Multiscale Problems and Methods

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- Pedro Pinheiro
- Lutz Tobiska
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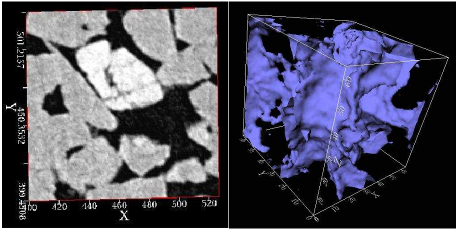
Outline

Outline

Example - Porous media flow

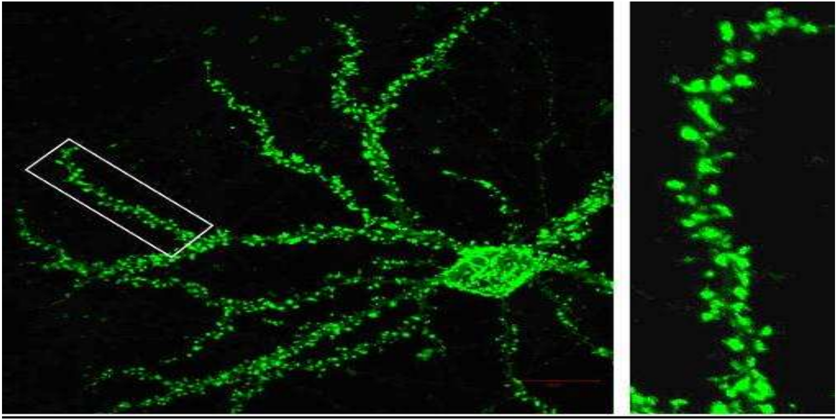


http://ccs.chem.ucl.ac.uk/research/

Water and oil flow in a porous rock

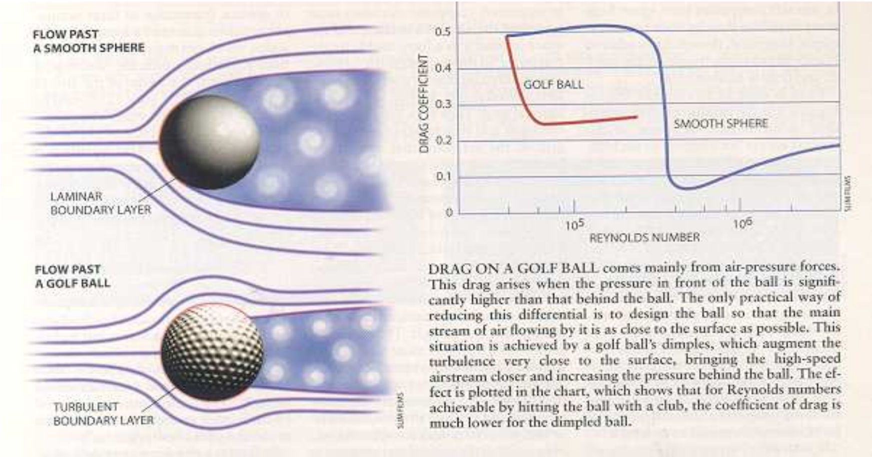
- X-ray microtomography to describe geometry (5 microns resolution)
- Computacional mesh with more than 100 millions nodes

Example - dendrites with synapses



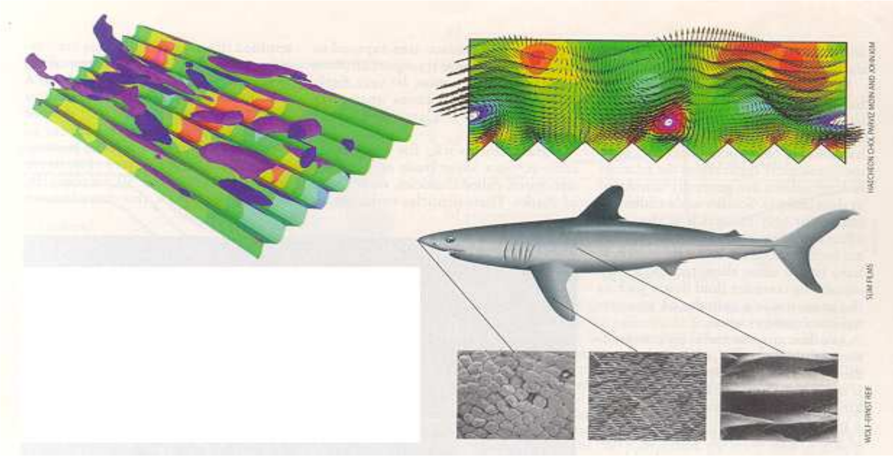
http://www.bristol.ac.uk/anatomy/research/staff/hanley.html

