Numerical homogenization for PDEs with nonseparable scales

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Outline

1. Introduction
2. Periodic media with scale separation.
3. Nonseparable scales
   - Homogenization via harmonic mapping – the solution space is 'low dimensional'
   - Homogenization via flux norm – optimality of the approximation order
   - Homogenization via localized basis – balancing accuracy and efficiency
4. Outlook

Model Problem

We want to homogenize:

- Scalar case:

$$\begin{cases} -\mathrm{div}(a\nabla u) = g & x \in \Omega \\ u = 0 & x \in \partial\Omega \end{cases} \quad (1)$$

$\Omega \subset \mathbb{R}^d$ bounded, open; $a = \{a_{ij}(x) \in L^\infty(\Omega)\}$ symmetric, uniformly elliptic; $g \in L^2(\Omega)$, $u \in H^1(\Omega)$.

- Vectorial case:

$$\begin{cases} -\mathrm{div}(C : \nabla u) = b & x \in \Omega \\ u = 0 & x \in \partial\Omega \end{cases} \quad (2)$$

$\Omega \subset \mathbb{R}^d$, $d \geq 2$, bounded, open; $C = \{C_{ijkl}(x) \in L^\infty(\Omega)\}$ symmetric elastic modulus, $b \in (L^2(\Omega))^d$ load; $u \in (H^1(\Omega))^d$ displacement field.

Classical homogenization theory

Typically, for homogenization, conditions on $a(x)$ are required

- Classical periodic homogenization: $a(y)$ periodic; $a\left(\frac{x}{\epsilon}\right)$, $\epsilon \to 0$ (Bachvalov, Sanchez-Palencia, Zhikov, Kozlov, Lions, Oleinik, Papanicolaou; ...)
  - in real life, no ϵ-family of media
- Random coefficients $a\left(\frac{x}{\varepsilon}; \omega\right)$: stationarity, ergodicity (Kozlov, Papanicolaou/Varadhan, ...)

General coefficients

- Abstract operator convergence – existence, justification of homogenized limit
- G-convergence Spagnolo
- H-convergence Murat-Tartar

Question:
Is there a constructive way to approximate solution in terms of *given data*?

Goal of Numerical Homogenization

scales $1 \gg H \gg \varepsilon$,

- ε: smallest scale of the problem.
- H: an artificial scale, determined by available computational power and desired precision, corresponding dof is N, $H \sim N^{-1/d}$.

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Goal:

Construct a finite dimensional space V_H, and approximate solution $u \in V$ by $u_H \in V_H$ in a certain norm, such that,

- want error estimate, e.g., $\|u - u_H\| \leq CH$
- V_H constructed via several precomputed problems which do not depend on RHS and BC (c.f., cell problems).

Note: Linear FEM can be arbitrarily slow (Babuška, Osborn, '99)

Model Problem

To solve for $g \in L^2(\Omega)$.

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Mapping from the RHS to solutions: $g \longrightarrow u$

- When $\mathrm{RHS} \in \mathrm{H}^{-1}(\cdot)$: $H^{-1}(\Omega) \longrightarrow H_0^1(\Omega)$
- When $\mathrm{RHS} \in \mathrm{L}^2(\cdot)$: $L^2(\Omega) \longrightarrow V$

$$\boxed{V := \{v \in H_0^1(\Omega) | \,\mathrm{div}(a\nabla v) \in L^2(\Omega)\}}$$

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Compactness of the solution space V:

$$V \subset\subset H_0^1(\Omega), \qquad V \sim H^2(\Omega)$$

Now the question is:

How to approximate V with a finite dimensional space?

Literature

Compute local effective conductivities

- HMM: Engquist, E, Abdulle, Runborg, et al. 2003-...
- Equation-free: Kevrekidis et al. 2003-...
- Stochastic Homogenization: Gloria, Otto, Le Bris, Legoll, et al. 2009-, Bal, Jing, 2010-...

Solve local cell problems

- MsFEM (Oscillating test functions): Murat-Tartar 1978, Babuska-Osborn 1984, Hou, Wu, Effendiev, et al. 1997-... Nolen, Papanicolaou, Pironneau, 2008
- Resonance Errors: Efendiev, Hou, Wu, 1999, Gloria 2010.

Literature

Pre-Computed Global Solutions

- White-Horne 1987, reservoir simulation
- Babuska-Caloz-Osborn 1994, $d = 1$
- Owhadi-Zhang 2005, harmonic coordinates, d arbitrary
- Efendiev-Hou 2006-..., two-phase flow simulations

Local Solutions

- Chu-Graham-Hou, 2010, finite number of inclusions
- Efendiev-Galvis-Wu, 2010, finite number of inclusions or masks
- Babuska-Lipton, 2010, local boundary eigenvectors
- Owhadi-Zhang, 2011, Green's function with exponential decay
- Grasedyck-Greff-Sauter, 2012, AL basis
- Malqvist-Peterseim, 2012, localized basis

Homogenization of Periodic Media

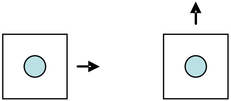
$$\begin{cases} -\operatorname{div}\left(a\left(\frac{x}{\varepsilon}\right)\nabla u^{\varepsilon}\right) = g & x \in \Omega \subset \mathbb{R}^d, \ a \text{ periodic in } y = x/\varepsilon, \\ u^{\varepsilon} = 0 & x \in \partial\Omega \end{cases}$$

$u^{\varepsilon} \rightharpoonup u_0$ in H^1; $u_0(x)$–coarse scale only, solves the homogenized problem

$$\begin{cases} -\operatorname{div}_x(\hat{a}\nabla_x u_0) = g & x \in \Omega \\ u_0 = 0 & x \in \partial\Omega. \end{cases} \tag{3}$$

u^{ε}–two scales, asymptotic expansion of $u^{\varepsilon} = u(x, x/\varepsilon)$ in ε
$\Rightarrow$ d cell problems (Y–periodicity cell, d dimension):

$$\begin{cases} -\operatorname{div}_y\left(a\left(\nabla_y \chi_i + e_i\right)\right) = 0 & x \in Y,\ 1 \leq i \leq d \\ \chi_i \in H^1_{\text{per}}(Y) \end{cases}$$



Homogenization of Periodic Media

Two objectives:

- Find effective coefficients $\hat{a}$.

