Operator Equations in High Dimensions II
Sparse Adaptive FEM
for
Elliptic Homogenization Problems

C. Schwab

Seminar for Applied Mathematics, ETH Zürich

joint w. V. Hoang, Cambridge and R. Stevenson, Utrecht

Outline

- Elliptic Homogenization Problems w. Multiple Scales
- Multiscale Convergence/ Unfolding Technique
- High-dimensional one-scale elliptic problem
- Sparse Tensor Product FEM
- Convergence vs. Complexity Analysis
- Numerical Examples
- Adaptivity
- Nonlinear, quasiconvex variational problems

$n + 1$-scale Homogenization Problem

Consider

$$\Omega \subset \mathbb{R}^d \quad \text{bounded, physical domain and} \quad n \geq 1 \quad \text{`cells'} \quad Y_1, \ldots, Y_n.$$

For $f \in L^2(\Omega)$, consider the elliptic homogenization problem

$$-\mathrm{div} A^{\varepsilon} \nabla u^{\varepsilon} = f \quad \text{in } \Omega, \quad u^{\varepsilon} = 0 \text{ on } \partial\Omega,$$

where $A^{\varepsilon}(x)$ is **elliptic with $n + 1$ scales**: there is

$$A(x, y_1, \ldots, y_n) \in L^{\infty}(\Omega \times Y_1 \times \ldots \times Y_n)^{d \times d}_{sym},$$

independent of ε and ex. $\gamma > 0$ such that for all $x \in \Omega$, $y_i \in Y_i$ holds

$$\forall \xi \in \mathbb{R}^d \qquad \gamma |\xi|^2 \leq \xi^{\top} A(x, y_1, \ldots, y_n) \xi \leq \gamma^{-1} |\xi|^2.$$

$n+1$-scale Homogenization Problem

We assume **Scale Separation**: *either* $n=1$ *or*

if $n>1$, ex. n functions $\varepsilon_1(\varepsilon),\dots,\varepsilon_n(\varepsilon)>0$ s.t.

$$\varepsilon_1(\varepsilon),\dots,\varepsilon_n(\varepsilon)\to 0 \quad \text{for} \quad \varepsilon\to 0, \qquad \lim_{\varepsilon\to 0}\frac{\varepsilon_{i+1}(\varepsilon)}{\varepsilon_i(\varepsilon)}=0, \qquad i=1,\dots,n-1.$$

and such that

$$\forall x\in\Omega, \quad \forall\varepsilon>0: \quad A^{\varepsilon}(x):=A\left(x,\frac{x}{\varepsilon_1},\dots,\frac{x}{\varepsilon_n}\right).$$

$n+1$-scale Homogenization Problem

Challenges:

- As $\varepsilon \to 0$, u^ε converges in $L^2(\Omega)$, but not in $H^1(\Omega)$ due to oscillations on “fine” scales (I. Babuška (1976), A. Bensoussan, J.L. Lions, G. Papanicolau (1978))
- $H^1(\Omega)$ physically relevant, “energy” norm.
- Describe numerically oscillations of u^ε to obtain $H^1(\Omega)$ convergence (“Correctors”)
- Numerical schemes to *resolve oscillations* with

robust performance, i.e accuracy / complexity independent of ε,

where

complexity = memory and float point operations versus

N**, the no. of macro discretization parameters**

$n+1$-scale Homogenization Problem

- Numerical Methods:
  - MSFEM (Babuška et al. 1975,..., Hou & al. 1997, 1999,..., Matache & CS 2000,...)
  - HMM (Engquist & E & al. "**HMM**" 2003, ..., Abdulle & CS 2005,...)

  all developed for $n = 1$, i.e 2-scale problems,

  ε-independent convergence rates in $H^1(\Omega)$ at **complexity** $O(N^{n+1})$
- Numerical solution of one 'cell' problem for each "macro degree of freedom"

Basic Question:

Robust, i.e. ε-independent, MSFEM in Complexity $O(N)$ for $n > 1$?

