Multiscale Modelling Applied to Fractured Oil Shale Rock

Rosangela Sviercoski

Bryan J. Travis

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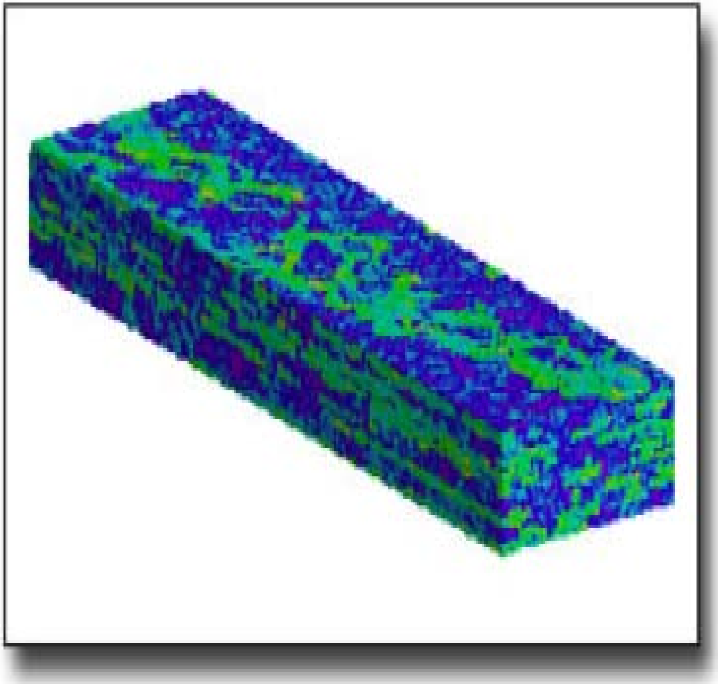
Motivation

Example of highly heterogeneous medium we use into the diffusion equation:

$$\nabla \cdot (K(x)\nabla u(x)) = f(x)$$



Permeability Field from SPE-10.

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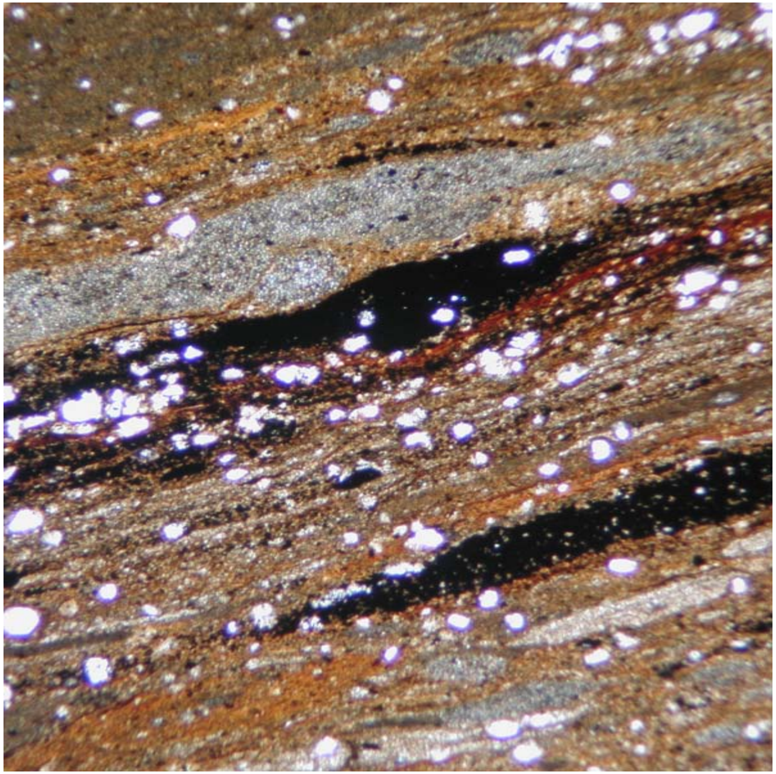
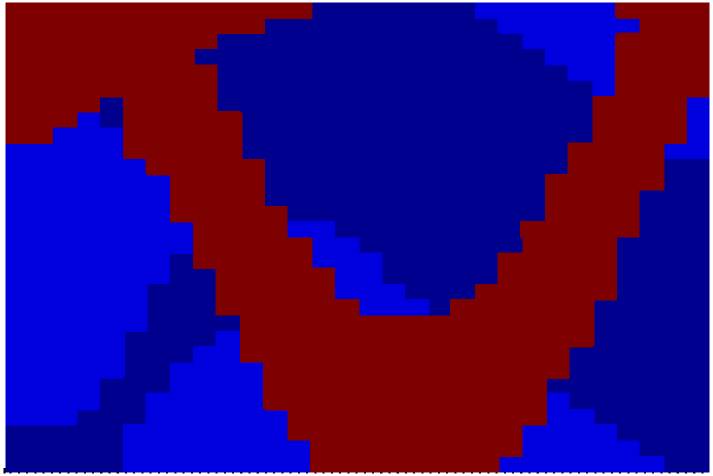


Microscopic Sample from a Oil-Shale Rock

Motivation



Heterogeneity built on the Computational Grid

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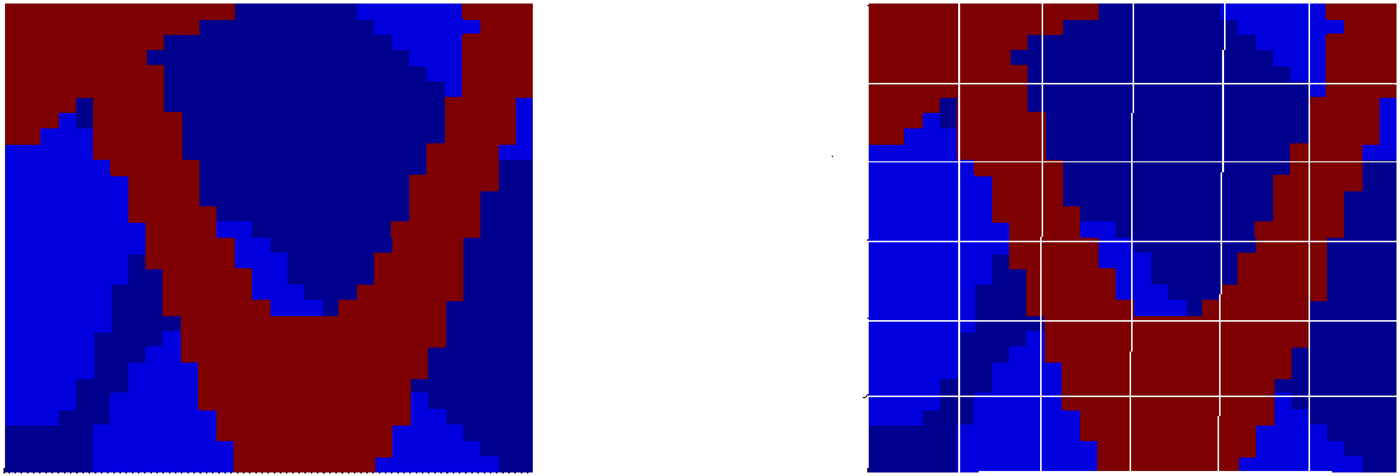

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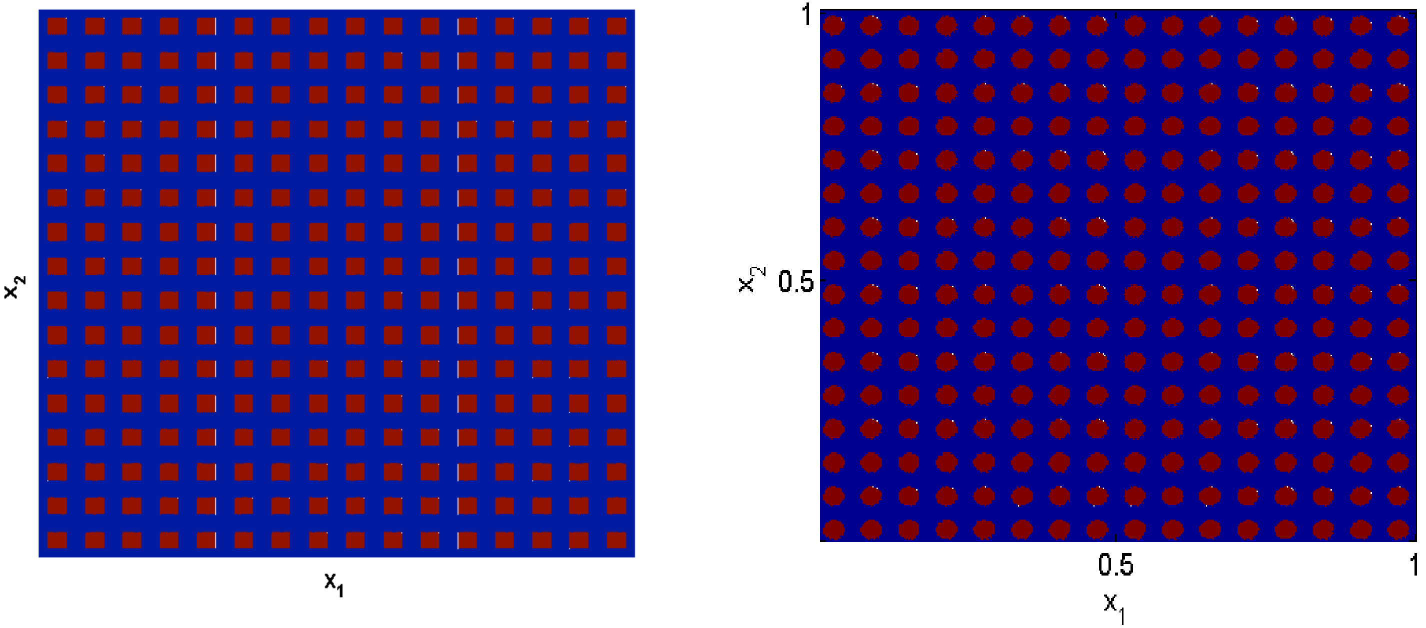

Computational Grid with Simplified Geometries

Outline

- Analytical Approach
- Zeroth-order Approximation for Diffusion Equations - Upscaled Coefficient
- Comparison with Theoretical and Numerical Results
- First-order Approximation for Diffusion Equations.
- Results of Convergence **Linear** and **Nonlinear**
- Analytical Upscaling for Generalized Geometries
- Application to **Transport** on Highly Heterogeneous Media
- Conclusion and Future Work

Analytical Approach

Each isotropic and heterogeneous media can be formalized

$$K_s^{\varepsilon}(x) = \begin{cases} \xi_1 & x \in \Omega_c^{\varepsilon} \\ \xi_2 & x \in \Omega^{\varepsilon} \backslash \Omega_c^{\varepsilon} \end{cases}$$

with ξ_1 at the inclusion Ω_c^{ε}, and $\xi_1 : \xi_2$ is the ratio: 10:1, 100:1, 1000:1 (for example).

