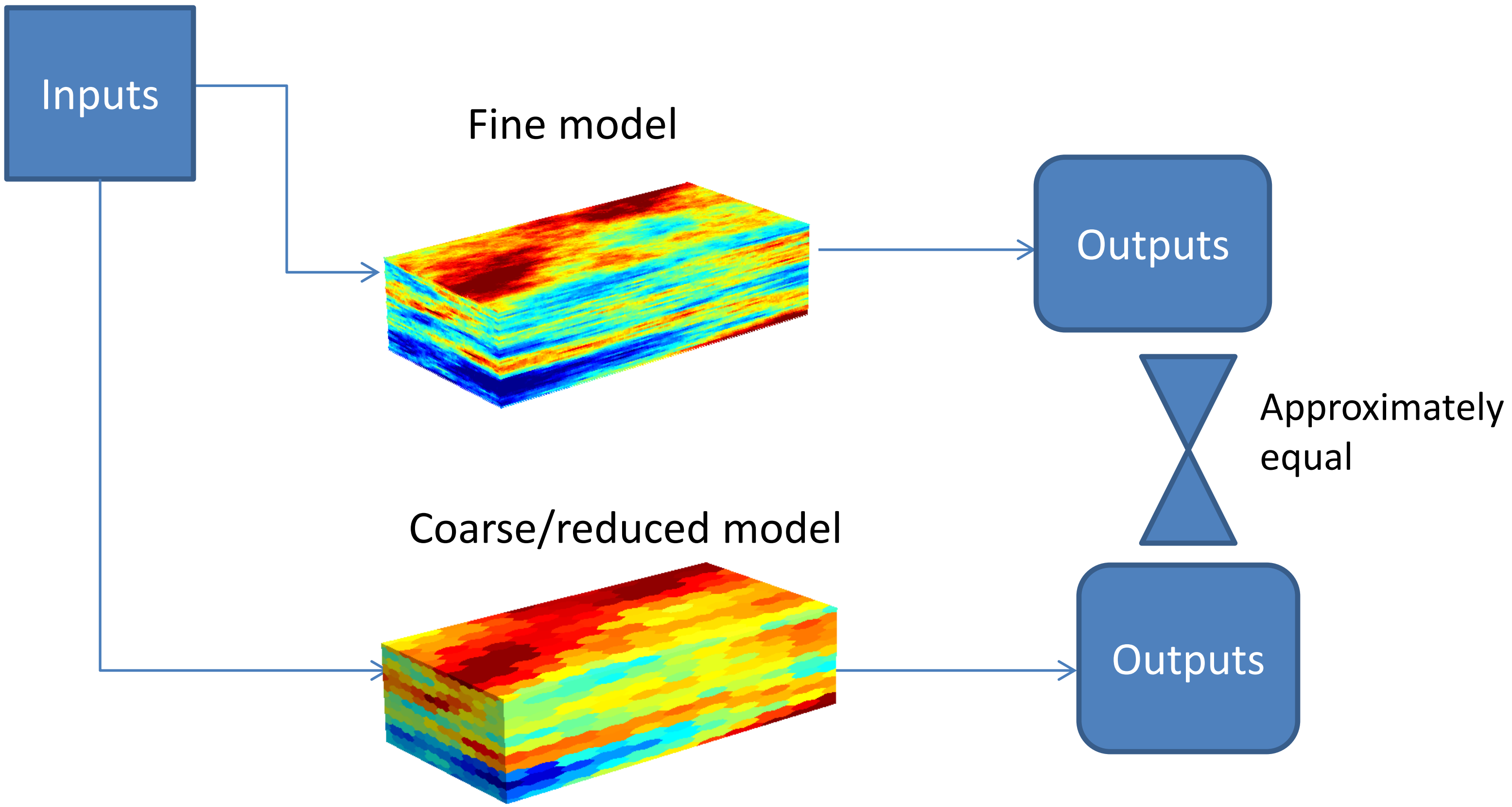
Acknowledgements: K. Sternlof, A. Ahmadov,

http://www.geoexpro.com/country_profile/mali/



- It is prohibitively expensive to resolve all scales and uncertainties. Some types of reduced models are needed.
- Objective: development of systematic reduced models for deterministic and stochastic problems

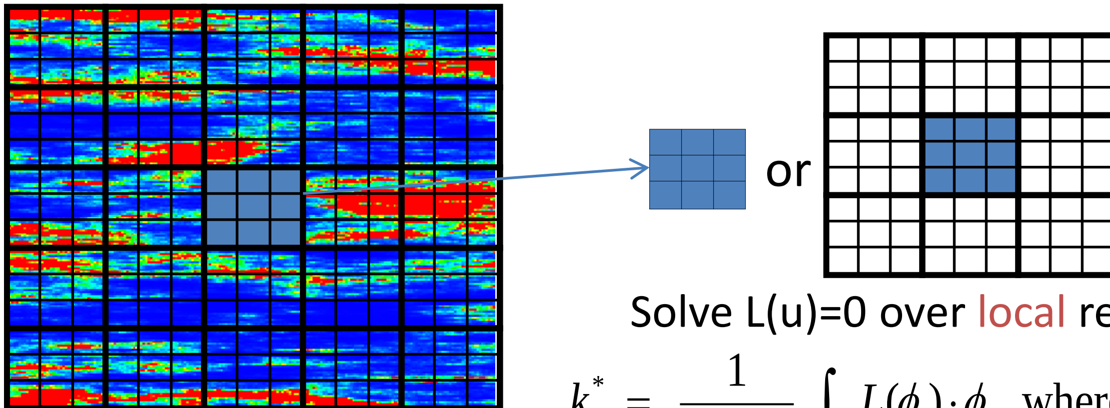
Coarse (reduced) modeling concepts

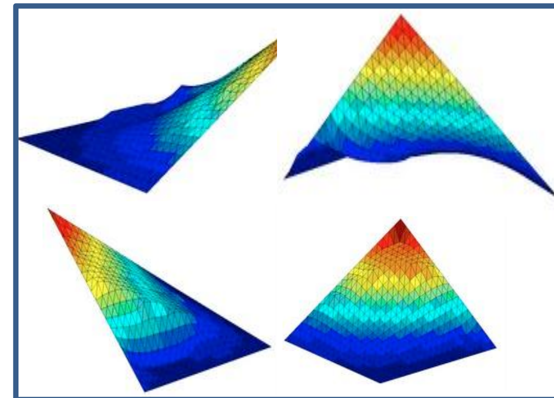


Reduced/coarse models

L
O
C
A
L

- Numerical upscaling/homogenization

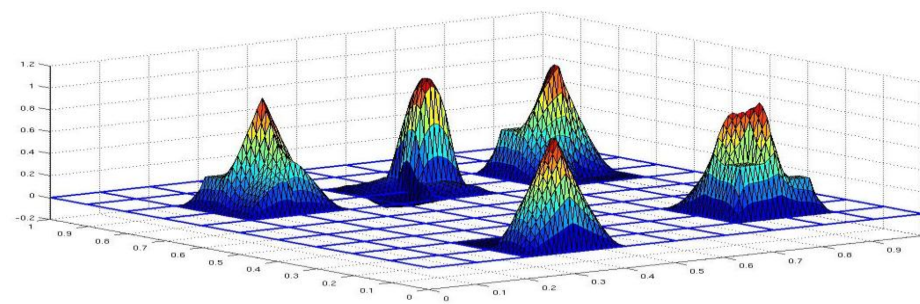




Solve L(u)=0 over local region for coarse scale $\mathbf{k}^*$

$$k^*_i = \frac{1}{|local|}\int_{local} L(\phi_i)\cdot\phi_i, \text{ where } \phi_i \text{ solves } L_k(\phi_i)=0 \text{ with BC } \phi_i = x_i.$$

- Multiscale (on a coarse grid) methods

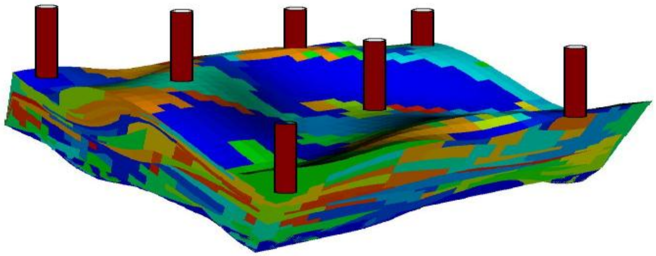


G
L
O
B
A
L

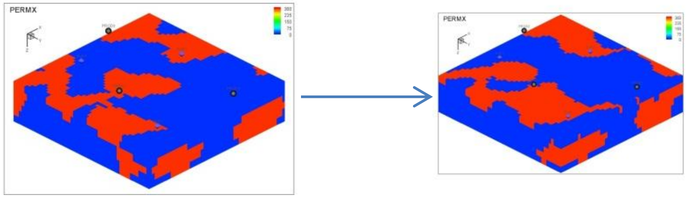
- POD, Reduced Basis, BT, … using global snapshots

Need for reduced models

- Forward problems are solved multiple times for different
  source terms
  boundary conditions
  mobilities (in multi-phase flow)
  ….