$(n+1)d$-dim. one-scale Problem (Allaire & Briane 96)

$\{u^\varepsilon\}_{\varepsilon>0} \subset H_0^1(\Omega)$ converges weakly to $u \in H_0^1(\Omega)$ and ∇u^ε $(n+1)-$scale converges to

$$\nabla u(x) + \sum_{i=1}^{n} \nabla_{y_i} u_i(x, y_1, \ldots, y_i),$$

where $(u, u_1, \ldots, u_n) = (u, \{u_i\}_{i=1}^n)$ is the unique solution in

$$\mathbf{V} = \{(\phi, \{\phi_i\}_{i=1}^n) : \phi \in H_0^1(\Omega), \phi_i \in L^2(\Omega \times Y_1 \times \ldots \times Y_{i-1}, H_\#^1(Y_i)/\mathbb{R}), i = 1, ..., n\}$$

of the **“unfolded”, $(n+1)d$-dimensional, one-scale limit problem**

$$\begin{aligned} & B\left((u, \{u_i\}_{i=1}^n); (\phi, \{\phi_i\}_{i=1}^n)\right) \\ &= \int_\Omega \int_{Y_1} \cdots \int_{Y_n} A\Big(\nabla_x u + \sum_{i=1}^n \nabla_{y_i} u_i\Big) . \Big(\nabla_x \phi + \sum_{i=1}^n \nabla_{y_i} \phi_i\Big) dy_n \ldots dy_1 dx \qquad (1) \\ &= \int_\Omega f \phi dx \quad \forall (\phi, \{\phi_i\}_{i=1}^n) \in \mathbf{V}. \end{aligned}$$

$(n+1)d$-dim. one-scale Problem (Allaire & Briane 96)

For example, for the *classical two-scale problem*, $n = 1$ and (1) becomes

$$\int_\Omega \int_Y A(x,y)\big(\nabla_x u(x) + \nabla_y u_1(x,y)\big) \cdot \big(\nabla_x \phi(x) + \nabla_y \phi_1(x,y)\big) dx dy = \int_\Omega f \phi dx$$

for all $\phi \in H_0^1(\Omega)$ and $\phi_1 \in L^2(\Omega, H_\#^1(Y)/\mathbb{R})$.

Corrector result: u^ε can be approximated in the physical domain Ω in terms of

- the homogenized solution $u(x) \in H_0^1(\Omega)$,
- the “scale-interaction terms” $u_1(x, y_1), \ldots, u_n(x, y_1, ..., y_n)$:

Assume that $(u, u_1, \ldots, u_n)$ in (1) are sufficiently smooth. Then,

$$\left\| u^\varepsilon(x) - \left[u(x) + \sum_{i=1}^{n} \varepsilon_i u_i\left(x, \frac{x}{\varepsilon_1}, \ldots, \frac{x}{\varepsilon_i}\right)\right] \right\|_{H^1(\Omega)} \to 0 \qquad \varepsilon \to 0$$

[Open Problem: convergence rates as $\varepsilon \to 0$ for $n > 1$ fast scales]

Full Tensor Product FEM for (1)

To approximate scale interaction terms $u_i(x, y_1, \dots, y_i)$, $i = 1, ..., n$, numerically, need

$$\text{Finite Element (FE) subspaces of } L^2(\Omega \times Y_1 \times \dots \times Y_{i-1}, H^1_\#(Y_i)/\mathbb{R}).$$

Assume (for ease of notation only!) that $Y_1 = Y_2 = ... = Y_n = Y$ and let

$$\{V_0^\ell\}_{\ell=0}^\infty \subset H_0^1(\Omega), \quad \{V_\#^\ell\}_{\ell=0}^\infty \subset H_\#^1(Y)$$

be nested (i.e. $V_0^\ell \subseteq V_0^{\ell+1} \subseteq ...$ etc.) sequences of fin. dim. subspaces.

Example:

continuous, piecewise polynomials of degree $p \geq 1$ on a quasiuniform mesh of width $h_\ell = O(2^{-\ell})$.

Full Tensor Product FEM for (1)

Since

$$u_i \in L^2(\Omega \times Y_1 \times \ldots \times Y_{i-1}, H^1_\#(Y_i)) \cong L^2(\Omega) \otimes L^2(Y_1) \otimes \ldots \otimes L^2(Y_{i-1}) \otimes H^1_\#(Y_i),$$

FE subspace $\mathbf{V}^L$ of $\mathbf{V}$ in (1) constructed as **tensor product of FE spaces** $V^\ell_\#$ in the scales:

$$\mathbf{V}^L = \{(u^L, \{u_i^L\}_{i=1}^n) : u^L \in V_0^L, u_i^L \in V_i^L, i = 1, \ldots, n\}$$

where

$$V_i^L := V^L \otimes \underbrace{V_\#^L \otimes \ldots \otimes V_\#^L}_{i \text{ times}}, \qquad i = 1, ..., n.$$