Example - Flows over Rough Surfaces

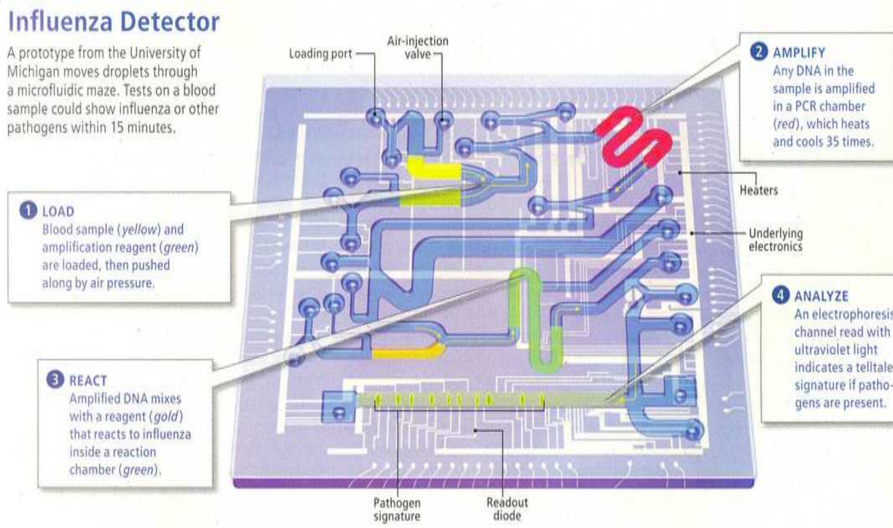


Source: Scientific America

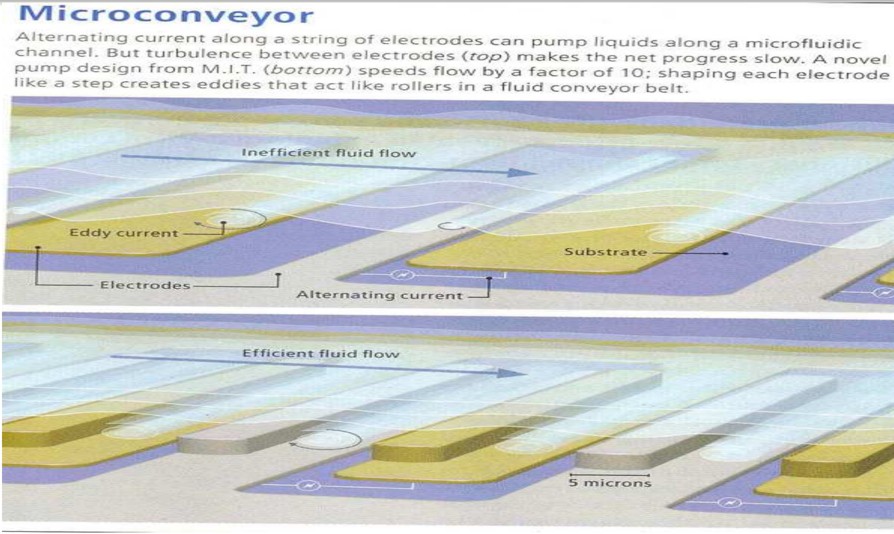
Example - Flows over Rough Surfaces



Source: Scientific America



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



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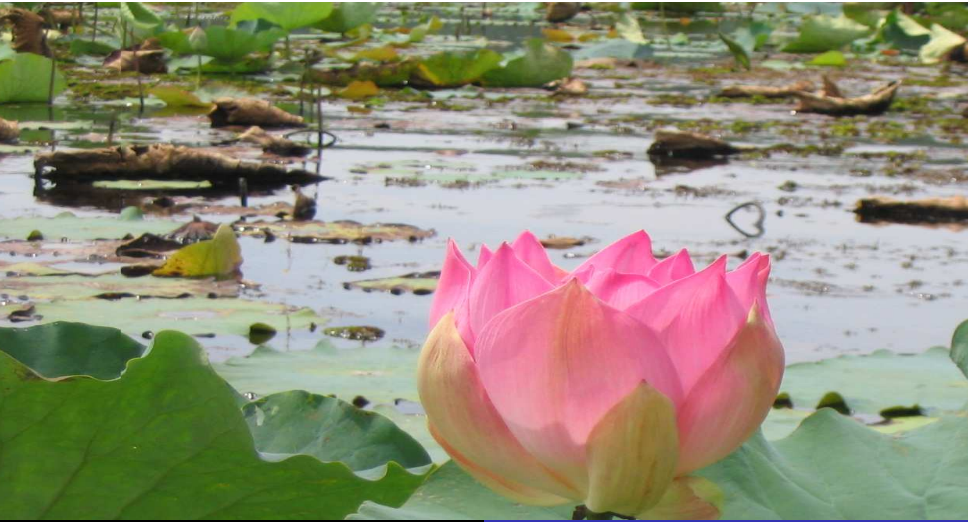
Example - Lotus Effect



Example - Lotus Effect

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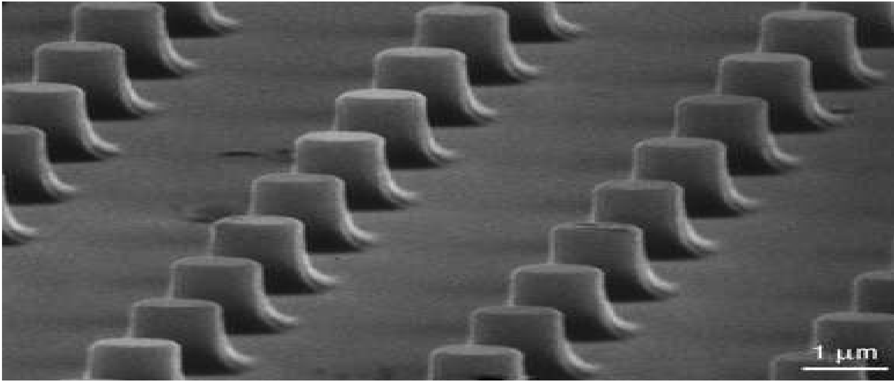


A designed rough surface, similar to a Fakir carpet

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

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

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

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

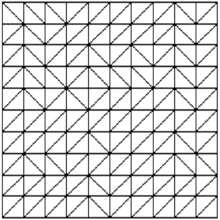
The weak solution $u_\epsilon \in H_0^1(\Omega)$ satisfies

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

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

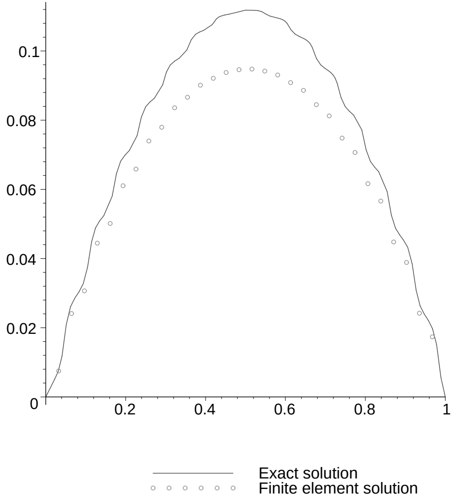
Consider a ϵ-independent partition of Ω into finite elements K:



