

Multiscale Problems and Methods

Alexandre Madureira
www.lncc.br/~alm

Laboratório Nacional de Computação Científica – LNCC

Brazil–France Workshop on HPC
September 10–13, 2012

Joint with

- Manuel Barreda
- Ana Carolina Carius
- Honório Fernando
- Leopoldo Franca
- Daniele Madureira
- Pedro Pinheiro
- Lutz Tobiska
- Frédéric Valentin

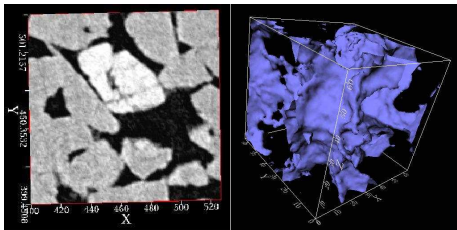
Outline

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

Outline

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

Example - Porous media flow

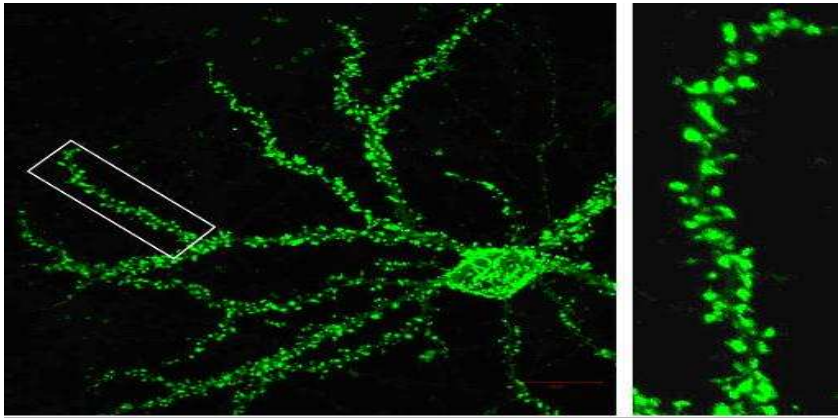


<http://ccs.chem.ucl.ac.uk/research/>

Water and oil flow in a porous rock

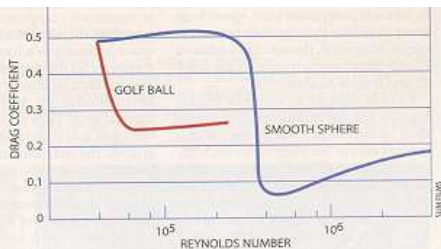
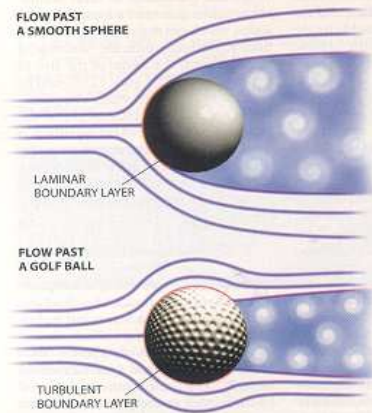
- X-ray microtomography to describe geometry (5 microns resolution)
- Computational mesh with more than 100 millions nodes

Example - dendrites with synapses



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

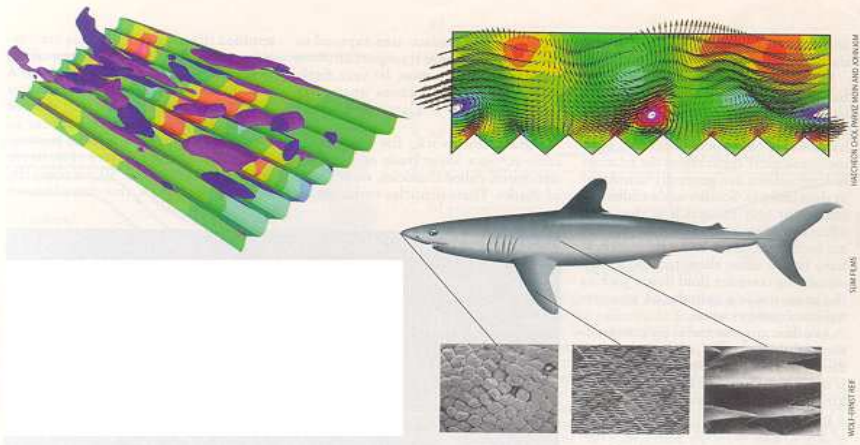
Example - Flows over Rough Surfaces



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

Influenza Detector

A prototype from the University of Michigan moves droplets through a microfluidic maze. Tests on a blood sample could show influenza or other pathogens within 15 minutes.