- In "uncertainty quantification", forward problem is solved for different realizations of permeability field (not necessarily log-Gaussian)

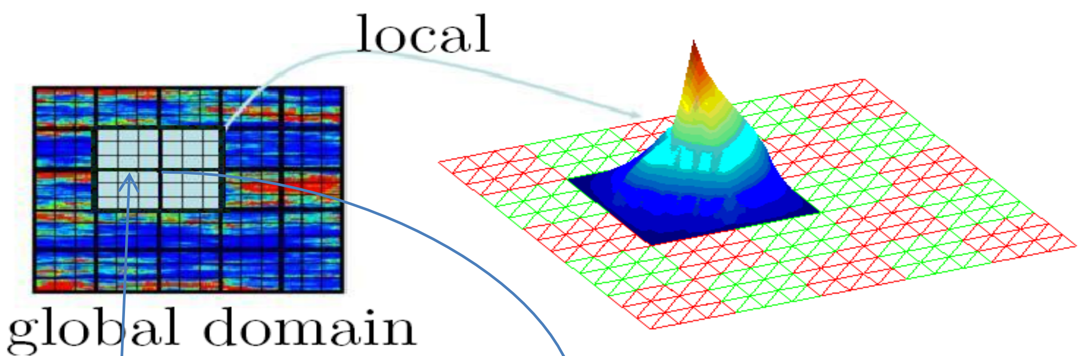


  - E.g., in MCMC, new realization is proposed and we need rapidly screen the new permeability and compute solution
  - It needs ensemble level multiscale model reduction, ensemble level preconditioners, solvers, ….

Multiscale FEM methods.

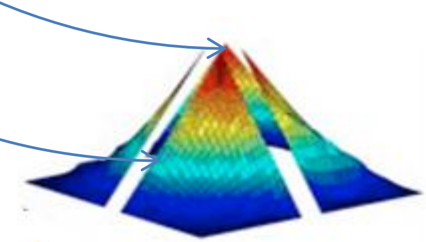
- We look for a reduced approximation of fine-scale solution $u = \sum_{i=1}^{fine} u_i \phi_i$

as $u^* = \sum_{i=1}^{coarse} u_i^* \Phi_i$, such that $\|u - u^*\|$ is small. Goal is to find Φ_i.



$L_k(\Phi_i) = 0$ in local region

- $L_k(\Phi_i) = 0$ in ω_{i}, $\Phi_i = \Phi_i^0$ on $\partial\omega_{\mathrm{i}}$.
- $L(u) = -div(k\nabla u)$

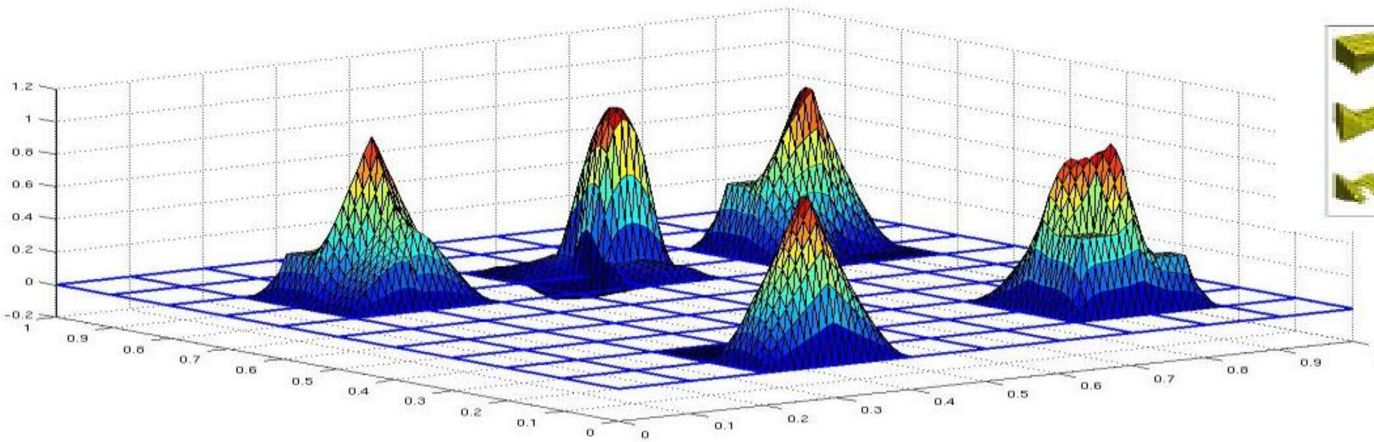


Multiscale FEM methods.

- $u = \sum_i u_i \Phi_i$, where u_i are found by a "Galerkin substitution" (Babuska et al. 1984, Hou and Wu, 1997),

$$\left\langle L\left(\sum_i u_i \Phi_i\right), \Phi_j \right\rangle = \left\langle f, \Phi_j \right\rangle.$$

- Integrals can be approximated for scale separation case.



From Aarnes et al.

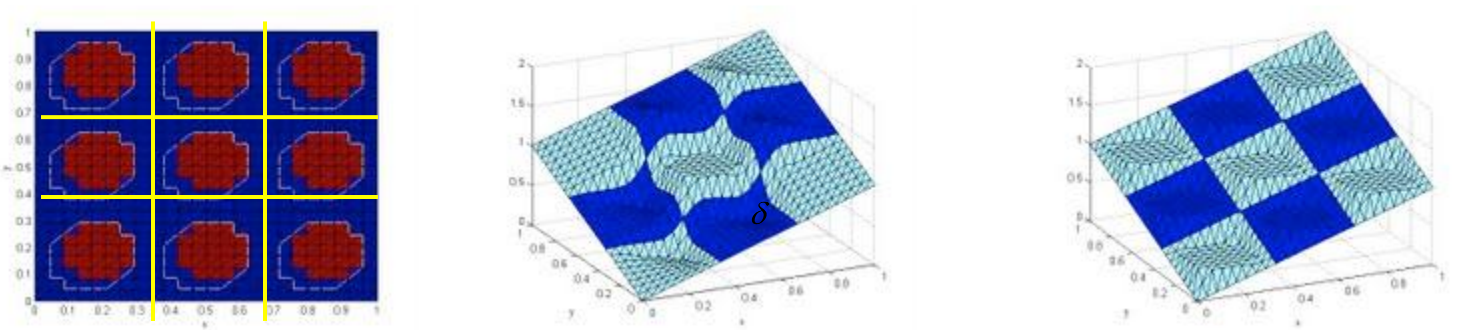
Some advantages of multiscale methods: (1) access to fine-scale information; (2) unstructured coarse gridding; (3) taking into account limited global information; (4) *systematic enrichment*

Literature (coarse-grid multiscale methods)

- Classical upscaling or numerical homogenization.
- Multiscale finite element methods (J. Aarnes, Z. Cai, Y. Efendiev, V. Ginting, T. Hou, H. Owhadi, X. Wu....)
- Mixed multiscale finite element methods (Z. Chen, J. Aarnes, T. Arbogast, K.A. Lie, S. Krogstad,...)
- MsFV (P. Jenny, H. Tchelepi, S.H. Lee, Iliev, ...)
- Mortar multiscale methods (T. Arbogast, M. Peszynska, M. Wheeler, I. Yotov,...)
- Subgrid modeling and stabilization (by T. Arbogast, I. Babuska, F. Brezzi, T. Hughes, ...)
- Heterogeneous multiscale methods (E, Engquist, Abdulle, M. Ohlberger, ...)
- Numerical homogenization (NH) using two-scale convergence (C. Schwab, V.H. Hoang, M. Ohlberger, ...)
- NH (Bourgeat, Allaire, Gloria, Blanc, Le Bris, Madureira, Sarkis, Versieux, Cao, ...)
- Component mode synthesis techniques (Lehoucq, Hetmaniuk)
- AMG coarsening (P. Vassilevski)
- Multiscale multilevel mimetic (Moulton, Lipnikov, Svyatskiy…)
- High-contast homogenization (G. Papanicolaou, L. Borcea, L. Berlyand, …)

Boundary conditions

- Local boundary conditions need to contain “correct” structure of small-scale heterogeneities. Otherwise, this can lead to large errors.



- Piecewise linear boundary conditions result to large discrepancies near the edges of coarse blocks (e.g., the solution is $u \approx u_0 + \varepsilon u_1(x, x/\varepsilon)$ along the coarse edge while MsFE solution is linear).