Where $\varepsilon = l/L$, l is the length of the inclusion and L the domain size.

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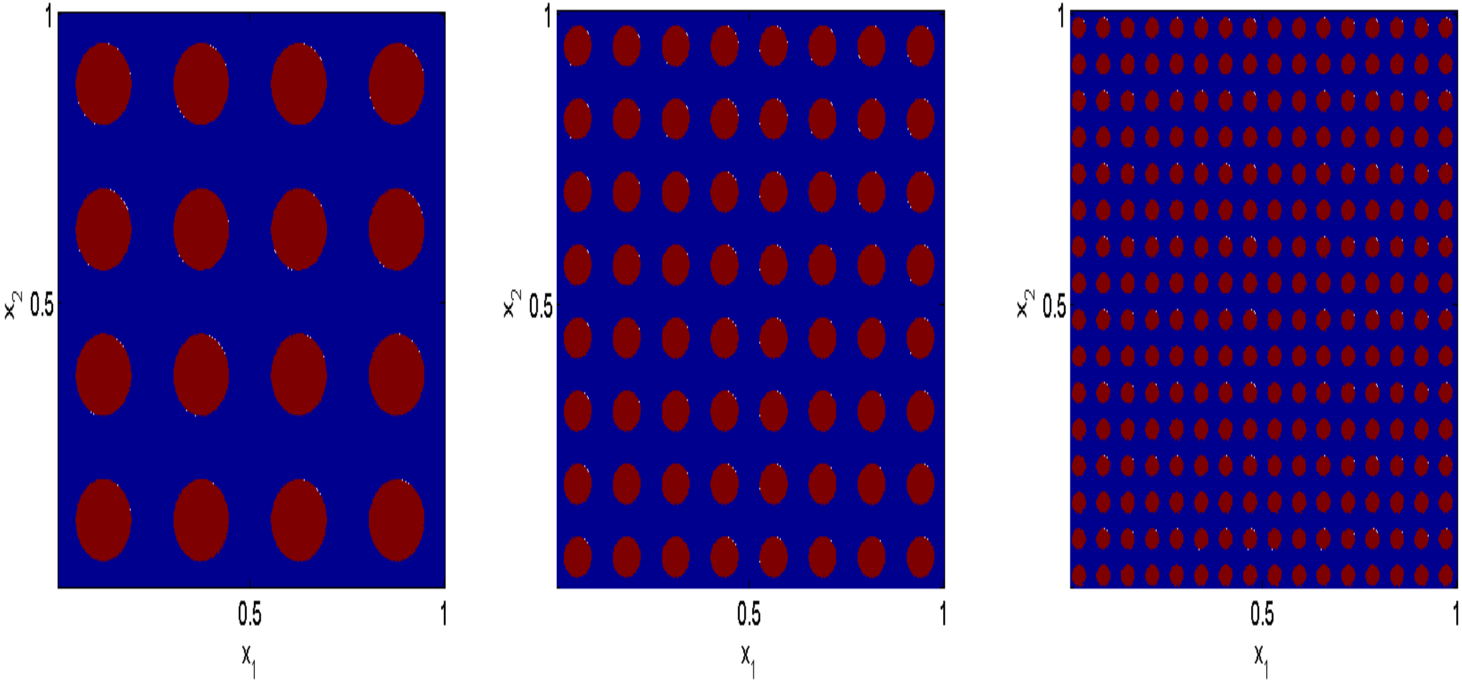
Goal: To propose an Upscaled Darcy's Law $q^0(x)$, the limit as $\varepsilon \to 0$:

$$q^{\varepsilon}(x) = -\frac{K_s^{\varepsilon}(x)\, k_r(u^{\varepsilon}(x))}{\rho g} \nabla u^{\varepsilon}(x) = -K^{\varepsilon}(x, u^{\varepsilon}(x)) \nabla u(x) \simeq -K^0(u^0) \nabla u^0(x) = q^0(x)$$

$$\nabla \cdot q^{\varepsilon}(x) = f(x) \simeq \nabla \cdot q^0(x) = f(x)$$

Sequence of $K^{\varepsilon}(x)$, as $\varepsilon \longrightarrow 0$

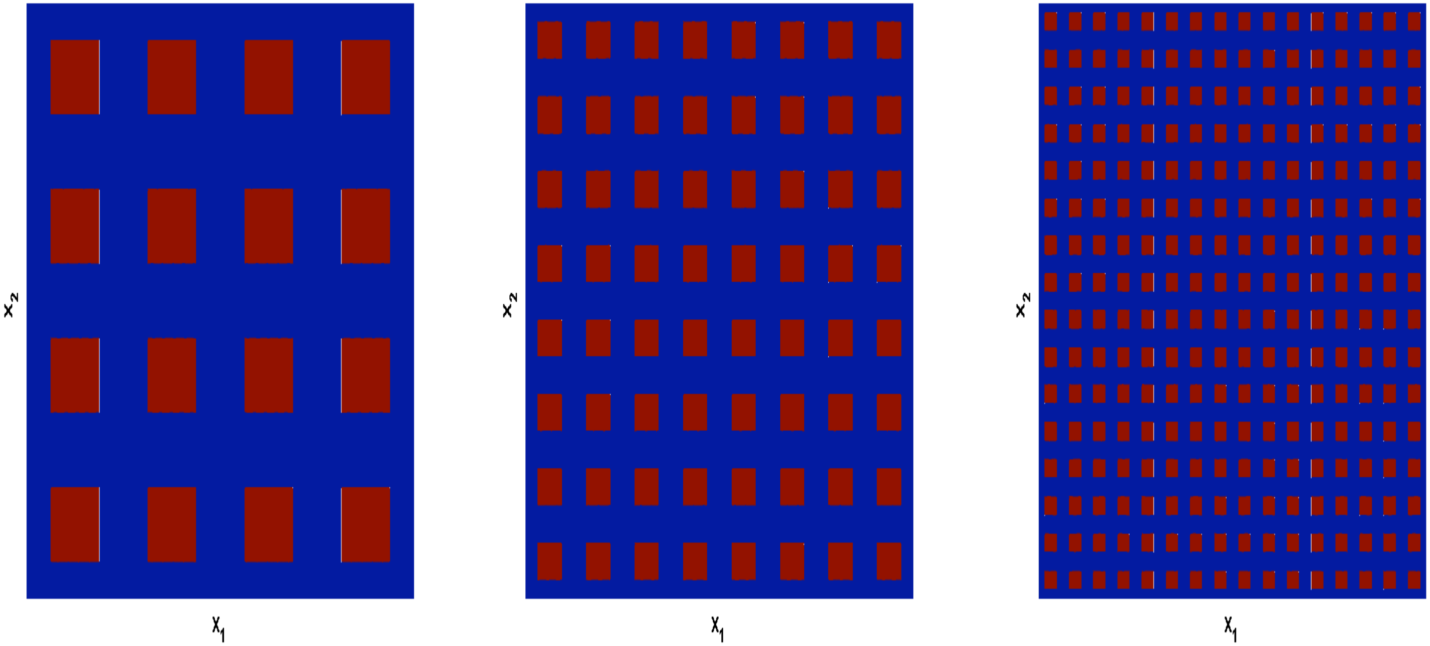
$$\nabla \cdot (K^{\varepsilon}(x)\nabla u^{\varepsilon}(x)) = f(x)$$



Highly oscillating media $K^{\varepsilon}(x)$, as $\varepsilon \longrightarrow 0$

Sequence of $K^\varepsilon(x)$, as $\varepsilon \longrightarrow 0$

$$\nabla \cdot (K^\varepsilon(x) \nabla u^\varepsilon(x)) = f(x)$$



Highly oscillating media as $\varepsilon \longrightarrow 0$

Diffusion in Periodic Media

From: Tartar, L. (1976), Keller, J. (1977), Bensoussan et al. (1978).