1 LOAD

Blood sample (*yellow*) and amplification reagent (*green*) are loaded, then pushed along by air pressure.

3 REACT

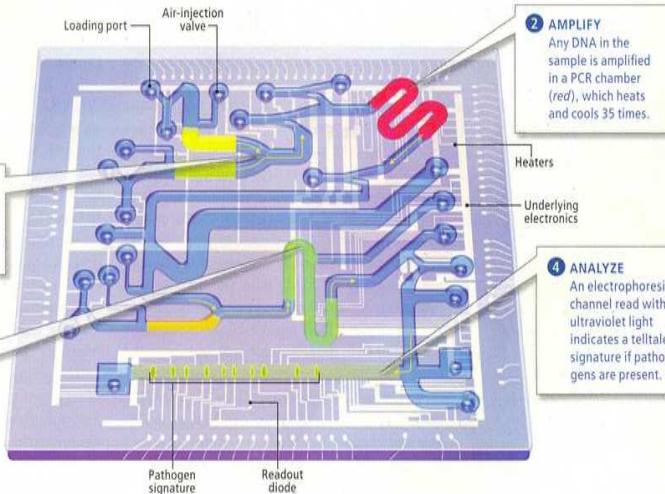
Amplified DNA mixes with a reagent (*gold*) that reacts to influenza inside a reaction chamber (*green*).

2 AMPLIFY

Any DNA in the sample is amplified in a PCR chamber (*red*), which heats and cools 35 times.

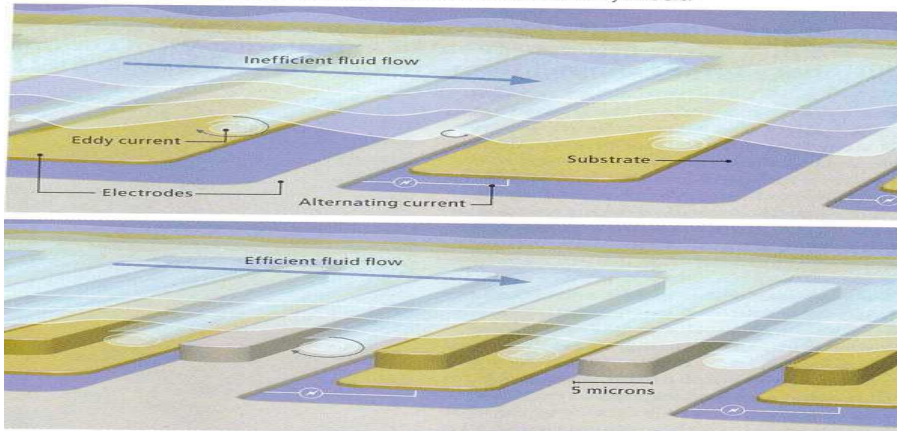
4 ANALYZE

An electrophoresis channel read with ultraviolet light indicates a telltale signature if pathogens are present.



