RFB methods: a consistent framework to derive multiscale finite element methods

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- Pedro Pinheiro
- Lutz Tobiska
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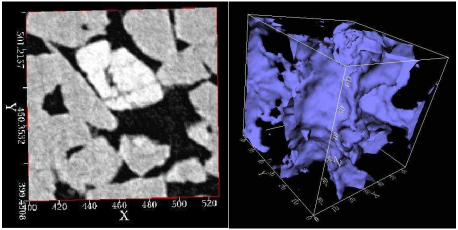
Outline

Outline

Example - Porous media flow

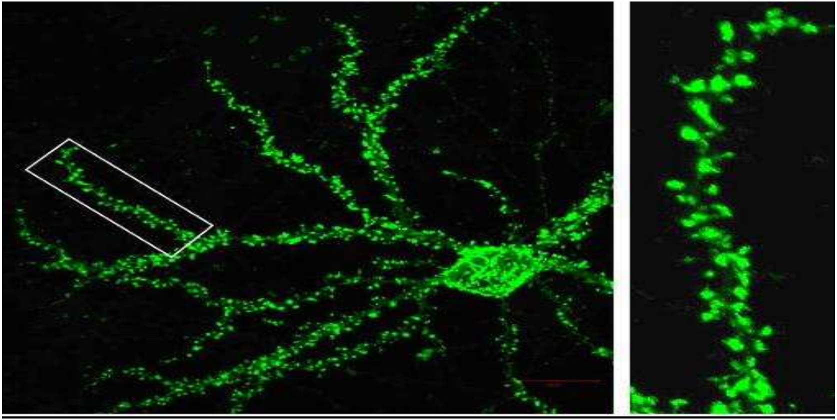


http://ccs.chem.ucl.ac.uk/research/

Water and oil flow in a porous rock

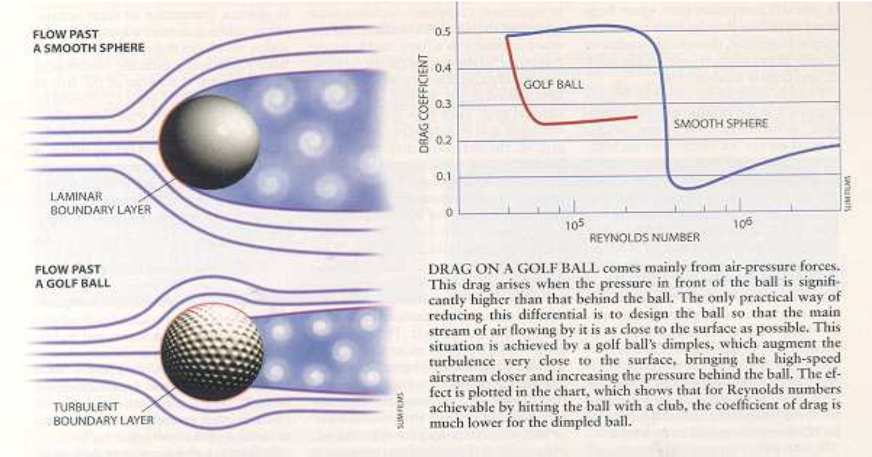
- X-ray microtomography to describe geometry (5 microns resolution)
- Computacional mesh with more than 100 millions nodes