Consider the family of BVP's

$$\begin{cases} \nabla \cdot \left(K^{\varepsilon}\left(x\right) \nabla u^{\varepsilon}\left(x\right)\right) = f(x) & x \in \Omega \\ u\left(x\right) = g(x) & x \in \partial\Omega \end{cases}$$

Let $y = \varepsilon^{-1} x$, and the expansion:

$$u^{\varepsilon}\left(x\right) \approx u^{0}\left(x, y\right) + \varepsilon u^{1}\left(x, y\right)$$

Definition 1 ***H-Convergence*** *A constant matrix K^0 is said to be the homogenized limit of K^{ε}, if and only if, in the limit as $\varepsilon \to 0$:*

$$u^{\varepsilon} \to u^{0} \quad in \quad L^{2}\left(\Omega\right)$$

$$K^{\varepsilon}\left(x\right) \nabla u^{\varepsilon}\left(x\right) \rightharpoonup K^{0} \nabla u^{0}\left(x\right) \quad in \quad L^{2}\left(\Omega\right)$$

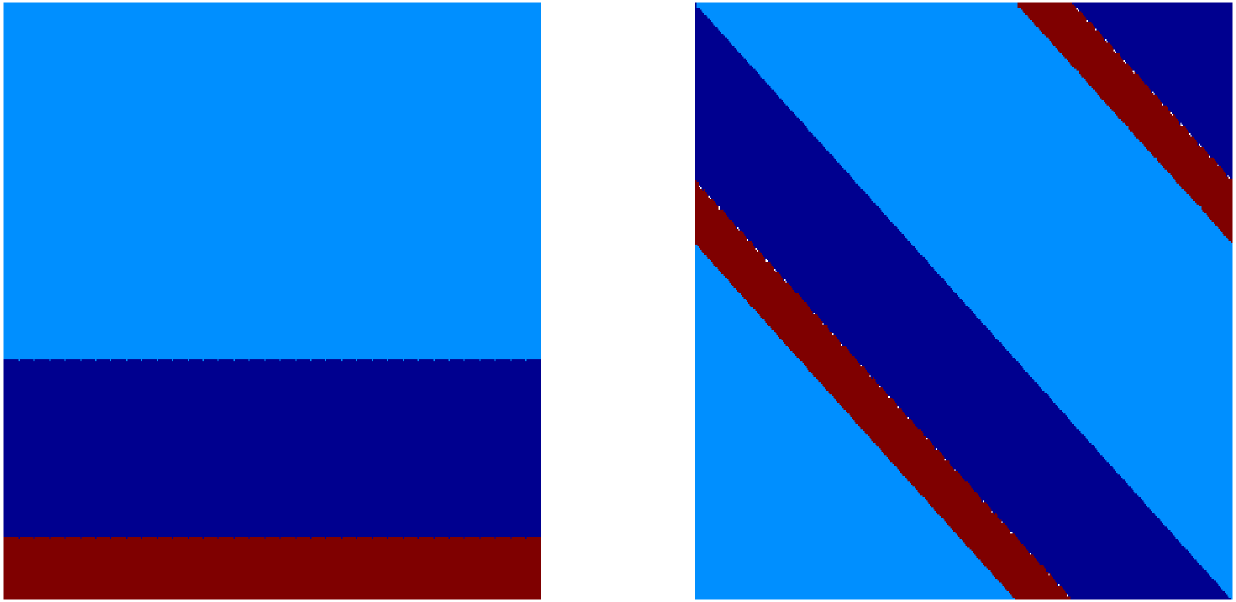
$$K_{ij}^{0} = \int_{Y} K\left(y\right)\left(\delta_{i,j} + \partial_{y_i} w_i\left(y\right)\right) dy$$

And $w_i \in H^1(Y)$ is the periodic solution of

$$\nabla \cdot (K(y) \nabla w_i(y)) = \nabla \cdot (K(y) e_i)$$

Known results for the n-dimensional case

If $K(x)$ is a Layered Media and/or Slanted Layered Media



Then K^0 is the arithmetic and harmonic averages **layered** and its rotation matrix.

Some Review on Numerical Methods

- Durlofsky et al. Numerical Calculation of Equivalent Grid Block Permeability Tensor (1991 and on)

  Idea To compute the effective numerically.

- Amaziane et al. Equivalent permeability and simulation of two-phase flow in heterogeneous media

  Idea Apply the idea of solving the cell-problem for generalized permeability field, under various BC and show agreement with fine-scale solution (1991)and (2001).

- MsFEM: initially proposed by Hou and Wu (JCP - 1997).

  Idea: To construct a finite element basis function, based on a solution of local problem. It has been improved and widely applied. (see Efendiev, Y. for references).

- Black Box Multigrid Numerical Homogenization Algorithm - Moulton, Dendy and Hyman (JCP-1998)

  Idea: Multiple length scales are captured by a multilevel iterative solver. It has not been extended to Nonlinear Equations.

Diffusion in Periodic Media

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Consider the family of BVP's

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Let $y = \varepsilon^{-1}x$, and the expansion:

$$u^{\varepsilon}(x) \approx u^{0}(x, y) + \varepsilon u^{1}(x, y)$$

Definition 2 ***H-Convergence*** *A constant matrix K^0 is said to be the homogenized limit of K^{ε}, if and only if, in the limit as $\varepsilon \to 0$:*

$$u^{\varepsilon} \to u^{0} \quad in \quad L^2(\Omega)$$

$$K^{\varepsilon}(x) \nabla u^{\varepsilon}(x) \rightharpoonup K^{0} \nabla u^{0}(x) \quad in \quad L^2(\Omega)$$

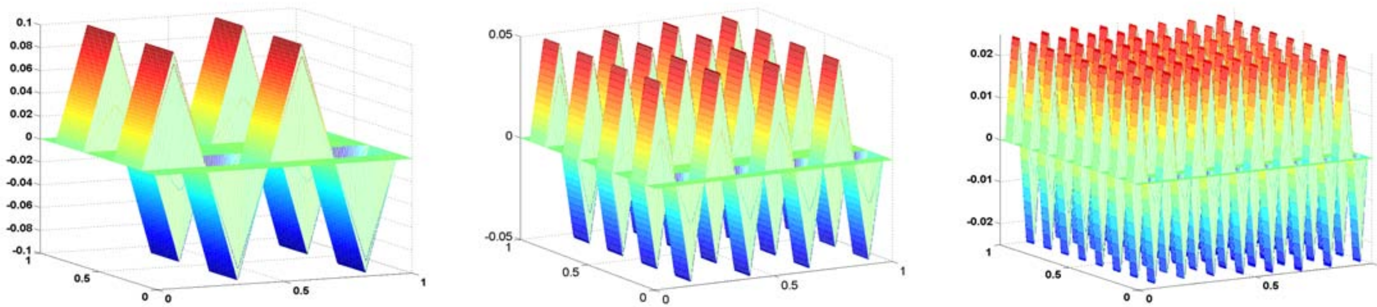
$$K^{0}_{ij} = \int_{Y} K(y) \left(\delta_{i,j} + \partial_{y_i} w_i(y)\right) dy$$

And $w_i \in H^1(Y)$ is the periodic solution of

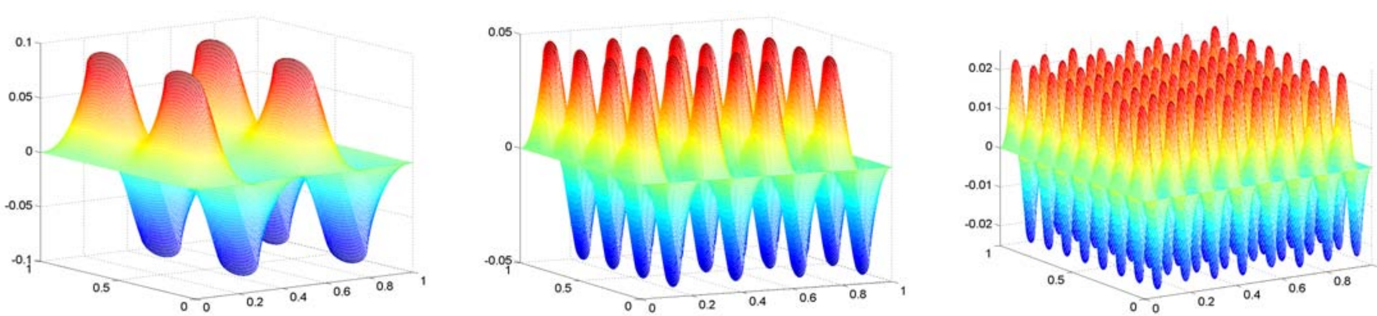
$$\nabla \cdot (K(y) \nabla w_i(y)) = \nabla \cdot (K(y) e_i)$$

Result*: $\tilde{w}^1(y) \in L^2(Y)$ approximates $w^1(y) \in H^1(Y)$

The analytical $\tilde{w}^1(y)$, are illustrated below:



And their respective **true** numerical solution:



4, 8 and 16 square inclusions, respectively.

* Sviercoski, Winter, Warrick, in: SIAM Journal of Applied Math, in press (2007).

Analytical Approx. for the Homogenized Coefficient

By assuming that, for each $i = 1, .., n$

$$\tilde{w}^i(y) = \left(\frac{\int_0^{y_i} \frac{d\tau}{K(y_1, y_2, \ldots, \tau, \ldots, y_n)}}{\int_0^1 \frac{d\tau}{K(y_1, y_2, \ldots, \tau, \ldots, y_n)}} - y_i \right)$$

One has that:

$$\tilde{K}^0 = \int_Y diag(R_1, R_2, \ldots R_n) dY$$

where:

$$R_i(y) = \frac{1}{\int_0^1 \frac{d\tau}{K(y_1, y_2, \ldots, \tau, \ldots, y_n)}}$$

One has that:

$$\tilde{K}^0 = \int_Y diag(R_1, R_2, \ldots R_n) dY$$

...$\tilde{K}^0$ is the arithmetic average of the harmonic average.

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One has that:

$$\tilde{K}^0 = \int_Y diag(R_1, R_2, \ldots R_n) dY$$

Result: $\tilde{K}^0$ is the lower bound of the Generalized Voig-Reiss Inequality:

$$\tilde{K}^0 \leq K^0 \leq K^u$$

where $K^u = \left(\int_Y \frac{dy_j}{\int_Y K(y) dy_i} \right)^{-1}$, with $j \neq i$ (Jikov et al. (1994)).

Defining* a Corrector to $\tilde{K}^0$

Let $\frac{\partial \tilde{w}^j}{\partial y_i} = 0$ a.e. in Y, for $i \neq j$, and define $C^{\varepsilon}_{ij}(x) = C_{ij}(y)$,

$$C^{\varepsilon}_{ij}(x) = \delta_{ij} + \frac{\partial \tilde{w}^j}{\partial y_i} = \frac{1}{K\,(y)} \left(\int_0^1 \frac{d\tau}{K\,(y_1, .., \tau, .., y_n)} \right)^{-1}$$

$$\nabla u^{\varepsilon}(x) = C^{\varepsilon}(x) \nabla u^0(x) + h.o.t$$

We define K^0, a corrector of $\tilde{K}^0$, as:

$$K^0 = ||C^{\varepsilon}_{ii}||_2\, \tilde{K}^0 = C_{ii} \tilde{K}^0$$

And the approximate solution has being **corrected** by a factor C.