Microconveyor

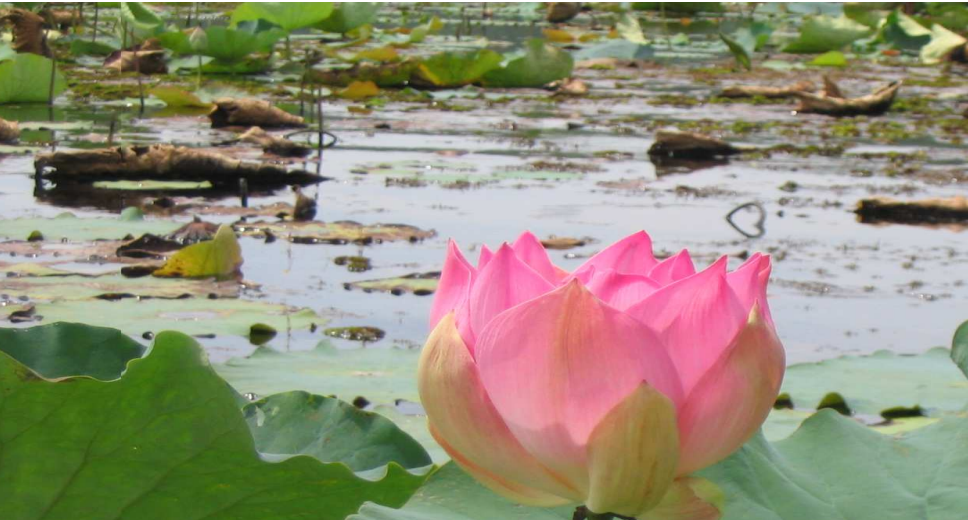
Alternating current along a string of electrodes can pump liquids along a microfluidic channel. But turbulence between electrodes (*top*) makes the net progress slow. A novel pump design from M.I.T. (*bottom*) speeds flow by a factor of 10; shaping each electrode like a step creates eddies that act like rollers in a fluid conveyor belt.



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

Numerical Multiscale Modeling: motivations
Modern Numerical Methods
Not so real life applications
Nonlinear RFB
Conclusions

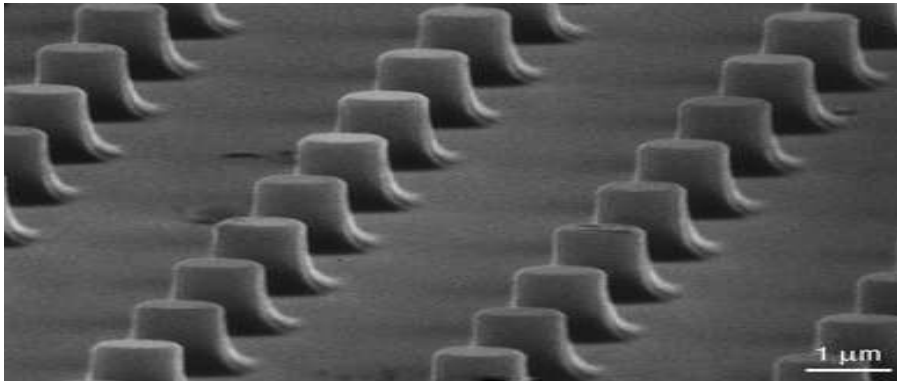
Example - Lotus Effect



Example - Lotus Effect



Example - Lotus Effect



A designed rough surface, similar to a Fakir carpet

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

Outline

- 1 Numerical Multiscale Modeling: motivations
- 2 Modern Numerical Methods**
 - A model PDE
 - Multiscale Finite Elements (MsFEM)
 - Linear RFB
 - Heterogeneous Multiscale Method (HMM)
- 3 Not so real life applications
- 4 Nonlinear RFB
- 5 Conclusions

PDE with Oscillatory coefficients

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

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

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

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

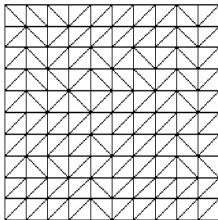
The weak solution $u_\epsilon \in H_0^1(\Omega)$ satisfies

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

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

Coarse Mesh

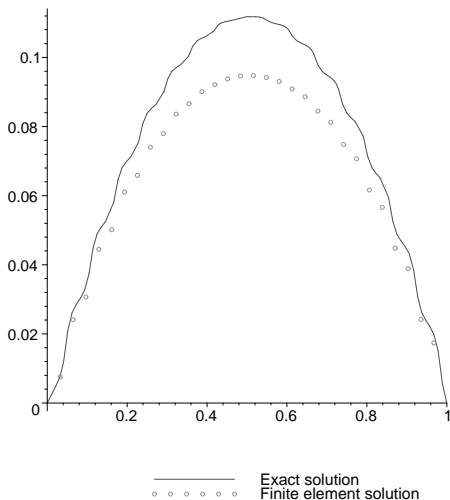
Consider a ϵ -independent partition of Ω into finite elements K :



Discretization

- nice

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



MsFEM Definition

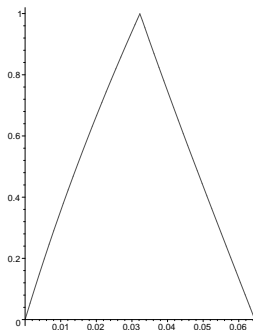
Such method [Babuška, Caloz, Osborn, 1994], [Hou, Wu, Cai, Effendiev 1997, 1999, 2000, 2011, 2012] uses basis function that are elementwise solutions