Example - dendrites with synapses



http://www.bristol.ac.uk/anatomy/research/staff/hanley.html

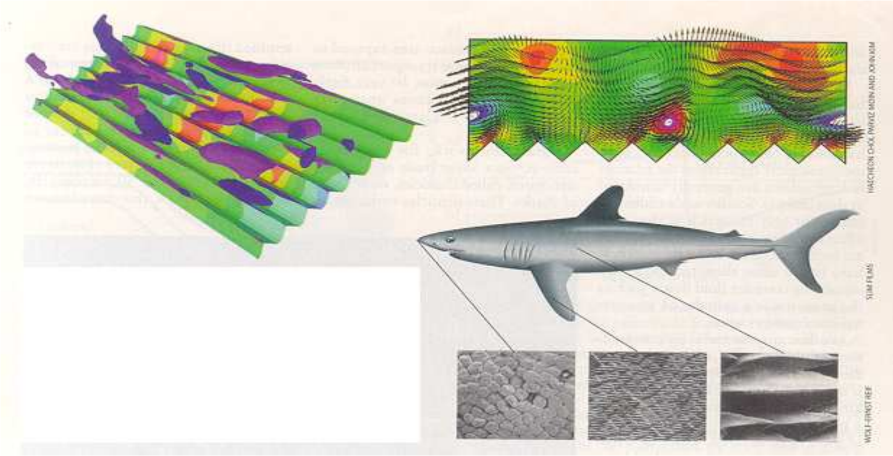
Example - Flows over Rough Surfaces



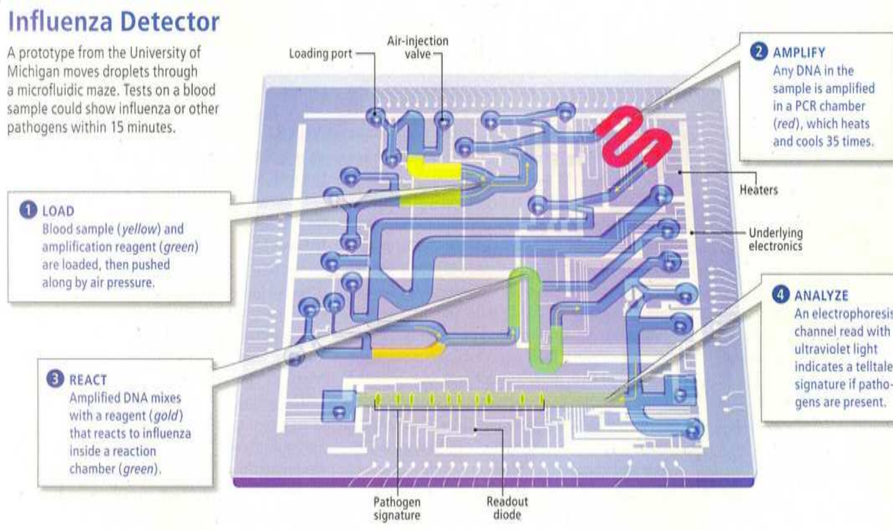
DRAG ON A GOLF BALL comes mainly from air-pressure forces. This drag arises when the pressure in front of the ball is significantly higher than that behind the ball. The only practical way of reducing this differential is to design the ball so that the main stream of air flowing by it is as close to the surface as possible. This situation is achieved by a golf ball's dimples, which augment the turbulence very close to the surface, bringing the high-speed airstream closer and increasing the pressure behind the ball. The effect is plotted in the chart, which shows that for Reynolds numbers achievable by hitting the ball with a club, the coefficient of drag is much lower for the dimpled ball.

Source: Scientific America

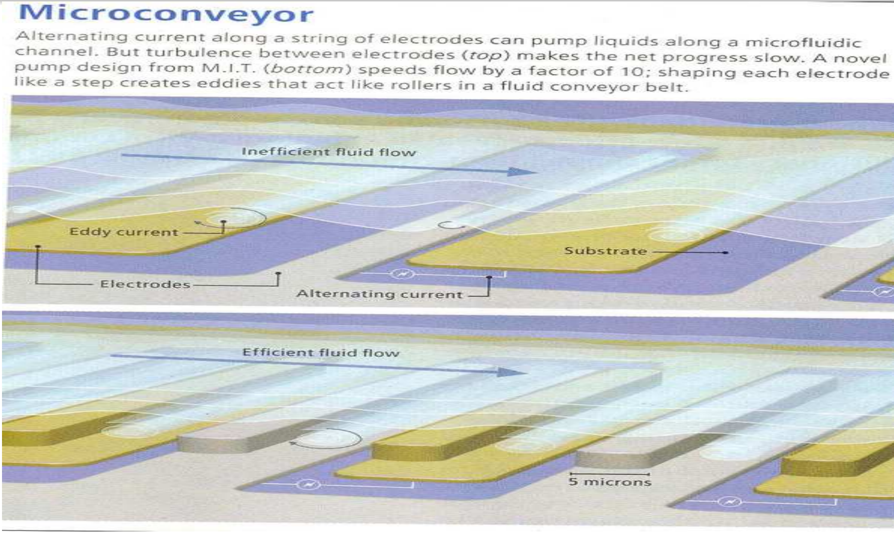
Example - Flows over Rough Surfaces



Source: Scientific America

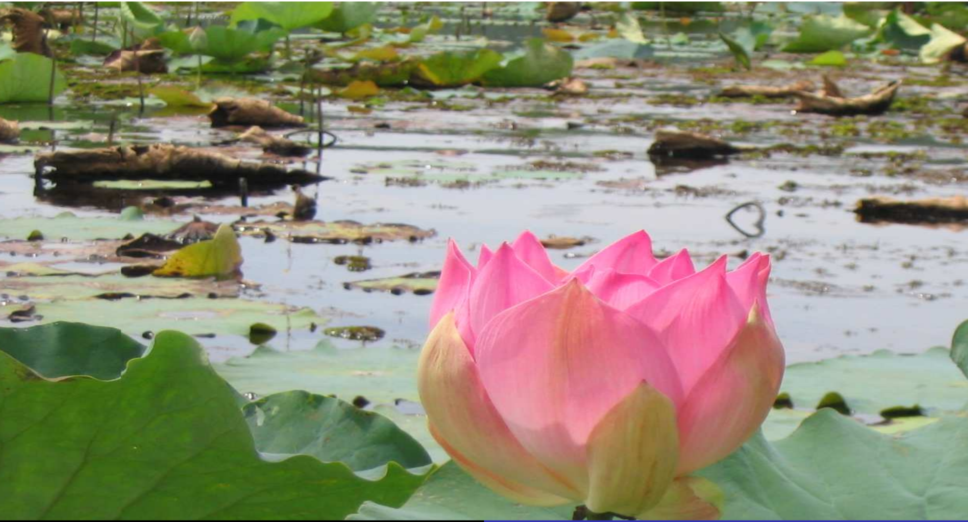


From *Big Lab on a Tiny Chip*, Charles Q. Choi, Scientific American, September 2007, 74 - 77



From *Big Lab on a Tiny Chip*, Charles Q. Choi, Scientific American, September 2007, 74 - 77

Example - Lotus Effect



Example - Lotus Effect

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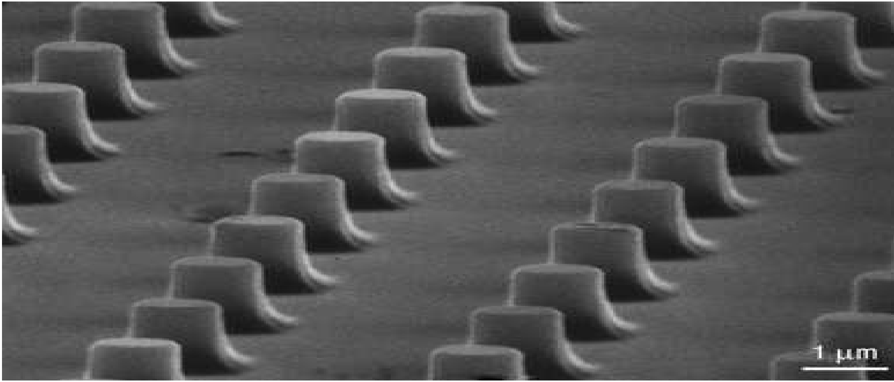


