Multiscale Modeling Using Goal-oriented Adaptivity and Numerical Homogenization

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August 8, 2008

Collaborators

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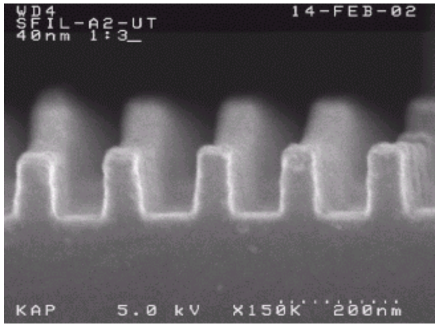
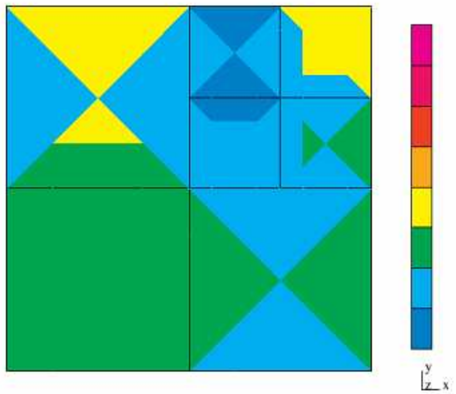
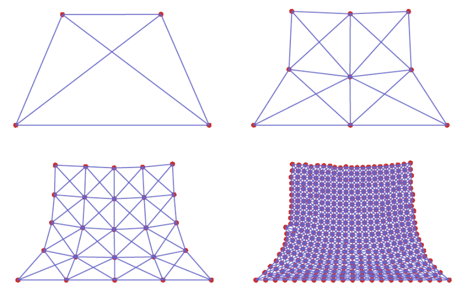
Financial support by the Department of Energy under Grant No. DE-FG02-05ER25701.

Outline

- Step and Flash Imprint Lithography, the base model and the goal of the modeling process
- The first approach: *hp*-adaptive Quasicontinuum Method (QCM), its success and its limitations
- Our method: Combining adaptivity with QCM and Numerical Homogenization

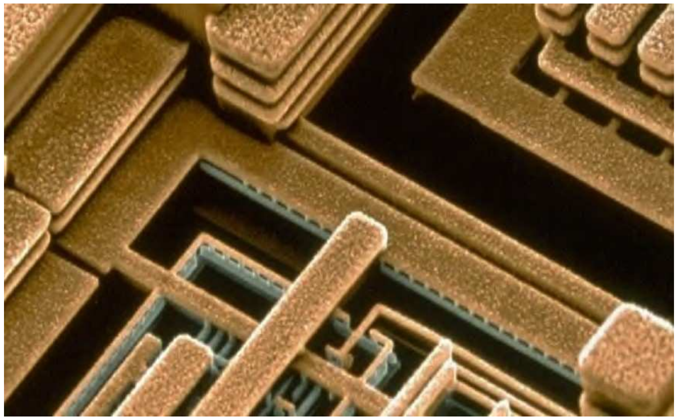




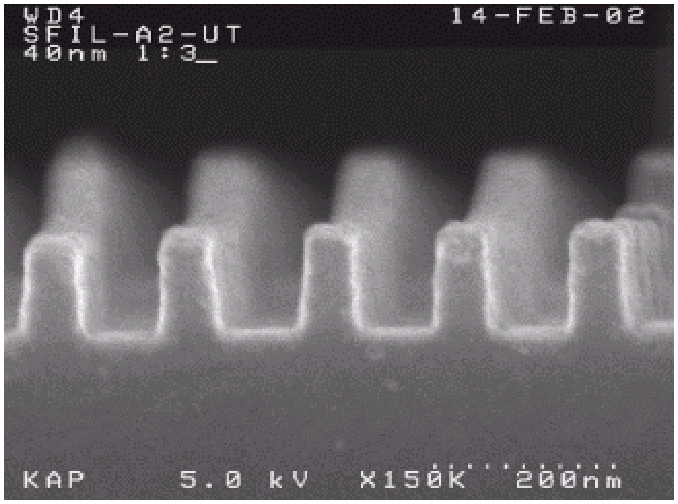


The Base Model

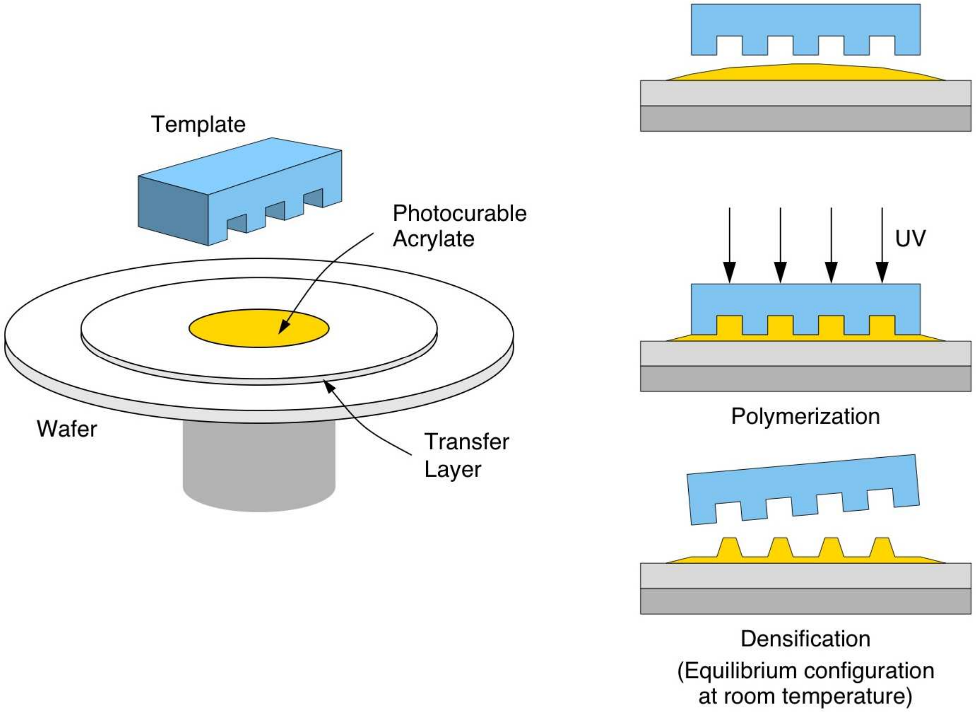
Step and Flash Imprint Lithography (SFIL)



A magnified chip



An electron microscope image of patterns in SFIL



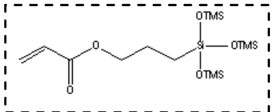
A schematic of the SFIL process

Step and Flash Imprint Lithography: A New Approach to High-resolution Patterning – Willson Research Group, The University of Texas at Austin, in Proceedings of SPIE/Emerging Lithographic Technologies III – 1999.