Determined by cell problems only, $\hat{a}_{ij} = \int_Y (e_i + \nabla\chi_i)^T a(y)(e_j + \nabla\chi_j)dy$ – bypass for arbitrary coefficients.

- Find approximate solution $\hat{u}^\varepsilon$–homogenization approximation.

$$\|u^\varepsilon - \hat{u}^\varepsilon\|_{H^1} \leq c\varepsilon^{\frac{1}{2}}, \text{where}$$

$$\begin{aligned} \hat{u}^\varepsilon &= u_0 - \varepsilon \sum \chi_i \left(\frac{x}{\varepsilon}\right) \frac{\partial u_0}{\partial x_i} \\ &= u_0 + \varepsilon u_1 \end{aligned}$$

χ_i are solutions of cell problems. To find approximation u_0 (and $u_0 + \varepsilon u_1$), solve coarse scale problem–requires precomputing d cell problems for χ_i which do not depend on f and Ω.

Numerical Homogenization of Periodic Media – Multiscale Finite Element Method

The oscillating basis function φ^ε is locally a-harmonic in the mesh $\mathcal{T}_H$ with size H
Babuška, Osborn; Hou, Efendiev, Wu, Chen; Allaire, Brizzi;...,

$$\begin{cases} -\operatorname{div} a\nabla\varphi^\varepsilon = 0 \quad \text{in} \quad K \in \mathcal{T}_H \\ \varphi^\varepsilon \quad \text{has boundary condition (linear, oscillatory, etc.)} \end{cases}$$

φ^ε has the similar two-scale expansion as u^ε

$$\varphi^\varepsilon = \varphi_0 + \varepsilon \sum_i^n \chi_i(\frac{x}{\varepsilon}) \frac{\partial \varphi_0}{\partial x_i}(x) + r^\varepsilon$$

$$\Rightarrow \|u^\varepsilon - u^\varepsilon_H\| \le C(H + \sqrt{\frac{\varepsilon}{H}})$$

- computation of φ can be done in parallel – crucial for efficiency
- error: resonance effect, boundary layer effect – oversampling technique
- justified for the periodic medium – non-periodic case?

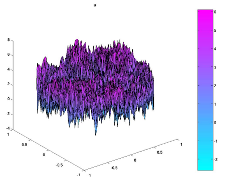
Homogenization via a-Harmonic mapping

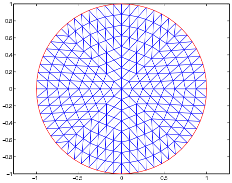
Harmonic coordinates F associated with $a(x)$.

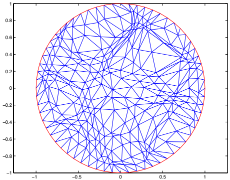
$$\begin{cases} -\operatorname{div} a \nabla F = 0 & \text{in} \quad \Omega \\ F(x) = x & \text{on} \quad \partial\Omega \end{cases}$$

$F = (F_1, F_2, \ldots, F_d)$, $x = (x_1, x_2, \ldots, x_d)$

- $d = 2$, F is a homeomorphism $\Omega \to \Omega$ Ancona, Alessandrini, Nesi.
- $\det(\nabla F) > 0$ a.e.
- $d \geq 3$, F can be non-injective (well chosen a).
- $\det(\nabla F)$ can become negative Briane, Milton, Nesi.







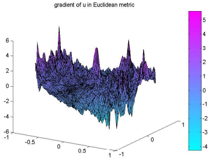
Homogenization via a-Harmonic mapping

Theorem (Finite element by composition rule, Owhadi-Zhang, '07)

Under Cordes type condition, $\exists C > 0$, the finite element solution $u_H \in V_H$ satisfies

$$\|u - u_H\|_{H^1(\Omega)} \leq CH\|g\|_{L^2(\Omega)}.$$

- While $u \in H^1(\Omega)$, $u \circ F^{-1} \in H^2(\Omega)$ – improved regularity – compact solution space in H^1!
- $u \circ F^{-1}$ can be approximated with $O(H)$ by $w_H \in P_1(\Omega)$ – piecewise linear finite element space on regular triangulation $\mathcal{T}_H$.
- u can be approximated with $O(H)$ by $u_H \in V_H := \left\{\phi \circ F \middle| \phi \in P_1(\Omega)\right\}$.



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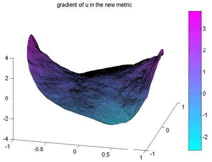

$\nabla u \circ F$

Homogenization via *a*-Harmonic mapping

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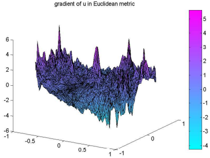

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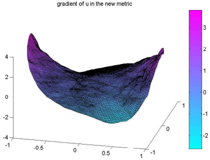

$\nabla u \circ F$

Remark:

- Cordes type condition restricts anisotropy in higher dimensions
- Harmonic coordinates approach cannot be extended to vectorial case

Homogenization via the Flux Norm

Key notion: the Flux Norm

For $k \in (L^2(\Omega))^d$, k_{pot} – potential part of k, i.e., the orthogonal projection of k onto $\{\nabla f \ : \ f \in H^1(\Omega)\}$.