For the i th node of element K , ψ_i is such that

$$\begin{aligned} -\operatorname{div}[\mathbf{a}^\epsilon \nabla \psi_i] &= 0 \quad \text{in } K, \\ \psi_i|_{\partial K} &\text{ linear,} \quad \psi_i(\mathbf{x}_j) = \delta_{ij} \quad \text{for every node } \mathbf{x}_j \end{aligned}$$

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:

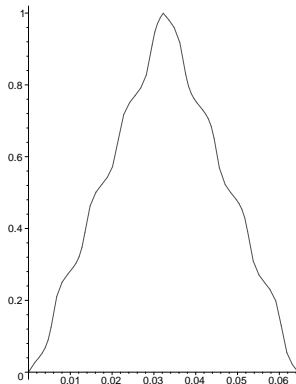
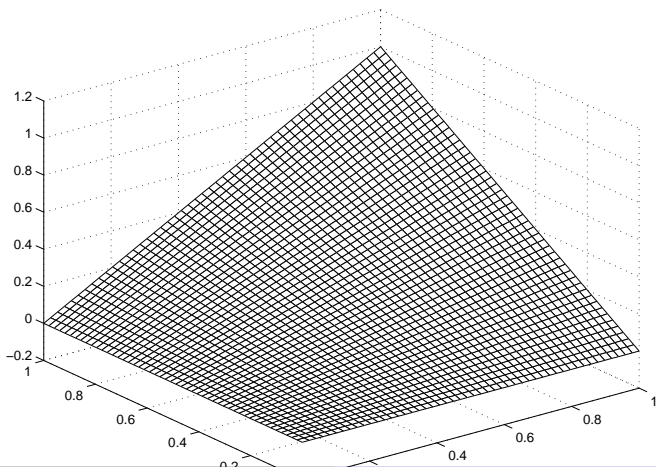


Figure: $\epsilon = 1/128$ e $h = 1/32$

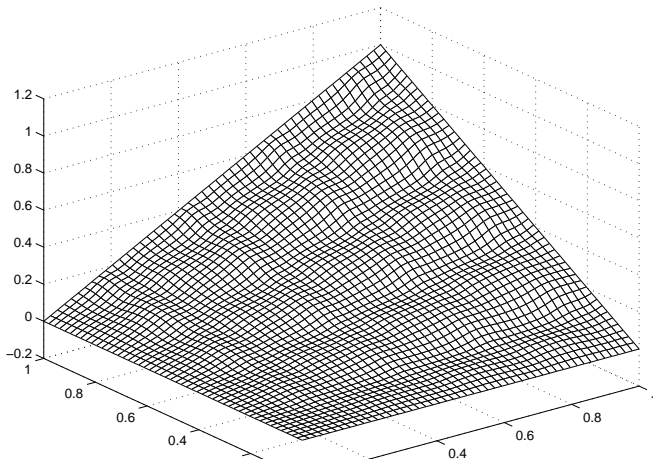
Two-dimensional Multiscale Basis Functions