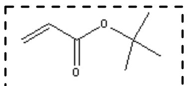
The SFIL Process

The etch barrier constituents

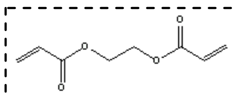
44% Gelest SIA-0210



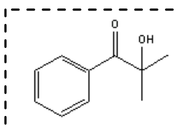
37% t-Butyl Acrylate

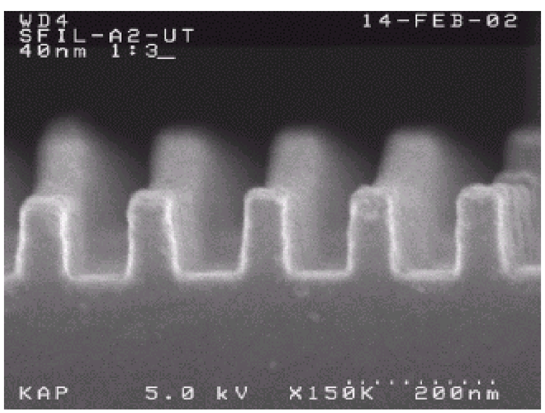


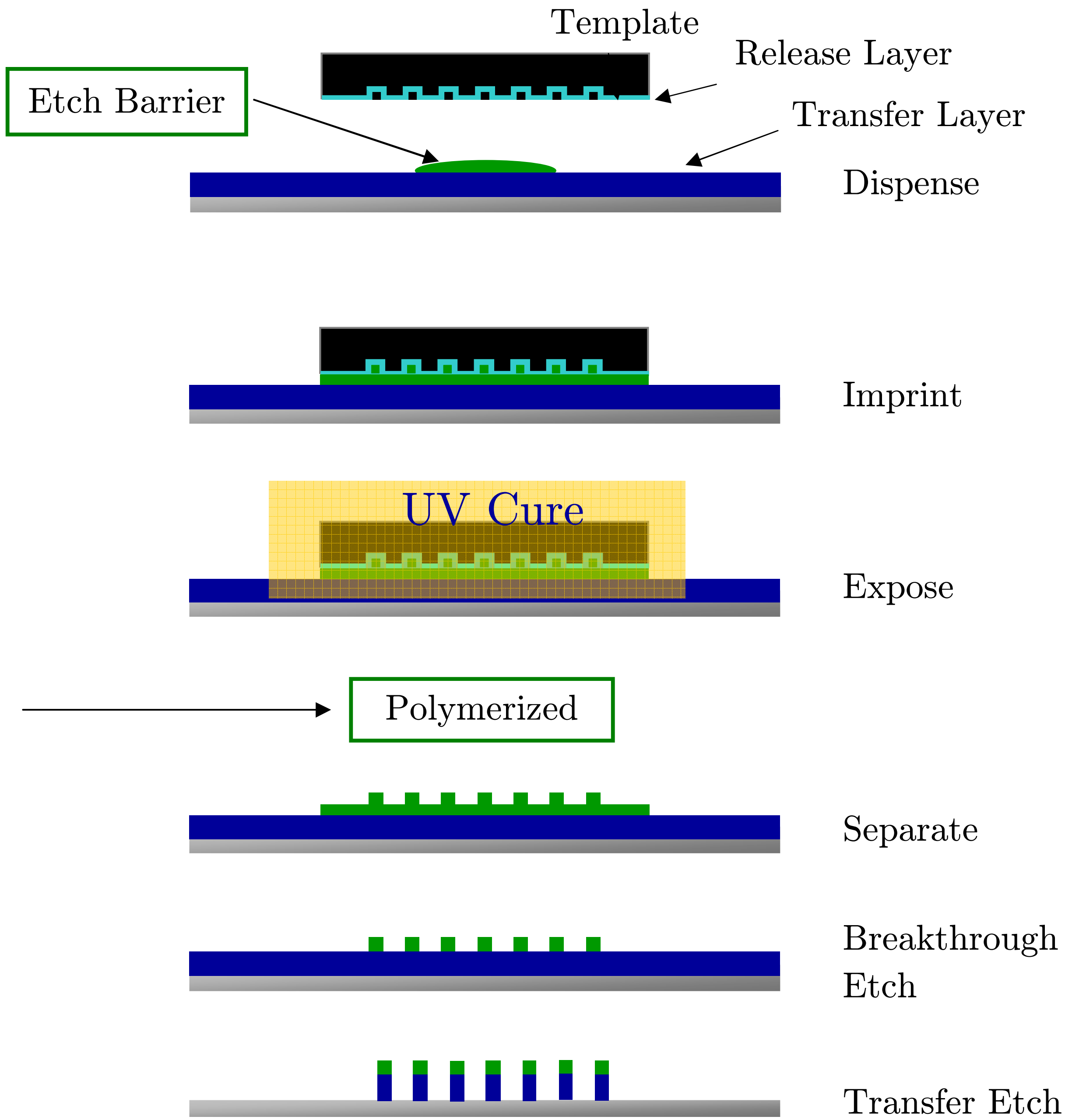
15% Ethylene Glycol Diacrylate



1-4% Darocur 1173

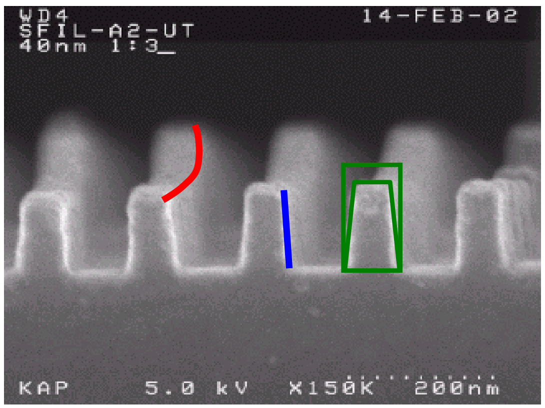






SFIL – The Goal and the Challenges

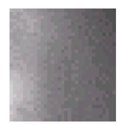
Analyze the mechanical behavior of the polymerized etch barrier solution forming the 3D relief patterns in SFIL



Slump due to volume change

Changes in side angle

Volume change


Surface roughness

Achieving this goal using just the base model is challenging due to

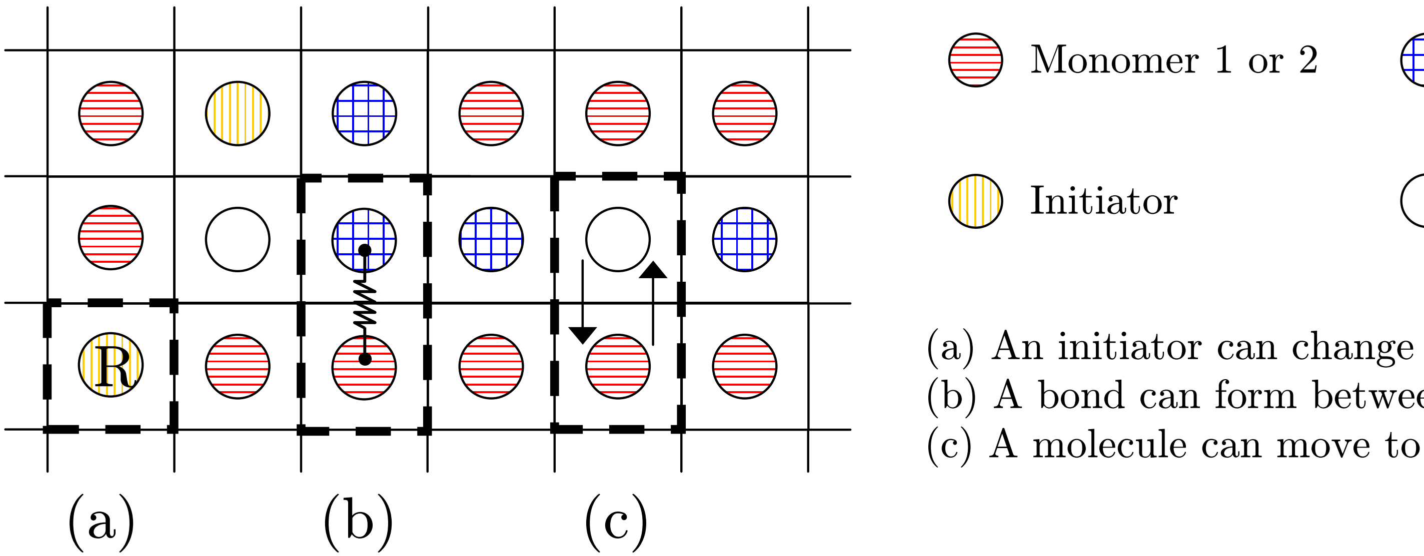
- Large number of DOFs, on the order of millions
- Geometric and material nonlinearity
- Fast variation in material properties
- Multiple scales – of the goal and that of the material
- Nonconvexity
- Stochasticity

The Base Model – Polymerization

$$
\left.\begin{array}{rcl} I & \xrightarrow{h\nu} & R^\bullet + R^\bullet \end{array}\right\} \text{Initiation}
$$

$$
\left.\begin{array}{rcl} R^\bullet + M & \rightarrow & P^\bullet \\ P^\bullet + M & \rightarrow & P^\bullet \end{array}\right\} \text{Propagation}
$$

$$
\left.\begin{array}{rcl} P^\bullet + P^\bullet & \rightarrow & P \end{array}\right\} \text{Termination by combination}
$$



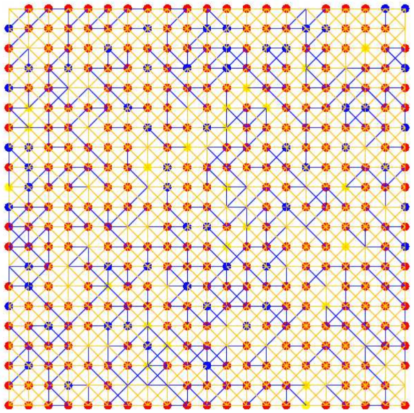
(a) An initiator can change to a radical
(b) A bond can form between two monomers or cross-linkers
(c) A molecule can move to an empty lattice site

J. E. Meiring, Mesoscale Simulation of the Photoresist Process and Hydrogel Biosensor Array Platform Indexed by Shape, PhD thesis, The University of Texas at Austin, 2005.

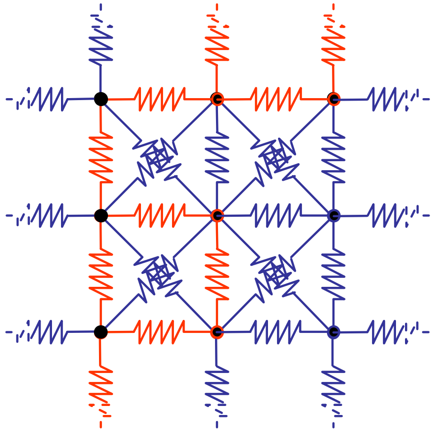
The Base Model – Lattice Topology

The output of the Monte Carlo polymerization model is

- A topological distribution of bonds and molecules but unknown geometry
- Monomers form the vertices of the cubical lattice
- Monomers interact via central pair potentials
- Bonds along 18 directions to nearest neighbors
- Covalent bonds forming the polymer backbone
- Weaker Lennard-Jones bonds where covalent bonds are absent



A small 2D lattice



A few “cells” in 2D

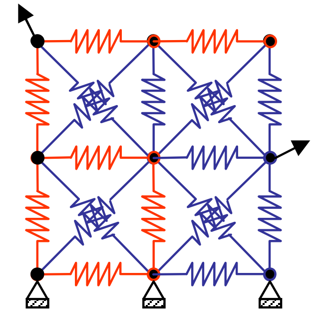
The Base Model – Molecular Statics

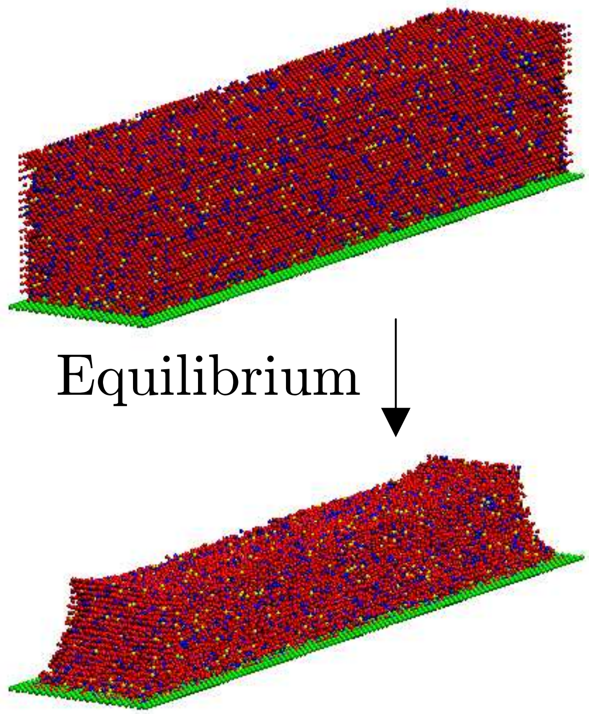
Let $\boldsymbol{x} := \{\{\{x^{ijk}\}_{i=0}^{N_1-1}\}_{j=0}^{N_2-1}\}_{k=0}^{N_3-1}$ be the set of all molecular positions (DOFs) for a cube and

$$J(\boldsymbol{x}) := \frac{1}{2} \sum_{x^{ijk} \in \boldsymbol{x}} \sum_{\substack{x^{lmn} \in \boldsymbol{x} \\ x^{lmn} \leftrightsquigarrow x^{ijk}}} E\left(\left|\left|x^{lmn} - x^{ijk}\right|\right|\right)$$

$$- \sum_{x^{ijk} \in x} \sum_{\substack{p=1 \\ (i,j,k,p)}}^{3} f_p^{ijk} x_p^{ijk}$$

E is a bond potential function and $\boldsymbol{f}$ denotes the set of forces. Equilibrium configuration is found by minimizing J as a function of $\boldsymbol{x}$.