Full Tensor Product FEM for (1)

Denote by $\{u^L, u_1^L, ..., u_n^L\} \in \mathbf{V}^L$ the FE solution

(p.w. polynomials of degree $p \geq 1$ on quasiuniform triangulations of Ω, Y_1, ..., Y_n of width h_L)

find $(u^L, \{u_i^L\}_{i=1}^n) \in \mathbf{V}^L$ such that

$$B(u^L, \{u_i^L\}; \phi, \{\phi_i\}) = \int_\Omega f\phi dx \quad \forall(\phi, \{\phi_i\}) \in \mathbf{V}^L.$$

Then

$$|||(u - u^L, \{u_i - u_i^L\}_{i=1}^n)||| \leq c(h_L)^p \left(\|u\|_{H^{p+1}(\Omega)} + \sum_{i=1}^n \|u_i\|_{\mathcal{H}_i^p} \right)$$

Here $||| \circ |||$ denotes the norm in $\mathbf{V}$ and

$$\mathcal{H}_i^p = \bigcap_{t_0+t_1+...+t_i=p} H^{t_0}(\Omega) \otimes H_\#^{t_1}(Y_1) \otimes ... \otimes H_\#^{t_{i-1}}(Y_1) \otimes H_\#^{t_i+1}(Y_i),$$

Full Tensor Product FEM for (1)

Note 1: c independent of ε and, as $\varepsilon \to 0$, $L \to \infty$, it holds

$$\left\| u^{\varepsilon}(x) - \left[u^{L}(x) + \sum_{i=1}^{n} \varepsilon_i u_i^{L}\left(x, \frac{x}{\varepsilon_1}, \dots, \frac{x}{\varepsilon_i} \right) \right] \right\|_{H^1(\Omega)} \to 0$$

Note 2: For fixed polynomial degree $p \geq 1$ holds asymptotically, as the meshwidth $h_L \to 0$,

$$\dim \mathbf{V}^{L} = O({h_L}^{-(n+1)d})$$

Note 3: HMM (Enquist and E (2003)) = full tensor FEM plus quadrature in slow scale

Convergence $O(h_L)$ ind. of ε

(Abdulle and Sc. $MMS(2005)$, Abdulle $M^3AS(2006)$),

Complexity of HMM at least $O({h_L}^{-(n+1)d})$ work and memory

Number of "macro" DOF is $N_L = O({h_L}^{-d})$

Sparse Tensor Product FEM for (1)

Recall: **Multigrid** for homogenized problem in $\Omega \subset \mathbb{R}^d$ has work $O(h_L^{-d})$, but

$$n + 1\text{-scale limit problem: } \dim \mathbf{V}^L = O(h_L^{-(n+1)d}), \quad h_L = 2^{-L}.$$

= complexity for FEM in dimension $(n+1)d$ — **"curse of dimension"**

– prohibitive for $n+1 > 2$ scales and dimension $d = 3$ even on large hardware

? Can we get complexity of "1-scale Problem in d dimensions" ?

3 Tools:

- Regularity of scale interaction terms u_i in spaces $\hat{\mathcal{H}}_i^p$ of mixed highest derivatives
- Hierarchic FE bases (Wavelet FEM/ Spectral FEM/ *hp*-FEM ...) in each scale
- Sparse Tensor Products (Zenger 1990/ Griebel et al/ ...) for scale-interactions u_i

Tool 1: Regularity of Scale Interaction Functions

A, $f(x)$ 'regular' $\rightarrow u_i(x, y_1, ..., y_i)$ regular *simultaneously in all scales*!

Consider scale interaction function $u_i(x, y_1, ..., y_i) \in L^2(\Omega \times Y_1 \times ... \times Y_{i-1}; H^1_\#(Y_i))$, $i = 1, ..., n$.

Theorem (V. Hoang & CS): Assume (for simplicity only)

- $A(x, y_1, ..., y_n)$ is smooth,
- $\partial\Omega$ smooth,
- $f(x) \in H^{t-1}(\Omega)$ for some smoothness order $t > 0$ ($t = 0$ corresponds to finite energy).