Discretization

- nice

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



MsFEM Definition

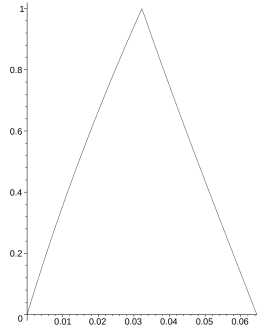
Such method [Babuška, Caloz, Osborn, 1994], [Hou, Wu, Cai, Effendiev 1997, 1999, 2000, 2011, 2012] uses basis function that are elementwise solutions

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:

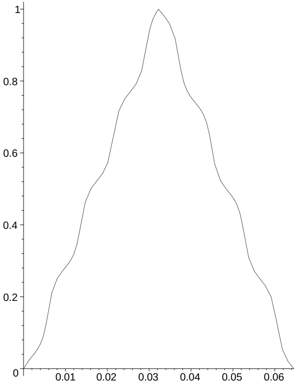
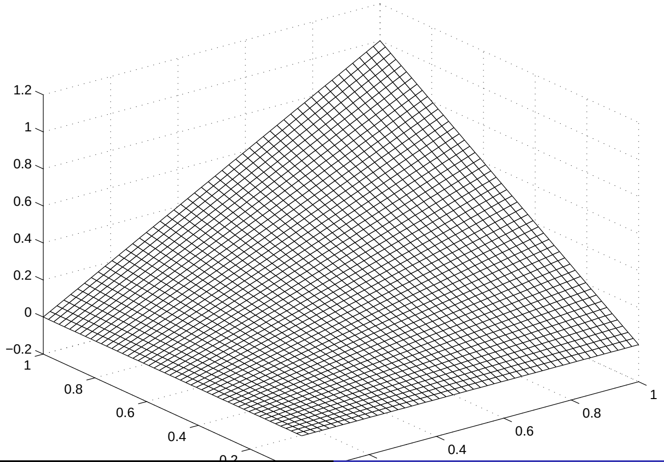


Figure: $\epsilon = 1/128$ e $h = 1/32$

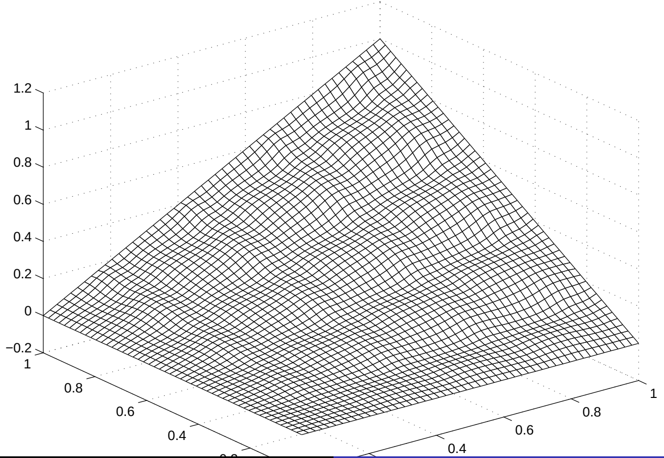
Two-dimensional Multiscale Basis Functions

