Upscaling Wave Computations

Xin Wang

2010 TRIP Annual Meeting

Outline

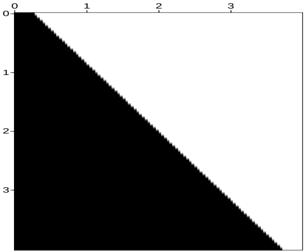
Wave Equations

scalar variable density acoustic wave equation

$$\frac{1}{\kappa}\frac{\partial^2 p}{\partial t^2} - \nabla \cdot \frac{1}{\rho}\nabla p = f \qquad p \equiv 0, t \ll 0$$

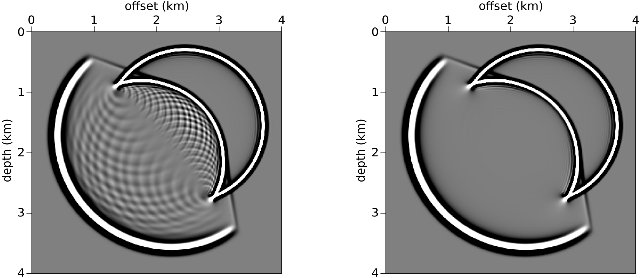
Lions, 1972: solution is continuous even when ρ, κ piecewise const or worse

careless data sampling on discrete grid can cause artifacts in FD, FEM method because of interface



Mass Lumping

- for constant density case, *Symes and Terentyev, 2009* used mass lumping in FE method to preserve sub-grid information



  even worse in elasticity (elastic tensor as density in AWE)
- for non-const case, direct averaging doesn't work: jumps in density (salt boundaries, sea floor) mean jumps in first order derivative of p. but $\mathbb{P}_1, \mathbb{Q}_1$ elements don't have such sub-grid feature

Wave Equation

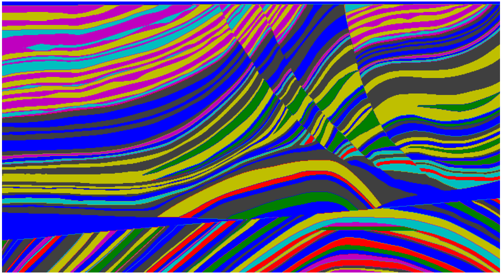
- conventional numerical methods work well for smooth $1/\rho$

$$\nabla \cdot \frac{1}{\rho} \nabla p = \frac{1}{\rho} \nabla^2 p + \nabla \frac{1}{\rho} \cdot \nabla p$$

  low order terms not important in convg analysis $\Rightarrow \nabla \cdot 1/\rho \nabla$ like $\nabla^2 \Rightarrow$ formally 2nd order scheme are actually 2nd order - RMS error$= O(\Delta x^2)$

Wave Equation

- BUT with small scale oscillation or jumps in $1/\rho$, $\nabla(1/\rho)$ can go to ∞, u has no continuous 1st order derivative. then no rate of convg for conventional methods



Current Upscaling Approaches

upscaling tries to use a coarse grid to resolve subgrid structure, such as jumps, small scale oscillation

- harmonic coordinates
- effective tensor for periodic media
- immersed interface method (IIM)
- other multiscale methods

same difficulty in steady-state problem:

$$-\nabla \cdot a(x)\nabla u = f$$

Harmonic Coordinates

observation: oscillatory $a \Rightarrow$ oscillatory u

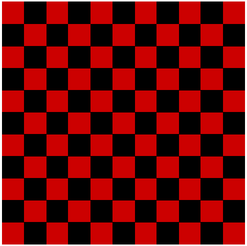


Figure: $a(x)$

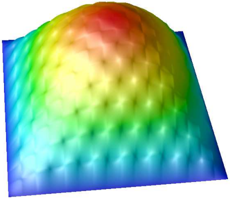


Figure: sol $u(x)$ for elliptic problem

Harmonic Coordinates

strategy: pull out $a(x)$ by the change of variable so as to transfer the orig prob to a non-divergence form (*Kozlov et al. 97, TRIP annual meeting 09, 10*)

global a-harmonic coordinates F solves: $j = 1, \cdots, n$

$$\begin{aligned} \nabla \cdot a(x) \nabla F_j = 0 \quad & \text{in } \Omega \\ F_j(x) = x_j \quad & \text{on } \partial\Omega \end{aligned}$$