Then the solution $(u, \{u_i\}_{i=1}^n)$ of limit problem (1) satisfies

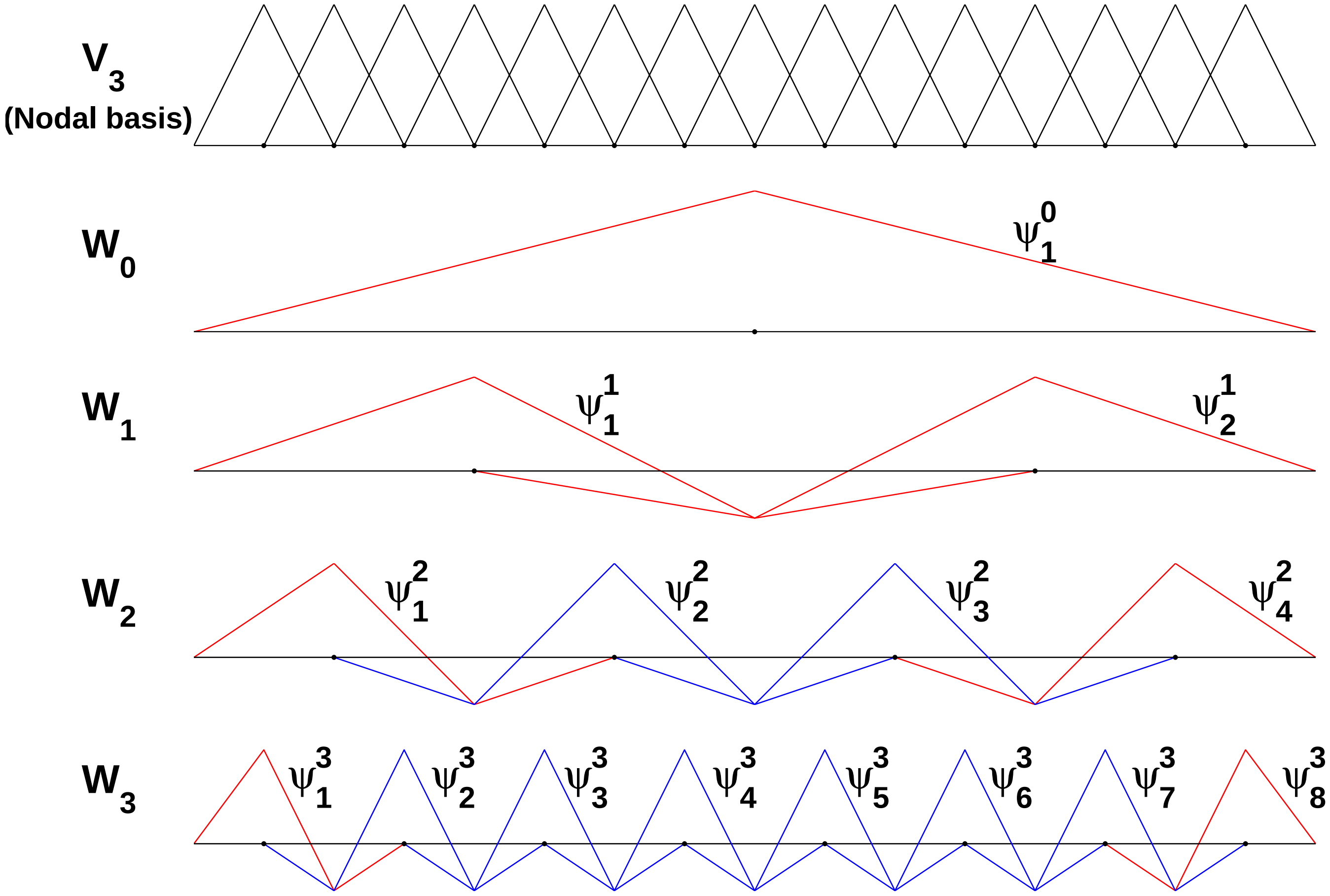
$$u \in H^{t+1}(\Omega),$$

and

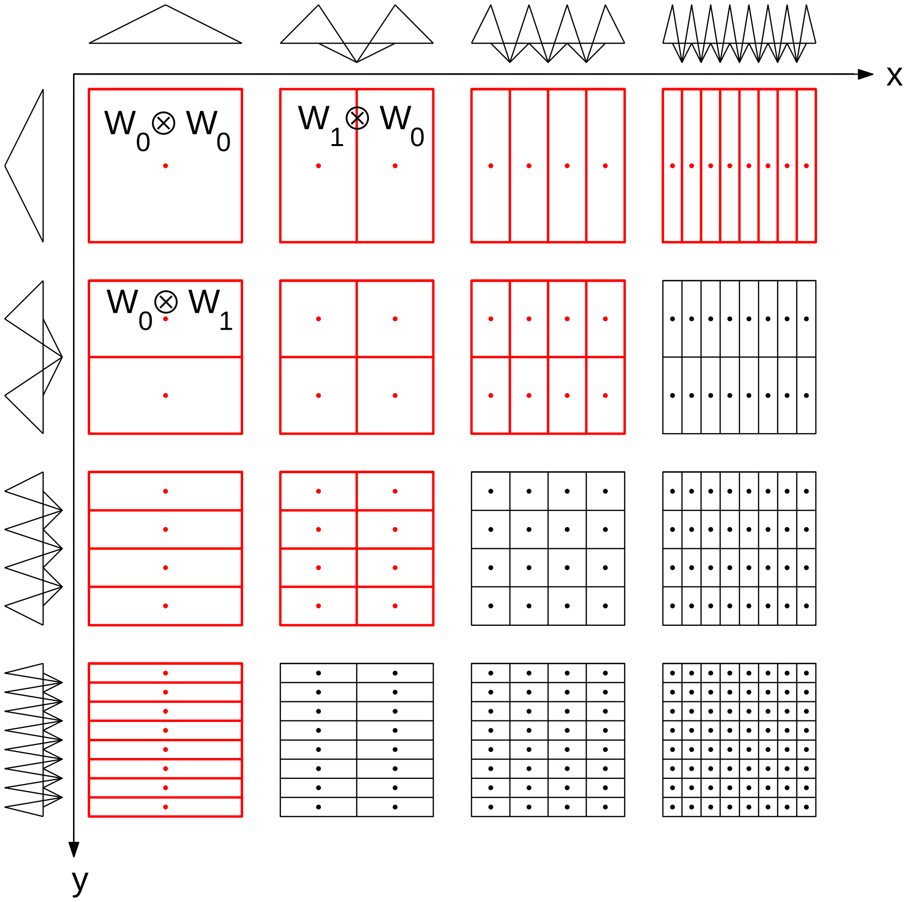
$$u_i \in \widehat{\mathcal{H}}_i^t := H^t(\Omega) \otimes H^t(Y_1) \otimes ... H^t(Y_{i-1}) \otimes H^{t+1}(Y_i) \qquad \text{for} \qquad i = 1, ..., n.$$

Tool 2: Hierarchic FE Basis

Finite Element wavelets, shown for $p = 1$, $d = 1$ (Dahmen, Urban, Canuto, Tabacco 2000 -)



Tool 3: Sparse Tensor Product



Convergence Rate

Theorem (V. Hoang & CS):

$$|||(u-\hat{u}^L, \{u_i-\hat{u}_i^L\}_{i=1}^n)||| \le c|\log h_L|^{n/2} h_L^p \left(\|u\|_{H^{p+1}(\Omega)} + \sum_{i=1}^n \|u_i\|_{\hat{\mathcal{H}}_i^p} \right).$$

Remark 1 The number of degrees of freedom of the sparse FE space $\hat{\mathbf{V}}^L$ as $L \to \infty$ is

$$\hat{N}_L := O(h_L^{-d}|\log h_L|^n) << O(h_L^{-(n+1)d})$$

Convergence Order and Complexity equal (up to logs of N) to mgFEM for the one-scale, *homogenized* problem in physical domain $\Omega \subset \mathbb{R}^d$ with $n = 0$.