For $\psi \in H_0^1(\Omega)$, define

$$\|\psi\|_{a\text{-flux}} := \|(a\nabla\psi)_{pot}\|_{(L^2(\Omega))^d}.$$

$\|\cdot\|_{a\text{-flux}}$ is a norm on $H_0^1(\Omega)$, for all $\psi \in H_0^1(\Omega)$,

$$\lambda_{\min}(a)\|\nabla\psi\|_{(L^2(\Omega))^d} \leq \|\psi\|_{a\text{-flux}} \leq \lambda_{\max}(a)\|\nabla\psi\|_{(L^2(\Omega))^d}.$$

Homogenization via the Flux Norm

Motivation for the flux norm:

- flux norm of solution of (1) is independent on a: rewrite (1) as $div(a\nabla u + \nabla\Delta^{-1} f) = 0 \Rightarrow a\nabla u + \nabla\Delta^{-1} f$ is a divergence free vector field, its potential part is 0. Thus $(a\nabla u)_{pot} + \nabla\Delta^{-1} f = 0 \Rightarrow \|u\|_{a\text{-flux}} = \|\nabla\Delta^{-1} f\|_{L^2}$.
- Why $(\cdot)_{\text{pot}}$? Fluxes ξ (heat, electric field, stress) are of interest

$$\int_{\partial\Omega} \xi \cdot n ds = \int_{\Omega} \text{div}(\xi) dx = \int_{\Omega} \text{div}(\xi_{\text{pot}}) dx.$$

- In classical homogenization convergence of energies (Γ-convergence) or convergence of fluxes (G-, H-convergence) $a^\varepsilon \nabla u^\varepsilon \rightharpoonup a^0 \nabla u^0$. Fluxes converge weakly, no flux norm was needed.

Transfer Property of Flux Norm

For a finite-dimensional linear subspace $V \subset H_0^1(\Omega)$, define $(\operatorname{div} a\nabla V)$, a finite-dim. subspace of $H^{-1}(\Omega)$, by

$$(\operatorname{div} a\nabla V) := \{\operatorname{div}(a\nabla v) \,:\, v \in V\}.$$

Theorem **(Transfer property of the flux norm)**, [Berlyand-Owhadi, '10]
Let V' and V be finite-dimensional (approximation) subspaces of $H_0^1(\Omega)$.
For $f \in L^2(\Omega)$

- let u solve $\operatorname{div}(a\nabla u) = f$ with conductivity $a(x)$,
- let u' sove $\operatorname{div}(a'\nabla u') = f$ with conductivity $a'(x)$.

If $(\operatorname{div} a\nabla V) = (\operatorname{div} a'\nabla V')$, then approximation errors are equal:

$$\sup_{f\in L^2(\Omega)} \inf_{v\in V} \frac{\|u-v\|_{a\text{-flux}}}{\|f\|_{L^2(\Omega)}} = \sup_{f\in L^2(\Omega)} \inf_{v\in V'} \frac{\|u'-v\|_{a'\text{-flux}}}{\|f\|_{L^2(\Omega)}}.$$

Transfer Property of the Flux Norm

Idea of the proof:

1. Show (recall $\|u-v\|_{a\text{-flux}} = \|(a\nabla u - a\nabla v)_{\text{pot}}\|_{(L^2(\Omega))^d}$)

$$\sup_{f\in L^2(\Omega)} \inf_{v\in V} \frac{\|(a\nabla u - a\nabla v)_{\text{pot}}\|_{(L^2(\Omega))^d}}{\|f\|_{L^2(\Omega)}} = \sup_{w\in H^2(\Omega)\cap H^1_0(\Omega)} \inf_{v\in V} \frac{\|(\nabla w - a\nabla v)_{pot}\|_{(L^2(\Omega))^d}}{\|\Delta w\|_{L^2(\Omega)}}. \tag{4}$$

   Proof of (4):
   Since $f\in L^2(\Omega)$, $\exists w\in H^2(\Omega)\cap H^1_0(\Omega)$ s.t. $-\Delta w = f$ for $x\in\Omega$.
   $\text{div}(a\nabla u) = -f = \text{div}(\nabla w) \Rightarrow (a\nabla u)_{\text{pot}} = (\nabla w)_{\text{pot}} = \nabla w$.
   Then, for any $v\in V$, $\|(\nabla w - a\nabla v)_{pot}\|_{(L^2(\Omega))^d} = \|(a\nabla u - a\nabla v)_{pot}\|_{(L^2(\Omega))^d}$.

2. Show

$$\sup_{w\in H^2(\Omega)\cap H^1_0(\Omega)} \inf_{v\in V} \frac{\|(\nabla w - a\nabla v)_{pot}\|_{(L^2(\Omega))^d}}{\|\Delta w\|_{L^2(\Omega)}} = \sup_{z\in(\text{div}\, a\nabla V)^\perp} \frac{\|z\|_{L^2(\Omega)}}{\|\nabla z\|_{(L^2(\Omega))^d}}. \tag{5}$$

   Proof: Appendix

3. The theorem then follows by combining (4) with (5) and noting that the RHS of (5) is the same for all pairs (a, V) and (a', V') whenever $\text{div}(a\nabla V) = \text{div}(a'\nabla V')$.

Optimal Approximation Space w.r.t Flux Norm

Kolmogorov n-width $d_n(A, X)$, measures how accurately a given set of functions $A \subset X$ can be approximated by a $n-$dim linear subspace $E_n \subset X$

$$d_n(A, X) = \inf_{E_n} \sup_{w \in A} \inf_{g \in E_n} \|w - g\|_X$$

for a normed linear space X.