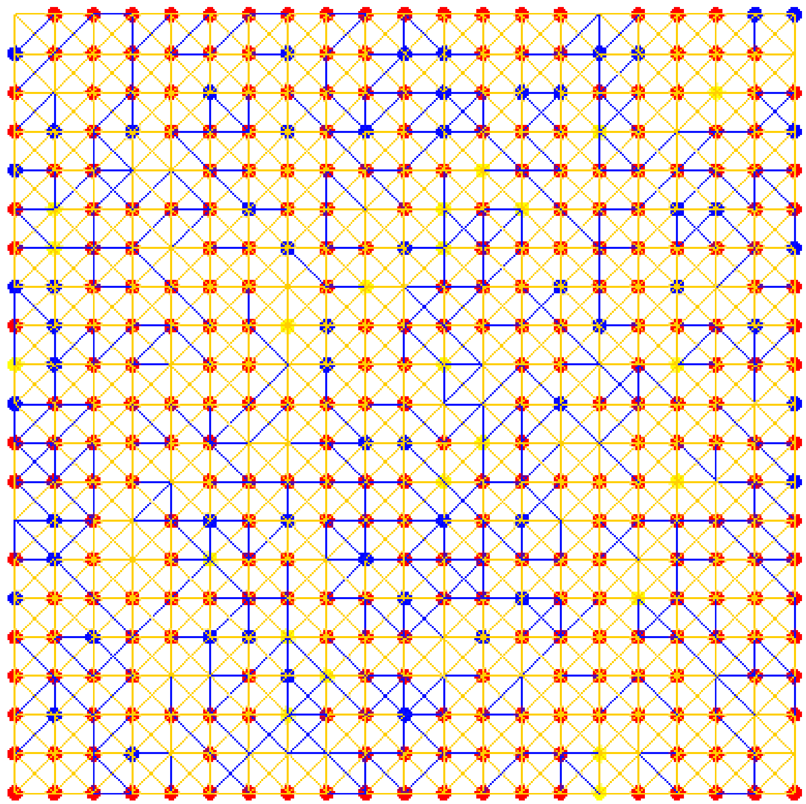




$21 \times 101 \times 21$ lattice

P. T. Bauman, Adaptive Multiscale Modeling of Polymeric Materials Using Goal-Oriented Error Estimation, Arlequin Coupling, and Goals Algorithms, PhD thesis, The University of Texas at Austin, 2008.

The Base Model – Trust-Region Iterations



The Research Goal

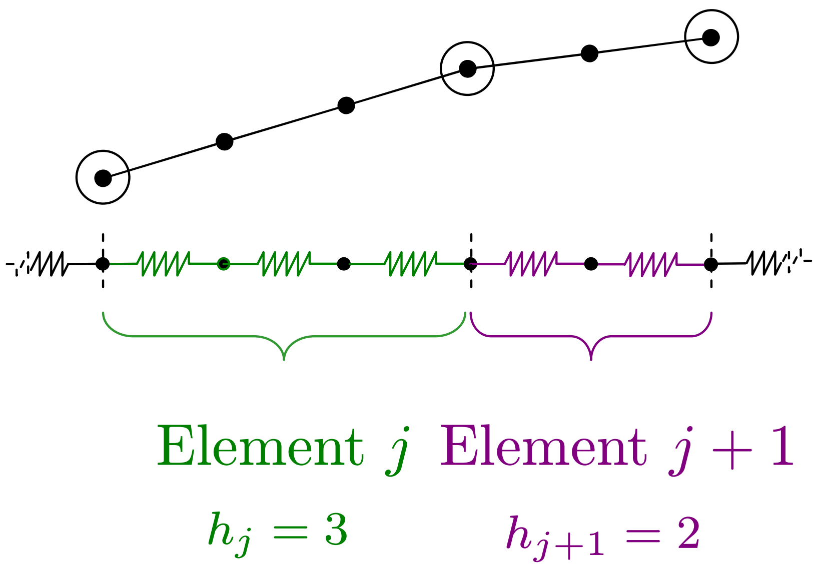
Devise an efficient numerical method for solving
large-scale nonlinear lattice-based problems
with fine-scale material features

(by combining homogenization and mesh-adaptivity)

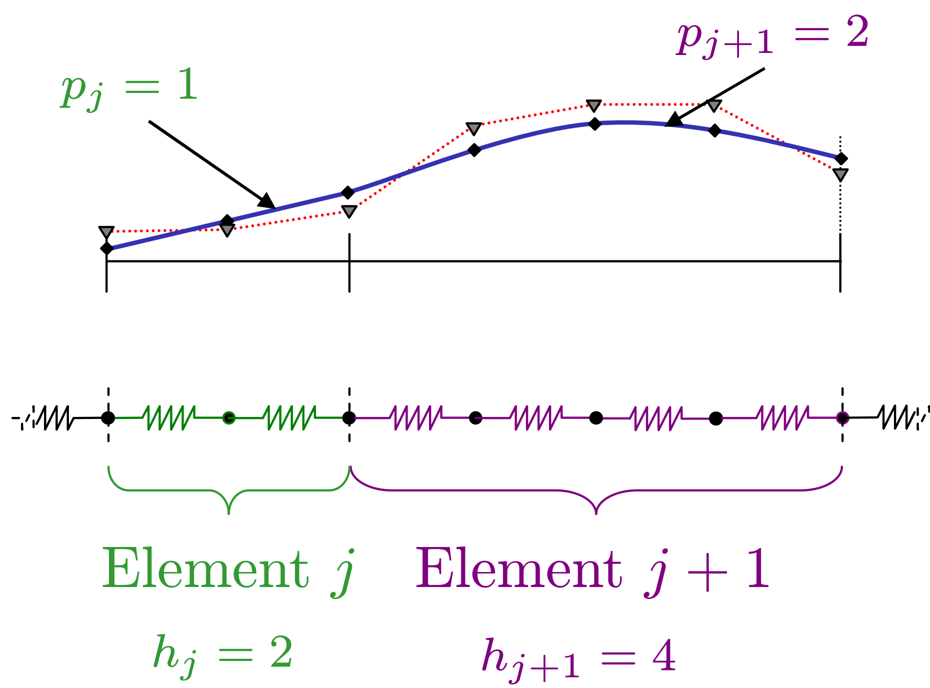
hp-adaptivity and QCM

Generalizing Quasicontinuum Method to *hp* meshes

The Quasicontinuum Method[1] is a dimensional reduction technique [2] that constrains element-interior DOFs by linearly interpolating the corner DOFs.



We have generalized the scheme to use higher order polynomial interpolation to constrain interior (edge/face/volume) DOFs[3].



1. R. E. Miller and E. B. Tadmor, The Quasicontinuum Method: Overview, applications, and current directions, Journal of Computer-Aided Design, v. 9, 2002.
2. C. Woźniak and M. Kleiber, Nonlinear Mechanics of Structures, Kluwer Academic Publishers, 1991
3. C. Jhurani and L. Demkowicz, Dimensional reduction for a lattice-like mass-spring polymer model using *hp*-adaptivity, Computer Methods in Material Science, v. 6, 2006.

Interpolation – Effective Stiffness and Load

Consider an abstract finite-dimensional minimization problem.

$$\min_{v \in \mathbb{R}^N} J(v) \quad \text{where} \quad J(v) := \frac{1}{2} v^T K v - v^T f$$

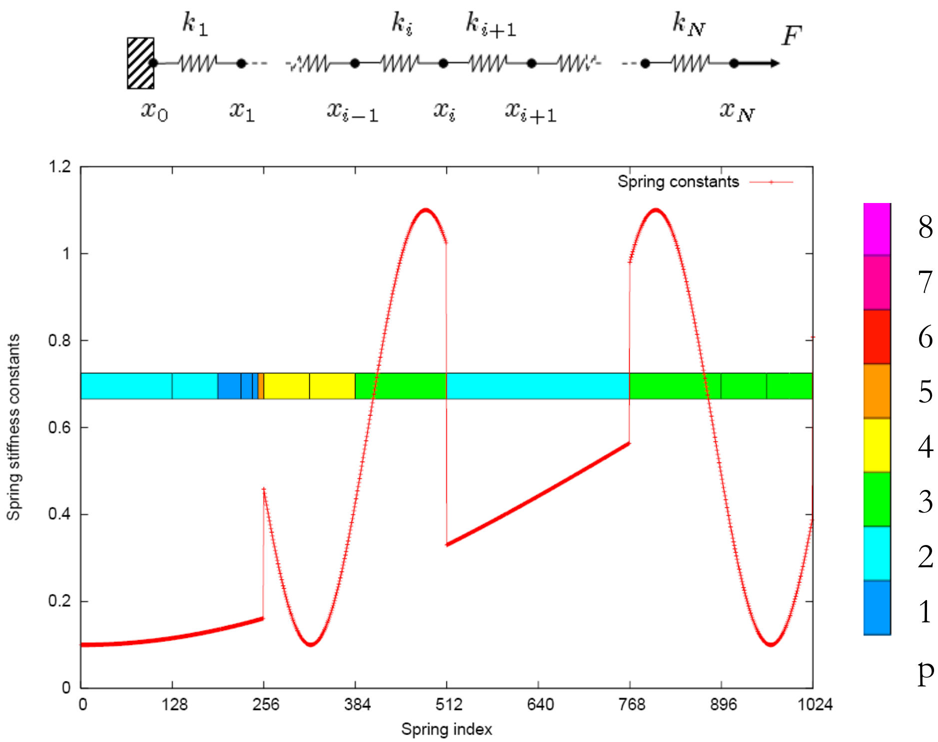
Let $A : \mathbb{R}^M \to \mathbb{R}^N$ be a global interpolation operator. We minimize in $range(A)$.