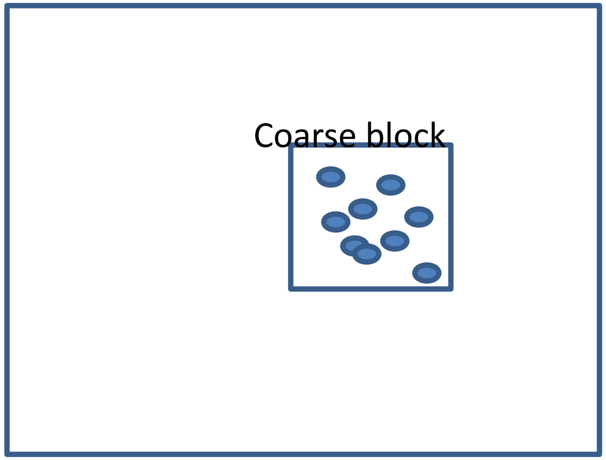
Error $\propto \frac{\varepsilon}{H}$, where ε is a physical scale and H is the coarse mesh size, $H \gg \varepsilon$.

Improving boundary conditions: Oversampling (Hou, Wu, Efendiev,…), local-global (Durlofsky, Efendiev, Ginting, ….), limited global information (Owhadi, Zhang, Berlyand…), …

Questions: (1) How to find these basis functions? How to define boundary conditions for basis functions? (2) How to systematically enrich the space ?

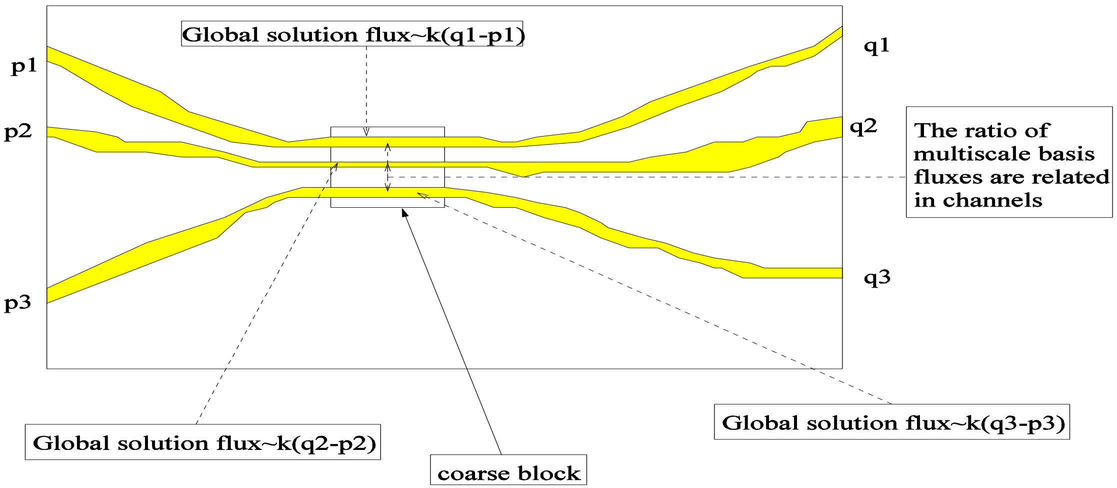
Systematic enrichment and initial multiscale space

- One basis per node is not sufficient.
- Many features can be localized, while some features need to be represented on a coarse grid.
- Initial basis functions are used to capture “localizable features” and construct a spectral problem that identifies “next” important features.
- Initial basis functions are important. Without a good choice of initial space, the coarse space can become very large.

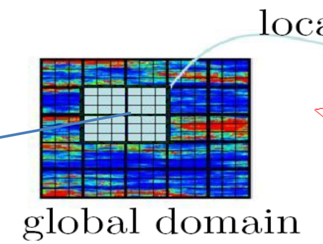


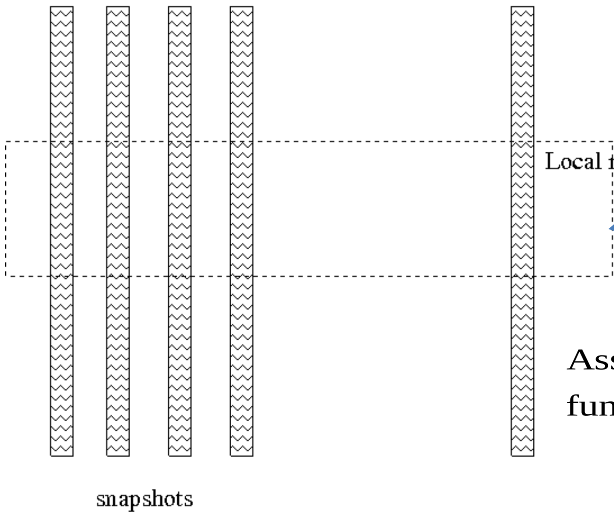
Localizable features

Non-localizable features



Local model reduction.





Assume ψ_1, $\psi_2, \ldots,$ ψ_N are local snapshots. How to generate local basis functions?

Denote by Φ_k initial multiscale basis functions. Basis functions for MsFEM are formed - $\Phi_i \bullet \psi_k$

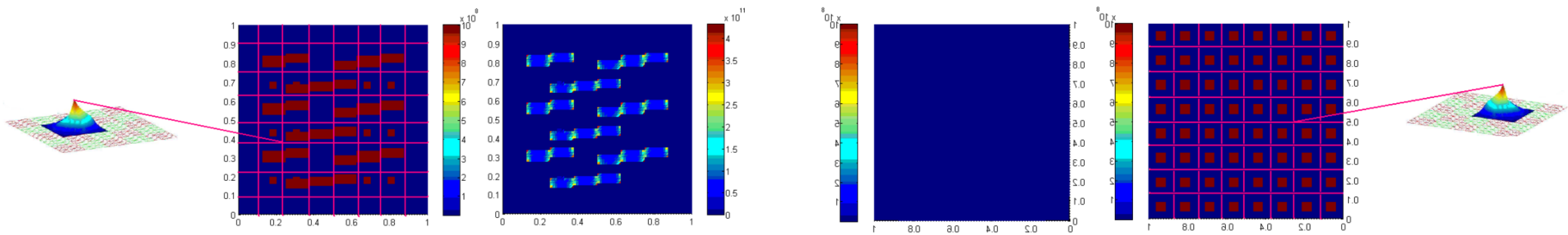
It can be shown that

$$\int_D k\,|\nabla(u-u_{ms})|^2 \leq \sum_i \int_{\omega_i} k\Phi_i^{\,2}\,|\nabla(u-u_0)|^2 + \sum_i \int_{\omega_i} k\,|\nabla\Phi_i|^2\,(u-u_0)^2,$$

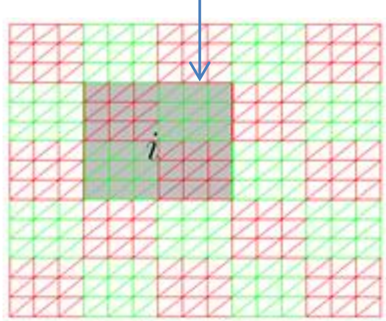
where u_0 is local coarse-grid approximation in Span(ψ_k), ω_i are coarse blocks sharing a vertex.

POD-type-reduction of snapshots can lead to large spaces.

Coarse space construction. Methodology



- Start with initial basis functions Φ_i and compute $k = \sum_i k\nabla\Phi_i \cdot \nabla\Phi_i$.
- For each ω_i, solve local spectral problem $-div(k\nabla\psi_i) = \lambda_i k\psi_i$ with zero Neumann bc and choose "small" eigenvalues and corresponding eigenvectors.

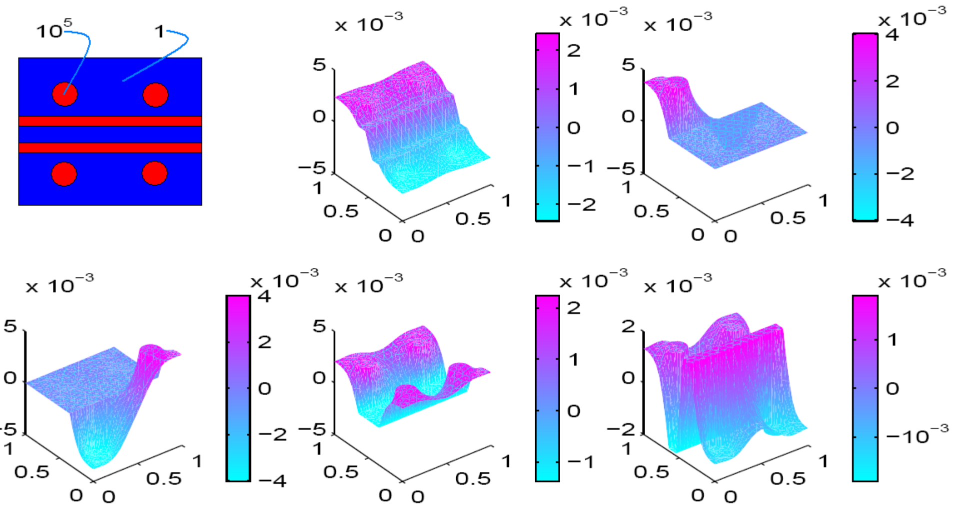


Systematic enrichment

- If Φ_i are bilinear functions, then $k \propto k$(the same high-cond. regions)