In our case:

- X: $H_0^1(\Omega)$ with $\|\cdot\|_{a-\text{flux}}$-norm,
- A: set of all solutions of (1) as f spans L^2

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The corresponding $n-$width is given by

$$d_n(A, X) = \frac{1}{\sqrt{\lambda_{n+1}}} \sim n^{-1/d} \operatorname{diam}(\Omega)$$

suppose that (u_i, λ_i) is the ith eigenpair for Dirichlet eigenvalue problem w.r.t $-\Delta$ in Ω, the optimal $n-$term approximation space is given by

$$V := \operatorname{span}\{v_i, -\operatorname{div} a \nabla v_i = \lambda_i u_i, v_i = 0\ \partial\Omega, i = 1 \cdots n\}$$

Localization of the Basis

Take $a' = I_d$ in the transfer property so that $\mathrm{div}(a'\nabla) = \Delta$

$$V' := \mathrm{span}\{\varphi_i\}$$

$$\begin{cases} -\nabla \cdot a \nabla \psi_i = -\Delta \varphi_i & \Omega, \\ \psi_i = 0 & \partial\Omega, \end{cases}$$

$$V_H := \mathrm{span}\{\psi_i\}$$

$$\sup_{g \in L^2(\Omega)} \inf_{v \in V_H} \frac{\|u - v\|_{a\text{-flux}}}{\|g\|_{L^2(\Omega)}} \leq CH$$

C independent of contrast.

Localization of the Basis

$$\begin{cases} -\nabla \cdot a\nabla\psi_i^l = -\Delta\varphi_i & \Omega_i, \\ \psi_i^l = 0 & \partial\Omega_i, \end{cases}$$

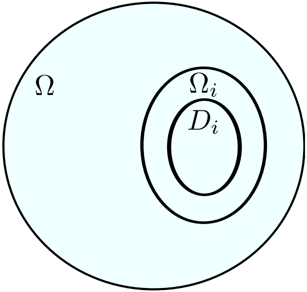
$$G(x,y) \sim \frac{1}{|x-y|^{d-2}}$$

$$\begin{cases} \frac{\psi_i^T}{T} - \nabla a \nabla\psi_i^T = -\Delta\varphi_i & \Omega_i \\ \psi_i^T = 0 & \partial\Omega_i \end{cases}$$

The zeroth-order term (a strange term from nowhere) makes Green's function decay exponentially.

$$G_T(x,y) \le \frac{C}{|x-y|^{d-2}} \exp\left(-\frac{|x-y|}{C\sqrt{T}}\right)$$

$D_i = \text{supp}\varphi_i$, $\Omega_i = \text{supp}\psi_i$,



Papanicolaou-Varadhan 1979, Yurinskii 1986, Gloria-Otto 2010.

Localization of the Basis

$X_h := \text{span}\{\varphi_i\}$, $\text{diam}(\text{supp}(\varphi_i)) = O(H)$,

$$\begin{aligned} \inf_{v\in X_H} \|w - v\|_{H^1} &\leq CH\|w\|_{H^2} \\ \inf_{v\in X_H} \|w - v\|_{H^1} &\leq CH^2\|w\|_{H^3} \end{aligned}$$

$\exists C_1 > 0$, $\Omega_i = B(x_i, C_1 H^{\frac{1}{2}} \log(\frac{1}{H}))$ (suboptimal), $T = H$,

$$\begin{cases} H^{-1}\psi_i - \nabla a \nabla \psi_i = -\Delta\varphi_i & \Omega_i \\ \psi_i = 0 & \partial\Omega_i \end{cases}$$

Theorem (Localized basis), [Owhadi-Zhang, '11]
$\exists C_0 > 0$, s.t. for $C > C_0$

$$\frac{\|u - u_H\|_{H^1}}{\|g\|_{L^2(\Omega)}} \leq C(H + \frac{H^2}{T}) \leq CH$$

New Idea: Approximate V by Interpolating its Elements.

Assume $d \leq 3$,

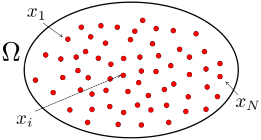
$$V := \{v \in H_0^1(\Omega) | \operatorname{div}(a\nabla v) \in L^2(\Omega)\}$$

- $d \leq 3$
- $\operatorname{div}(a\nabla v) \in L^2(\Omega)$

$\xrightarrow{\text{De Giorgi, Stampacchia}} v \in C^\alpha(\Omega).$

Elements of V are continuous and have well defined point values

1. Pick N points $(x_1, x_2, \cdots, x_N)$
2. For $(v_1, \ldots, v_N) \in \mathbb{R}^N$,
   find $v \in V$, s.t. $v(x_i) = v_i$.



Question: Which v to pick? Choice is not unique.

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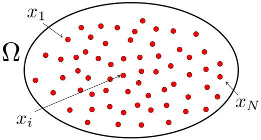

Answer: Pick v minimize the $\|\cdot\|_V$-norm.
where $\|\cdot\|_V^2 := \int_\Omega |\operatorname{div}(a\nabla\phi)|^2$.

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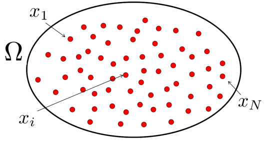


Answer: Pick v minimize the $\|\cdot\|_V$-norm.

The elements of V have bounded $\|\cdot\|_V$ norm implies the compactness of V in $H_0^1(\Omega)$.

New Idea: Approximate V by Interpolating its Elements.