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

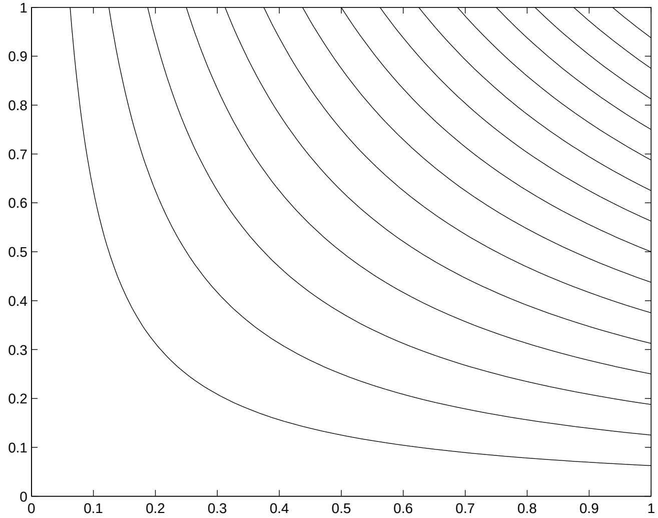


Two-dimensional Multiscale Basis Functions

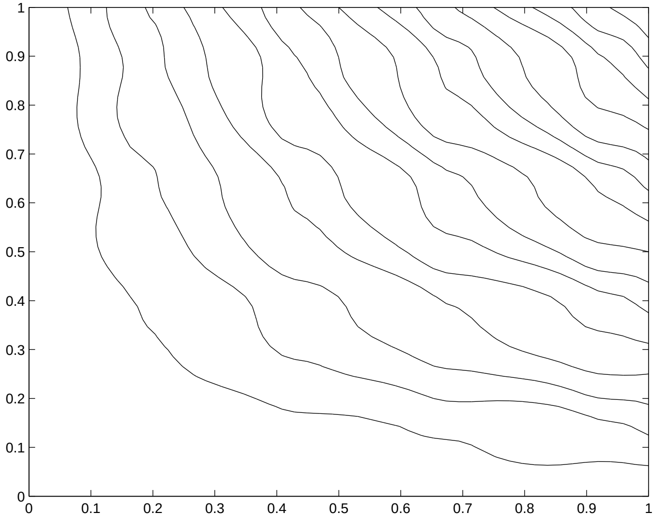
And for $\epsilon/h = 1/64$:



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

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

In the Residual Free Bubbles (RFB),

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

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:

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

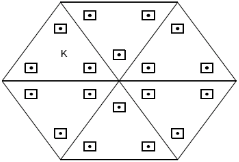
- Static condensation: write u_b in terms of u_1, yielding a formulation in terms of u_1 only
- For a^ϵ periodic: $\|u_\epsilon - u_h\|_{H^1(\Omega)} \le c(\epsilon h^{-1/2} + h)$

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

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

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

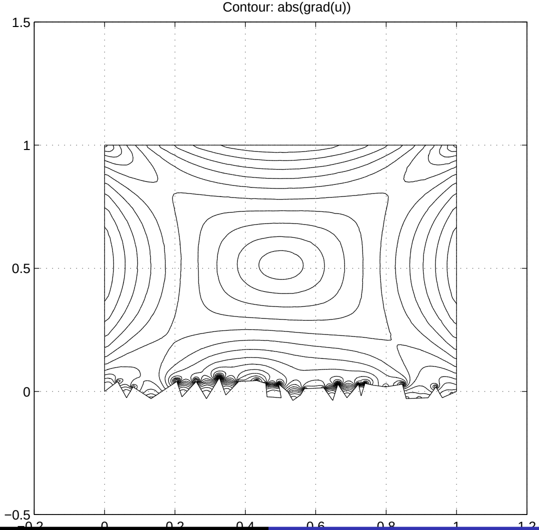
- Periodic case: $\|u_{\text{homog}} - u_{\text{HMM}}\|_{H^1(\Omega)} \leq c(h+\epsilon)$
- Several papers by Abdulle, E, Engquist, Huang, Ming, Li, Vanden-Eijnden, Vilmart, Yue, Zhang, from 2003 on

Outline

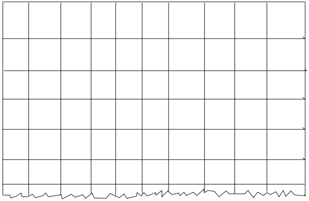
1. Numerical Multiscale Modeling: motivations
2. Modern Numerical Methods
3. Not so real life applications
   - MsFEM: Oscillatory boundary
   - MsFEM: Neuroscience
   - RFB: Reaction Diffusion
   - RFB: Heterogeneous Plates
4. Nonlinear RFB
5. Conclusions

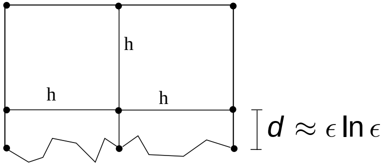
MsFEM: Oscillatory boundary

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:

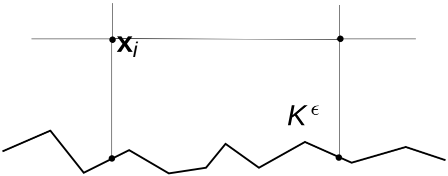




[M., 2009] proposes a Multiscale Finite Element Method.