Remark 2 *Let $n = 1$ (2-scale problem) and $p = 1$ (piecewise linear, continuous FEM). Then:*

$$\|\nabla_x u^\varepsilon(x) - \left[\nabla_x \hat{u}^L(x) + \nabla_y \hat{u}_1^L(x, x/\varepsilon)\right]\|_{L^2(\Omega)} \le c(\varepsilon^{1/2} + L^{1/2} h_L).$$

Example: 2-scale Model Problem

$$A(x,y) = a_0(x)a_1(y), \quad a_0(x) = 1 + x \text{ and } a_1(y) = (2/3)(1 + \cos^2 2\pi y), f = -1$$

in $\Omega = (0,1)$

Exact (homogenized) solution

$$u(x) = \frac{3}{2\sqrt{2}}(x - \frac{\log(1+x)}{\log 2}),$$

Scale interaction term

$$u_1(x,y) = \frac{3}{2\sqrt{2}}(1 - \frac{1}{(1+x)\log 2})(\frac{1}{2\pi}\tan^{-1}(\frac{\tan 2\pi y}{\sqrt{2}}) - y + C),$$

Example: 2-scale Model Problem

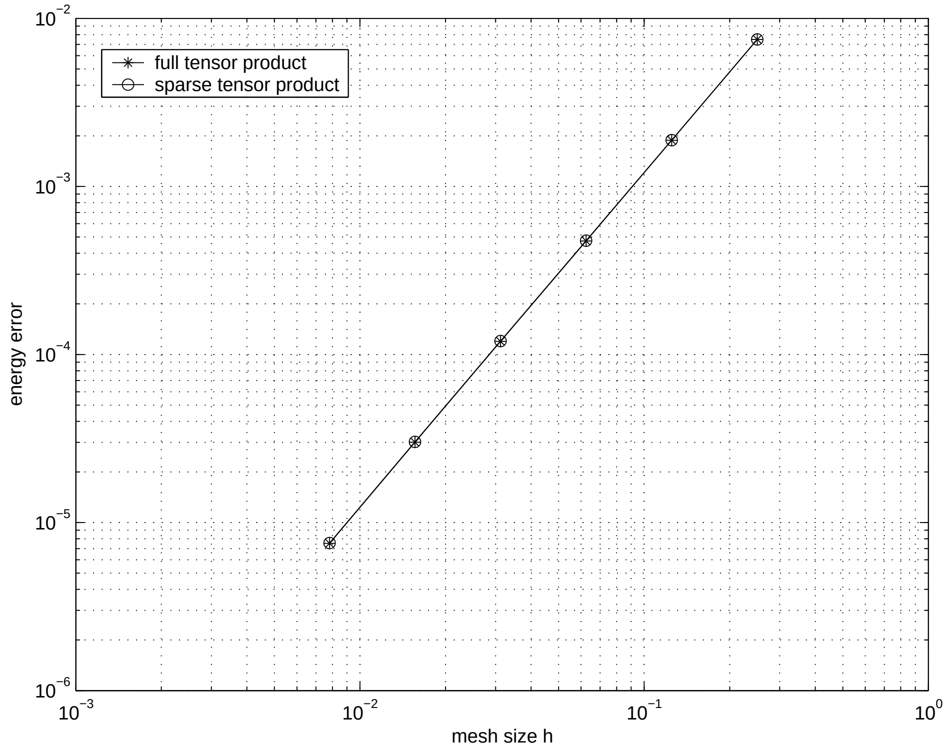


Figure 1: Energy error versus the mesh size h

Example: 2-scale Model Problem

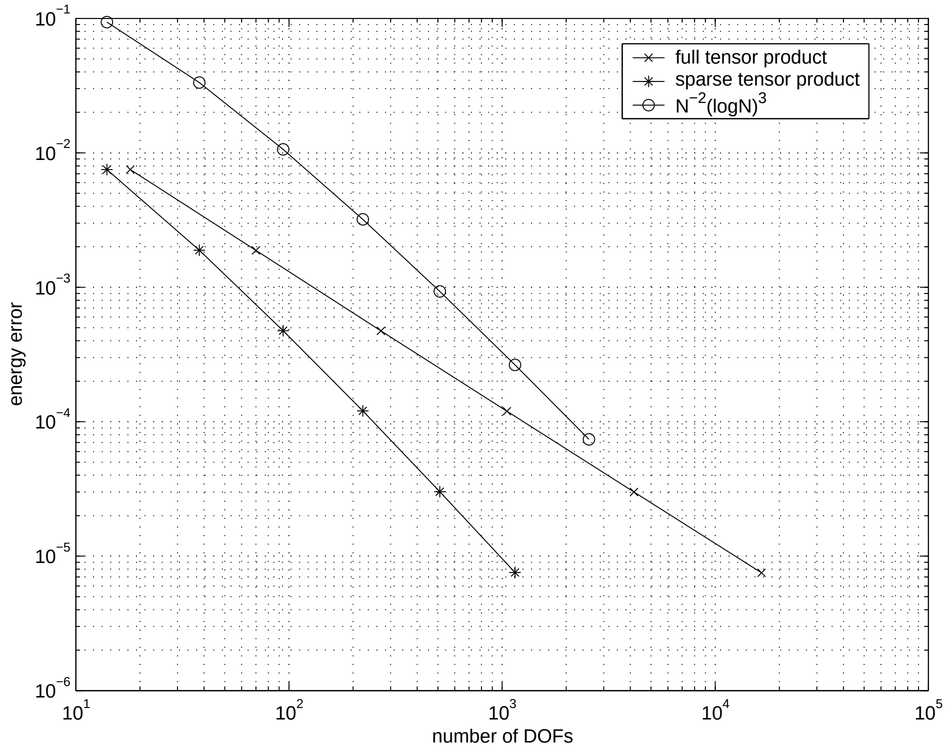


Figure 2: Energy error versus the number of degrees of freedom

Conclusions

- Elliptic Multiscale Problems with $n+1$ separated scales in phys. domain $\Omega \subset \mathbb{R}^d$
- Multiscale convergence: elliptic single scale problem in dimension $(n+1)d$
- Discretization by tensor product FEM plus quadrature = **HMM** of Engquist and E.
- Multilevel FEM on each scale → sparse tensor product FEM
- Anisotropic regularity of single scale limit problem →

  full convergence rate of sparse tensor product FEM
- Resolution of all $n+1$ scales in $H^1(\Omega)$ with complexity $O(N(\log N)^n)$ where

  N = work for MG Poisson solve in Ω rather than $O(N^{(n+1)})$ for e.g. **HMM**.
- A-posteriori error estimation: Ohlberger SIAM MMS Journal (2005)

  (full tensor product FEM only)

- Adaptivity: anisotropic → standard error indicators/ estimators?