- Interpolation Problem:
  For $(v_1, \dots, v_N) \in \mathbb{R}^N$, find $v \in V$, s.t. $v(x_i) = v_i$.
- Answer: Pick v as the minimizer of

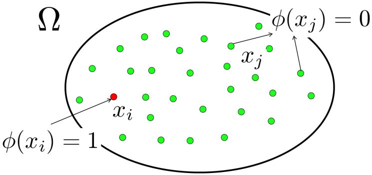
$$\begin{cases} \text{Minimizer } \|\operatorname{div}(a\nabla\omega)\|_{L^2(\Omega)}. \\ \text{Subject to } \omega(x_i) = v_i. \end{cases}$$

- Questions:
  - Is the minimization problem well-posed? Existence & Uniqueness?
  - Is the interpolation space linear?
  - Is there an interpolation basis?

Existence of an Interpolation Basis

Formulation: For each i, find $\phi_i \in V$, s.t.

$$\begin{cases} \text{Minimize } \|\operatorname{div}(a\nabla\phi)\|_{L^2(\Omega)}. \\ \text{Subject to } \phi_i(x_j) = \delta_{ij}. \end{cases} \quad (6)$$



$$\boxed{V := \{v \in H_0^1(\Omega) | \operatorname{div}(a\nabla v) \in L^2(\Omega)\}}$$

$$\boxed{V_i := \{\phi \in V | \phi(x_j) = \delta_{ij}, \text{for } j \in \{1, \dots, N\}\}}$$

Theorem [Well-posedness of ϕ_i]:

- V_i is a non-empty closed affine subspace of V.
- (6) is a strictly convex (quadratic) minimization problem over V_i.
- ϕ_i is the unique minimizer of (6).

Representation Theorem for the Interpolation Basis

Theorem [Representation of ϕ_i]:

$$\phi_i(x) = \sum_j^N P_{ij}\tau(x, x_j)$$

where

$$\tau(x, y) := \int_\Omega G(x, z)G(z, y)dz$$

G: Green's function of (1)

$$\begin{cases} -\mathrm{div}_x(a\nabla_x G(x, y)) = \delta(x - y) & x \in \Omega \\ G(x, y) = 0 & x \in \partial\Omega \end{cases}$$

τ: fundamental solution of $(\mathrm{div}(a\nabla\cdot))^2$

$$\begin{cases} -\mathrm{div}_x(a\nabla_x(\mathrm{div}_x\, a\nabla_x \tau(x, y)))) = \delta(x - y) & x \in \Omega \\ \tau(x, y) = \mathrm{div}_x(a\nabla_x \tau(x, y)) = 0 & x \in \partial\Omega \end{cases}$$

Representation Theorem for the Interpolation Basis

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Θ: $N \times N$ pos. def. sym. matrix

$$\Theta_{i,j} := \tau(x_i, x_j)$$

P: $N \times N$ pos. def. sym. matrix

$$P := \Theta^{-1}$$

Representation Theorem for the Interpolation Basis

$$\boxed{\Theta_{i,j} := \tau(x_i, x_j)}$$

$$\Downarrow$$

$$\boxed{\Theta_{i,j} = \int_\Omega G(y, x_i) G(y, x_j) dy}$$

Theorem [Property of Θ]: Θ is symmetric positive definite. For $l \in \mathbb{R}^d$, $l^T \Theta l = \|v\|^2_{L^2(\Omega)}$, where v is the solution of

$$\begin{cases} -\operatorname{div}(a\nabla v) = \sum_{j=1}^N l_j \delta(x - x_j) & x \in \Omega \\ v(x) = 0 & x \in \partial\Omega \end{cases}$$

Representation Theorem for the Interpolation Basis

P: Discretization of $(\mathrm{div}(a\nabla\cdot))^2$ over $(x_i)_{i\in\mathcal{N}}$

- $\Theta_{i,j} := \tau(x_i, x_j)$
- τ: fundamental solution of $L := (\mathrm{div}(a\nabla\cdot))^2$.
- $P := \Theta^{-1}$, $L := \tau^{-1}$,

$\Rightarrow P = L_d$.

Representation Theorem for the Interpolation Basis

P: Discretization of $(\mathrm{div}(a\nabla\cdot))^2$ over $(x_i)_{i\in\mathcal{N}}$

- $\Theta_{i,j} := \tau(x_i, x_j)$
- τ: fundamental solution of $L := (\mathrm{div}(a\nabla\cdot))^2$.
- $P := \Theta^{-1}$, $L := \tau^{-1}$,

$\Rightarrow P = L_d$.

ϕ_i : Approximation of a Dirac at x_i.

- $P = L_d$, P discretization of L over $(x_i)_{i\in\mathcal{N}}$.
- $\phi_i(x) := \sum_{j=1}^{N} P_{ij}\tau(x, x_j)$
- $\phi_i = L_d\tau$

$\Rightarrow \phi_i \simeq \delta(x - x_i)$.

Rough Polyharmonic Splines

- for $d \leq 3$. ϕ_i is biharmonic

$$(\mathrm{div}(a\nabla\cdot))^2\phi_i(x) = 0 \text{ for } x \neq x_j$$

- Generalization to $d \geq 4$, $m > d/2$. ϕ_i minimizer of

$$\int_\Omega |\,\mathrm{div}(a\nabla\phi)|^m$$

subject to $\phi \in H_0^1(\Omega)$ and $\phi(x_j) = \delta_{i,j}$.