A designed rough surface, similar to a Fakir carpet

From *Self-cleaning surfaces — virtual realities*, Ralf Blossey, Nature Materials 2, 301 - 306 (2003)

Outline

PDE with Oscillatory coefficients

Let $\Omega \subset \mathbb{R}^2$, and

$$-\operatorname{div}[a^\epsilon(x)\,\nabla u_\epsilon] = f \quad \text{in } \Omega,$$
$$u_\epsilon = 0 \quad \text{on } \partial\Omega,$$

where $\epsilon \ll 1$ is the lenght scale of a^ϵ, and for some α_0 and α_1,

$$0 < \alpha_0 \le a^\epsilon(x) \le \alpha_1.$$

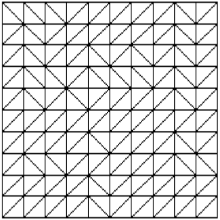
The weak solution $u_\epsilon \in H_0^1(\Omega)$ satisfies

$$a(u_\epsilon, v) = (f, v) \quad \text{for all } v \in H_0^1(\Omega),$$

where $a(u_\epsilon, v) = \int_\Omega a^\epsilon(x)\,\nabla u_\epsilon \cdot \nabla v$ and $(f, v) = \int_\Omega fv\,dx$.

Coarse Mesh

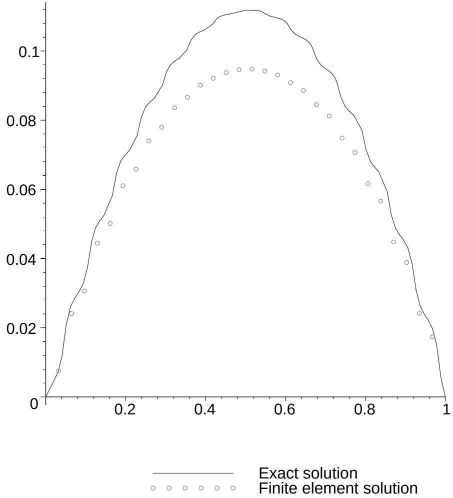
Consider a ϵ-independent partition of Ω into finite elements K:



Discretization

- nice

Then, unless mesh size $h \ll \epsilon$, classical finite element fails:



MsFEM Definition

Such method [Babuška, Caloz, Osborn, 1994], [Hou, Wu, Cai, Effendiev 1997, 1999, 2000, 2011, 2012] uses basis function that are elementwise solutions

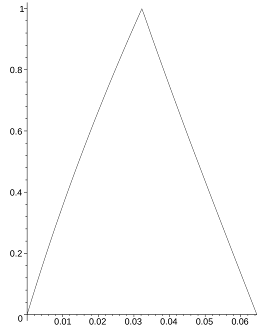
For the ith node of element K, ψ_i is such that

$$-\operatorname{div}[a^\epsilon \nabla \psi_i] = 0 \quad \text{in } K,$$

$$\psi_i|_{\partial K} \quad \text{linear}, \qquad \psi_i(\mathbf{x}_j) = \delta_{ij} \quad \text{for every node } \mathbf{x}_j$$

One-dimensional Multiscale Basis Functions

Multiscale basis functions for $\epsilon = 1/4$ and $h = 1/32$:



Similar to linear by parts since $h \ll \epsilon$.

One-dimensional Multiscale Basis Functions

For $\epsilon \ll h$ however:

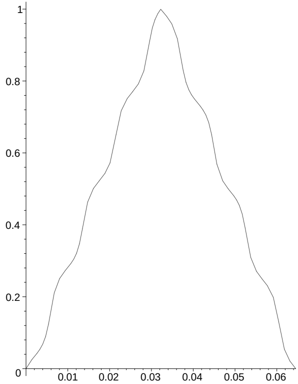
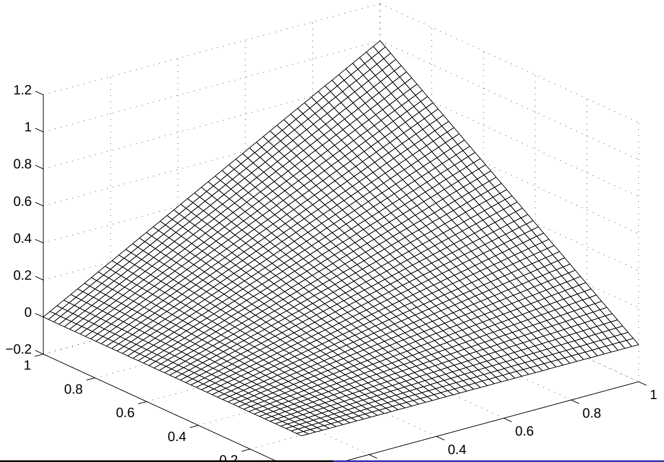


Figure: $\epsilon = 1/128$ e $h = 1/32$

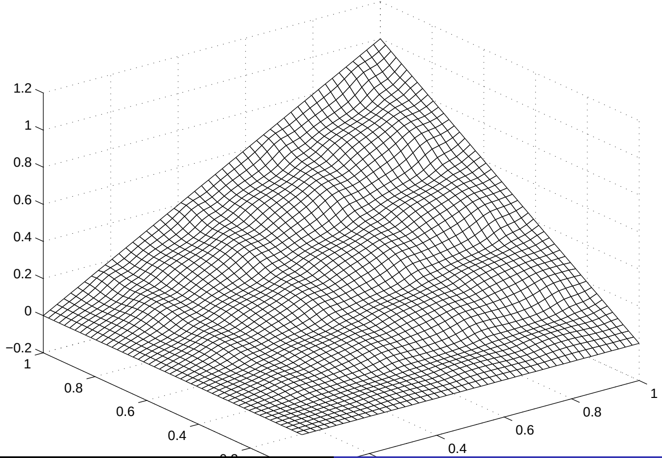
Two-dimensional Multiscale Basis Functions