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

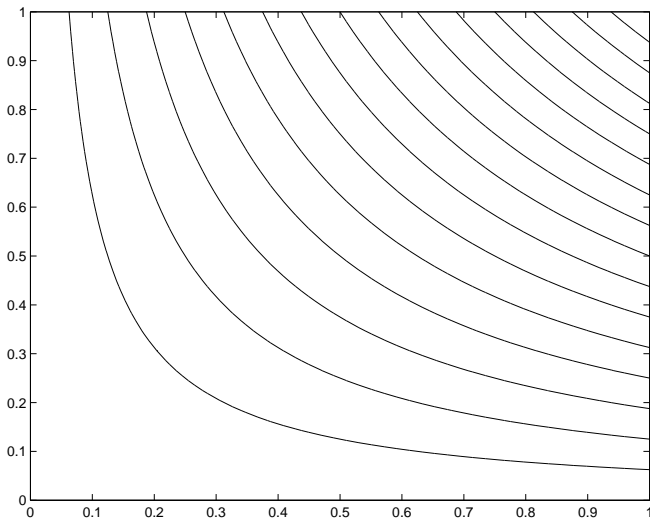


Two-dimensional Multiscale Basis Functions

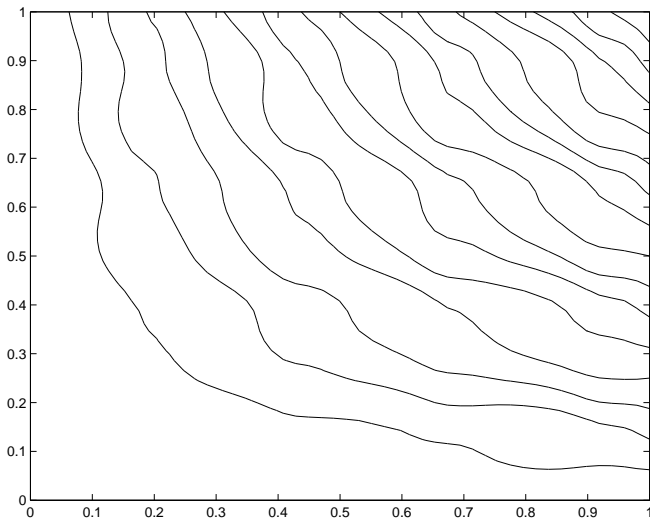
And for $\epsilon/h = 1/64$:



Level curves for $h < \epsilon$:



Level curves for $\epsilon \ll h$:



MsFEM Definition

Define the multiscale space

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

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

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

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

The error estimate:

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

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

MsFEM Definition

Define the multiscale space

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

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:

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

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

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),

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

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
- $B = \bigoplus_K H_0^1(K)$ 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 :

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

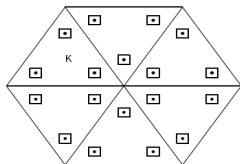
- Static condensation: write u_b in terms of u_1 , yielding a formulation in terms of u_1 only
- For a^ϵ periodic: $\|u_\epsilon - u_h\|_{H^1(\Omega)} \leq c(\epsilon h^{-1/2} + h)$

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)

Approximate $\int_K A \nabla V \cdot \nabla W$ 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

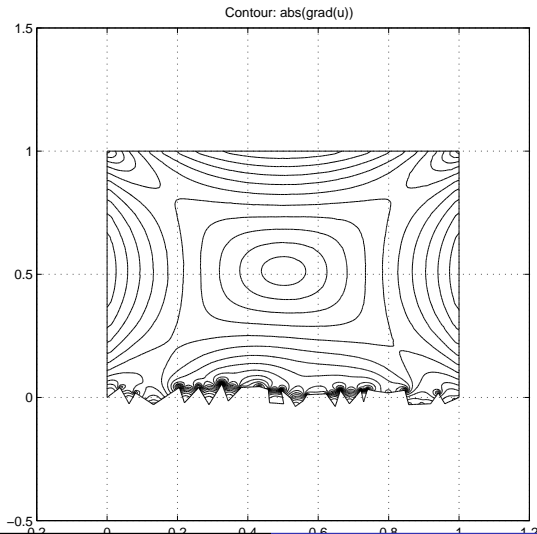
- Periodic case: $\|u_{\text{homog}} - u_{\text{HMM}}\|_{H^1(\Omega)} \leq c(h + \epsilon)$
- Several papers by Abdulle, E, Engquist, Huang, Ming, Li, Vanden-Eijnden, Vilmart, Yue, Zhang, from 2003 on

Outline

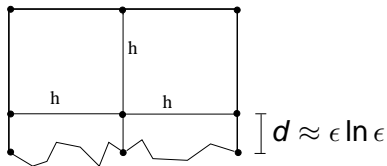
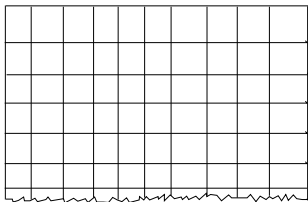
- 1 Numerical Multiscale Modeling: motivations
- 2 Modern Numerical Methods
- 3 Not so real life applications**
 - MsFEM: Oscillatory boundary
 - MsFEM: Neuroscience
 - RFB: Reaction Diffusion
 - RFB: Heterogeneous Plates
- 4 Nonlinear RFB
- 5 Conclusions