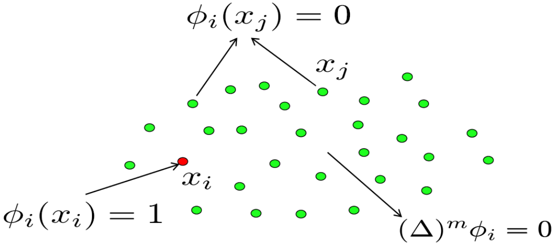
$$(\mathrm{div}(a\nabla\cdot))^m\phi_i(x) = 0 \text{ for } x \neq x_j$$

ϕ_i: is polyharmonic (m-harmonic).

Rough Polyharmonic Splines (RPS)

We call $\{\phi_i\}_{i\in\mathcal{N}}$ Rough Polyharmonic Splines (RPS), a generalizeation of polyharmonic splines to PDEs with rough coefficients.

Polyharmonic Splines:



ϕ_i minimizes

$$\Big(\int_{\mathbb{R}^d} \sum_{\alpha\in\mathbb{N}^d, |\alpha|=m} c_\alpha \big(\frac{\partial^\alpha \phi}{\partial x^\alpha}\big)^2 \,\mathrm{d}x\Big)^{\frac{1}{2}}$$

$c_\alpha > 0$ are usually chosen to be equal to $m!/\alpha!$ to ensure the rotational invariance of the semi-norm (sometimes chosen as 1)

Literature on Polyharmonic Splines

- Harder-Desmarais, 1975: Interpolation of functions of two variables based on the minimization of a quadratic functional corresponding to the bending energy of a thin plate.
- Atteia 1970: fonctions splines.
- Schoenberg 1973: Cardinal spline interpolation (1d case)
- Duchon 1976, 1977, 1978: Seminal work and extensions to higher dimensions.
- Madych-Neslon 1990: Cardinal polyharmonic splines.

Example: $d = 1$

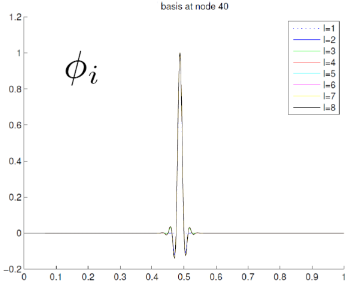
$d = 1$, $\Omega = (0, 1)$.

$$a(x) := 1 + \frac{1}{2}\sin\Big(\sum_{k=1}^{K} k^{-\alpha}\big(\zeta_{1k}\sin(kx) + \zeta_{2k}\cos(kx)\big)\Big)$$

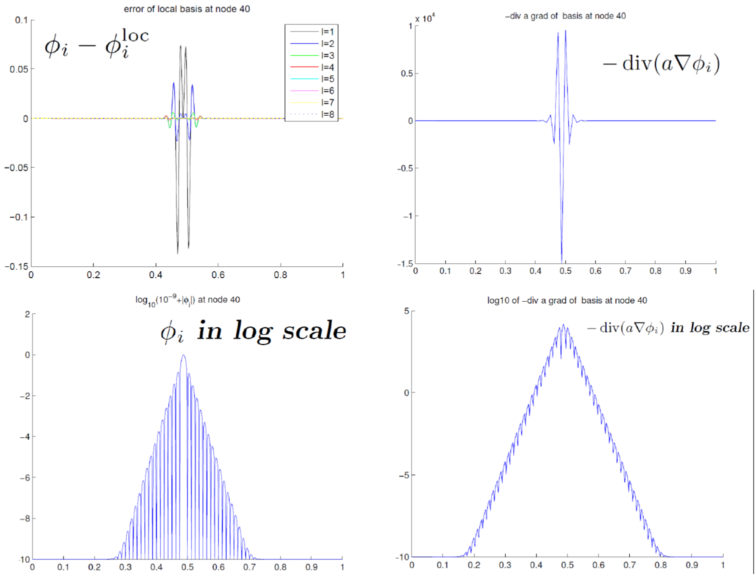
$\{\zeta_{1k}\}$, $\{\zeta_{2k}\}$: i.i.d. uniformly distributed in $[-\frac{1}{2}, \frac{1}{2}]$.

$$\langle|\hat{a}(k)|^2\rangle \simeq |k|^{-\alpha}$$

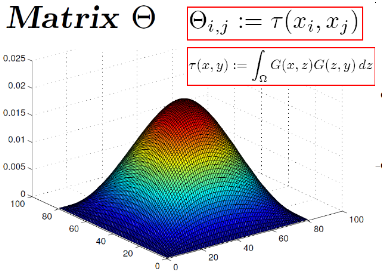
Example taken out of [Hou-Wu 1997] and [Ming-Yue 2006].

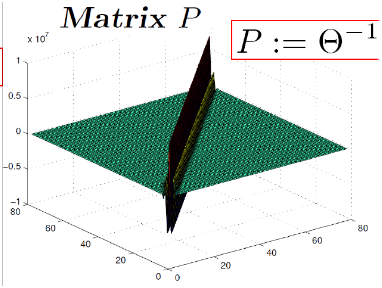


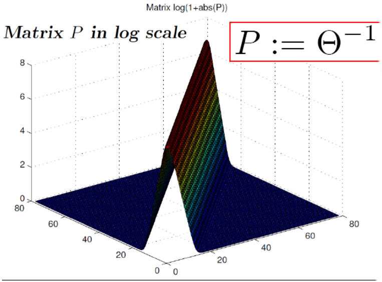
Example: $d = 1$


error of local basis at node 40
$\phi_i - \phi_i^{\text{loc}}$
l=1
l=2
l=3
l=4
l=5
l=6
l=7
l=8
x 10^4
–div a grad of basis at node 40
$-\operatorname{div}(a\nabla\phi_i)$
log10(10^−9+|φi|) at node 40
ϕ_i in log scale
log10 of –div a grad of basis at node 40
$-\operatorname{div}(a\nabla\phi_i)$ in log scale