For $h < \epsilon$, it looks like the bilinear:

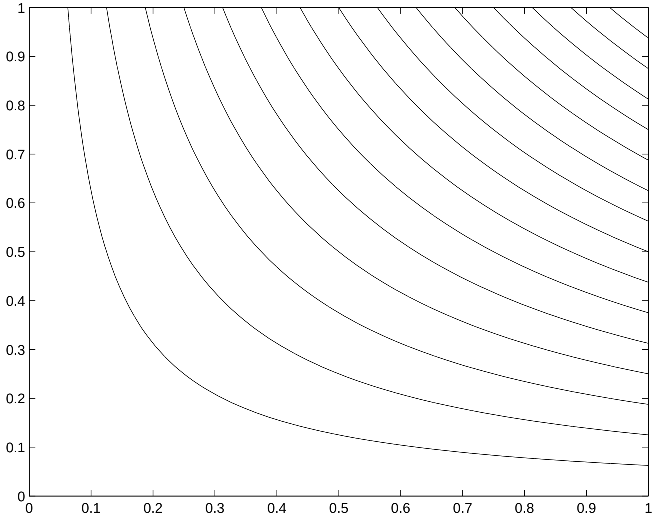


Two-dimensional Multiscale Basis Functions

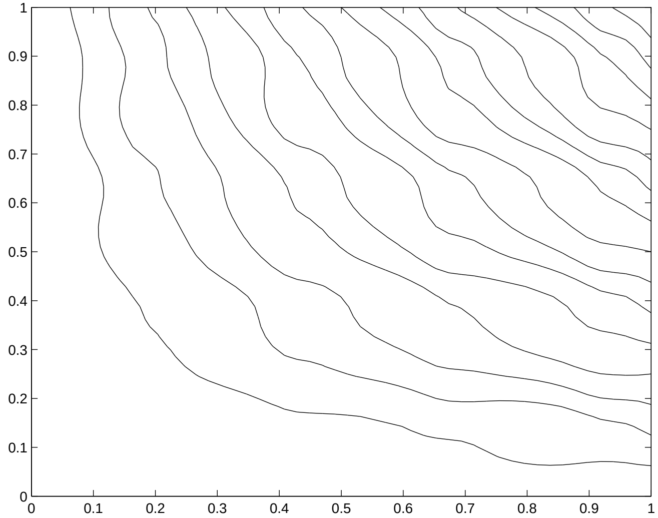
And for $\epsilon/h = 1/64$:



Level curves for $h < \epsilon$:



Level curves for $\epsilon \ll h$:



MsFEM Definition

Define the multiscale space

$$V_0^{h,\epsilon} = \text{span}\,\{\psi_1, \ldots, \psi_N\},$$

and the solution $u^{h,\epsilon} \in V_0^{h,\epsilon}$ is obtained by the Galerkin projection:

$$\int_\Omega \left(a^\epsilon(\mathbf{x}) \nabla u^{h,\epsilon}(\mathbf{x}) \nabla v^{h,\epsilon} \right) d\mathbf{x} = \int_\Omega f(\mathbf{x}) v^{h,\epsilon}(\mathbf{x})\, d\mathbf{x}$$

for all $v^{h,\epsilon} \in V_0^{h,\epsilon}$.

The error estimate:

$$\|u^\epsilon - u^{h,\epsilon}\|_{H^1(0,1)} \leq c(f)\left[h + (\epsilon/h)^{1/2}\right].$$

Note the sign of trouble if $\epsilon \approx h$.

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Residual Free Bubbles (RFB)

For many multiscale problems, the solution behaves as

$$u_{\text{sol}} = u_{\text{macro}} + u_{\text{micro}}$$

In the Residual Free Bubbles (RFB),

$$u_{\text{RFB}} = u_{linear} + u_b$$

where u_{linear} is the piecewise linear part, and the bubble u_b "captures" the microstructure.

Residual Free Bubbles (RFB)

Consider a nice partition of the domain into elements $\{K\}$ and add "bubbles" to the piecewise linears:

$$V_h := V_1 \oplus B,$$

where

- $V_1 \subset H_0^1(\Omega)$ is the space of piecewise linear functions
- $B = \oplus_K H_0^1(K)$ is the space of bubbles

The method looks for $u_h \in V_1 \oplus B$ such that

$$a(u_h, v_h) = (f, v_h) \quad \text{for all } v_h \in V_1 \oplus B.$$

Residual Free Bubbles (RFB)

Decomposing $u_h = u_1 + u_b \in V_1 \oplus B$, after some easy algebra:

$$a(u_1, v_1) + a(u_b, v_1) = (f, v_1) \quad \text{for all } v_1 \in V_1,$$

and for each element K:

$$\begin{aligned} -\operatorname{div}[\alpha_\epsilon(x)\nabla u_b] &= f + \operatorname{div}[\alpha_\epsilon(x)\nabla u_1] \quad \text{in } K, \\ u_b &= 0 \quad \text{on } \partial K, \end{aligned}$$