MsFEM: Oscillatory boundary

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



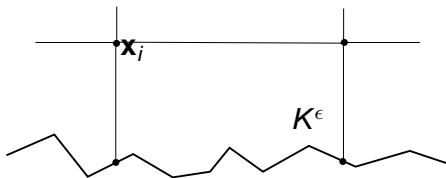
"Coarse mesh" for Ω , and a patch of elements at the bottom:



[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

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

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 :

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

Main Properties:

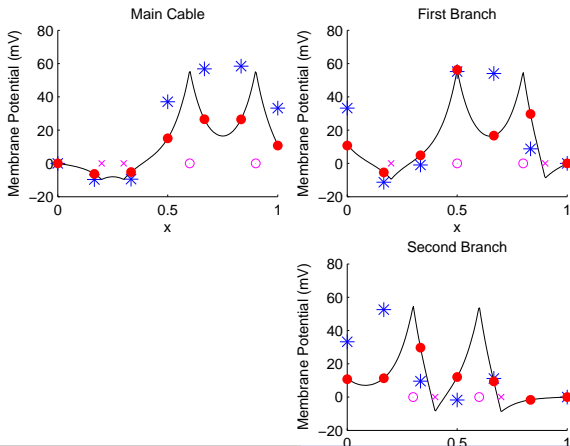
- Conforming method
- Local problems depend on ϵ
- Use of parallel computation to find basis functions
- Size of final system independent of ϵ
- Not restricted to periodic wrinkles
- Analysis of "periodic case": $\|u^\epsilon - u_h^\epsilon\|_{H^1(\Omega)} \leq c(h + \epsilon h^{-1/2})$

MsFEM: Neuroscience

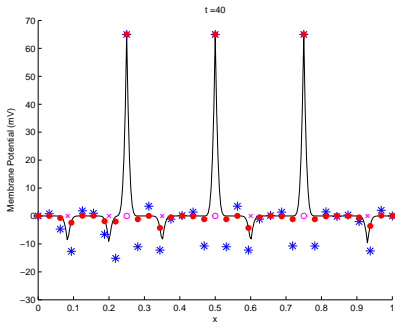
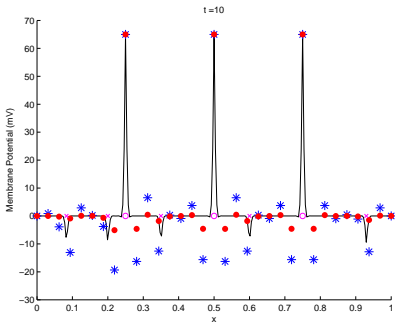
Joint with

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

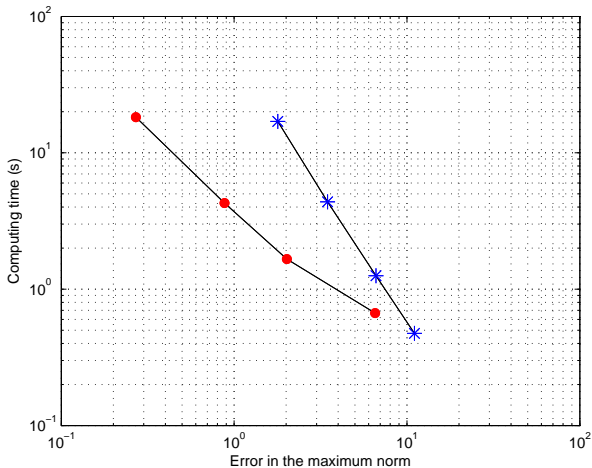
Steady-state problem: reaction-diffusion equation with Dirac Deltas, in a Y-shaped domain



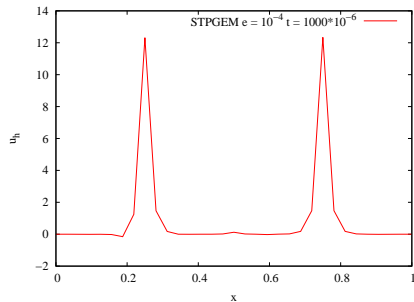
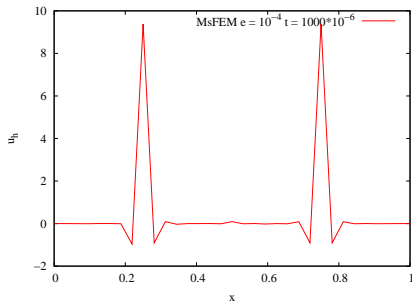
Transient Problem