* Sviercoski and Travis in Transport in Porous Media, (submitted)

*First-Order and Upper Bound Estimate for the Error

The **first order approximation** comes readily as:

$$u^{\varepsilon}(x) \simeq u^{0}(x) + \sum_{i} C_{ii}\tilde{w}^{i}\frac{\partial u^{0}}{\partial x_i}$$

And the **Error** for the zeroth order approximation:

$$E = \left|\left|u^{\varepsilon}(x) - u^{0}(x)\right|\right|_2 \leq \left|\left|\sum_{i} C_{ii}\tilde{w}^{i}\frac{\partial u^{0}}{\partial x_i}\right|\right|_2 = UBE$$

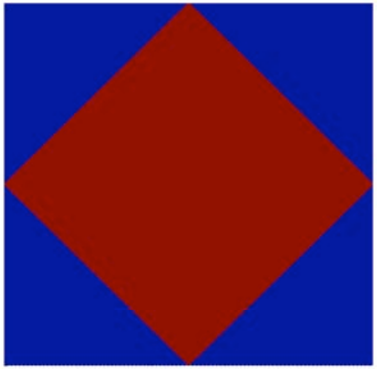
And,

$$\nabla u^{\varepsilon}(x) \simeq \left[\delta_{i,j} + \textstyle\sum_{i=1}^{n} C_{ii}\nabla_y \tilde{w}_i(y)\right]\frac{\partial u^0}{\partial x_i} + \ldots.$$
$$\nabla u^{\varepsilon}(x) \simeq P^{\varepsilon}(x)\nabla u^{0}(x) + \varepsilon \textstyle\sum_{i=1}^{n} \tilde{w}_i(y)\nabla\left(\frac{\partial u^0}{\partial x_i}\right) + \ldots.$$

* Sviercoski, Travis, Hyman in: Comp. Math. & Appl.: In press (2007)

Comparing with Theoretical Results

For the checkerboard case, the **geometric average** is obtained:



$\xi_1 : \xi_2$	K^h	K^g	$C\tilde{K}^0 = K^0$	K^u	K^a
5:20	8.02	10	$\mathbf{1.0725}\times 9.31 = 9.98$	10.79	12.56
1:10	1.82	3.16	$\mathbf{1.1732}\times 2.60 = 3.05$	3.94	5.53
2:8	3.21	4	$\mathbf{1.0725}\times 3.722 = 3.99$	4.35	5.02
4:16	6.40	8	$\mathbf{1.0725}\times 7.4451 = 7.985$	8.69	10.05
16:4	6.39	8	$\mathbf{1.0725}\times 7.38 = 7.91$	8.64	10.00

Comparison with Published Numerical Results

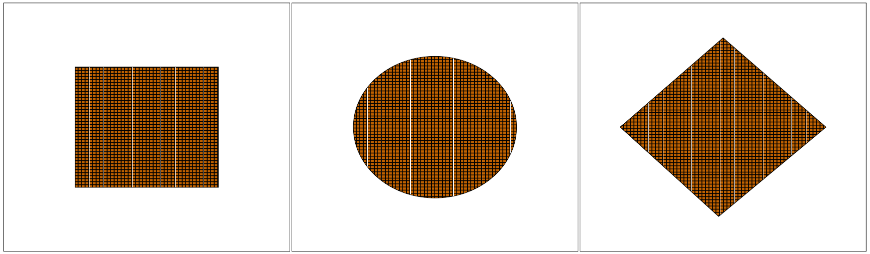


Figure 1: Ratio - 10:1 and all have area equals $\frac{1}{4}$

Shape	K^h	K^{num}	$C\tilde{K}^0 = K^0$	K^u	K^a
square	1.3	1.548	$\mathbf{1.0937}\times 1.4091=1.5411$	1.695	3.2952
circle	1.29	1.516	$\mathbf{1.08}\times 1.403=1.5156$	1.791	3.2511
lozenge	1.29	1.573	$\mathbf{1.069}\times 1.417=1.5148$	1.936	3.2361

K^{num} : Bourgat, J.F. in: Comp. Meth. in App. Sci. and Engin.(1978)

Comparison with published numerical results

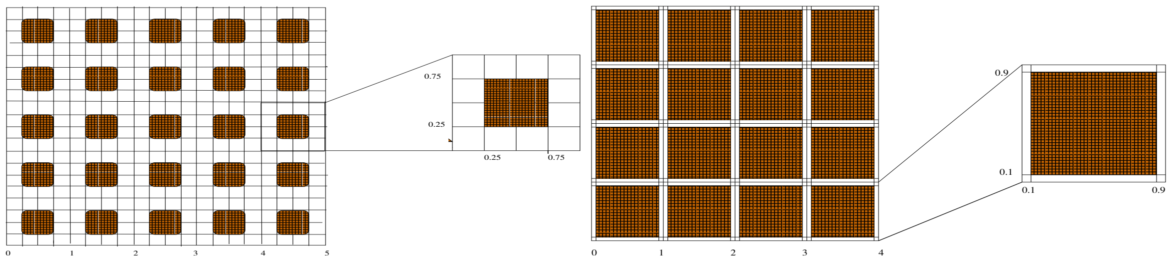


Figure 2: Tests 1 - 1:10, Test 2 - 1:10 and Test 3 - 1:100 (left) and Test 4 - 1:10 (right)

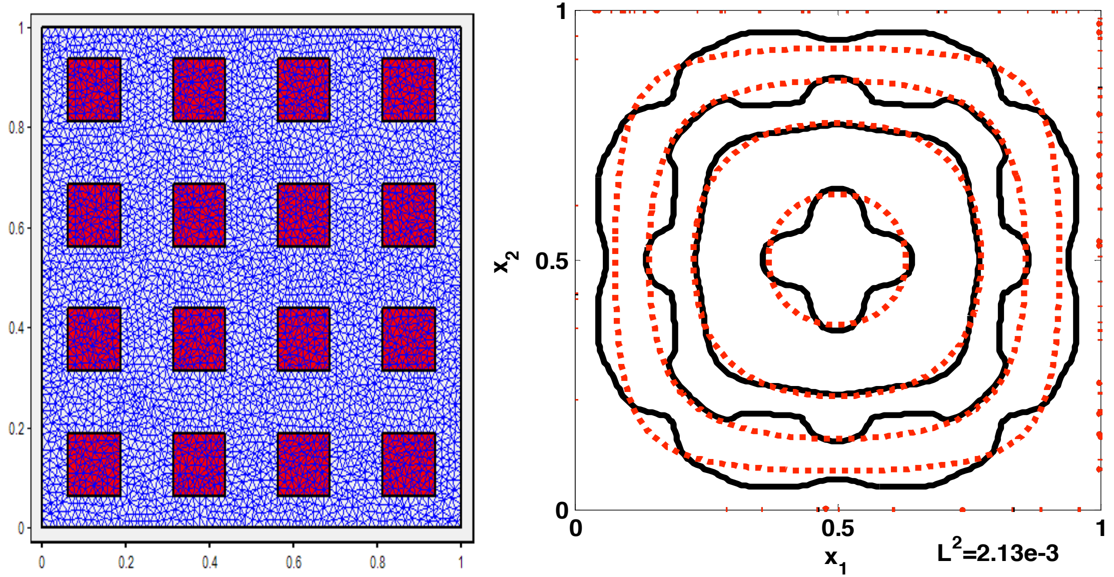
	K^h	$K^\#$	$C\tilde{K}^0 = K^0$	K^u	K^a
Test 1	3.09	6.52	$\mathbf{1.093}\times 5.91=6.459$	7.09	7.75
Test 2	3.09	6.52	$\mathbf{1.093}\times 5.91=6.459$	7.09	7.75
Test 3	3.89	59.2	$\mathbf{1.1378}\times 51=58.03$	67	76.0
Test 4	1.48	3.106	$\mathbf{1.0663}\times 2.98=3.177$	3.27	4.24

$K^\#$: Amaziane, B., Bourgeat, A., Koebbe, J., in Transp. in P. Media 6:519-547,(1991)

Error Analysis

Consider the following BVP in $\Omega = [0,1]^2$:

$$\begin{cases} \nabla \cdot (K^\varepsilon(x)\nabla u^\varepsilon(x)) = 1 & x \in \Omega \\ u^\varepsilon(x) = 0 & x \in \partial\Omega \end{cases} \approx \begin{cases} \nabla \cdot (K^0 \nabla u^0(x)) = 1 & x \in \Omega \\ u^0(x) = 0 & x \in \partial\Omega \end{cases}$$



$K^\varepsilon(x)$ (left), $u^\varepsilon(x) \simeq u^0(x)$ (right)

$u^\varepsilon(x)$, fine-scale (solid) and Approximations (dashed)