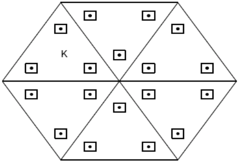
- Static condensation: write u_b in terms of u_1, yielding a formulation in terms of u_1 only
- For a^ϵ periodic: $\|u_\epsilon - u_h\|_{H^1(\Omega)} \leq c(\epsilon h^{-1/2} + h)$

Some Comments about RFB

- Formal framework induces the method, prone to parallelization
- Derivation based on problem's linearity
- Connections: Stabilized, Multiscale, and Variational Multiscale finite elements
- Lots of good work on RFB: reaction–advection–diffusion (Brezzi, Franca, M., Russo, Sangalli, Valentin, . . .), but also Helmholtz (Franca, Farhat, Lesoinne, Macedo, . . .)
- Oscillatory PDEs: converges as MsFEM (Sangalli)
- Numerics for nonlinear problem: Ramalho & Valentin

Heterogeneous Multiscale Method (HMM)

Aproximate $\int_K A \nabla V \cdot \nabla W$ by a "multiscale quadrature"



Given V linear find v_l such that

$$
\begin{aligned}
-\operatorname{div}[a^\epsilon(\mathbf{x}) \nabla v_l(\mathbf{x})] &= 0 \quad \text{in } I_\delta(\mathbf{x}_l), \\
v_l &= V \quad \text{on } \partial I_\delta(\mathbf{x}_l).
\end{aligned}
$$

Let $[A \nabla V \cdot \nabla W](\mathbf{x}_l) \approx \frac{1}{\delta} \int_{I_\delta(\mathbf{x}_l)} [a^\epsilon(\mathbf{x}) \nabla v_l(\mathbf{x})] \cdot \nabla w_l(\mathbf{x})\, d\mathbf{x}.$

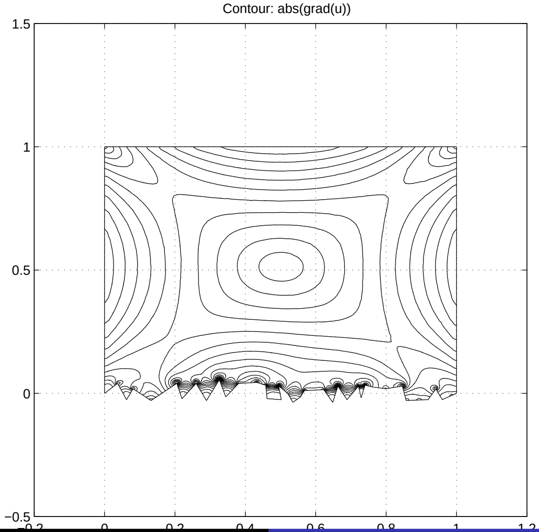
Comments on HMM

- Periodic case: $\|u_{\text{homog}} - u_{\text{HMM}}\|_{H^1(\Omega)} \leq c(h + \epsilon)$
- Several papers by Abdulle, E, Engquist, Huang, Ming, Li, Vanden-Eijnden, Vilmart, Yue, Zhang, from 2003 on

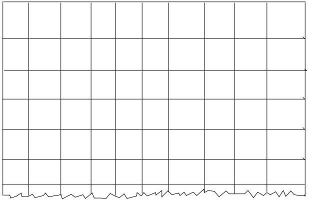
Outline

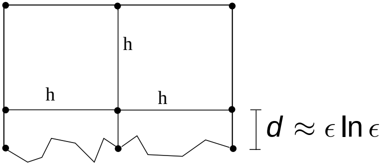
MsFEM: Oscillatory boundary

Absolute value of the gradient of the solution of $\Delta u^\epsilon = 1$:



"Coarse mesh" for Ω, and a patch of elements at the bottom:

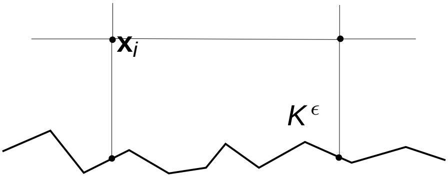




[M., 2009] proposes a Multiscale Finite Element Method.

Consider the basis functions $\lambda_i \in H_0^1(\Omega)$:

- $\lambda_i(\mathbf{x}_j) = \delta_{ij}$ at nodes $\mathbf{x}_j$.
- λ_i linear at edges
- λ_i bilinear at elements *not* intercepting the bottom



Impose

$$-\Delta\lambda_i = 0 \quad \text{in } K^\epsilon,$$
$$\lambda_i(\mathbf{x}_j) = \delta_{ij} \quad \text{for nodes } \mathbf{x}_j, \qquad \lambda_i \text{ linear on } \partial K^\epsilon \cap \Omega,$$
$$\lambda_i = 0 \quad \text{on } \partial\Omega.$$

Using such functions, we set $V_h^\epsilon = \text{span}\{\lambda_i\} \subset H_0^1(\Omega)$.

MsFEM soltn $u_h^\epsilon \in V_h^\epsilon$ is the Galerkin approximation of u^ϵ in V_h^ϵ:

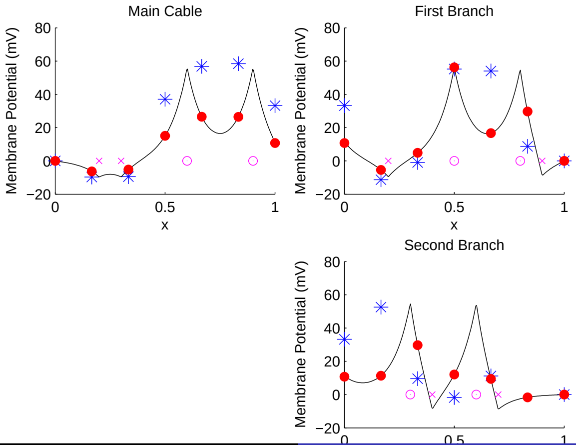
$$\int_\Omega u_h^\epsilon(\mathbf{x}) v_h(\mathbf{x})\, d\mathbf{x} = \int_\Omega f(\mathbf{x}) v_h(\mathbf{x})\, d\mathbf{x} \qquad \text{for all } v_h \in V_h^\epsilon.$$