Example: $d = 1$

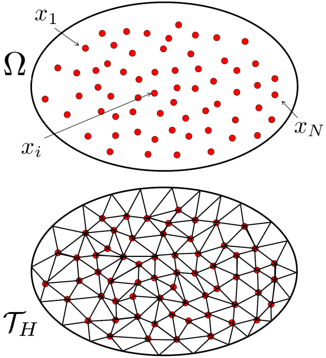

Matrix Θ
$\Theta_{i,j} := \tau(x_i, x_j)$
$\tau(x,y) := \int_\Omega G(x,z)G(z,y)\,dz$
0.025
0.02
0.015
0.01
0.005
0
100
80
60
40
20
0
0
20
40
60
80
100


Matrix P
$P := \Theta^{-1}$
x 10^7
1
0.5
0
−0.5
−1
80
60
40
20
0
0
20
40
60
80


Matrix log(1+abs(P))
Matrix P in log scale
$P := \Theta^{-1}$
8
6
4
2
0
80
60
40
20
0
0
20
40
60
80

Accuracy of the Rough Polyharmonic Splines

- Need: A measure of regularity of the distribution of the points $(x_i)_{i\in\mathcal{N}}$.
- The accuracy depends on the property of the discrete set $(x_i)_{i\in\mathbb{N}}$, i.e., the constant $H := \sup_{x\in\Omega} \min_{i\in\mathbb{N}} |x - x_i|$.
  meshless method, does not depend on the aspect ratio of the mesh



Accuracy of the Rough Polyharmonic Splines

Variational Property of the Interpolation Basis

$$V := \{v \in H_0^1(\Omega) | \operatorname{div}(a\nabla v) \in L^2(\Omega)\}$$

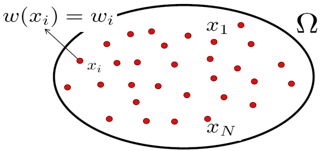
$$V_0 := \{v \in V | v(x_i) = 0 \text{ for all } i\}$$

Theorem [variational property]:

- The basis ϕ_i is orthorgonal to V_0 w.r.t the product $\langle \cdot, \cdot \rangle$ associated with V-norm.
- $\sum_{i=1}^N \omega_i \phi_i$ is the unique minimizer of

$$\int_\Omega (\operatorname{div}(a\nabla\omega))^2$$

over all $\omega \in V$ such that $\omega(x_i) = \omega_i$.



Accuracy of the Rough Polyharmonic Splines

Higher order Poincare Inequality

$$V := \{v \in H_0^1(\Omega) | \operatorname{div}(a\nabla v) \in L^2(\Omega)\}$$

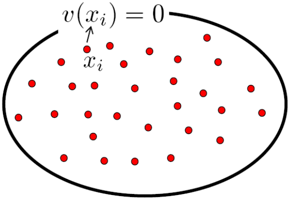
$$V_0 := \{v \in V | v(x_i) = 0 \text{ for all } i\}$$

Theorem [Higher Order Poincare]: Let $f \in V_0$. It holds true that

$$\|\nabla f\|_{L^2(\Omega)} \leq CH \| \operatorname{div}(a\nabla f)\|_{L^2(\Omega)}$$

C depends on $\lambda_{\min}(a)$.

Proof by contradiction.



Accuracy of the Rough Polyharmonic Splines

$$\begin{cases} -\operatorname{div}(a\nabla v) = g & x \in \Omega \\ v(x) = 0 & x \in \partial\Omega \end{cases}$$

u: Solution of (1)
$u^{in} := \sum_{i=1}^{N} u(x_i)\phi_i(x)$.

Theorem [Accuracy of RPS]:

$$\|u - u^{in}\|_{H_0^1(\Omega)} \leq CH\|g\|_{L^2(\Omega)}$$

C depends on $\lambda_{\min}(a)$.

Accuracy of the Rough Polyharmonic Splines

$V_0 := \{v \in V | v(x_i) = 0 \text{ for all } i\}$

Proof [Accuracy of RPS]:

$$u - u^{in} \in V_0$$

Higher order Poincare inequality

$$\|\nabla f\|_{L^2(\Omega)} \leq CH \|\operatorname{div}(a\nabla f)\|_{L^2(\Omega)}$$

Variational property of the interpolation basis

$$\|\operatorname{div}(a\nabla u^{in})\|_{L^2(\Omega)} \leq \|\operatorname{div}(a\nabla u)\|_{L^2(\Omega)}$$

Accuracy of the FEM

$$\begin{cases} -\operatorname{div}(a\nabla v) = g & x \in \Omega \\ v(x) = 0 & x \in \partial\Omega \end{cases}$$

u: Solution of (1)
u^H: F.E. solution of (1) over span(ϕ_i)

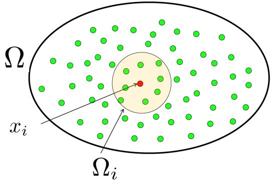
Theorem [Accuracy of the FEM]:

$$\|u - u^H\|_{H_0^1(\Omega)} \leq CH\|g\|_{L^2(\Omega)}$$

C depends on $\lambda_{\min}(a)$, $\lambda_{\max}(a)$, does not depend on the aspect ratio of the mesh.

Localization of the RPS

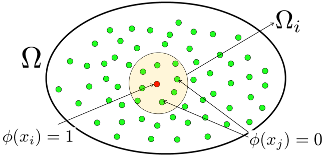
- Subdomain Ω_i around x_i.