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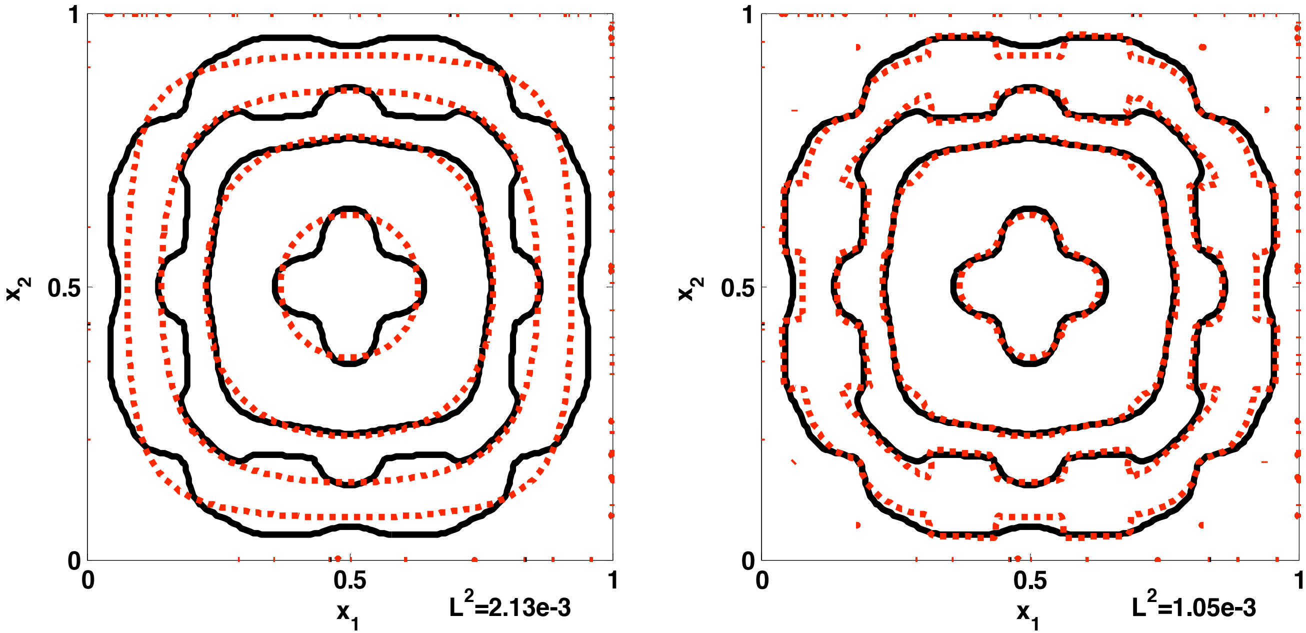
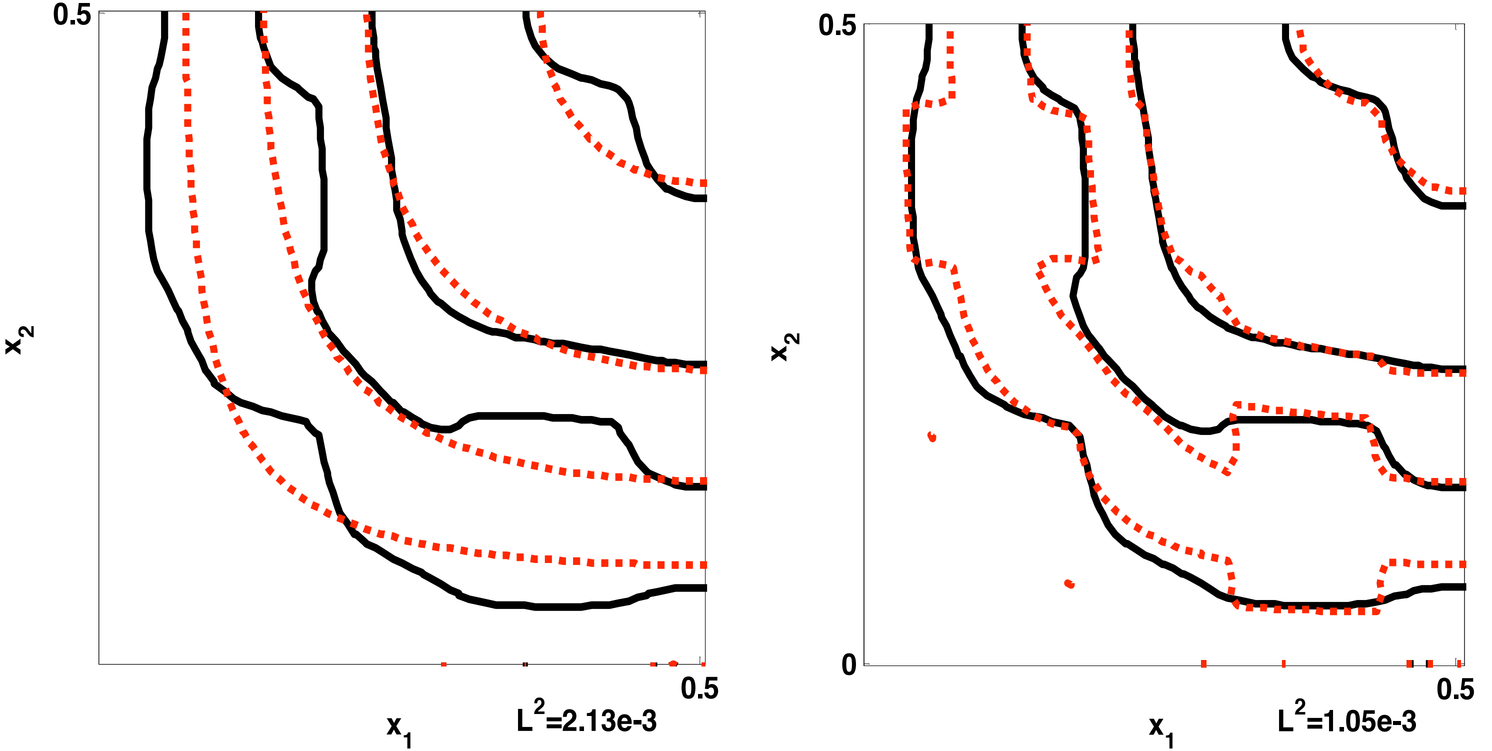


$u^\varepsilon(x) \simeq u^0(x)$ (left), $u^\varepsilon(x) \simeq u^0(x) + \sum_i C_{ii}\tilde{w}^i \frac{\partial u^0}{\partial x_i}$(right).

$u^\varepsilon(x)$ fine-scale (solid) and approximations (dashed)



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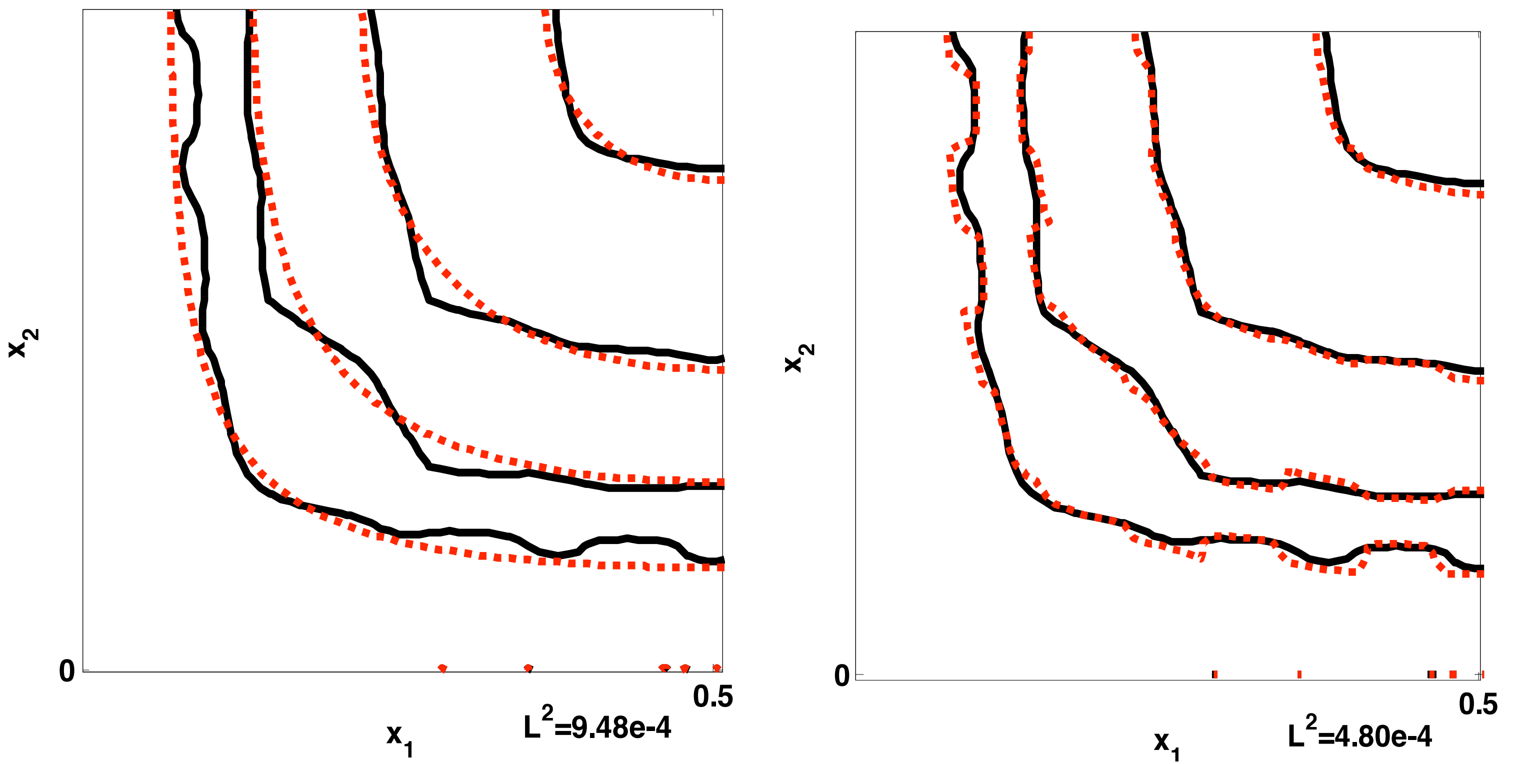