F: identity operator on boundaries

Harmonic Coordinates

suppose F invertible, $u(x) = \tilde{u}(F(x)) = \tilde{u} \circ F(x)$. then

$$\frac{\partial u}{\partial x_i} = \sum_j \frac{\partial F_j}{\partial x_i} \frac{\partial}{\partial F_j} \tilde{u} \circ F$$

$$\nabla \cdot a \nabla u = \sum_j [\nabla \cdot a \nabla F_j] \frac{\partial}{\partial F_j} \tilde{u} \circ F + \sum_{j,k} [a \nabla F_j \cdot \nabla F_k] \frac{\partial^2}{\partial F_j \partial F_k} \tilde{u} \circ F$$

now let $A_{jk} = [a \nabla F_j \cdot \nabla F_k] \circ F^{-1}$ defined on new coordinates F. then

$$-\sum_{j,k} A_{jk} \frac{\partial^2 \tilde{u}}{\partial F_j \partial F_k} = f \circ F^{-1}$$

Harmonic Coordinates

- 1D harmonic coordinate: $F(x) = \int_0^x 1/a(z)\,\mathrm{d}z / \int_0^1 1/a(z)\,\mathrm{d}z$

$$-\frac{\mathrm{d}^2\tilde{u}}{\mathrm{d}F^2} = \Big(\int_0^1 1/a(z)\,\mathrm{d}z\Big)^2 (fa)\circ F^{-1}$$

  in 1D smoothness recovered automatically

- smoothness of $\tilde{u}$ in higher-D assured by Bernstein theorem, 1906 requiring the stability of matrix A

  to use this strategy F must be invertible; this is guaranteed in 2D (see Alessandrini 2001), but not always hold in 3D (see Owhadi and Zhang 2006)

Harmonic Coordinates

- *Babuška, Caloz and Osborn 1994* used the harmonic coordinate change to build base functions for special (unidirectional varied) coefficient functions: apply to curved interface without implementation
- *Muir, Dellinger, Etgen and Nichols 1992* applied Schoenberg-Muir averaging to gridding problem

we claim that Muir et al. actually implement equivalent upscaling rule as in Babuška et al.

Effective Tensor for Periodic Media

by *Bensoussan et al. 1978*, consider a family of problems

$$-\nabla \cdot a^{\epsilon}(x)\nabla u^{\epsilon} = f$$

where $a^{\epsilon}(x) = a(x/\epsilon)$, $a(y)$ a Y-periodic function ($Y = (0,1)^n$)

want to identify the effective coefficient a^* such that as $\epsilon \to 0$, $u^{\epsilon} \to u^*$:

$$-\nabla \cdot a^* \nabla u^* = f$$

Two-scale Asymptotic Expansion

- sol u^ϵ in the form of a power series expansion in ϵ

$$u^\epsilon = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \cdots$$

- $\{u_i\}$ depend explicitly on x and $y = x/\epsilon$ and 1-periodic w.r.t. y (idea of multiple scales)

$$\Rightarrow u^\epsilon(x) = u_0\left(x, \frac{x}{\epsilon}\right) + \epsilon u_1\left(x, \frac{x}{\epsilon}\right) + \epsilon^2 u_2\left(x, \frac{x}{\epsilon}\right) + \cdots$$

Effective Tensor for Periodic Media

- $u_0(x, x/\epsilon) = u^*(x)$ is the sol of the homogenized prob

$$-\nabla \cdot a^* \nabla u^* = f \qquad \text{in } \Omega$$
$$u^* = 0 \qquad \text{on } \partial\Omega$$

where a^* is a constant effective tensor

$$a^* = \int_Y a(y)(I + \nabla\chi(y)^T)\,\mathrm{d}y$$

- χ_i solves cell problem

$$-\nabla_y \cdot a(y)(e_i + \nabla_y \chi_i) = 0 \qquad \text{in Y}$$
$$y \to \chi_i(y) \qquad \text{Y} - \text{periodic}$$