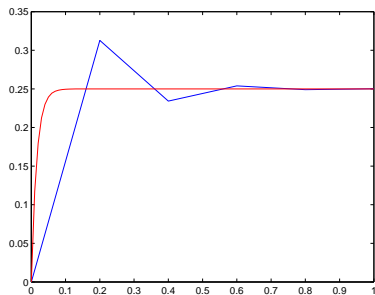
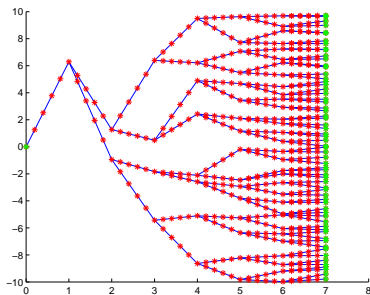
Transient Problem: computational costs



Eliminating further oscillations



Modeling dendritic trees



RFB: Reaction Diffusion

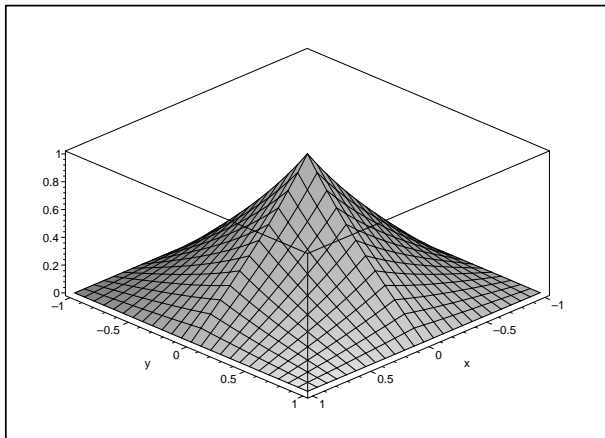
(joint with F. Valentin)

The problem

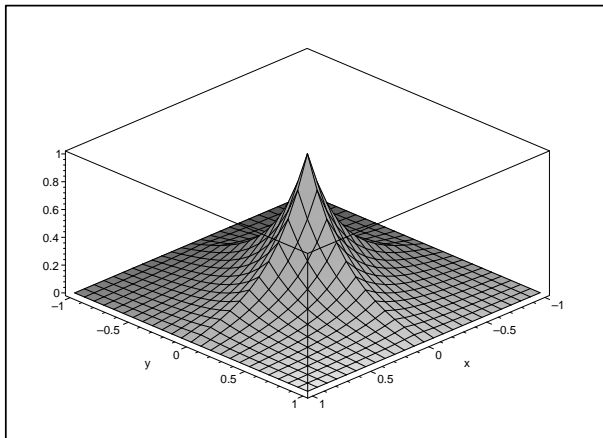
Consider Ω a polygon, $\epsilon > 0$ a small parameter, and

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

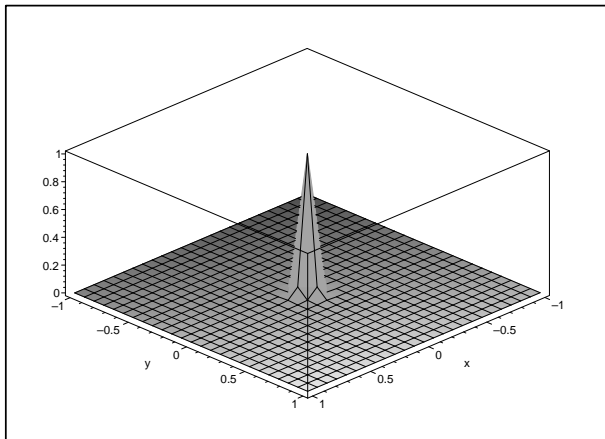
Typical basis functions θ for $\epsilon = 1.0$