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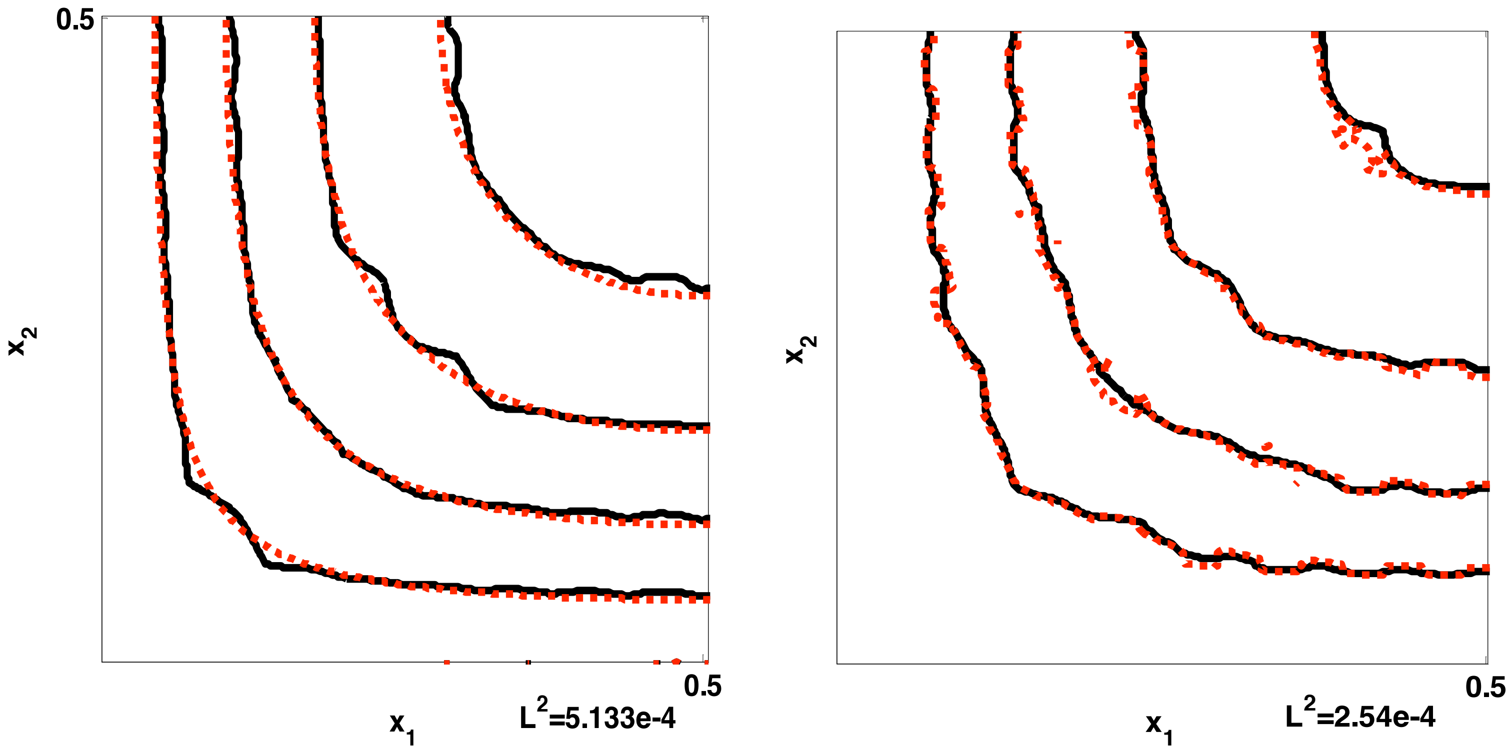


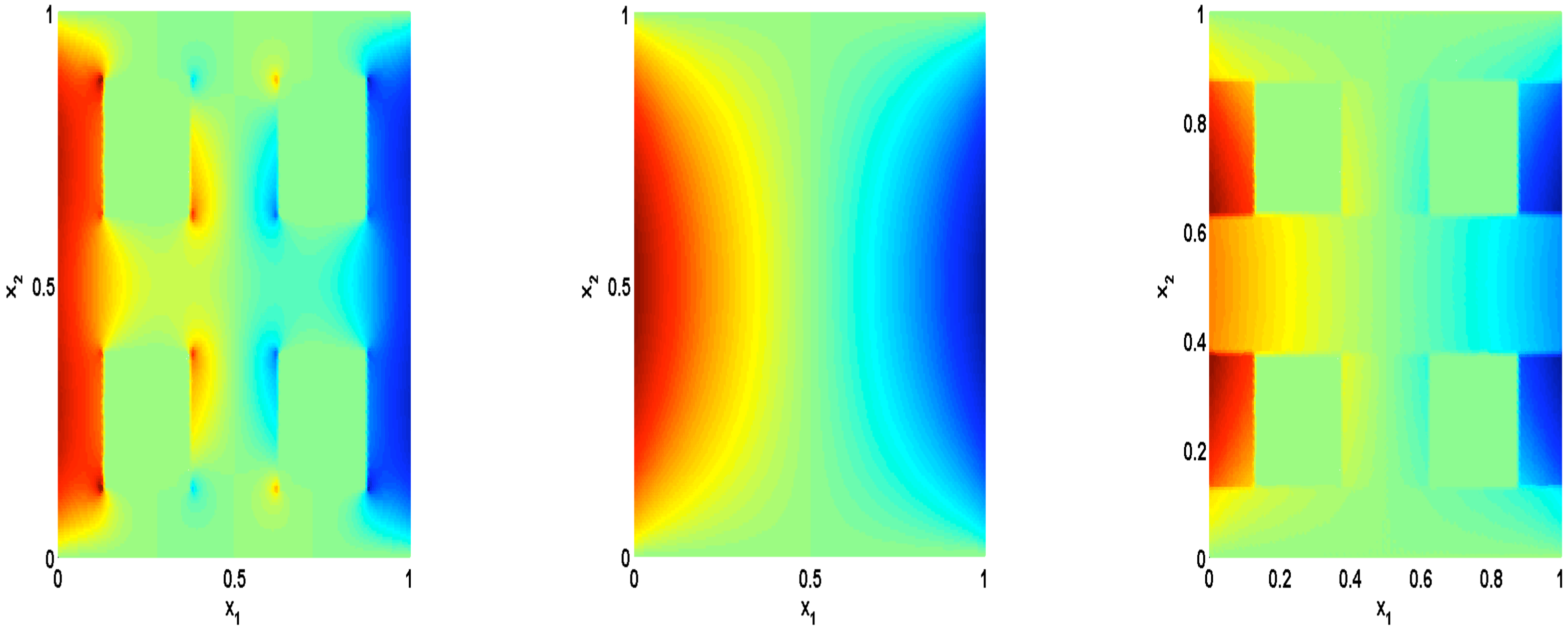
$u^{\varepsilon}(x) \simeq u^0(x)$ (left), $u^{\varepsilon}(x) \simeq u^0(x) + \sum_i C_{ii}\tilde{w}^i \frac{\partial u^0}{\partial x_i}$(right).

Ratio 10:1 on $[0,1]^2$ with $K^0 = \mathbf{1.0937} \times 1.4091 = 1.5411$

ε	$\|\|u^\varepsilon - u^0\|\|_2$	UBE	$\|\|u^\varepsilon - (u^0 + u^1)\|\|_2$	$\|\|\nabla u^\varepsilon - P^\varepsilon \nabla u^0\|\|_2$	$\|\|K^\varepsilon \nabla u^\varepsilon - K^0 P^\varepsilon \nabla u^0\|\|_2$	#nodes
$(0.5)^1$	1.10e-2	**1.61e-2**	4.43e-3	6.91e-2	2.36e-1	16641
$(0.5)^2$	4.92e-3	**7.48e-3**	2.31e-3	5.75e-2	2.11e-1	16641
$(0.5)^3$	2.13e-3	**3.74e-3**	1.05e-3	4.53e-2	1.97e-1	16641
$(0.5)^4$	9.48e-4	**1.80e-3**	4.80e-4	3.89e-2	1.88e-1	16265
$(0.5)^5$	5.13e-4	**9.33e-4**	2.54e-4	3.65e-2	1.87e-1	161393

$$E = \left|\left|u^\varepsilon(x) - u^0(x)\right|\right|_2 \leq C \left|\left| \sum_i \tilde{w}^i \frac{\partial u^0}{\partial x_i} \right|\right|_2 = UBE$$

Comparison between Gradients of the approximations



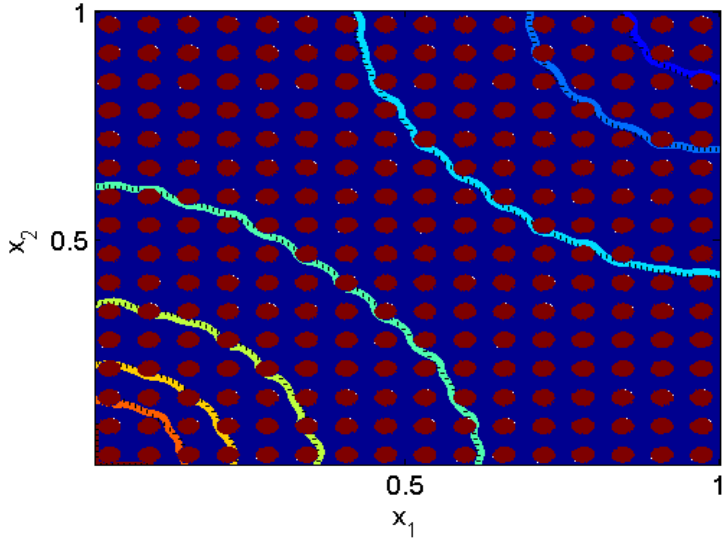
$\nabla u^{\varepsilon}(x)$ (left) and $\nabla u^{0}(x)$ (center) and $P^{\varepsilon}(x)\nabla u^{0}(x)$ (right).

* Nonlinear Equations - Circular Inclusion - $K_s^\varepsilon(x)$ ratio 1:1000

The conductivity is given by the Van Genuchten's relationship:

$$K^\varepsilon\left(x, u_\varepsilon(x)\right) = K_s^\varepsilon\left(x\right)\left(\left(1+|\alpha u_\varepsilon(x)|^n\right)^{-m}\right)^p\left[1-\left(1-\left(\left(1+|\alpha u_\varepsilon(x)|^n\right)^{-m}\right)^{\frac{1}{m}}\right)^m\right]^2$$

and parameters: $\alpha = 1.04\ m^{-1}$, $m = 0.283$, $n = 1/(1-m)$ and $p = 0.5$.



* Sviercoski, Popov, Travis in preparation to JCP.