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:

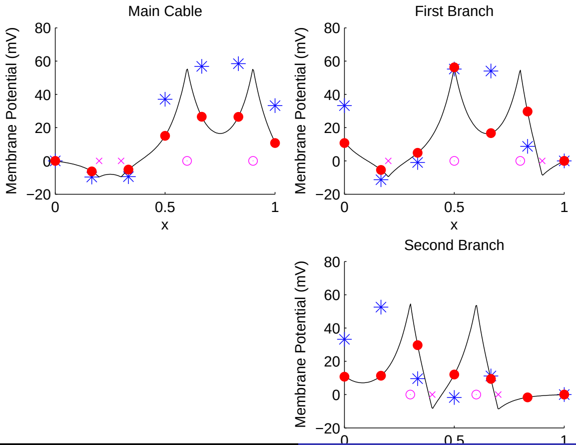
- Conforming method
- Local problems depend on ϵ
- Use of parallel computation to find basis functions
- Size of final system independent of ϵ
- Not restricted to periodic wrinkles
- Analysis of "periodic case": $\|u^\epsilon - u_h^\epsilon\|_{H^1(\Omega)} \leq c(h + \epsilon h^{-1/2})$

MsFEM: Neuroscience

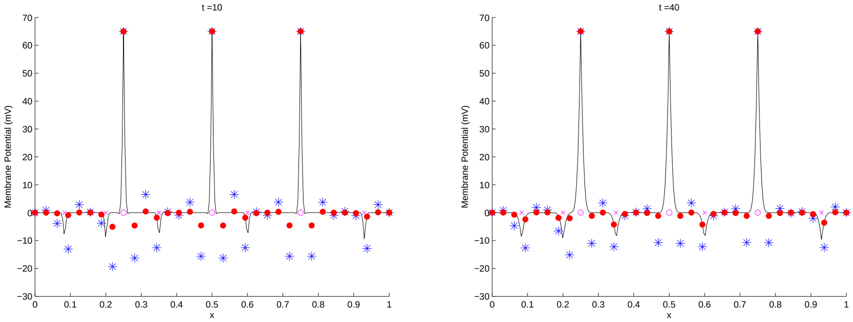
Joint with

- Honório Fernando
- Daniele Madureira
- Pedro Pinheiro
- Matheus Rinaldi
- Frédéric Valentin

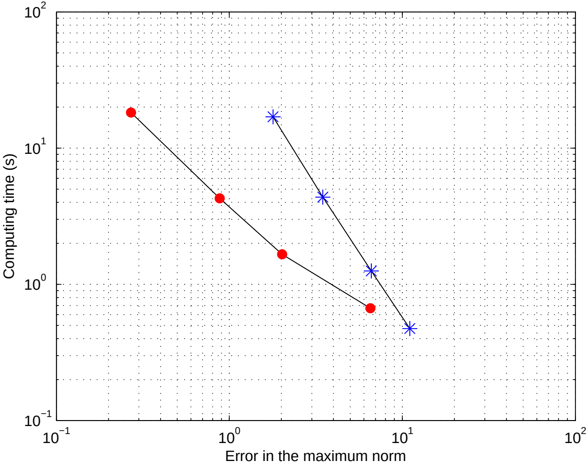
Steady-state problem: reaction-diffusion equation with Dirac Deltas, in a Y-shapped domain