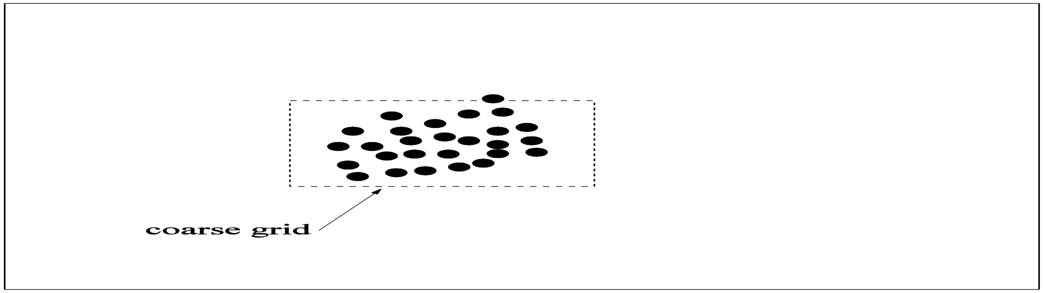
$$k = \sum_i k \nabla \Phi_i \cdot \nabla \Phi_i$$

- $-div(k\nabla \psi_i) = \lambda_i k \psi_i$ with zero Neumann bc
- Identify $\lambda_1 = 0 \leq \lambda_2 \leq \ldots \leq \lambda_n$.
- There are 6 small (inversely $\propto$ to high-contrast) eigenvalues.
- Eigenfunctions represent piecewise smooth functions in high-conductivity regions
- "Gap" in the spectrum --- $\dfrac{\int k |\nabla \psi|^2}{\int k \psi^2}$.
- $-div(k\nabla \psi_i) = \lambda_i \psi_i$ - too many contrast-dependent eigenvalues.

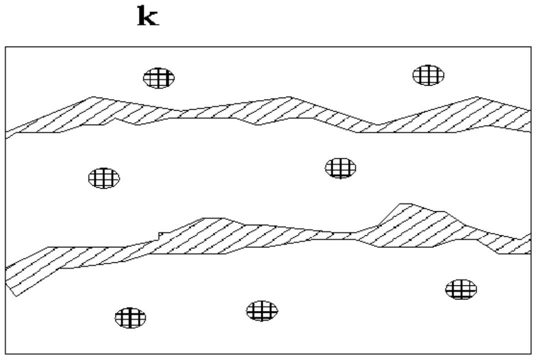


Systematic enrichment

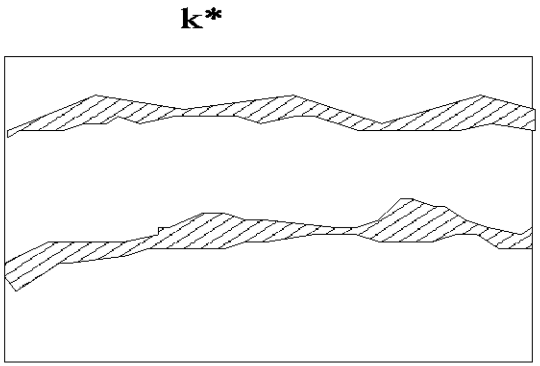
- If there are many inclusions, we may have many basis functions. We know "many isolated inclusion domain" can be homogenized (one basis per node).



- What features can be localized? Channels vs. inclusions.

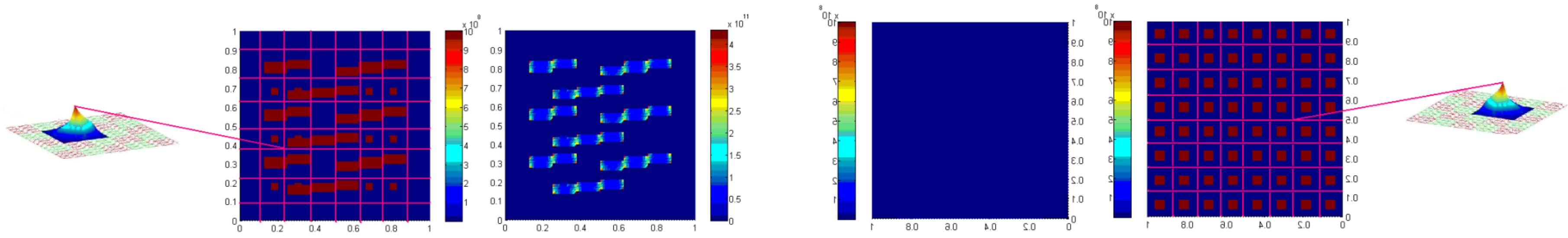


Coarse grid with isolated inclusions and channels

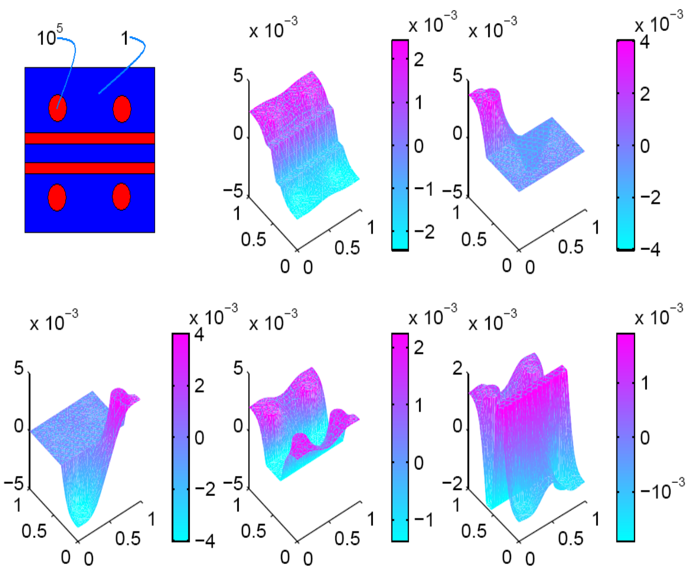


Coarse grid without isolated inclusions

Systematic enrichment

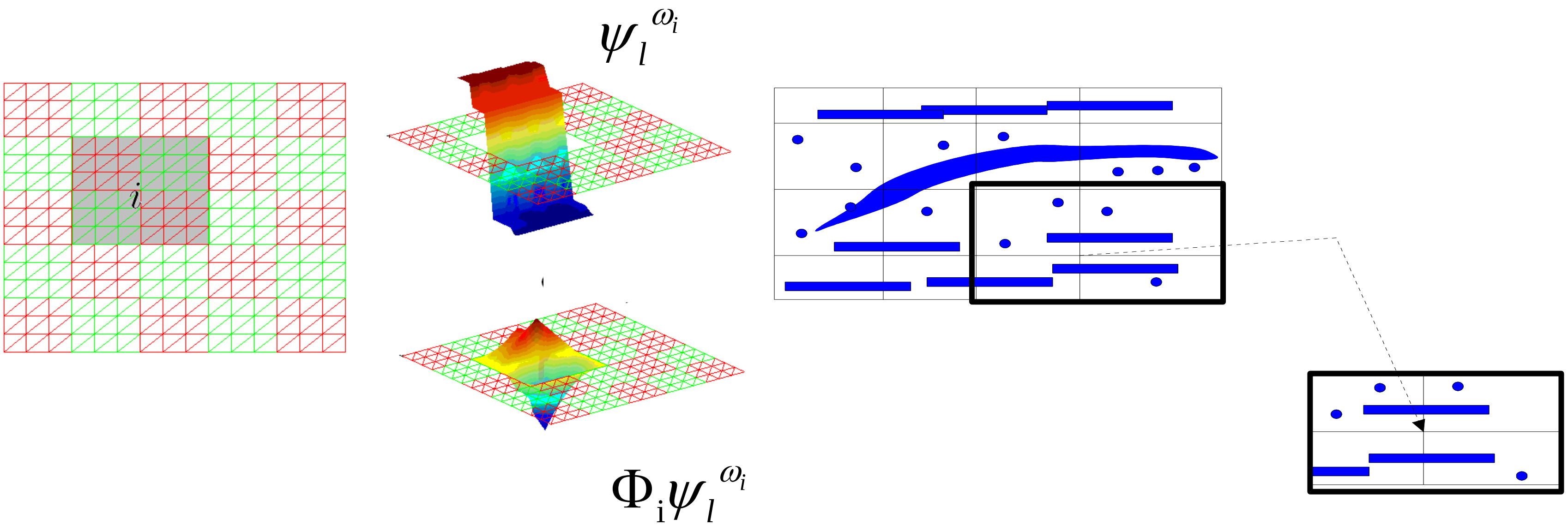


- Φ_i are multiscale FEM functions - $k = \sum_i k\nabla\Phi_i \cdot \nabla\Phi_i$
- $-div(k\nabla\psi_i) = \lambda_i k\psi_i$ with zero Neumann bc
- Identify $\lambda_1 = 0 \le \lambda_2 \le \ldots \le \lambda_n$.
- There are 2 small (inversely $\propto$ to high-contrast) eigenva
- Eigenfunctions represent piecewise smooth functions in high-conductivity channels
- "Gap" in the spectrum --- $\dfrac{\int k\,|\nabla\psi|^2}{\int k\psi^2}$.