$$\min_{\widehat{v} \in \mathbb{R}^M} J(A\widehat{v})$$

This can be written as

$$\min_{\widehat{v} \in \mathbb{R}^M} \frac{1}{2} \widehat{v}^T \underbrace{(A^T K A)}_{\text{Effective stiffness matrix}} \widehat{v} - \widehat{v}^T \underbrace{(A^T f)}_{\text{Effective load}}.$$

Goal-driven *hp*-adaptivity Results in 1D



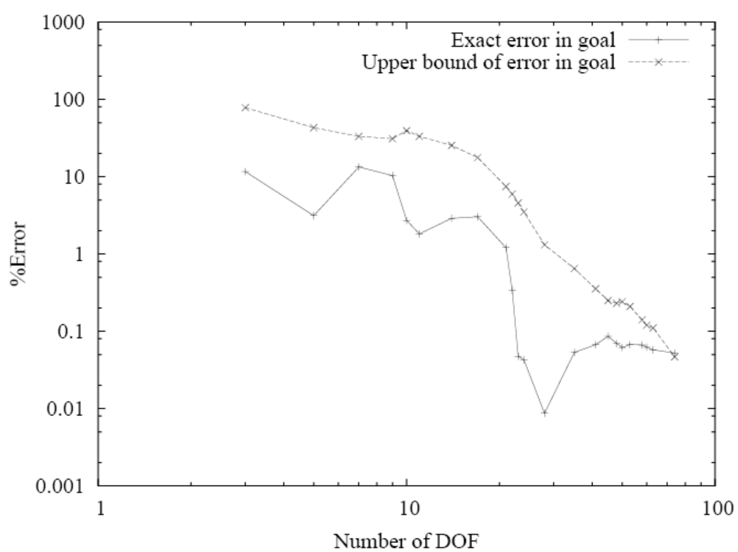
(a)

1024 harmonic springs in 1D with variable stiffnesses, goal $= u_{341} - u_{682}$ (relative displacement).

(a) Mesh with 2.5% error

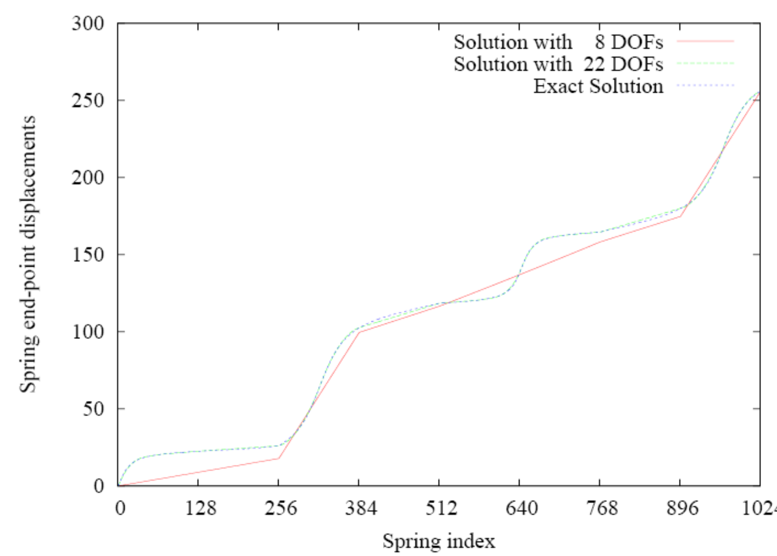
(b) Error in goal

(c) Solution



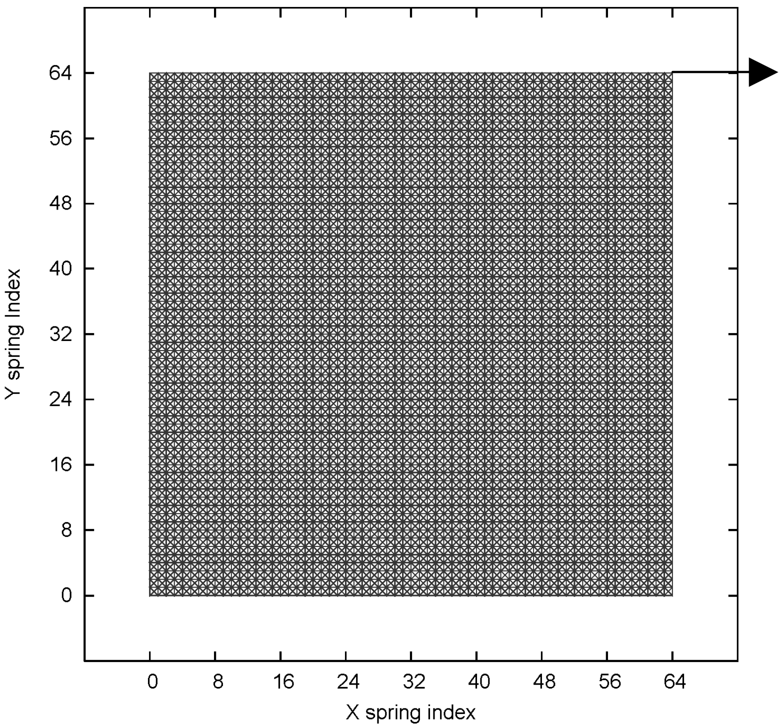
(b)

(c)

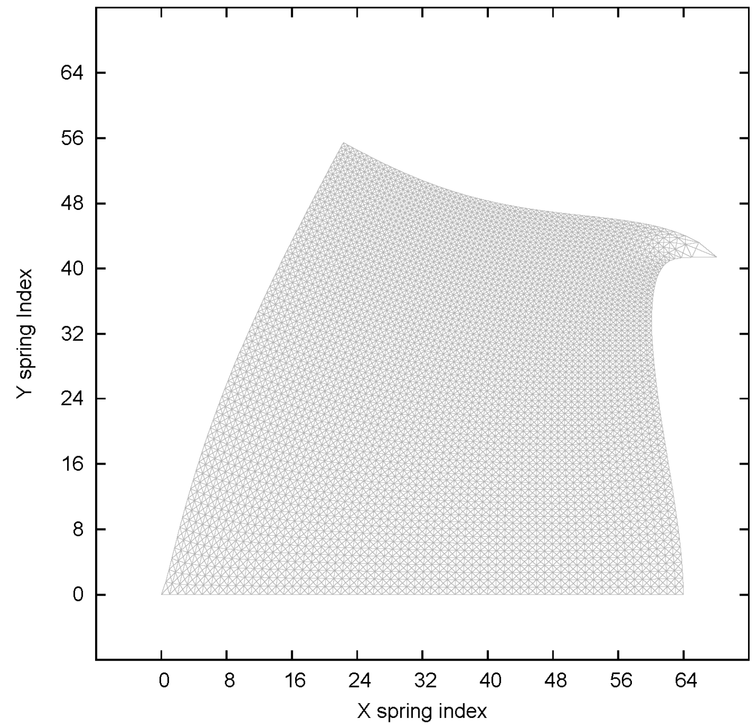


A 2D Linear Test Problem and Adaptivity

- 64 cells on each side
- pre-strain $l\left[1-\sin\left(y/64\right)\right]/2$ in each spring.
- Spring constants depend on y. $k = 1 + \sin\left(y/64\right)$.
- A force $1\hat{i}$ on the top-right corner.