Numerical Convergence for Nonlinear Equations

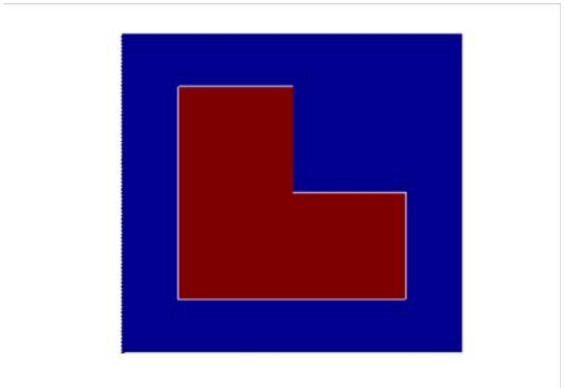
ε	$\|\|u_\varepsilon - u_0\|\|_2$	UBE	$\|\|\nabla u_\varepsilon - \nabla u_0\|\|_2$	$\left\|\left\|K^\varepsilon \nabla u_\varepsilon - K^0 \nabla u_0\right\|\right\|_2$	grid
$(0.5)^1$	2.22e-2	3.65e-2	1.58e-1	3.10e+0	88X88
$(0.5)^2$	1.08e-2	2.17e-2	1.50e-1	2.85e+0	94X94
$(0.5)^3$	4.00e-3	1.21e-2	1.45e-1	2.60e+0	104X104
$(0.5)^4$	3.25e-3	5.92e-3	1.41e-1	2.47e+0	114X114
$(0.5)^5$	1.34e-3	2.31e-3	1.22e-1	2.21e+0	130X130

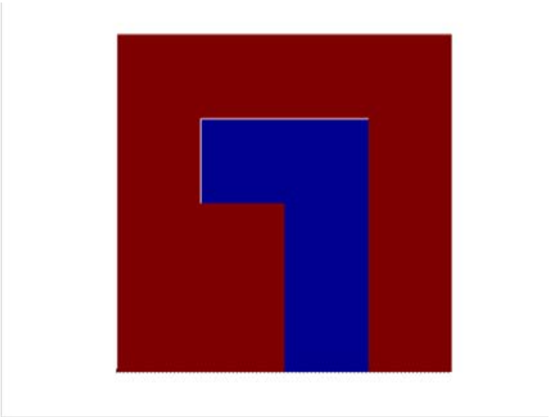
Table 1: **Zeroth-order Approximation for $K_s^\varepsilon(x)$ with circular inclusions, ratio 1:1000; $K_s^0 = \mathbf{1.1866} \times 436.60 = 518.09$.**

ε	$\left\|\left\|u_\varepsilon - u^{fo}\right\|\right\|_2$	UBE	$\|\|\nabla u_\varepsilon - P^\varepsilon \nabla u_0\|\|_2$	$\left\|\left\|K^\varepsilon \nabla u_\varepsilon - K^0 P^\varepsilon \nabla u_0\right\|\right\|_2$
$(0.5)^1$	1.34e-2	3.65e-2	2.45e-1	3.47e+0
$(0.5)^2$	8.56e-3	2.17e-2	2.28e-1	3.35e+0
$(0.5)^3$	4.57e-3	1.21e-2	2.28e-1	3.26e+0
$(0.5)^4$	2.89e-3	5.92e-3	2.10e-1	2.96e+0
$(0.5)^5$	1.09e-3	2.31e-3	1.01e-1	2.57e+0

Table 2: **The Respective First-order Approximation**

Generalized Geometries - Work in Progress...





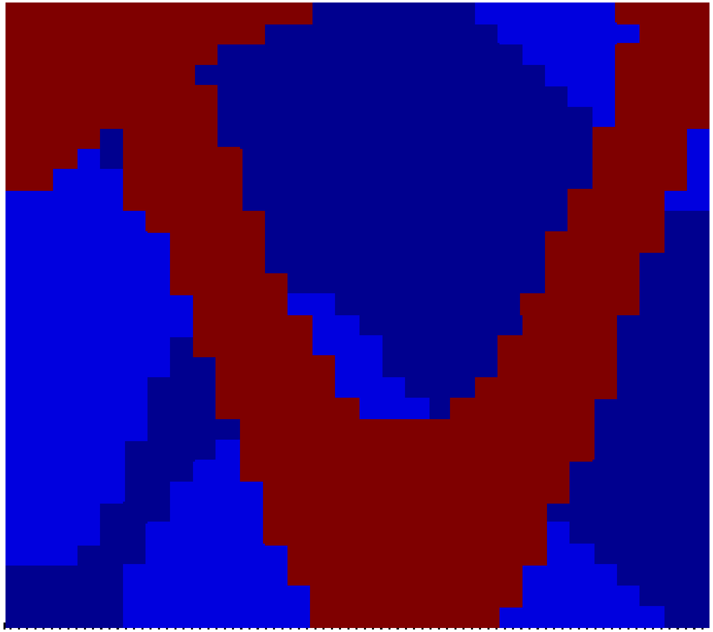
$$Num^{*} = \begin{bmatrix} 1.91 & -0.101 \\ -0.101 & 1.91 \end{bmatrix} \qquad Num^{\bullet} = \begin{bmatrix} 5.33 & -0.286 \\ -0.286 & 6.761 \end{bmatrix}$$

$$Anal = \begin{bmatrix} 1.86 & -0.102 \\ -0.102 & 1.86 \end{bmatrix} \qquad Anal = \begin{bmatrix} 5.73 & -0.212 \\ -0.212 & 6.55 \end{bmatrix}$$

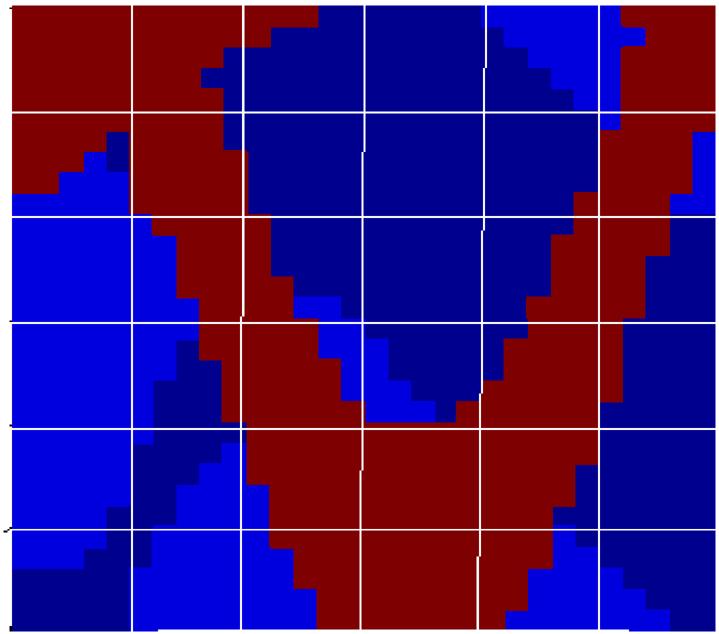
*Bourgat, J.F. in: Comp. Meth. in Ap. Sci. and Eng. (1978)

• Amaziane et al. in: Comp. Geoscience (2001)

Generalized Geometries - Work in Progress...



Generalized Geometries - Work in Progress...



Generalized Geometries - Work in Progress...

$$Num^{\bullet} = \begin{bmatrix} 3.8292 & 0.1912 \\ 0.1912 & 2.7202 \end{bmatrix}$$

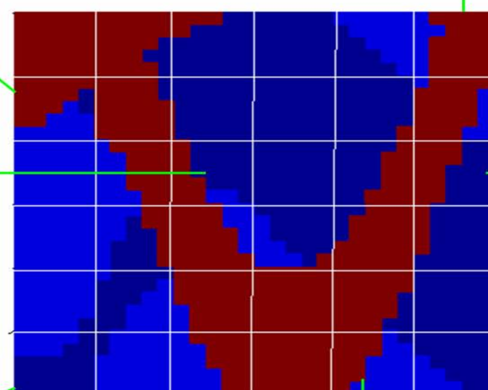
$$Anal = \begin{bmatrix} 3.7713 & 0.0979 \\ 0.0979 & 2.7517 \end{bmatrix}$$

$$Num^{\bullet} = \begin{bmatrix} 3.4402 & 0.0000 \\ 0.0000 & 7.4172 \end{bmatrix}$$

$$Anal = \begin{bmatrix} 3.5072 & 0.0029 \\ 0.0029 & 7.1862 \end{bmatrix}$$

$$Num^{\bullet} = \begin{bmatrix} 0.2432 & -0.0101 \\ -0.0101 & 2.3542 \end{bmatrix}$$

$$Anal = \begin{bmatrix} 0.2259 & -0.0137 \\ -0.0137 & 2.2065 \end{bmatrix}$$



$$Num^{\bullet} = \begin{bmatrix} 0.2179 & 0.0001 \\ 0.0001 & 4.3325 \end{bmatrix}$$

$$Anal = \begin{bmatrix} 0.2640 & 0.0056 \\ 0.0056 & 4.1289 \end{bmatrix}$$

$$Num^{\bullet} = \begin{bmatrix} 0.2060 & 0.0047 \\ 0.0047 & 0.1466 \end{bmatrix}$$

$$Anal = \begin{bmatrix} 0.1922 & 0.0054 \\ 0.0054 & 0.1526 \end{bmatrix}$$

$$Num^{\bullet} = \begin{bmatrix} 1.6822 & 0.0479 \\ 0.0479 & 3.9697 \end{bmatrix}$$

$$Anal = \begin{bmatrix} 1.7663 & 0.03608 \\ 0.0368 & 3.4894 \end{bmatrix}$$

$Num^{\bullet}$ - Amaziane et al. in: Comp. Geoscience (2001).