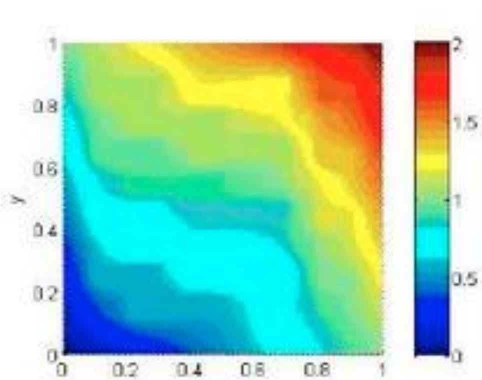
Coarse space construction

- Coarse space: $V_0 = Span\left\{\Phi_i \psi_l^{\omega_i}\right\}$

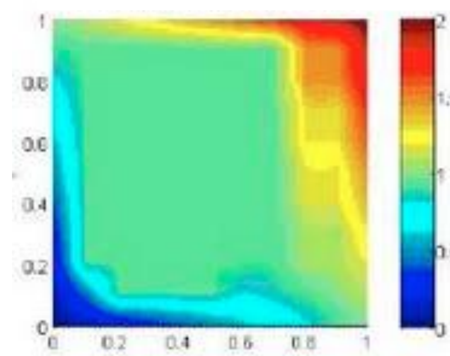


Coarse grid approximation

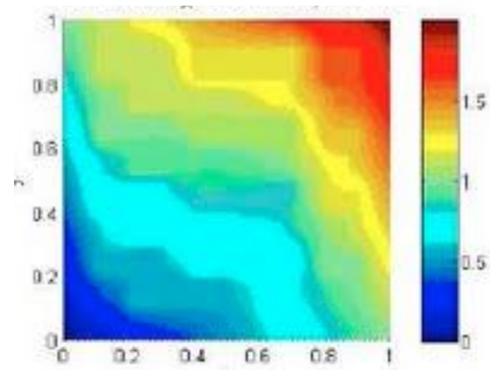
Fine-scale solution



MSwith initial space, error=90%



MS with systematically enriched space, error=6%



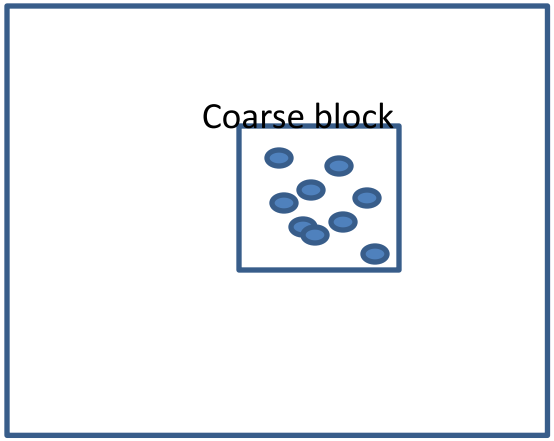
	H=1/10	H=1/20
+0	0.2 (Λ=0.2)	0.12 (Λ=0.11)
+1	0.036 (Λ=0.95)	0.034 (Λ=0.9)
+2	0.03 (Λ=1.46)	0.02 (Λ=1.54)
+3	0.027 (Λ=3.15)	0.01 (Λ=1.9)

$\int k\,|\nabla(u-u_{Ms})|^2 \le C\frac{H^\gamma}{\Lambda}$ (YE, Galvis, Wu, 2010), where Λ is the smallest eigenvalue that the corresponding eigenvector is not included in the coarse space.

Larger spaces give same convergence rate.

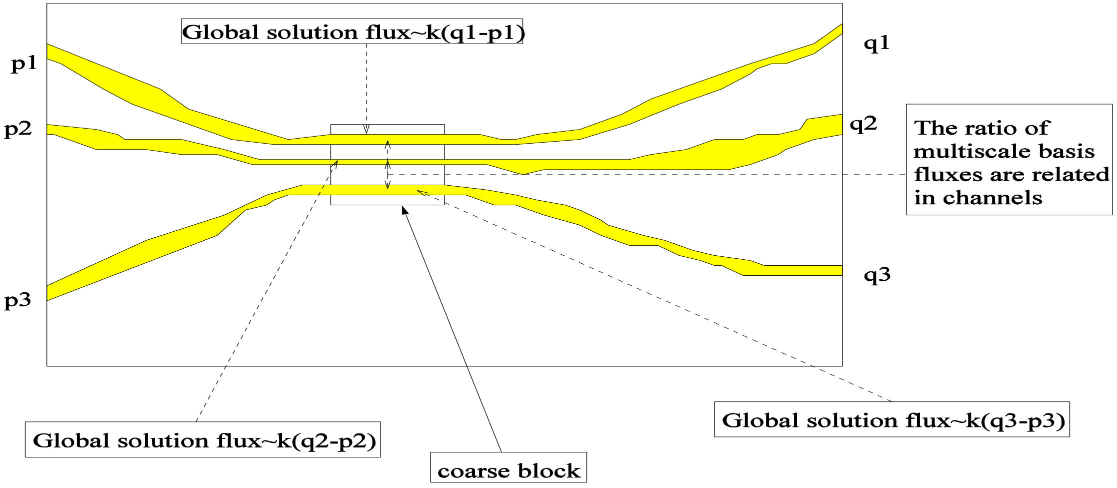
Dimension reduction

- Without appropriate initial multiscale space, the dimension of the coarse space can be large.
- Dimension reduction for channels (channels need to be included in the coarse space).



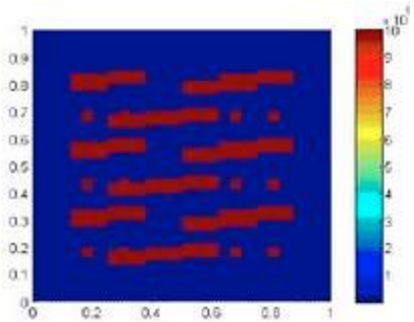
Localizable features

Non-localizable features



Applications to preconditioners

Permeability



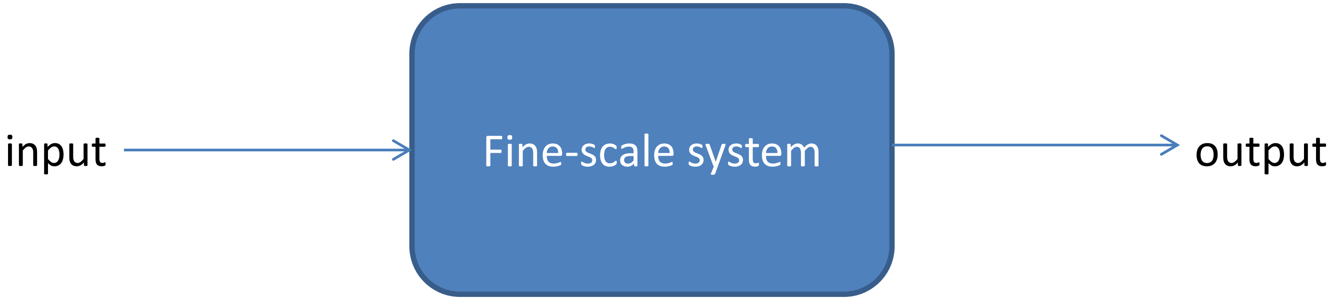
contrast	Initial MS space	Enriched (w. incl)	Enriched (opt.)
10^4	98(2490.75)	27(6.19)	28(7.34)
10^5	123(24866.24)	28(6.19)	29(7.35)
10^6	144(248621.33)	29(6.19)	29(7.35)
10^7	174(2486172.35)	29(6.19)	30(7.35)
Dim	49	102	69

We show that $cond(B^{-1}A) \leq \frac{1}{\Lambda}$ (Galvis and YE, 2010), where Λ is (rescaled) smallest eigenvalue that the corresponding eigenvector is not included in the coarse space. For optimality, all eigenvectors corresponding to asymptotically small eigenvalues need to be included. Here B^{-1} is two-level additive Schwarz preconditioner ($B^{-1} = R_0^T A_0 R_0 + \sum_i R_i^T A_i^{-1} R_i$)

- Multilevel methods (YE, Galvis, Vassilevski, 2010).