Main Properties:

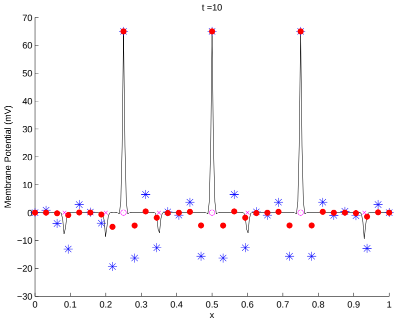
- Conforming method
- Local problems depend on ϵ
- Use of parallel computation to find basis functions
- Size of final system independent of ϵ
- Not restricted to periodic wrinkles
- Analysis of "periodic case": $\|u^\epsilon - u_h^\epsilon\|_{H^1(\Omega)} \le c(h + \epsilon h^{-1/2})$

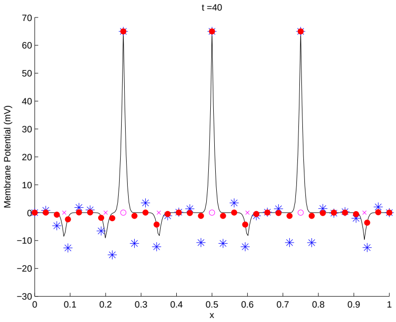
MsFEM: Neuroscience

Steady-state problem: reaction-diffusion equation with Dirac Deltas, in a Y-shapped domain

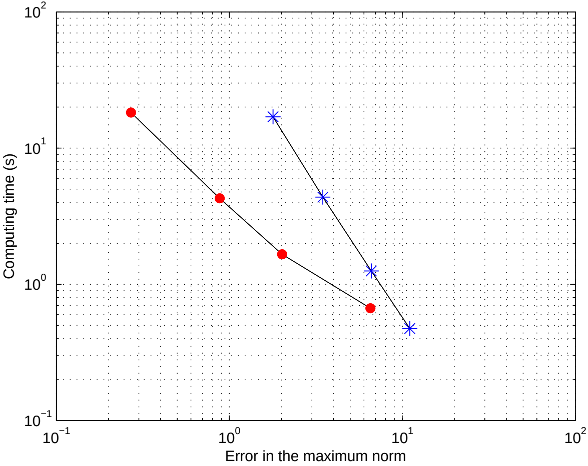


Transient Problem

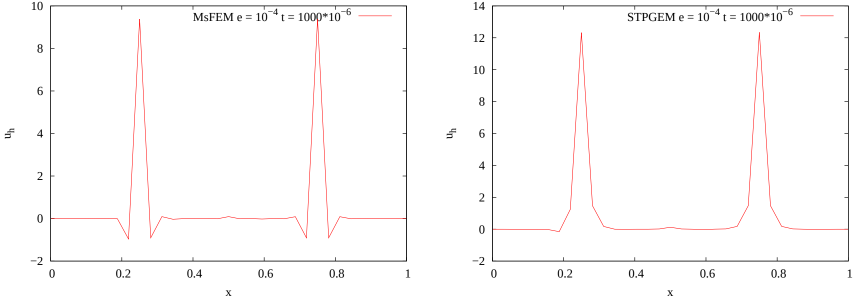




Transient Problem: computational costs



Eliminating further oscillations



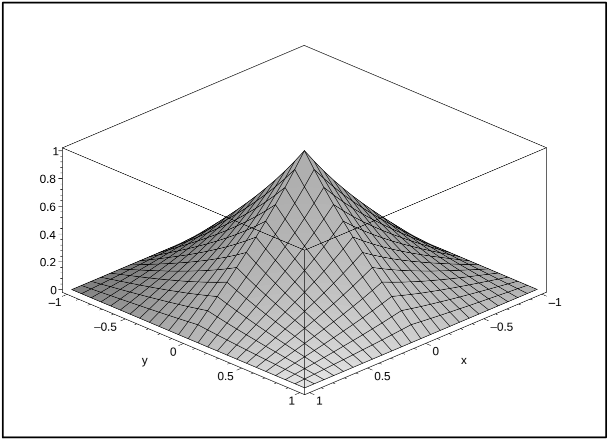
RFB: Reaction Diffusion

The problem

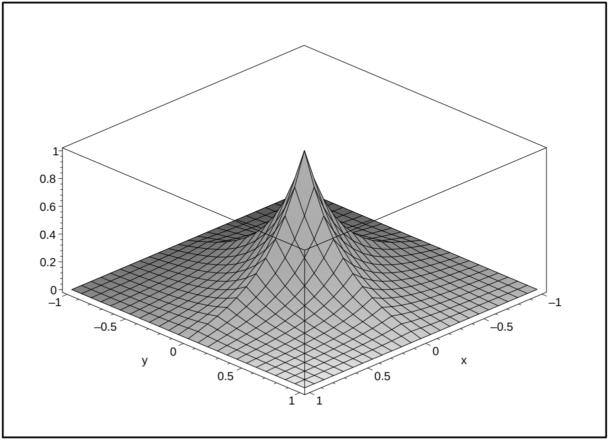
Consider Ω a polygon, $\epsilon > 0$ a small parameter, and

$$-\epsilon \Delta u + u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega,$$