- $u_1(x, x/\epsilon) = \sum_i \chi_i(\frac{x}{\epsilon})\frac{\partial u^*}{\partial x_i}(x)$

Effective Tensor and Harmonic Coordinates

χ_i solves cell problem: $y = x/\epsilon$, $\nabla_y x_i = \epsilon e_i$

$$-\nabla_y \cdot a(y) \nabla_y (x_i + \epsilon \chi_i) = 0 \qquad \text{in Y}$$
$$y \to \chi_i(y) \qquad \mathrm{Y-periodic}$$

$x + \epsilon\chi \to$ harmonic coordinates F

rewrite two-scale asymptotic expansion as:

$$u^\epsilon(x) \approx u^*(x) + \epsilon \sum_{i=1}^{n} \chi_i\left(\frac{x}{\epsilon}\right) \frac{\partial u^*}{\partial x_i}(x) \approx u^*(x + \epsilon\chi) = u^* \circ F(x)$$

Effective Tensor in 1D is Harmonic Average

the cell problem in 1D

$$-\frac{\mathrm{d}}{\mathrm{d}y}\Big(a(y)\frac{\mathrm{d}\chi}{\mathrm{d}y}\Big) = \frac{\mathrm{d}}{\mathrm{d}y}a(y) \quad y \in [0,1]$$

$$\chi \text{ is periodic}$$

$$\chi(y) = \int_0^y \frac{1}{a(y)}\,\mathrm{d}y \Big/ \int_0^1 \frac{1}{a(y)}\,\mathrm{d}y - y$$

1D effective coefficient is harmonic average

$$a^* = \int_0^1 (a(y) + a(y)\frac{\mathrm{d}\chi(y)}{\mathrm{d}y})\,\mathrm{d}y = \Big(\int_0^1 1/a(y)\,\mathrm{d}y\Big)^{-1}$$

Backus Averaging

Backus 1962:

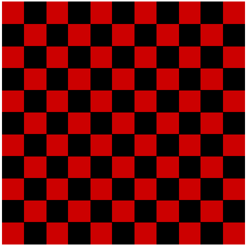
"A horizontally layered inhomogeneous medium, isotropic or transversely isotropic, is considered, whose properties are constant or nearly so when averaged over some vertical height l. For waves longer than l the medium is shown to behave like a homogeneous, or nearly homogeneous, transversely isotropic medium ..."

2D Checkerboard Example

example in Eymard and Gallouët 04,

$$a^{\epsilon}(x,y) = \begin{cases} a_r, & \mathrm{Int}(x/\epsilon) + \mathrm{Int}(y/\epsilon) \text{ odd} \\ a_b, & \mathrm{Int}(x/\epsilon) + \mathrm{Int}(y/\epsilon) \text{ even} \end{cases} \rightarrow a^*(x,y) = \sqrt{a_r a_b}$$

note: a^* is not harmonic average



$a_r = 1.0, a_b = 0.4, \epsilon = 0.25$

$\|u^* - u^\epsilon\|_{L^2} = 0.026$

Figure: u^* (left) and u^ϵ (right)

$a_r = 1.0, a_b = 0.4, \epsilon = 0.125$

$\|u^* - u^\epsilon\|_{L^2} = 0.0149$

Figure: u^* (left) and u^ϵ (right)

$a_r = 1.0, a_b = 0.4, \epsilon = 0.0625$

$\|u^* - u^\epsilon\|_{L^2} = 0.0096$

Figure: u^* (left) and u^ϵ (right)

Immersed Interface Method

- designed for interface problem
- both FD and FEM implementations
- need to know interface location explicitly
- successfully apply to waves (acoustic and elastic) by R. LeVeque and his student, remove staircase diffraction $\Rightarrow$ full order convergence