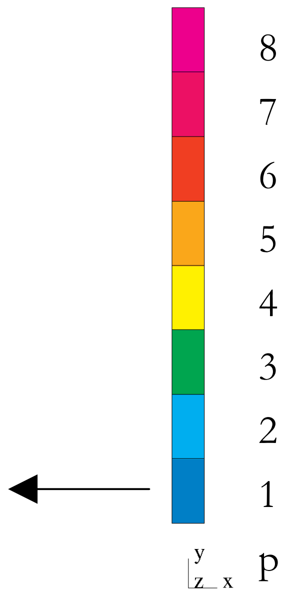
Lattice topology



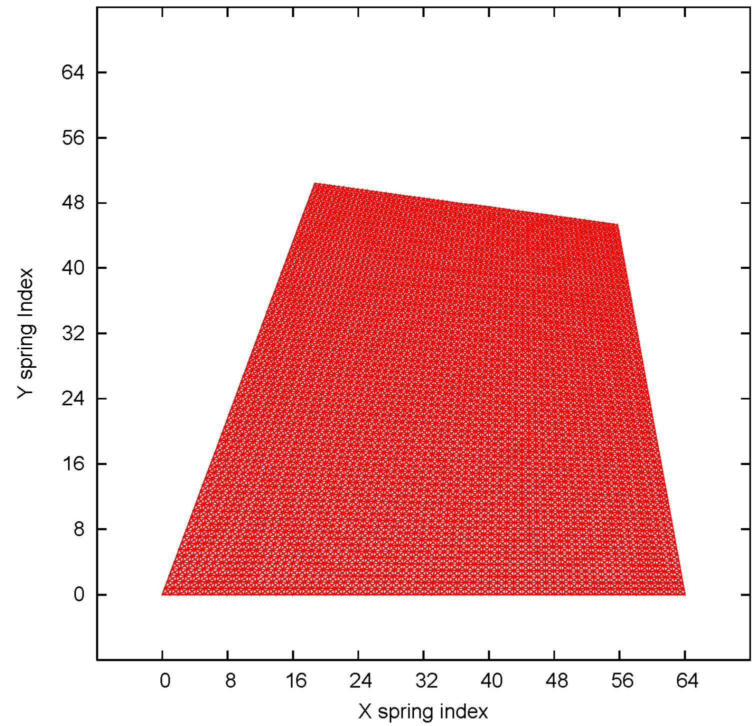
Exact solution

hp-adaptivity – Iteration 1

hp mesh



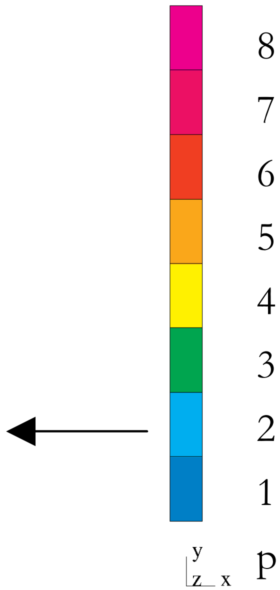
Polynomial degree



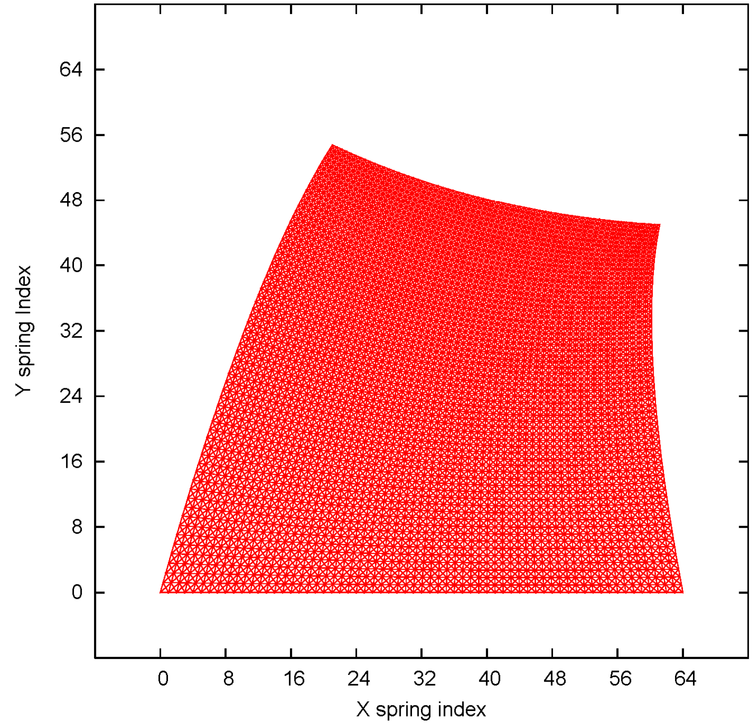
Current solution

hp-adaptivity – Iteration 2

hp mesh



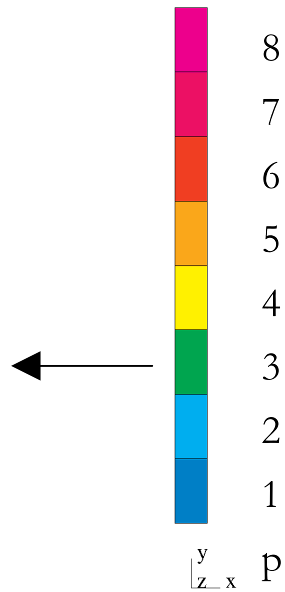
Polynomial degree



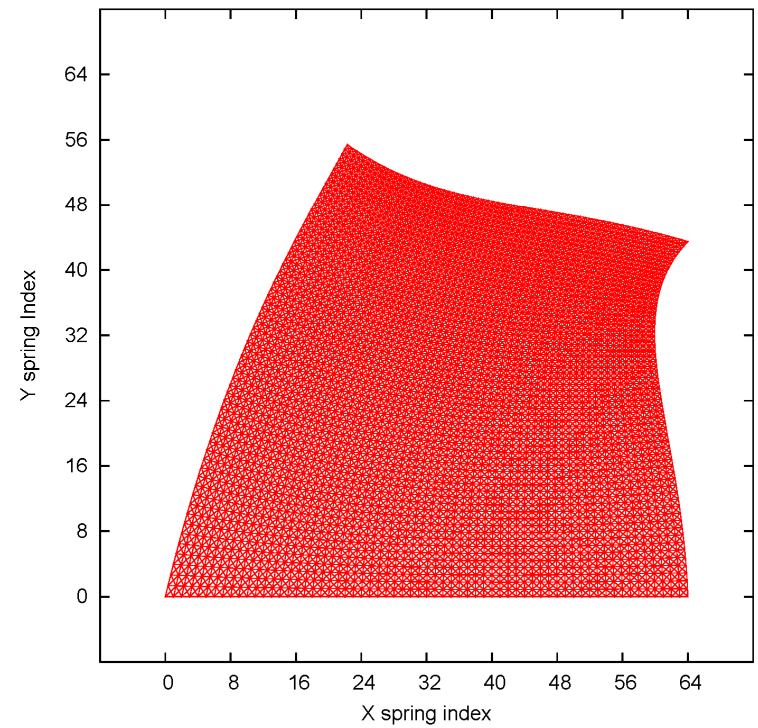
Current solution

hp-adaptivity – Iteration 3

hp mesh

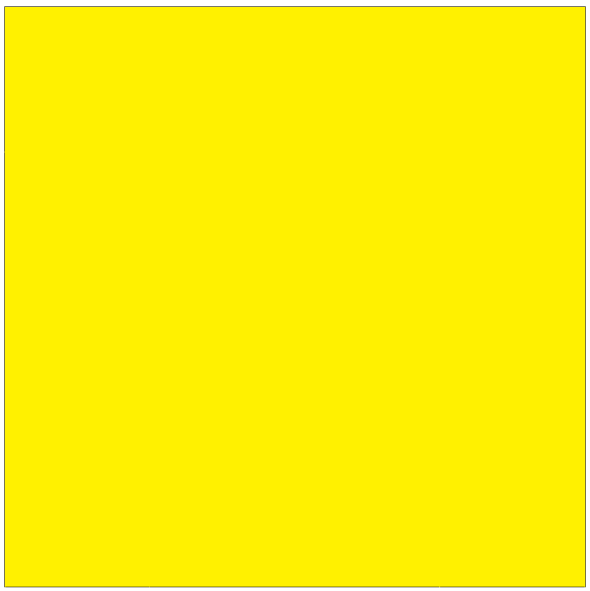


Polynomial degree

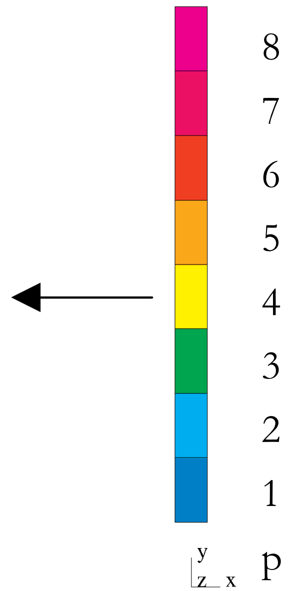


Current solution

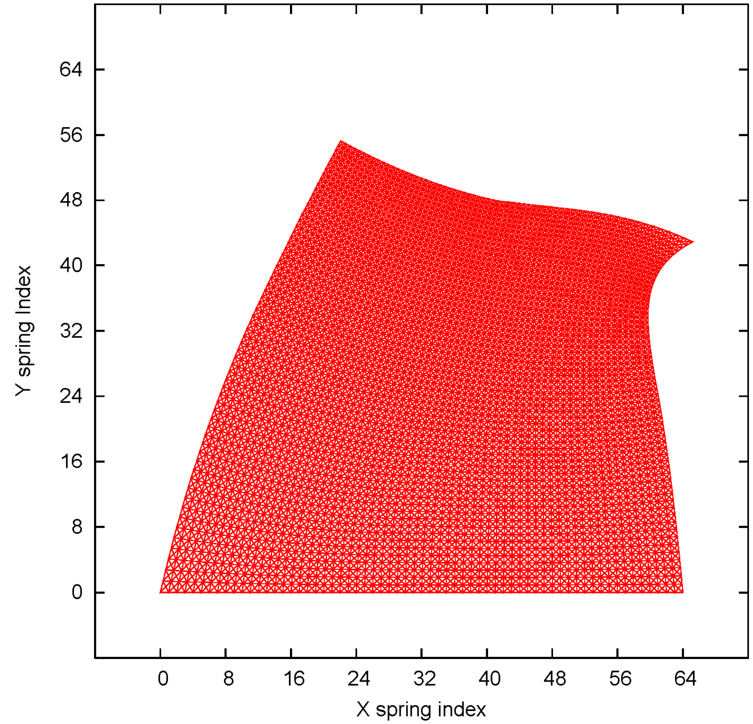
hp-adaptivity – Iteration 4



hp mesh

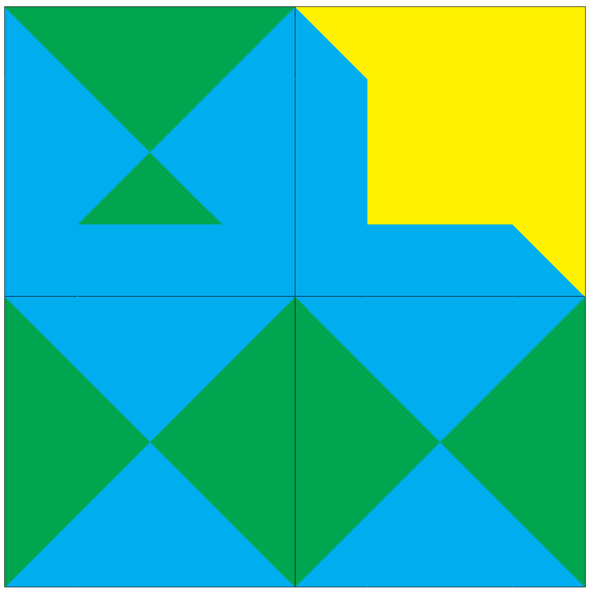


Polynomial degree

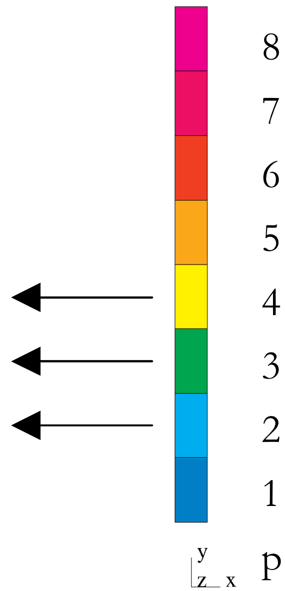


Current solution

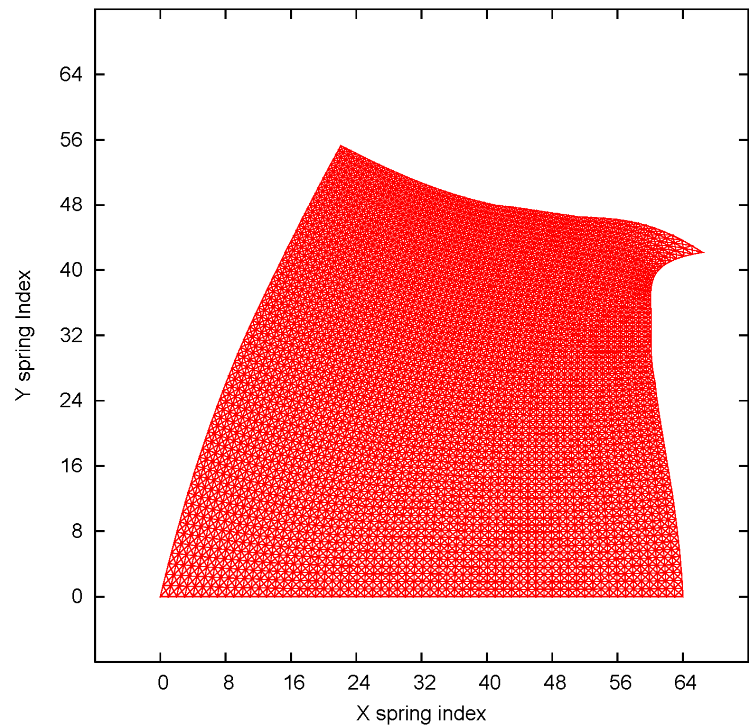
hp-adaptivity – Iteration 5



hp mesh

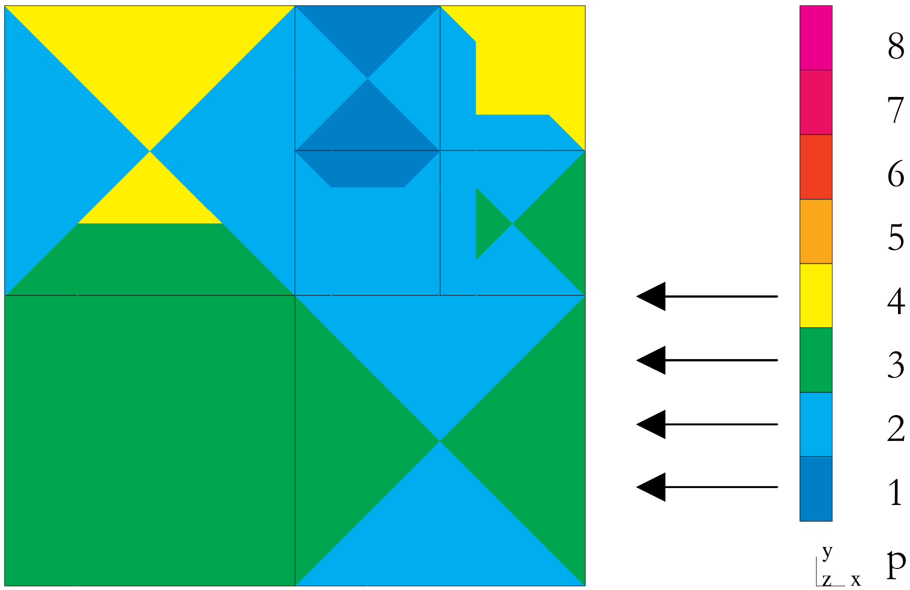