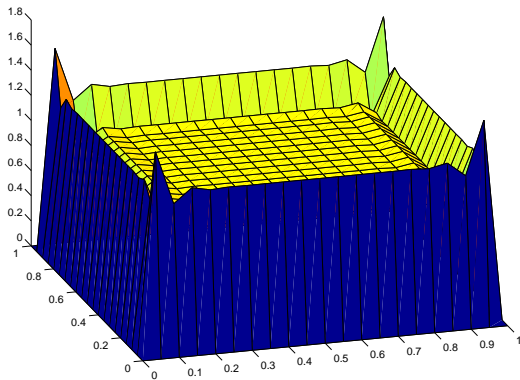
Typical basis functions θ for $\epsilon = 0.1$



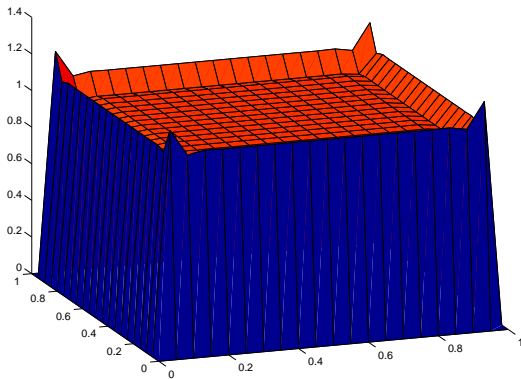
Typical basis functions θ for $\epsilon = 10^{-3}$



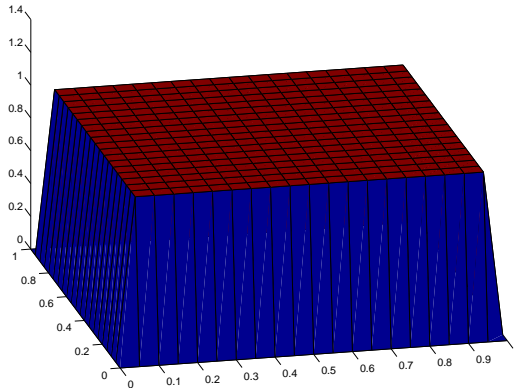
Piecewise Linear Galerkin ($\epsilon = 10^{-6}$):



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



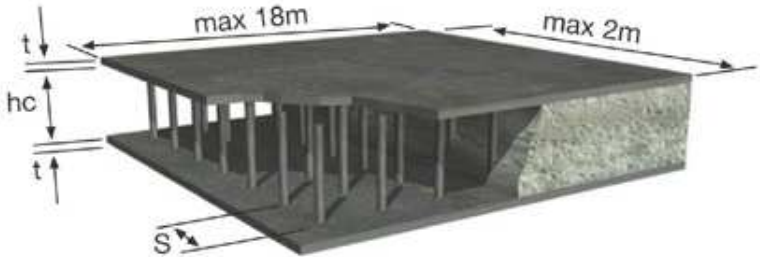
New Formulation ($\epsilon = 10^{-6}$):



RFB: Heterogeneous Plates

(joint with A. Carius)

Linearized Elasticity in a heterogeneous Plate



$t = 5$ to 20mm
 $hc = 200$ to 700mm
Bar diameter = 25mm
Min $S = 200\text{mm}$
Min $R = 1500\text{mm}$

The Romans knew:



Numerics for an oscillatory Reissner-Mindlin model

Use dimensional reduction technique to obtain

$$\begin{aligned} -\frac{\delta^2}{3} \operatorname{div} \mathcal{C}^* \underline{\underline{\phi}} + \lambda(\underline{\underline{\phi}} - \underline{\underline{\nabla}}\omega) &= -\underline{\underline{g}}^{odd} \quad \text{em } \Omega, \\ \lambda \operatorname{div}(\underline{\underline{\phi}} - \underline{\underline{\nabla}}\omega) &= \underline{\underline{g}}_3^{even} \quad \text{em } \Omega, \\ \underline{\underline{\phi}} = 0 \quad \omega = 0 &\quad \text{on } \partial\Omega. \end{aligned}$$

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 (with M. Barreda)

Consider

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

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

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

Variational 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 :

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

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.

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

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

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

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

Theorem

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

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.

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

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

That's nice:

Note that it's easy to iterate.

Reduced Version

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

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

and

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

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 nonlinear multiscale problems
- Cea's Lemma for the *full version*
- Convergence to the homogenized solution for the *reduced version*

Outline

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

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

Obrigado!