Immersed Interface Method

1d elliptic interface problem

$$(\beta u_x)_x = f \quad 0 \leq x \leq 1, \qquad u(0) = u(1) = 0$$

$f \in L^2(0,1)$, β has discontinuity at $x = \alpha$

$$\beta(x) = \begin{cases} \beta^- & x < \alpha \\ \beta^+ & x > \alpha \end{cases}$$

displacement u is continuous as well as normal stress βu_x at α

$\Rightarrow [u]_{x=\alpha} = u^+(\alpha) - u^-(\alpha) = 0$, and

$[\beta u_x]_{x=\alpha} = \beta^+ u_x^+(\alpha) - \beta^- u_x^-(\alpha) = 0$

if f is continuous,

$\beta_x^+ u_x^+(\alpha) + \beta^+ u_{xx}^+(\alpha) = f_x(\alpha) = \beta_x^- u_x^-(\alpha) + \beta^- u_{xx}^-(\alpha)$.

$$\Rightarrow \beta^+ u_{xx}^+(\alpha) = \beta^- u_{xx}^-(\alpha)$$

Immersed FD

- generate a Cartesian grid, $x_i = ih, \ i = 0, 1, \cdots, N$ and $x_j \leq \alpha \leq x_{j+1}$ for some j
- at a grid point $x_i, i \neq j, j+1$, IFD use the 3-point central FD

$$\frac{1}{h^2}\Big(\beta_{i+1/2}(U_{i+1} - U_i) - \beta_{i-1/2}(U_i - U_{i-1})\Big) = f_i$$

  where $\beta_{i+1/2} = \beta(x_{i+1/2})$ and $f_i = f(x_i)$
- at points x_j and x_{j+1}, IFD use

$$\gamma_{0,1} U_{j-1} + \gamma_{0,2} U_j + \gamma_{0,3} U_{j+1} = f_j$$
$$\gamma_{1,1} U_j + \gamma_{1,2} U_{j+1} + \gamma_{1,3} U_{j+2} = f_{j+1}$$

  the coefficients minimize local truncation error
- solve the system to get $u_i, i = 0, 1, \cdots, N$

Immersed FD

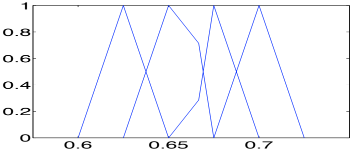
- improve accuracy near interfaces
- additional memory for coefficients, conditional branch (code inefficiency) or post process

Immersed FEM

immersed FEM is to modify the base functions so that the jump conditions are satisfied, that is, in 1D

$$\phi_i(x_k) = \begin{cases} 1 & \text{if } i = k \\ 0 & \text{otherwise} \end{cases} \qquad [\phi] = 0, \quad [\beta\phi_i'] = 0$$

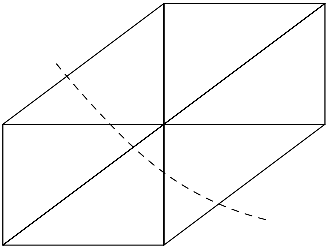
$\Rightarrow (\beta\phi_i')' = 0 \quad jh \le x \le (j+1)h$, ϕ_i: local harmonic mapping, piecewise lin on harmonic coordinate

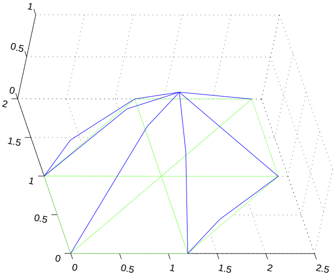


the numeric error between true sol and sol by FE method on the piecewise linear FE space with this modification is $O(h^2)$ (optimal)

Immersed FEM in Higher-D

- partition not have to align with interfaces
- base function may not continuous because of the jump conditions $\Rightarrow$ nonconforming FE space (not always 2nd order convergence in L^∞)





Other Multiscale Methods

- multiscale finite element method by Hou and Wu 1997: work for general $a(x)$, but convg analysis only for periodic media
- heterogeneous multiscale method by E and Engquist 2003, apply to acoustic wave propagation by Engquist et al. 2009: focus on the case when $a(x)$'s small scales have special features such as scale separation, self-similarity, periodicity
- operator-based upscaling by Vdovina, Minkoff et al. 2005
- ...