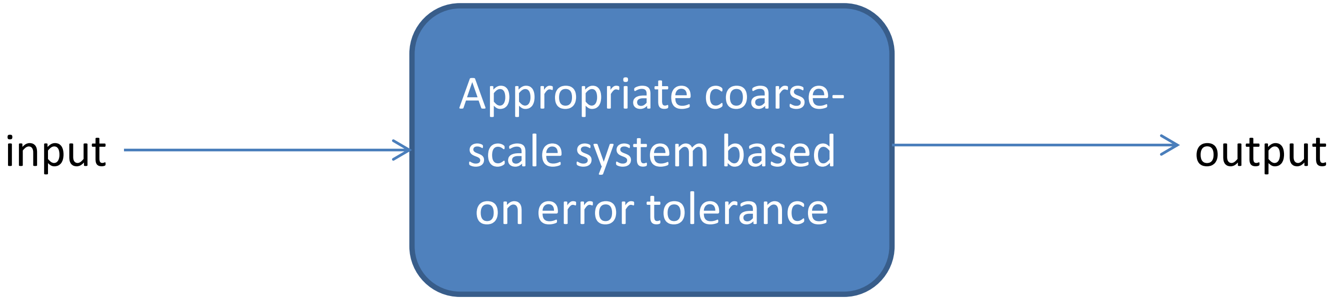
Local-global model reduction

- "Multiscale methods" are typically designed to provide approximations for arbitrary coarse-level inputs
- How can we take an advantage if inputs belong to a smaller dimensional spaces?



Local-global model reduction

- Multiscale methods are typically designed to provide approximations for arbitrary coarse-level inputs
- How can we take an advantage if inputs belong to a smaller dimensional spaces?



- We use balanced truncation approach to select reduced global modes. We consider

$$\frac{dp}{dt} = Ap + Bu, \; q = Cp, \text{ where } u \text{ is input, q is observed quantity.}$$

- "Balanced truncation" allows obtaining reduced models; however, it is very expensive and involves solving Lyapunov equation $AP + PA^T + BB^T = 0, \; A^T Q + QA + C^T C = 0.$

- We choose an appropriate local coarse-scale model given a tolerance and combine it to a global model reduction and guarantee a smallest dimensional reduced model.

Numerical results

- Approach: Apply Balanced Truncation (BT) on a coarse grid with a careful choice of MS (red – BT with 10 SV, black – BT with 3 SV).

- $\left\| q - q_o{}^r \right\| \leq \left\| q - q_o \right\| + \left\| q_0 - q_o{}^r \right\|$, where q_o is coarse approx., and $q_o{}^r$ is a reduced coarse approx.

$$\left\| q - q_0{}^r \right\| \leq \left\| C \right\|_A \frac{H^{\gamma}}{\lambda^{*}{}_{L+1}} + \sum_{i=l+1} \sigma_i^0 .$$

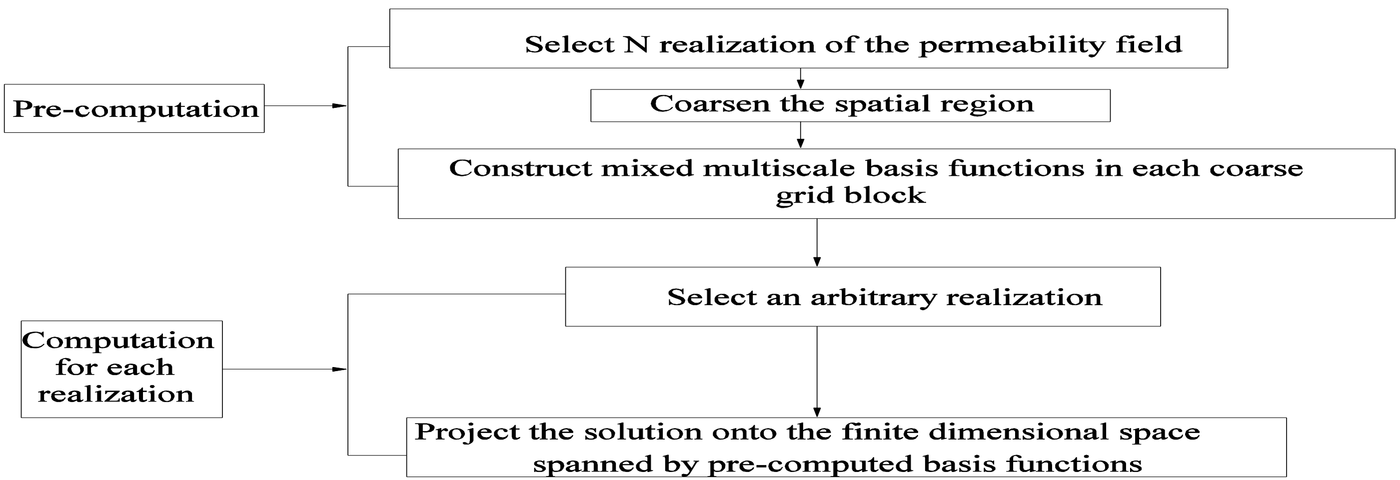
MS Dim	MS Error	BT Error	Total Error
69	0.12(0.12)	0.23(0.04)	0.29(0.12)
150	0.08(0.08)	0.25(0.06)	0.29(0.11)
231	0.06(0.06)	0.26(0.06)	0.29(0.09)

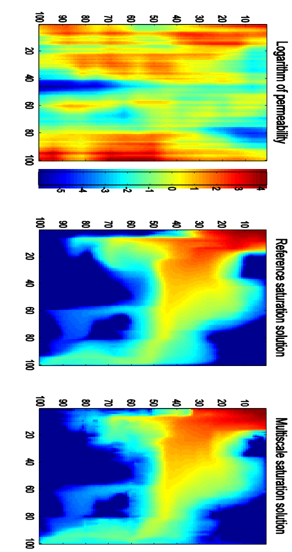
Stochastic (parameter-dependent) problems

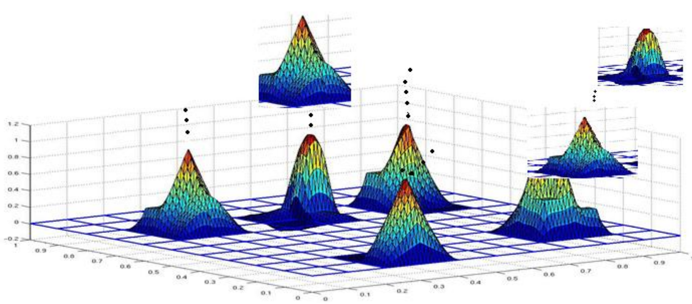
- Permeability fields are usually stochastic (variogram-based, channelized permeability,…). Uncertainties are typically parameterized
- Basis (subgrid representation) computations can be expensive if performed realization-by-realization. Can we construct “ensemble” level approaches?
- Fast ensemble-level multiscale methods (ensemble level preconditioners) are needed for many Monte Carlo simulations. E.g., Markov chain Monte Carlo for uncertainty quantification in inverse problems,…

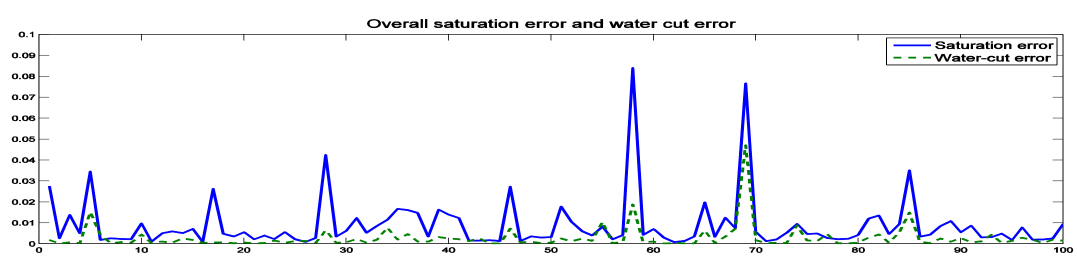
Ensemble level multiscale methods

- Objective is to construct coarse spaces for "an ensemble (Aarnes and YE, 2008)
- Construct basis functions by selecting a few realizations in the ensemble





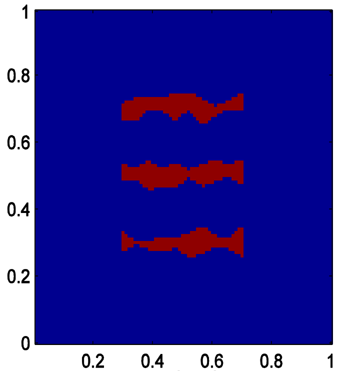




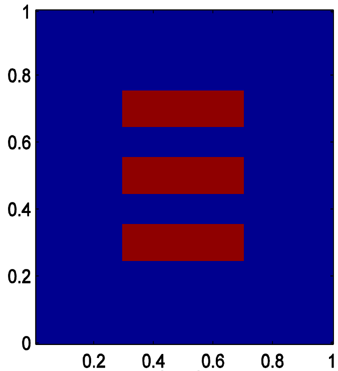
Ensemble level multiscale

- Ensemble level multiscale spaces for coarse-grid approximation and preconditioning.
- For channelized permeability fields, we propose using largest channels within coarse-grid block and constructing multiscale basis functions based on it.
- These multiscale spaces are used in preconditioning for each proposal of the ensemble (joint work with J. Galvis , P. Vassilevski, J. Wei)

contrast	Ms-no enrich	Ms spectral
1e+3	2.76e+2	1.06e+1
1e+6	2.61e+5	1.24e+1
1e+9	2.6e+8	1.24e+1



Permeability Realization from ensemble



Permeability used constucting multiscale casis functions

- How to generalize this method? The main idea is to construct a small dimensional local problems offline that can be used for each online parameter.