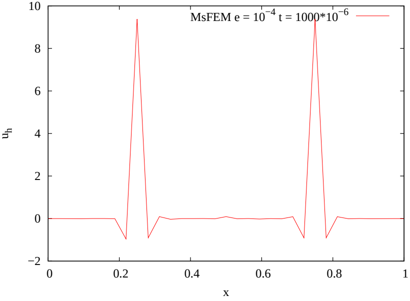
Transient Problem

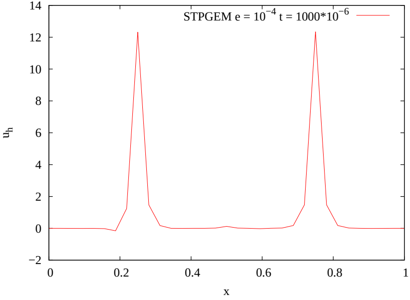


Transient Problem: computational costs

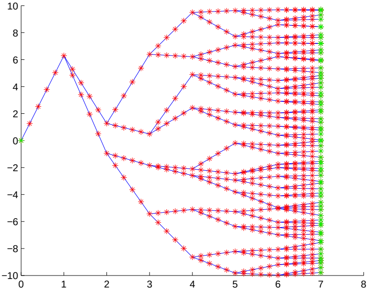


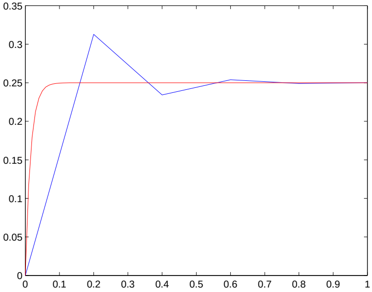
Eliminating further oscillations





Modeling dendritic trees





RFB: Reaction Diffusion

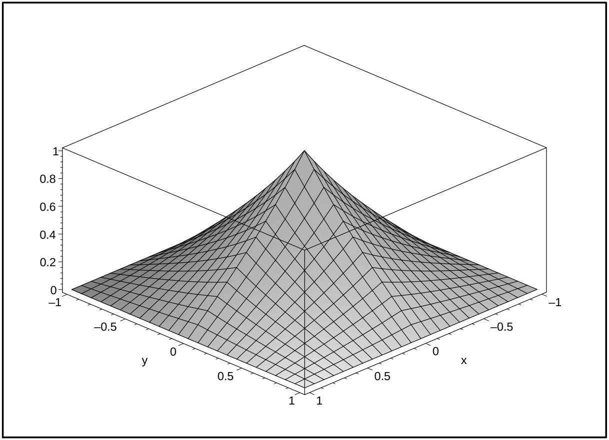
(joint with F. Valentin)

The problem

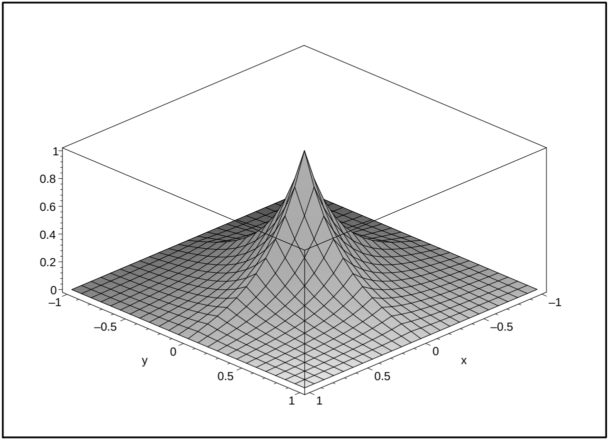
Consider Ω a polygon, $\epsilon > 0$ a small parameter, and

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

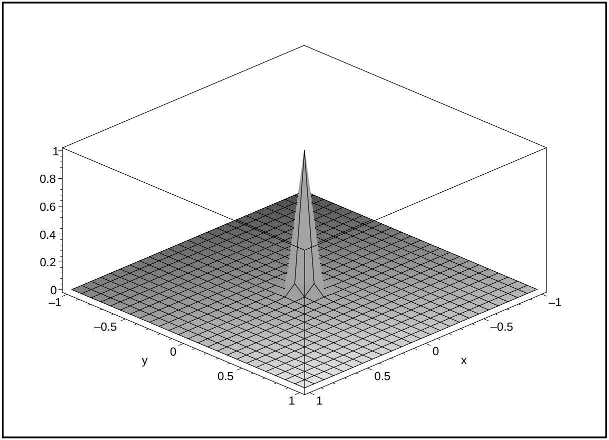
Typical basis functions θ for $\epsilon = 1.0$