Future Plan

upscale wave equation:

- use local harmonic mapping to encode sub-grid feature into base functions
  - lots of ideas based on this approach
  - with this approach, Owhadi and Zhang 2005's upscaling approach is the only one without requirement of media structure, such as smoothness of interface, scale separation, ergodicity at small scales
  - locally in space and time according to finite speed propagation
  - parallel

Future Plan (Cont.)

- nonconforming approximation space (DG space)
  - from immersed FEM, nonconforming FEM likely more successful
  - advantages of DG
  - leading experts of DG in this building
- regular grid approach, not include geometry of interface in method
  - computational efficiency
  - apply this method in inversion

References

G. Allaire and R. Brizzi.
A multiscale nite element method for numerical homogenization.
Multiscale Model. Sim., 4(3):790–812, 2005.

I. Babuška, G. Caloz, and J. E. Osborn.
Special finite element methods for a class of second order elliptic problems with rough coefficients.
SIAM Journal on Numerical Analysis, 31(4):945–981, 1994.

G. E. Backus.
Long-wave elastic anisotropy produced by horizontal layering.
J. Geophys. Res., 67(11):44274440, 1962.

A. Bensoussan, J. L. Lions, and G. Papanicolaou.
Asymptotic analysis of periodic structures.
North-Holland Publ., 1978.

W. E, B. Engquist, X. Li, W. Ren, and E. Vanden-Eijnden.
Heterogeneous multiscale methods: A review.
Communications in Computational Physics, 2(3):367–450, 2007.

B. Engquist, H. Holst, and O. Runborg.
Multi-scale methods for wave propagation in heterogeneous media.
2009.

R. Eymard and T. Gallouët.
H-convergence and numerical schemes for elliptic problems.
SIAM J. OF NUM. ANAL, 41(2):539–562, 2004.

References (cont.)

Thomas Y. Hou and Xiao hui Wu.
A multiscale finite element method for elliptic problems in composite materials and porous media.
Journal of Computational Physics, 134:169–189, 1997.

Thomas Y. Hou, Xiao-Hui Wu, and Zhiqiang Cai.
Convergence of a multiscale finite element method for elliptic problems with rapidly oscillating coefficients.
Math. Comp, 68:913–943, 1999.

V.A. Kozlov, V.G. Maz'ya, and J. Rossmann.
Elliptic Boundary Value Problems in Domains with Point Singularities.
AMS, 1997.

Zhilin Li and Kazufum Ito.
The Immersed Interface Method – Numerical Solutions of PDEs Involving Interfaces and Irregular Domains.
SIAM Frontiers in Applied mathematics, 33, 2006.

F. Muir, J. Dellinger, J. Etgen, and D. Nichols.
Modeling elastic fields across irregular boundaries.
Geophysics, 57(9):1189–1193, 1992.

H. Owhadi and L. Zhang.
Metric based up-scaling.
Communications on Pure and Applied Mathematics, 60:675–723, 2006.

H. Owhadi and L. Zhang.
Homogenization of the acoustic wave equation with a continuum of scales.
Computer Methods in Applied Mechanics and Engineering, 198(3-4):397–406, 2008.

References (cont.)

G.A. Pavliotis and A.M. Stuart.
Multiscale Methods: Averaging and Homogenization.
Springer, 2008.

M. Schoenberg and F. Muir.
A calculus for finely layered anisotropic media.
Geophysics, 54(5):581589, 1989.

T. Vdovina, S. Minkoff, and O. Korostyshevskaya.
Operator upscaling for the acoustic wave equation.
SIAM Journal on Multiscale Modeling and Simulation, 4(4):1305–1338, 2005.

C. Zhang and R. J. LeVeque.
The immersed interface method for acoustic wave equations with discontinuous coefficients.
Wave Motion, 25(3):237–263, 1997.

Thank You

Q&A