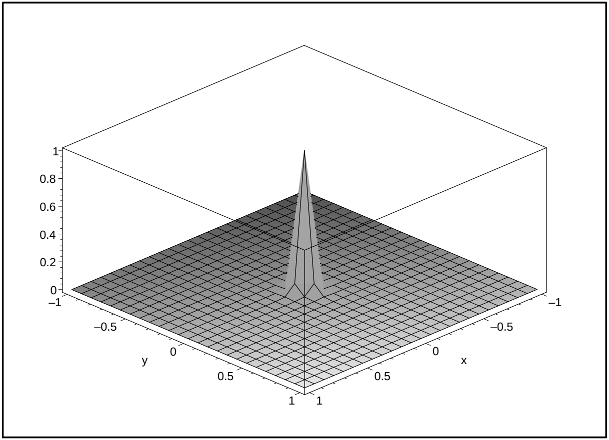
Typical basis functions θ for $\epsilon = 1.0$



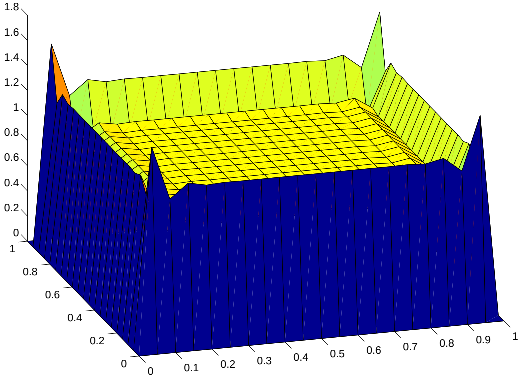
Typical basis functions θ for $\epsilon = 0.1$



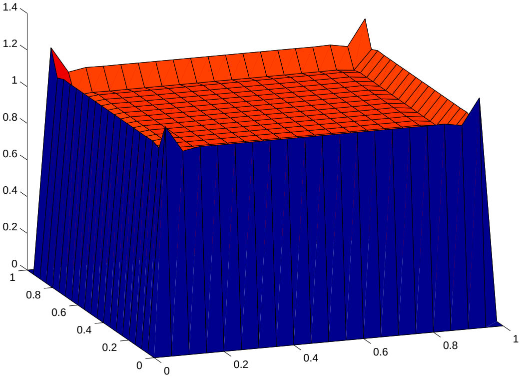
Typical basis functions θ for $\epsilon = 10^{-3}$



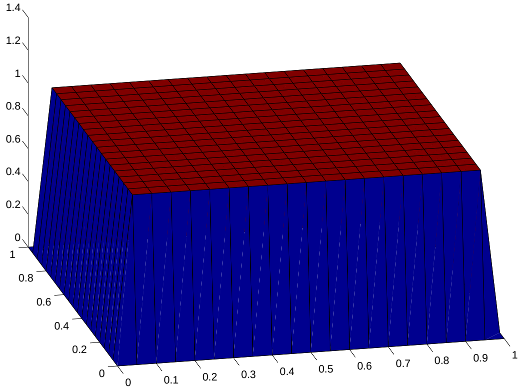
Piecewise Linear Galerkin ($\epsilon = 10^{-6}$):



RFB ($\epsilon = 10^{-6}$):

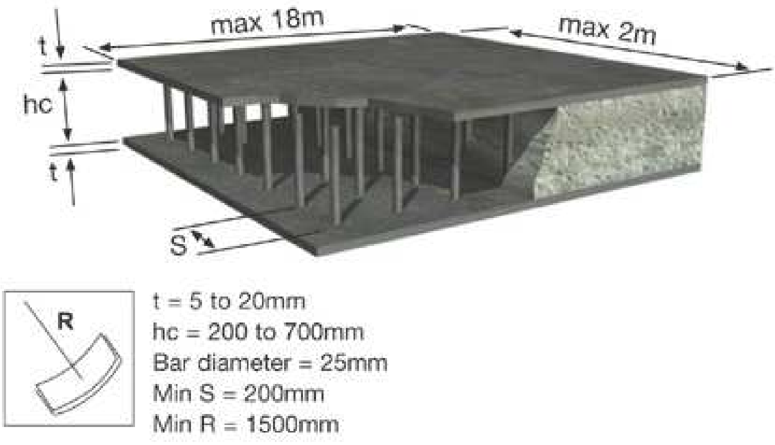


New Formulation ($\epsilon = 10^{-6}$):



RFB: Heterogeneous Plates

Linearized Elasticity in a heterogeneous Plate



www.tatasteelconstruction.com/

Numerics for an oscillatory Reissner-Mindlin model

Use dimensional reduction technique to obtain

$$-\frac{\delta^2}{3}\,\underset{\sim}{\mathbf{div}}\,\mathcal{C}^*\,\underset{\approx}{e}(\underset{\sim}{\phi}) + \lambda(\underset{\sim}{\phi} - \underset{\sim}{\nabla}\omega) = -\underset{\sim}{\boldsymbol{g}}^{odd} \quad \text{em } \Omega,$$

$$\lambda\,\text{div}(\underset{\sim}{\phi} - \underset{\sim}{\nabla}\omega) = g_3^{even} \quad \text{em } \Omega,$$

$$\underset{\sim}{\phi} = 0 \quad \omega = 0 \quad \text{on } \partial\Omega.$$

Special numerics needed

- Oscillatory coefficients along with numerical locking, for small thickness
- Helmholtz decomposition to obtain a Stokes-like system
- Bubbles to stabilize and capture the oscillations

Outline

1. Numerical Multiscale Modeling: motivations
2. Modern Numerical Methods
3. Not so real life applications
4. Nonlinear RFB
   - Complete version
   - Reduced version
5. Conclusions

The nonlinear version

Consider

$$-\operatorname{div}[\alpha_\epsilon(x) b(u_\epsilon) \nabla u_\epsilon] = f \quad \text{in } \Omega, \qquad u_\epsilon = 0 \quad \text{on } \partial\Omega,$$

where α_ϵ is uniformly bounded, and $b(\cdot)$ is nice and:

$$0 < b_0 \leq b(\cdot) \quad \text{in } \mathbb{R}. \tag{1}$$

Variacional formulation:

$$a(u_\epsilon, v) = (f, v) \quad \text{for all } v \in H_0^1(\Omega),$$

where $a(u, v) = \int_\Omega \alpha_\epsilon(x) b(u) \nabla u \cdot \nabla v \, dx$.