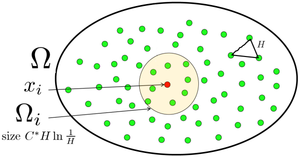
- Define localized basis ϕ_i^{loc} in Ω_i.
  ϕ_i^{loc}: minimizer of $\int_{\Omega_i} |\operatorname{div}(a\nabla\phi)|^2$,
  subject to $\phi \in H_0^1(\Omega_i)$ and $\phi(x_j) = \delta_{ij}$

  $$(\operatorname{div}(a\nabla\cdot))^2\phi_i^{\text{loc}}(x) = 0 \text{ for } x \neq x_j$$

  –minimizing variational problem, thus sparse and elliptic, numerically stable



- Ω_i is of size $CH\log(\frac{1}{H})$ – super localization.
  $(B(x_i, C^*H\log\frac{1}{H}) \cap \Omega) \subset \Omega_i$



Localization of the RPS

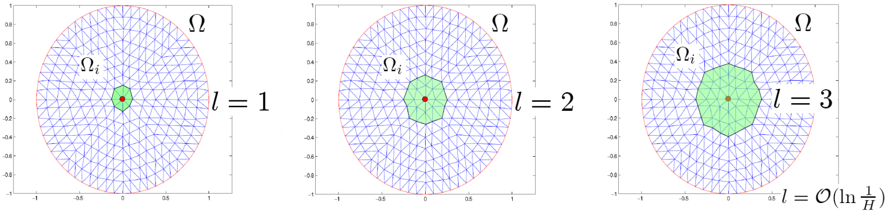
u: solution of PDE (1) $\begin{cases} -\operatorname{div}(a\nabla u) = f & x \in \Omega \\ u = 0 & x \in \partial\Omega \end{cases}$.

$u^{H,\mathrm{loc}}$: Finite Element solution of (1) over span(ϕ_i^{loc}).

Theorem [Accuracy of the FEM]: If $(B(x_i, CH\log(\frac{1}{H}) \cap \Omega) \subset \Omega_i$, then

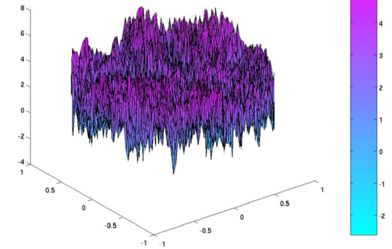
$$\|u - u^{H,\mathrm{loc}}\|_{H_0^1(\Omega)} \leq CH\|g\|_{L^2(\Omega)}$$

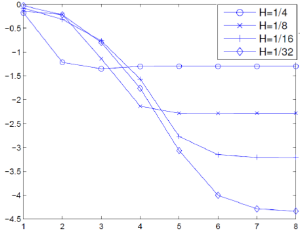
C depends on $\lambda_{\min}(a)$, $\lambda_{\max}(a)$.



Numerical Results: $d = 2$

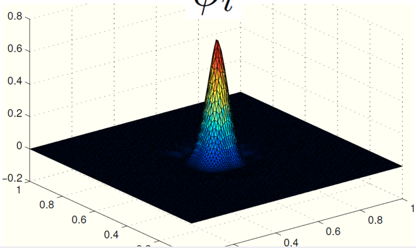
a



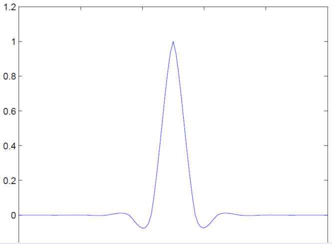


$\|u - u^{H,\mathrm{loc}}\|_{\mathcal{H}^1(\Omega)}$ vs number of layers l in $\log_{10}$ scale

ϕ_i



Slice of ϕ_i along the x-axis



Outlook: Straightforward Applications

- Domain decomposition preconditioner
- A posteriori error estimate
- Hyperbolic equations

$$\begin{cases} \rho(x)\partial_t^2 u(x,t) - \text{div}(a\nabla u(x,t)) = g(x,t) & x \in \Omega_T \\ \text{B.C.} + \text{I.C.} \end{cases} \tag{7}$$

$$u^{H,\text{loc}}(x,t) = \sum_i c_i(t)\phi_i^{\text{loc}}(x)$$

$$\|\partial_t(u - u^{H,\text{loc}})\|_{L^2(\Omega)} + \|u - u^{H,\text{loc}}\|_{L^2(0,T,H_0^1(\Omega))} \le CH$$

up to $T = O(1)$.

- Linear elasticity and elastodynamics
- Coarse graining of atomistic systems

Outlook: Further Questions

- Effective Equation of $-\operatorname{div} a(x)\nabla u = f$ on scale $H \gg \varepsilon$, could it be a non-local equation?
- Nonlinear Problem, $-\operatorname{div} W(x, \nabla u) = f$ or $-\operatorname{div} W(\frac{x}{\varepsilon}, \nabla u) = f$, how to obtain a low-dimensional approximating space?
- Wave equation
$$u_{tt} = \operatorname{div} a(x)\nabla u$$
using basis from elliptic problem might be problematic, approximating H-measure?
- Coarse graining atomistic system, incorporating finite temperature effect?

Happy Birthday Professor Tartar!
Thanks for Your Attention!

- The method is local and the support $H \log(1/H)$.
- The interpolation is nodal (so it solves the inverse problem from going from point measurements to the actual function).
- Even after localization the method remains variational and of the form: minimize $x^T Ax$ where A is sparse.
- Because it is sparse AND elliptic it has the smallest cost we know of in terms of number of operations to find the localized basis: $((H(\log(1/H))/h)^{-d})$ (H=size of coarse mesh, h=size of fine mesh).
- Because it is sparse and a minimization problem it is robust with respect to the contrast of the medium (no proof there but we observe it numerically at this stage).