  CDD2000 adaptive anisotropic wavelet-based FEM can yield optimal rates, indep. of n, under much weaker (anisotropic Besov-type) regularity, allowing for singularities / layers on each scale (P.A. Nitsche: Constr. Approx. 2006),

- Stiffness matrix for anisotropic, sparse adaptive FEM for the limit problem (1) is *compressible* and *computable* in linear complexity: C. Schwab and R. Stevenson (2006)

Adaptive Wavelet Algorithms

$A : V \to V'$ boundedly invertible, and some $f \in V'$,

$$\text{find} \quad u \in V : \quad Au = f. \tag{2}$$

Write $u = \boldsymbol{u}^T \Psi$ where $\Psi = \{\psi_\lambda : \lambda \in \Lambda\}$ Riesz basis for V. Then (2) equivalent to

$$\text{find} \quad \boldsymbol{u} \in \ell_2 = \ell_2(\Lambda) : \quad \boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}. \tag{3}$$

Here the "stiffness" matrix

$$\boldsymbol{A} := \langle \Psi, A\Psi \rangle : \ell_2 \to \ell_2$$

is boundedly invertible,

$$\boldsymbol{u} := \langle \Psi, u \rangle, \quad \boldsymbol{f} := \langle \Psi, f \rangle \in \ell_2, \quad \langle \cdot, \cdot \rangle \text{ duality on } V \times V'.$$

Adaptive Wavelet Algorithms

If, for some $s > 0$ solution $\boldsymbol{u}$ of (3) is in the *Approximation Class*

$$\mathcal{A}^s_\infty = \{\boldsymbol{v} \in \ell_2 : \sup_N N^s \|\boldsymbol{v} - \boldsymbol{v}_N\| < \infty\},$$

[CDD01,CDD02,GHS05]: Algorithms that produce sequence $\boldsymbol{u}^\ell$, $\ell = 0, 1, 2, \ldots$ converging with *this rate* s, provided $\boldsymbol{A}$ *is* s^**-computable* for some $s^* > s$, ie.

- for each $q \in \mathbb{N}$, an infinite matrix $\boldsymbol{A}_q$ can be constructed, s.t. in each row and column there are at most $\mathcal{O}(2^q)$ non-zero entries,
- computable in $\mathcal{O}(2^q)$ operations, and such that
- $\|\boldsymbol{A} - \boldsymbol{A}_q\| \lesssim 2^{-q\bar{s}}$ for any constant $\bar{s} < s^*$.