Upscaling the Transport Equation

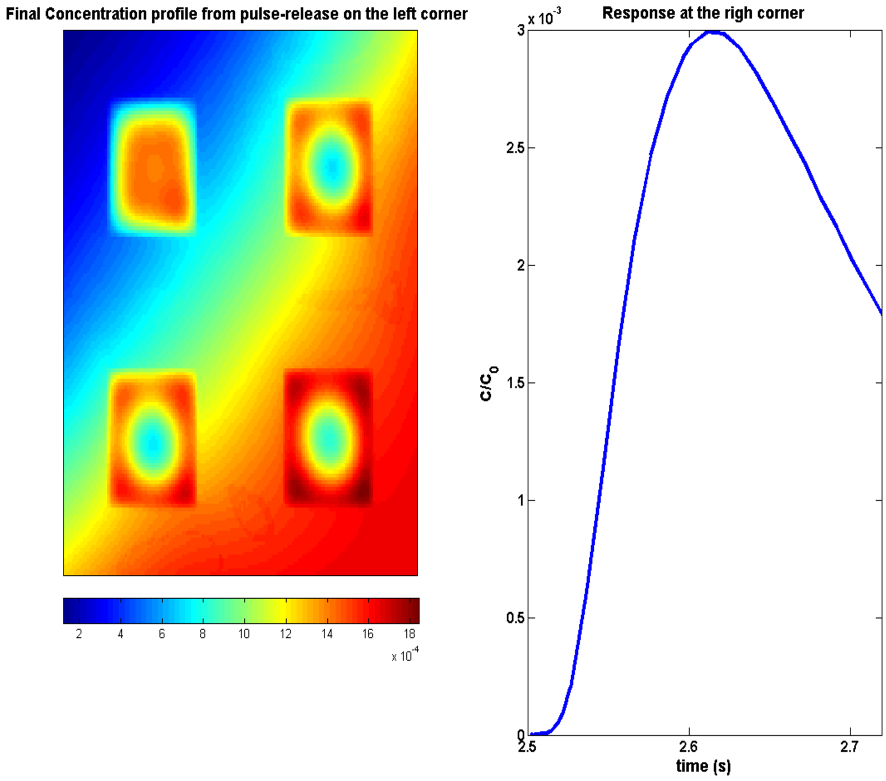
$$\begin{cases} \nabla \cdot v^{\varepsilon}(x) = 0 \\ \nabla \cdot (D \nabla C^{\varepsilon}(x)) - v^{\varepsilon} \cdot \nabla C^{\varepsilon}(x) = \frac{\partial C^{\varepsilon}}{\partial t} \\ C\left(t_a, x_2\right) = f(x_2) \end{cases} \approx \begin{cases} \nabla \cdot v^{0}(x) = 0 \\ \nabla \cdot \left(D \nabla C^{0}(x)\right) - v^{0} \cdot \nabla C^{0}(x) = \frac{\partial C^{0}}{\partial t} \\ C\left(t_a, x_2\right) = f(x) \end{cases}$$

Where D is the diffusivity $[L^2/T]$ and $f(x)$ is a pulse-type loading:

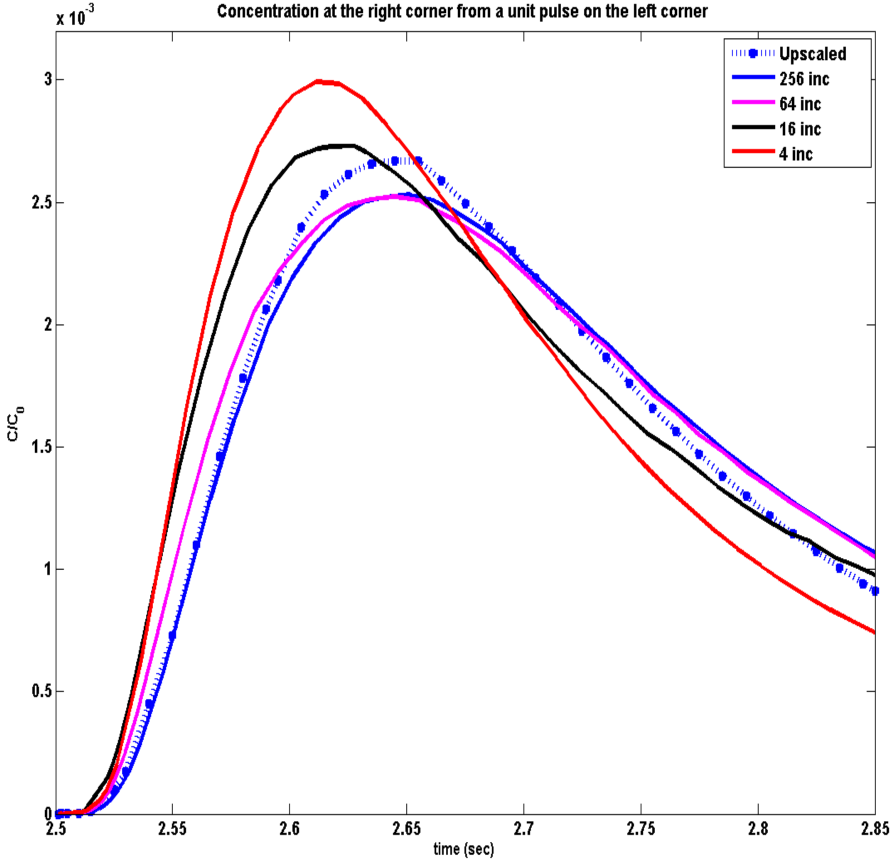
$$f(x) = \begin{cases} 1 & t_0 < t_a \leq t_1 \\ 0 & otherwise \end{cases}$$

And $v^0(x)$ is the **Upscaled Darcy's velocity**

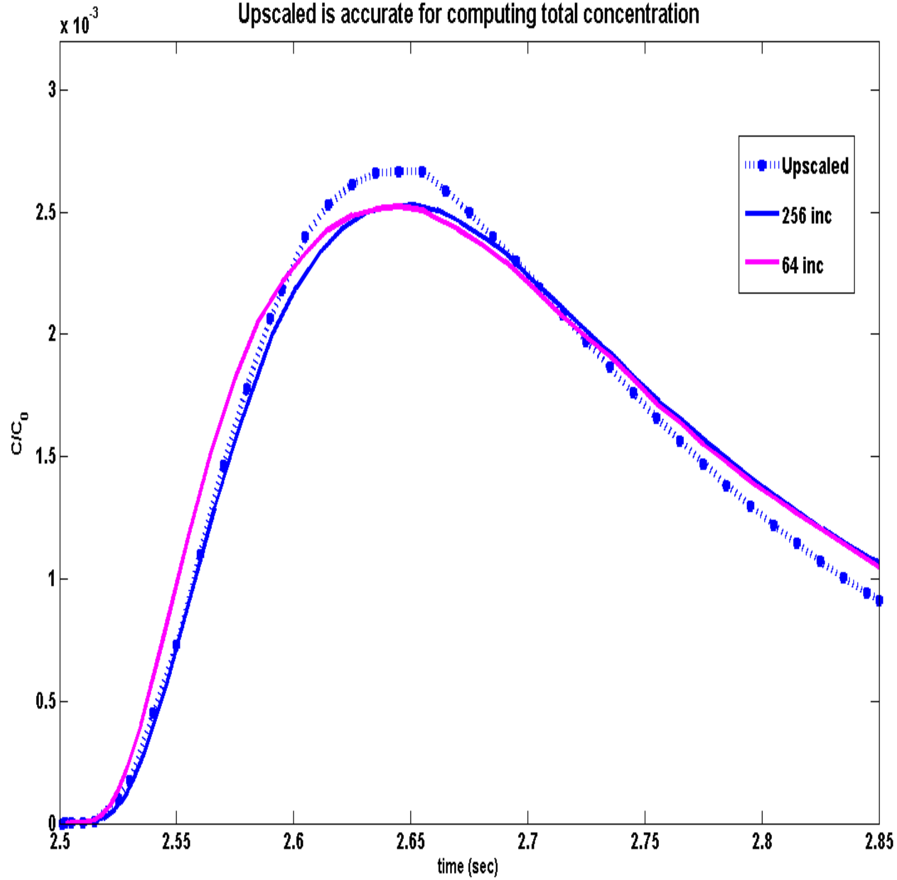
Upscaling the Transport Equation



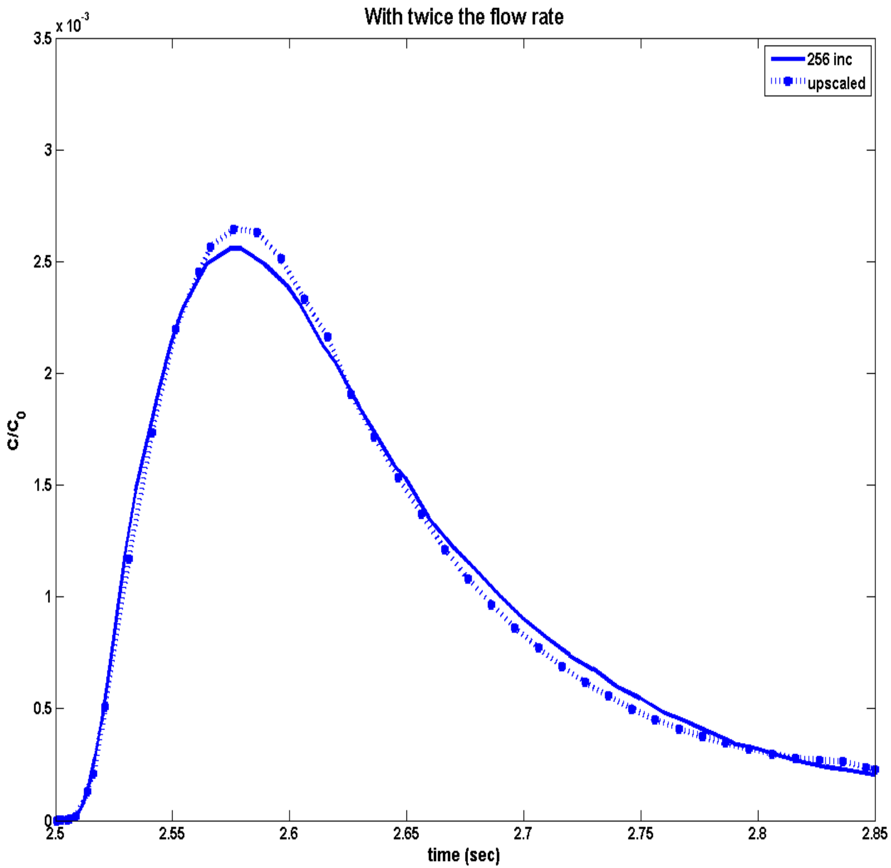
Pulse's Response with Time



Pulse's Response with Time



Pulse's Response with Time



Conclusions - Future Work

- An analytical upscaling method was presented having the advantage of being computationally attractive and portable.
- The method applies to analogous Diffusion systems.
- The method applies to random media.
- Extension to Flow in Deformable Media is possible.
- Extension to Reaction-Diffusion equations is work in progress.
- Matching the results with experiments in an ongoing work.