Polynomial degree



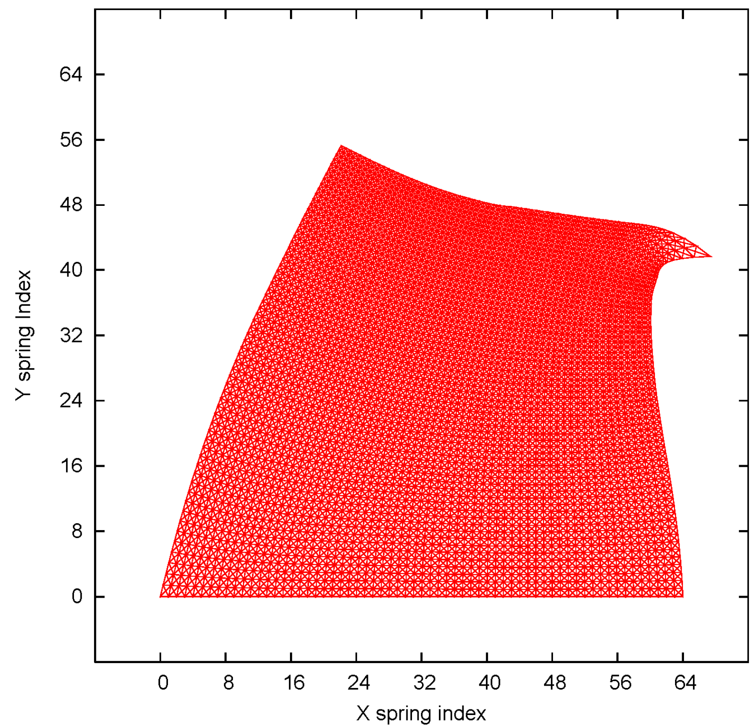
Current solution

hp-adaptivity – Iteration 6



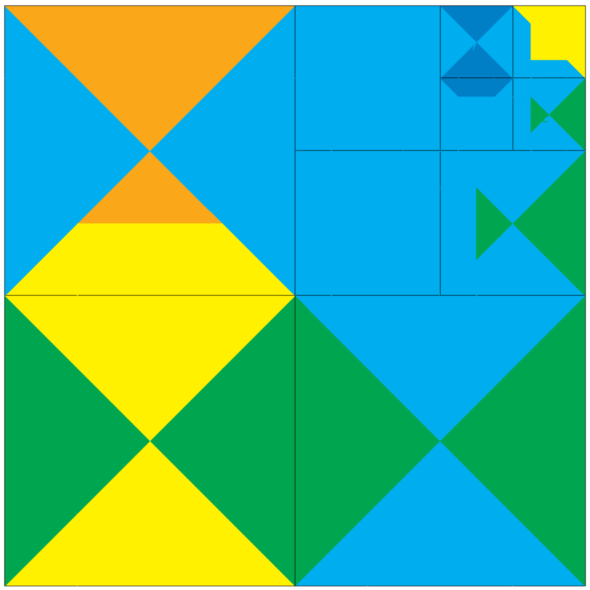
hp mesh

Polynomial degree

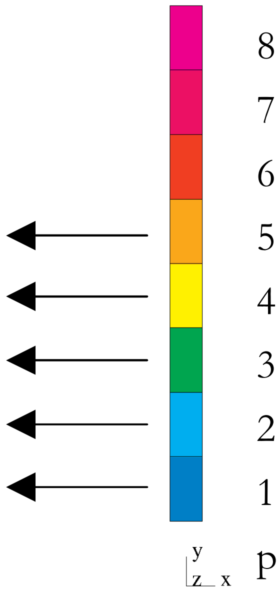


Current solution

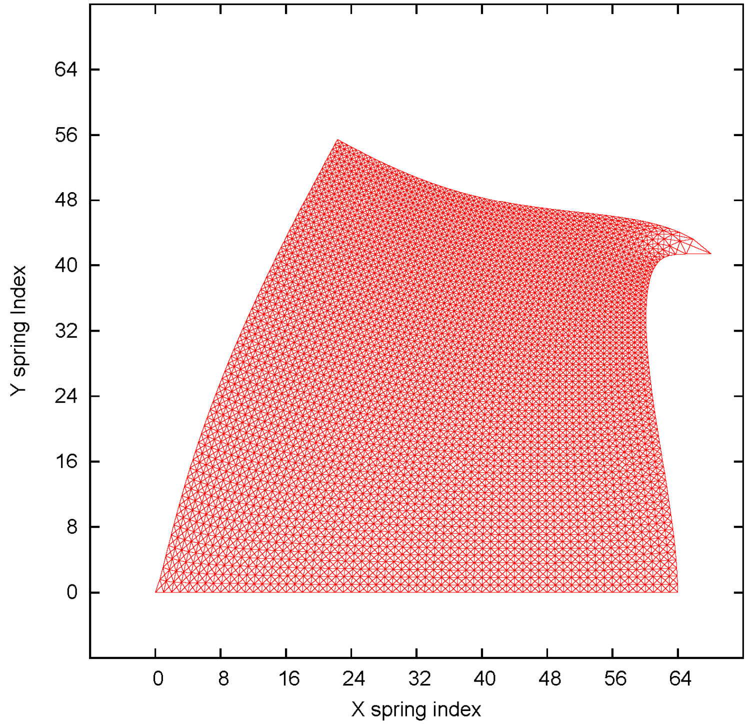
hp-adaptivity – Iteration 7



hp mesh

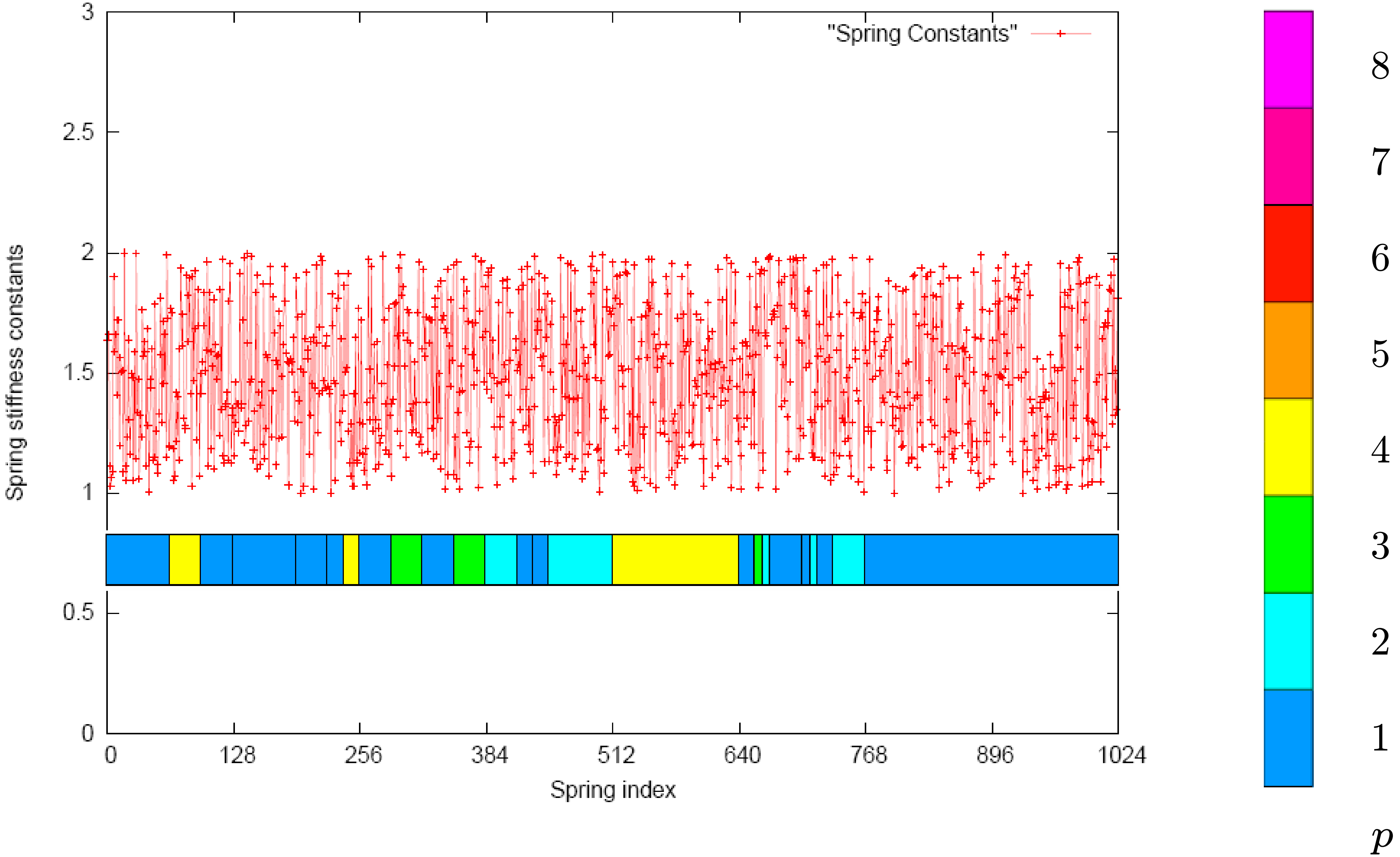


Polynomial degree



Current solution
Error estimate = 1.5%

hp-adaptivity – Limitations



Rough material data leads to refinements everywhere

Numerical Homogenization

Homogenization – A Classical Example

Consider the linear second order ODE

$$(a(x)u'(x))' = 0, \quad x \in (0,1),$$

with boundary conditions $u(0) = 0$ and $a(1)u'(1) = F$.

Assume periodic material properties.

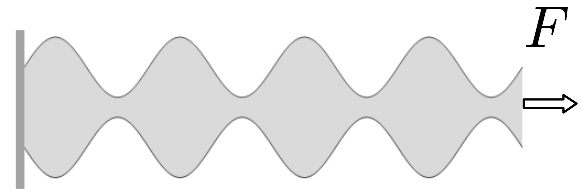
$$a(x) := 1 + \alpha \sin(2\pi n x)$$

where $|\alpha| < 1$ and $n \in \mathbb{N}$.

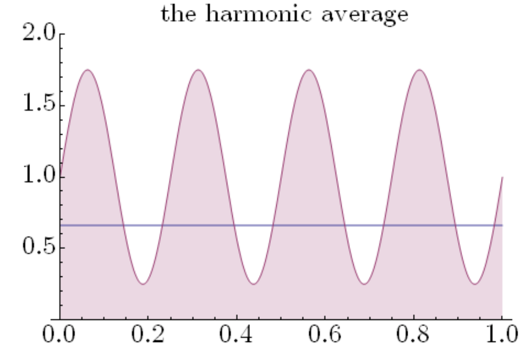