Tool 2: Wavelet FE Basis

Let $\{\psi_\lambda^{(m)} : \lambda \in \Lambda_m\}$ be wavelets of order $p \geq 1$ in Y_m, such that for $\ell' = 0$ or $\ell' = 1$,

$$\{2^{-|\lambda|\ell'}\psi_\lambda^{(m)} : \lambda \in \Lambda_m\} \text{ is a Riesz basis for } L_2(Y_m) \text{ or } \tilde{H}^1(Y_m), \text{ respectively.}$$

With $\boldsymbol{u}_m$ denoting the representation of $u_m \in L_2(Y_m)$ or $u_m \in \tilde{H}^1(Y_m)$, respectively, it holds

$$u_m \in B^{sd+\ell'}_{\tau,\tau}(Y_m) \text{ for } s \in (0, \tfrac{p-\ell'}{d}) \text{ with } \tau = (s + \frac{1}{2})^{-1} \quad \text{if and only if} \quad \boldsymbol{u}_m \in \mathcal{A}^s_\tau.$$

where, for $\tau \in (0, \infty)$,

$$\mathcal{A}^s_\tau := \{\boldsymbol{v} \in \ell_2 : \sum_{N \in \mathbb{N}} (N^s \|\boldsymbol{v} - \boldsymbol{v}_N\|)^\tau N^{-1} < \infty\}.$$

Tool 2: Wavelet FE Basis

Then, with $\boldsymbol{e}^{(m)} := (0,0,0,...,0,1) \in \mathbb{N}^{m+1}$, $m = 0, ..., n$,

$$\boldsymbol{\Psi}^{(m)} := \{2^{-|\boldsymbol{\lambda}_m|} \bigotimes_{k=0}^{m} \psi^{(k)}_{\boldsymbol{\lambda}_k} : \boldsymbol{\lambda} \in \prod_{k=0}^{m} \Lambda_k\} \text{ is a Riesz basis for } H^{\boldsymbol{e}^{(m)}}(\Omega \times Y_1 \times ... \times Y_m)\,.$$

and

$$\boldsymbol{\Psi} := \boldsymbol{\Psi}^{(0)} \times \boldsymbol{\Psi}^{(1)} \times ... \boldsymbol{\Psi}^{(n)}$$

is a Riesz basis for $\mathbf{V}$.

Proposition

$$\operatorname{cond}(\boldsymbol{A}) = \operatorname{cond}(\langle \boldsymbol{\Psi}, A\boldsymbol{\Psi} \rangle) \leq c < \infty.$$

s^*-approximability

With $\boldsymbol{U} = (\boldsymbol{u}_0, \dots, \boldsymbol{u}_n)$ representation of $U = (u_0, \dots, u_n)$ w.r.to $\boldsymbol{\Psi}$ have

$$\boldsymbol{U} \in \mathcal{A}^s \quad \text{if and only if} \quad \boldsymbol{u}_m \in \mathcal{A}^s, \quad 0 \le m \le n.$$

Theorem (P.A. Nitsche *Constr.Approx.*2006):

Set $Y_0 := \Omega$. Then

- $\boldsymbol{u}_m \in \mathcal{A}^s$ holds for $s \in (0, \frac{p-1}{d})$ with $\tau = (s + \frac{1}{2})^{-1}$ if and only if

$$u_m \in (\bigotimes_{k=0}^{m-1}{}_{\tau} B^{sd}_{\tau,\tau}(Y_k)) \bigotimes_{\tau} B^{sd+1}_{\tau,\tau}(Y_m),$$

- $\boldsymbol{U} \in \mathcal{A}^s$ for $s > \frac{p-1}{d}$ cannot be expected.

s^*-computability

For $O(N)$ dimension-independent adaptive MSFEM, $\boldsymbol{A}$ has to be s^* computable with

$$s^* > p/d$$

Much stronger condition than w. isotropic wavelets in $\mathbb{R}^{(n+1)d}$ where only

$$s^* > p/[(n+1)d]$$

is needed.

Theorem (Sc. & Stevenson (*Preprint*2006))

There is a compression strategy and a (sparse, adaptive) tensor product quadrature strategy such that for any number n of fast scales in (1), $\boldsymbol{A}$ is s^* computable with

$$s^* > p/d$$