Reduced Basis (RB) Multiscale FEM Approach

- S. Boyoval, A. Cohen, R. DeVore, , C. LeBris , Y. Maday , A. Pattera,…

$$-\mathrm{div}(k(x;\mu)\nabla p) = f, \quad \mu \in \Lambda, \quad k(x;\mu) = \sum_i k_q(x)\Theta_q(\mu)$$

- Reduced basis discretizes the manifold Ω=Span$\{p(x;\mu),\ \mu \in \Lambda\}$ via
  $\Omega_{\mathrm{N}} = \mathrm{Span}\{p(x;\mu_i),\ i \leq N\},$ for small N.
- RB uses snapshots of global solutions (offline) to construct a reduced model for solving the global system for an online value of μ
- Aposteriori error estimates are used to find snapshots with greedy algorithm
- Affine form of $k(x;\mu)$ is needed to compute bilinear forms offline and make online computations fast
- Extensions to corrector problems Boyoval et al., 2009,...

Reduced basis MsFEM

$$-\mathrm{div}(k(x;\mu)\nabla p) = f, \quad \mu \in \Lambda, \quad k(x;\mu) = \sum_i k_q(x)\Theta_q(\mu)$$

- Define initial basis functions

$$\mathrm{div}(k(x;\mu_0)\nabla\Phi_i) = 0, \; \Phi_i = \Phi_i^0$$

- Define $v^T A_q^{\omega_i} u := \int_{\omega_i} k_q(x)\nabla u \nabla v;$

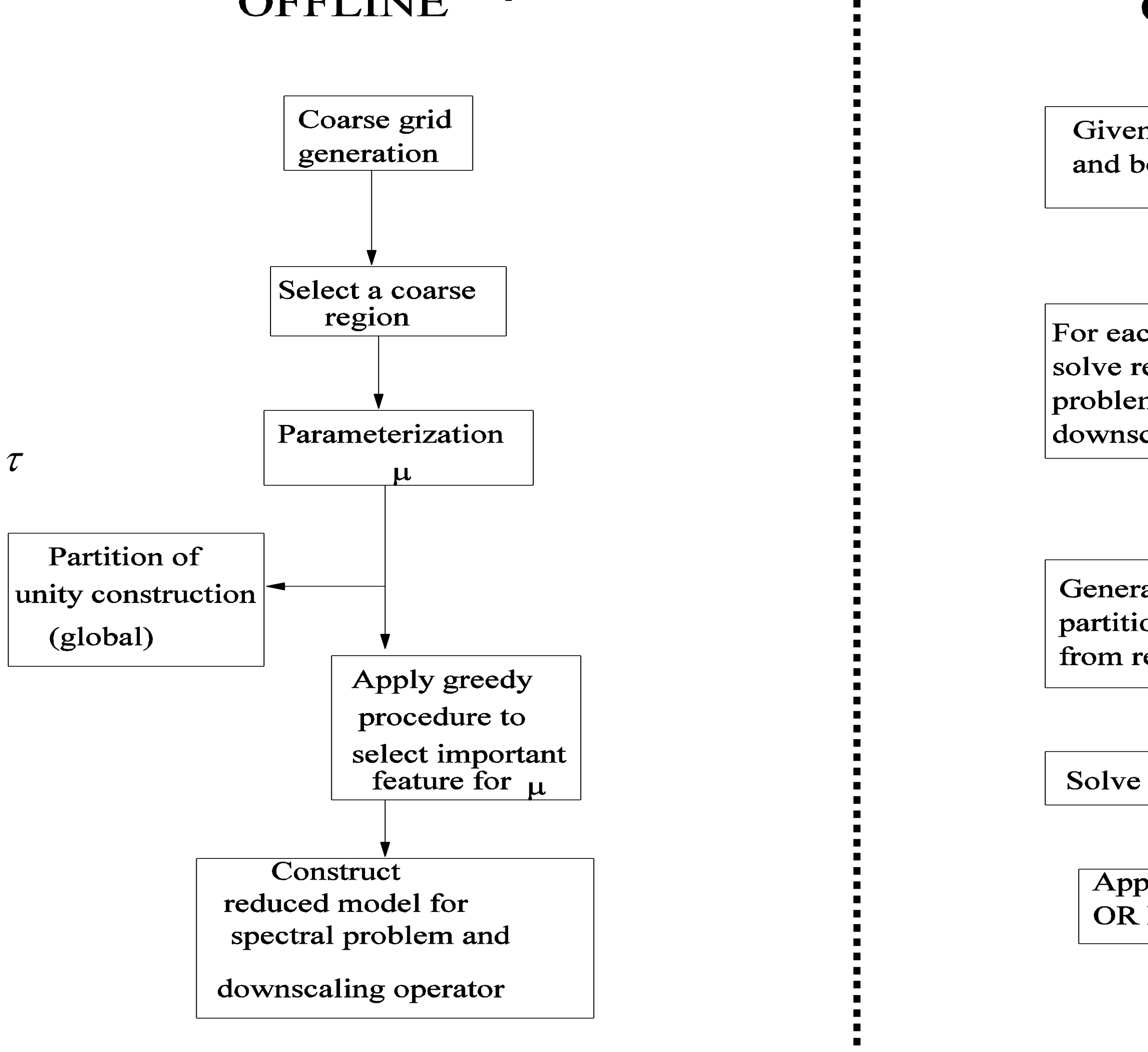
$$v^T M_q^{\omega_i} u := \int_{\omega_i} k_q(x) \sum_i |\nabla \Phi_i|^2 uv$$

- Define the sequence μ_j such that

$$\sum_q \Theta_q(\mu_j)(A_q^{\omega_i} - \lambda_l^{\omega_i} M_q^{\omega_i})\phi_l^{\omega_i} = 0, \; \lambda_l^{\omega_i} < \tau$$

- Outputs of offline stage: $A_q^{\omega_i}$, $M_q^{\omega_i}$, and

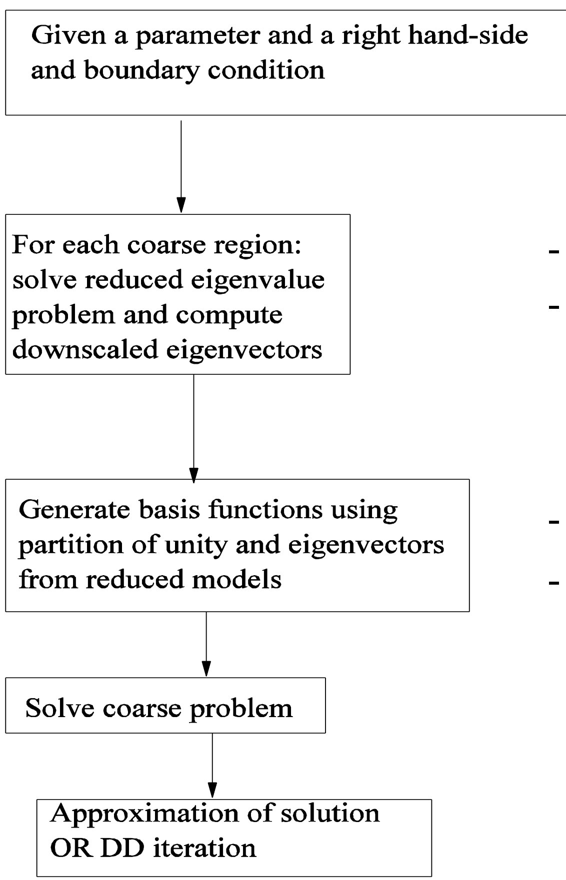
$$R^{\omega_i} = [\phi_1^{\omega_i} \dots \phi_M^{\omega_i}] \text{ and } R_0^T = [\Phi_1 \dots \Phi_L].$$



Reduced basis MsFEM

$$-\mathrm{div}(k(x;\mu)\nabla p) = f, \quad \mu \in \Lambda, \quad k(x;\mu) = \sum_i k_q(x)\Theta_q(\mu)$$