$$u(1) = F \int_0^1 \frac{1}{1 + \alpha \sin(2\pi n s)} ds = \frac{F}{\sqrt{1-\alpha^2}}$$

The *effective* "a", defined here as $F/u(1)$, is $\sqrt{1-\alpha^2}$.

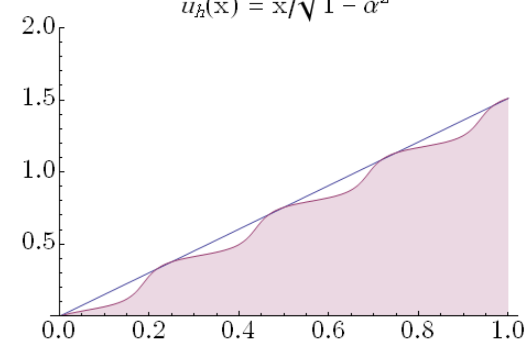
A bar with variable stiffness or area



a(x) for α = 0.75 and n = 4 and the harmonic average



u(x) for α = 0.75 and n = 4 and $u_h(x) = x/\sqrt{1-\alpha^2}$



Homogenization – Interpolate & Minimize?

Energy functional for the previous ODE is

$$J(u) := \frac{1}{2}\int_0^1 a(x)u'(x)^2 dx - Fu(1).$$

The exact solution can be found by solving

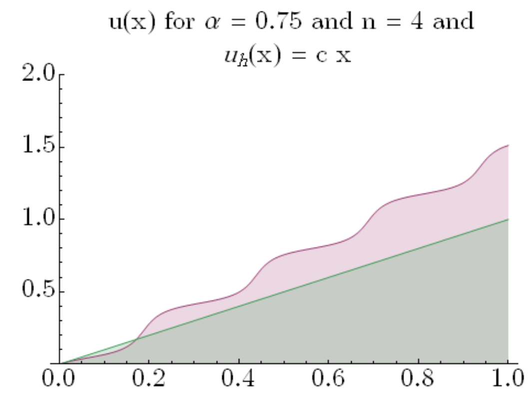
$$\min_u J(u) \text{ such that } u(0) = 0.$$

We try an approximate solution of the form $u_h(x) := cx$.

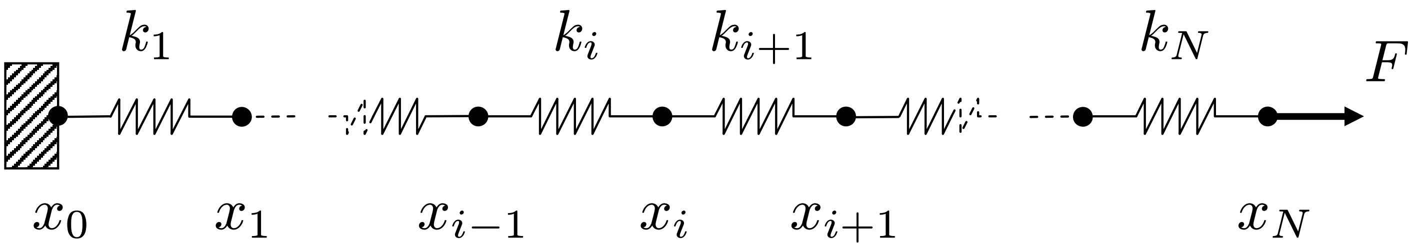
$$\min_c \frac{1}{2}\int_0^1 a(x)c^2 dx - Fc.$$

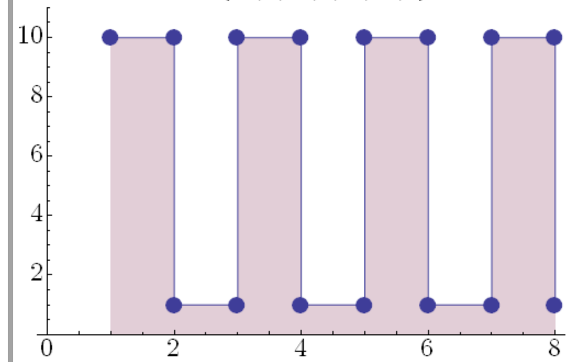
$c = F\int_0^1 a(x)dx = F$ and *effective* "a" is $F/u(1) = 1$.