The RFB

Consider a partition of Ω into elements $\{K\}$, and again let $V_h = V_1 \oplus B$. Thus, $u_h = u_1 + u_b \in V_1 \oplus B$ solves

$$\int_\Omega \alpha_\epsilon(x) b(u_1+u_b)\,\nabla(u_1+u_b)\cdot\nabla\, v_1\,dx = \int_\Omega f v_1\,dx \quad \text{for all } v_1 \in V_1,$$

and for each element K:

$$-\operatorname{div}[\alpha_\epsilon(x) b(u_1+u_b)\,\nabla(u_1+u_b)] = f \quad \text{in } K, \ \text{for all elements } K,$$
$$u_b = 0 \quad \text{on } \partial K,$$

Theoretical results (J. Douglas, T. Dupont, J. Xu)

Theorem

- *Existence and uniqueness for the continuous problem*
- *RFB existence. RFB uniqueness for h small*
- *Cea's Lemma:* $\|u_\epsilon - u_h\|_{1,\Omega} \leq C\|u_\epsilon - w_h\|_{1,\Omega}$ *for all* $w_h \in V_h$

Proof.

- For existence: fixed point arguments (continuous and RFB)
- For uniqueness: Kirchhoff transform (continuous), and "robust stability" of the linearization (for RFB)
- For Cea: usual coercivity estimate, then duality estimates, then compactness w.r.t. h

□

How to linearize

So, $u_1 \in V_1$ and $u_b \in B$ solves

$$\int_\Omega \alpha_\epsilon(x) b(u_1 + u_b) \nabla(u_1 + u_b) \cdot \nabla v_1 \, dx = \int_\Omega f v_1 \, dx \quad \text{for all } v_1 \in V_1$$

$$-\operatorname{div}[\alpha_\epsilon(x) b(u_1 + u_b) \nabla(u_1 + u_b)] = f \quad \text{in } K, \text{ for all elements } K$$

First option: replace $b(u_h)$ by

- $b(\int_K u_h \, dx)$ (Hou, Efendiev, Ginting) or
- $b(u_h(x_K))$ for some $x_K \in K$ (Chen, Savchuk)

Other option

Fixed point approach: let $u_\epsilon^{n-1} \in H_0^1(\Omega)$, find $u_\epsilon^n \in H_0^1(\Omega)$ s.t.

$$\int_\Omega \alpha_\epsilon(x) b(u_\epsilon^{n-1}) \nabla(u_\epsilon^n) \cdot \nabla v \, dx = \int_\Omega fv \, dx \quad \text{for all } v \in H_0^1(\Omega).$$

Given $u_h^{n-1} \in V_h$, find $u_h^n \in V_h$ s.t.

$$\int_\Omega \alpha_\epsilon(x) b(u_h^{n-1}) \nabla(u_h^n) \cdot \nabla v_h \, dx = \int_\Omega fv_h \, dx \quad \text{for all } v_h \in V_h.$$

In the above scheme, *discretization* and *linearization* comutte

Theorem

$\lim_{n\to\infty} u_\epsilon^n = u_\epsilon$ *and* $\lim_{n\to\infty} u_h^n = u_h$.

Other option

Given $u_1^{n-1} \in V_1$ e $u_b^{n-1} \in V_b$, find $u_1^n \in V_1$ e $u_b^n \in V_b$ s.t.

$$\int_\Omega \alpha_\epsilon(x) b(u_1^{n-1} + u_b^{n-1}) \nabla(u_1^n + u_b^{n-1}) \cdot \nabla v_h \, dx = \int_\Omega f v_h \, dx ,$$

$$-\operatorname{div}[\alpha_\epsilon(x) b(u_1^n + u_b^{n-1}) \nabla(u_1^n + u_b^n)] = f \quad \text{em } K ,$$

for all $v_h \in V_h$ and all K.

That's nice:

Note that it's easy to iterate.

Reduced Version

Use that $b(u_1 + u_b) \approx b(u_1)$:

$$\int_\Omega \alpha_\epsilon(x) b(u_1)\, \nabla(u_1 + u_b) \cdot \nabla v \, dx = (f, v) \quad \forall v \in V_1$$

and

$$-\operatorname{div}[\alpha_\epsilon(x) b(u_1)\, \nabla u_b] = f + \operatorname{div}[\alpha_\epsilon(x) b(u_1)\, \nabla u_1] \quad \text{in } K$$

Theorem

- *Existence and uniqueness for the reduced version.*
- *For periodic α_ϵ, let $u \in H_0^1(\Omega) \cap W^{2,\infty}(\Omega)$ be the homogenized solution. For $\epsilon \ll h \ll 1$:*

$$\|u - u_1\|_{1,\Omega} \leq C\left(\sqrt{\frac{\epsilon}{h}} + h\right).$$

- Extended the RFB for noninear multiscale problems
- Cea’s Lemma for the *full version*
- Convergence to the homogenized solution for the *reduced version*

Outline

- Both RFB and MsFEM are powerfull methodologies for both linear and nonlinear problems
- Both methods have parallelization at their DNAs

Merci!