ONLINE

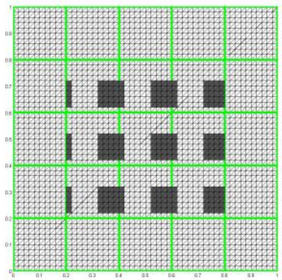


- For each μ
- For each ω_{i}, solve

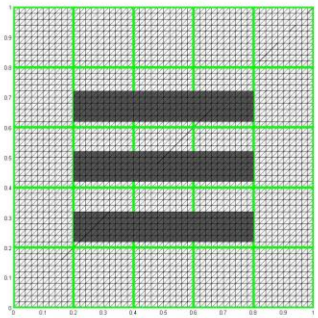
$$\sum_{\mathrm{q}} \Theta_{\mathrm{q}}(\mu)(R_{\omega_i}{}^T A_q{}^{\omega_i} R_{\omega_i} - \lambda_l{}^{N_{rb}}(\mu) R_{\omega_i}{}^T M_q{}^{\omega_i} R_{\omega_i})\phi_l{}^{N_{rb},\omega_i}(\mu) = 0$$

  for eigenvalues below a threshold
- Compute multiscale basis functions $\Phi_{\mathrm{i}}{}^j := \Phi_i \phi_j{}^{N_{rb},\omega_i}$
- Solve the coarse system

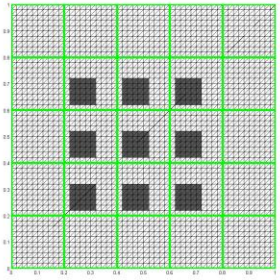
Numerical results



Mu=0



Mu=1/2



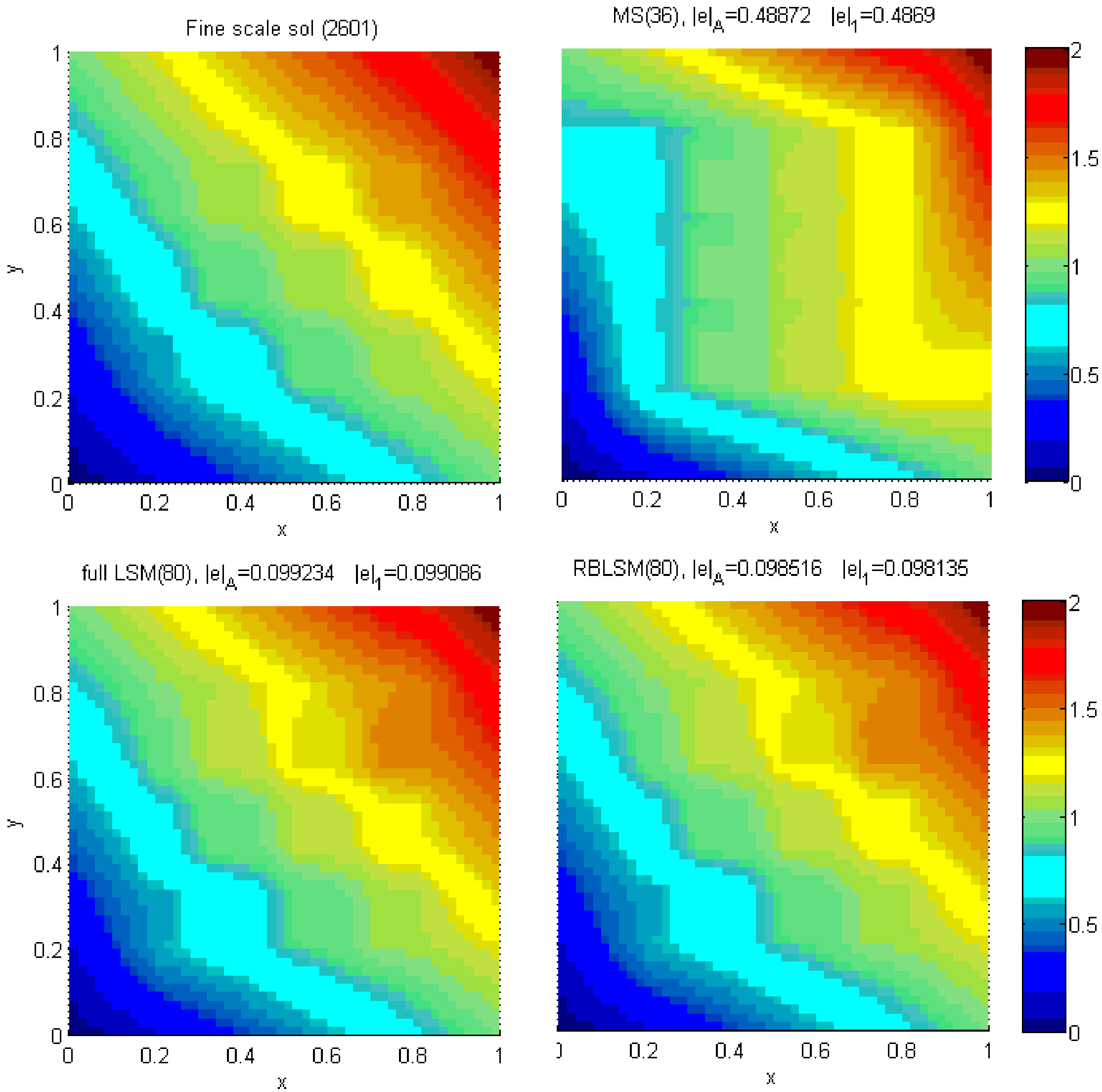
Mu=1

$$k = \mu k_0 + (1-\mu) k_1$$

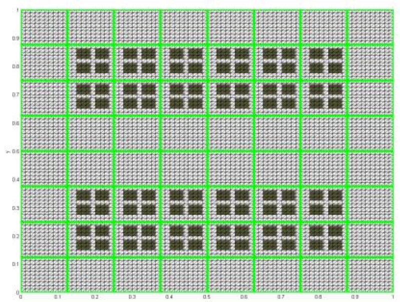
	True	Nrb=1	Nrb=2	Nrb=3	Nrb=4
LSM+0	13.6 (44)	39.3(36)	39.3(36)	13.6(44)	13.6(44)
LSM+1	4.01 (80)	39.2(72)	38.6(72)	4.01(80)	4.01(80)
LSM+2	3.93(116)	39.18(108)	26.5(108)	3.93(116)	3.93(116)

Eta	MS	True	Nrb=1	Nrb=2	Nrb=3
1e+5	47(1.4e+4)	27(8.8)	42(2e+4)	45(1.8e+4)	26(9.34)
1e+5	57(1.4e+6)	31(7.8)	52(2e+6)	53(2e+6)	28(9.34)
Dim	16	24	16	16	24

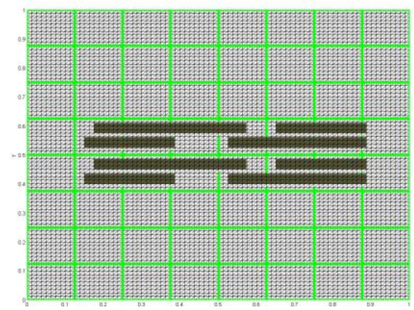
Numerical results



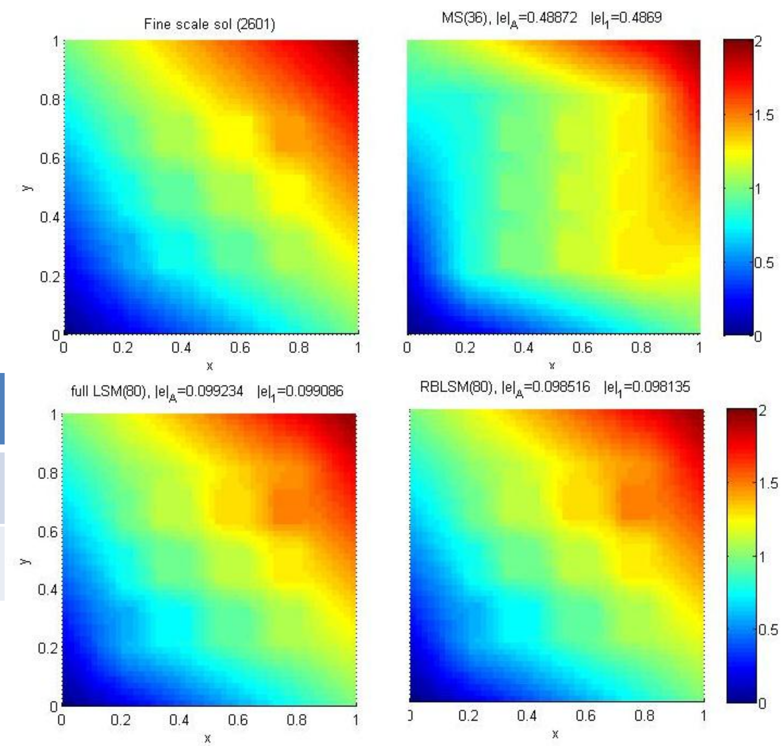
Numerical results



Mu=0



Mu=1



	Lin. Init. Basis	Ms. Init. Basis
LSM+0	9.9 (300)	10.36 (120)
LSM+1	6.28 (415)	2.45 (201)

Computational cost

- RB-MsFEM CPU gain is due to the fact that many features are eliminated at the coarse-grid level before involving a global solve

Conclusions

- Local multiscale methods.
- Systematic enrichment. A choice of initial multiscale basis functions.
- Local-global approaches
- Parameter-dependent problems.