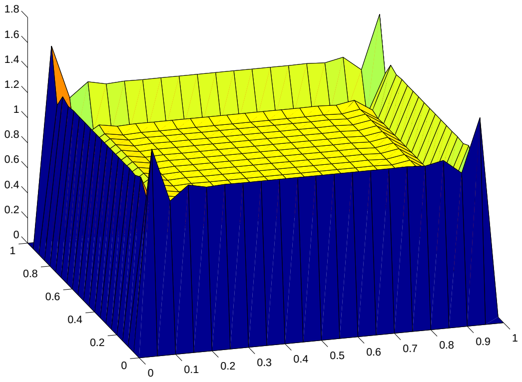
Typical basis functions θ for $\epsilon = 0.1$



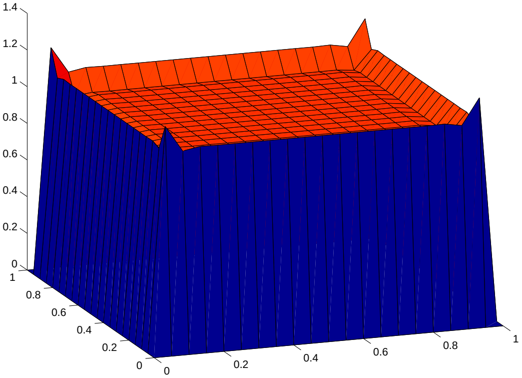
Typical basis functions θ for $\epsilon = 10^{-3}$



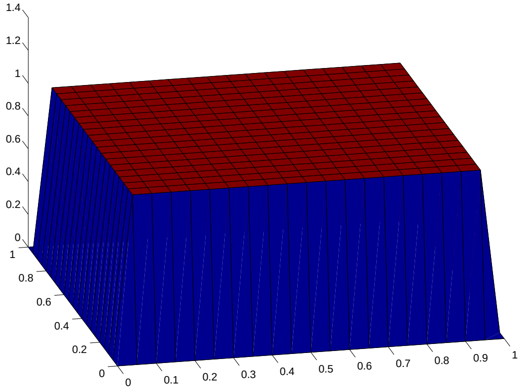
Piecewise Linear Galerkin ($\epsilon = 10^{-6}$):



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



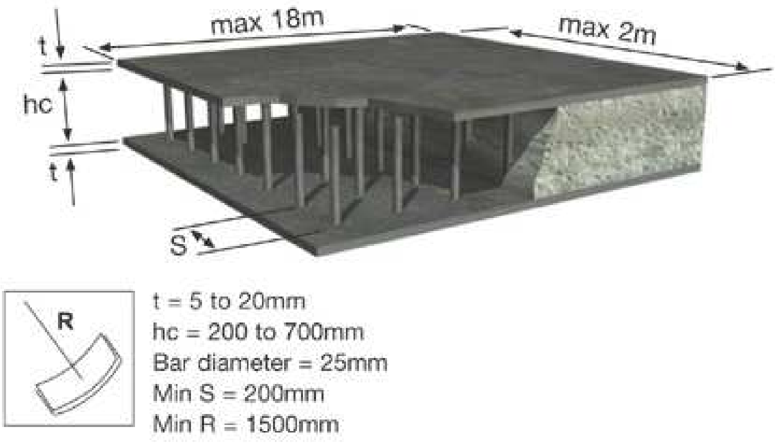
New Formulation ($\epsilon = 10^{-6}$):



RFB: Heterogeneous Plates

(joint with A. Carius)

Linearized Elasticity in a heterogeneous Plate



www.tatasteelconstruction.com/

The Romans knew:

Numerics for an oscillatory Reissner-Mindlin model

Use dimensional reduction technique to obtain

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

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

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

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

The nonlinear version (with M. Barreda)

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:

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

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

$\square$

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

Obrigado!