$\Longrightarrow$ The relative error is unbounded as $\alpha \to 1$.



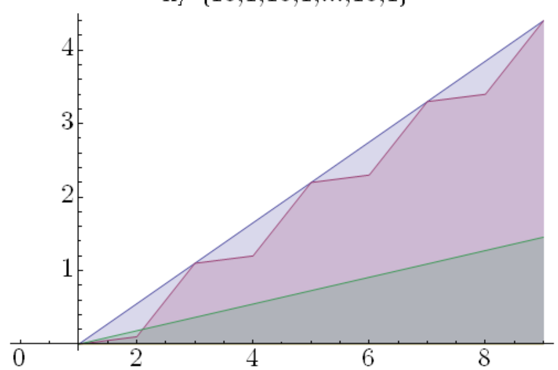
Homogenization – A Discrete 1D Problem





For N springs in 1D connected in series and pulled on end-points, matching the end-point displacements leads to averaging of the inverse stiffnesses.

$$\frac{1}{k_{\text{eff}}} = \sum_{i=1}^{N} \frac{1}{k_i}$$



Instead, if we linearly interpolate and minimize energy, we get the wrong effective stiffness.

$$k_{\text{eff}} = \frac{1}{N^2} \sum_{i=1}^{N} k_i$$

Homogenization – Effects of Interpolation

Problems with minimizing in a subspace (via simple interpolation)

- Not suitable for fast variations in material properties
- Effects of fine-scale ignored
- Interpolation averages the stiffness and not the solution
- It gives meaningful results even if a spring constant tends to zero (or if '$a(x)$' is zero in a region for the continuous problems)

Homogenization – A Literature Review

Classical Homogenization – Effective equations in periodic/random media

Numerical Homogenization – Upscaling – Subgrid modeling – Multiscale FEM

- Variational multiscale method and projections – Hughes et al.
- Wavelets to compute effective homogenized operators – Dorobantu, Engquist et al.
- Numerical upscaling for two-phase flow in porous media – Arbogast
- Solve local problems to get operator-dependent basis functions – Hou et al.
- Operator-dependent interpolation for multigrid methods – Knapek
- Estimate effective stiffness matrix at quadrature points (heterogeneous multiscale methods) – E and Engquist

Homogenization – Change of Focus

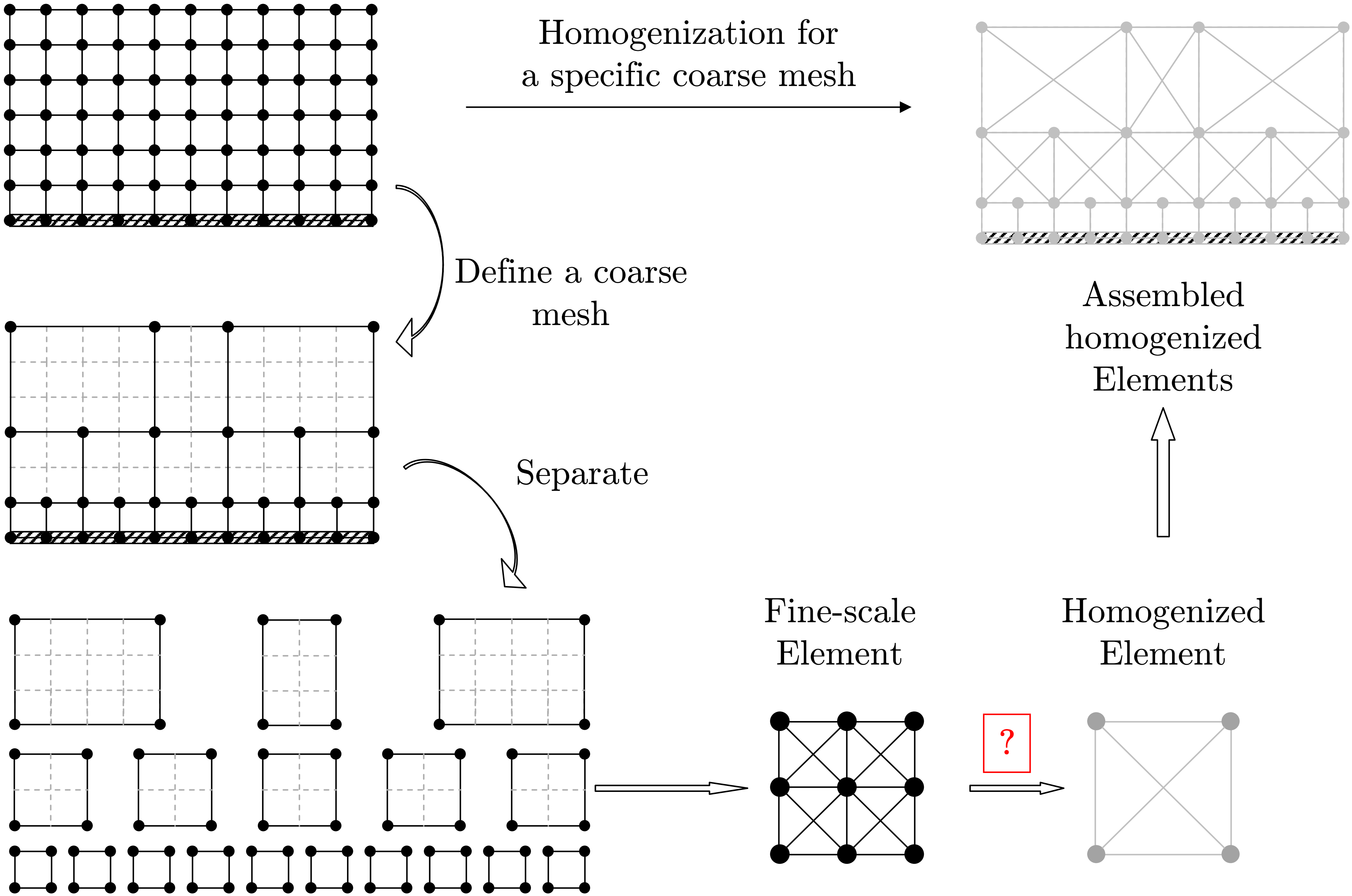
We change our focus to get locally best effective material properties

Classical homogenization approach

$$
\begin{tikzcd}
\text{Fine-scale problem} \arrow[r, "\text{Homogenize}"] \arrow[d, "\text{Discretize}"'] & \text{A global coarse-scale problem} \arrow[d, "\text{Discretize}"] \\
\text{Local coarse-scale problems} \arrow[r, "\text{Homogenize}"] & \text{Solution}
\end{tikzcd}
$$

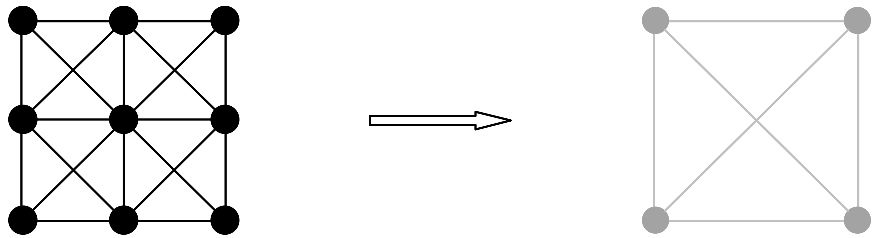
Our approach

Homogenization – A Schematic



Homogenization – The Linearized Problem

Fine-scale Element
$N = 18$



Homogenized Element
$M = 8$

- $K \in \mathbb{R}^{N \times N}$, symmetric.
- K has a non-trivial null-space.
- $u, f \in \mathbb{R}^N$.
- f is self-equilibrated.
- f is sum of internal load and unknown interaction with the rest of the lattice.

Local fine scale equation:

$$Ku = f.$$

- $\widehat{K} \in \mathbb{R}^{M \times M}$, symmetric.
- $\widehat{K}$ has a non-trivial null-space.
- $\widehat{u}, \widehat{f} \in \mathbb{R}^M$.
- $\widehat{f}$ is self-equilibrated.
- $\widehat{f}$ is sum of internal load and unknown interaction with the rest of the coarse mesh.

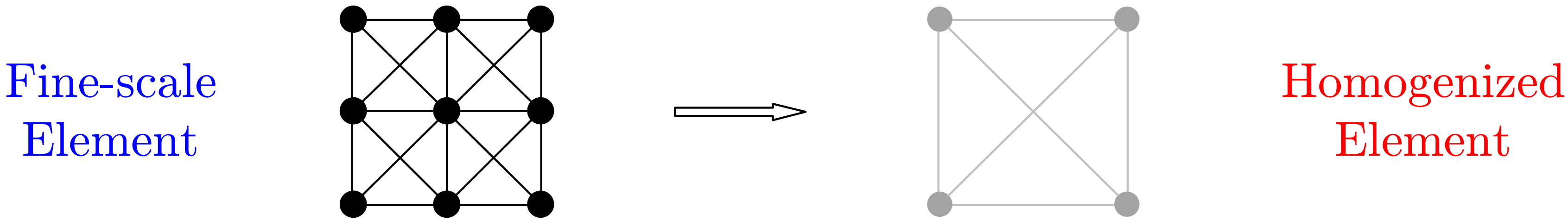
Local coarse scale equation:

$$\widehat{K}\widehat{u} = \widehat{f}.$$

What should $\widehat{K}$ be?

Let $A \in \mathbb{R}^{N \times M}$ be the bilinear interpolation operator.
Approximate fine scale solution $= A\widehat{u}$.
Restriction of fine scale load to the coarse scale $= A^T f =: \widehat{f}$.

Homogenization – A Definition of the Error



$$K\,u = f \qquad\qquad \color{red}{\widehat{K}}\widehat{u} = A^T f$$

$$\Longrightarrow \quad u = K^\dagger f + u_0. \qquad\qquad \Longrightarrow \quad \widehat{u} = \color{red}{\widehat{K}^\dagger}A^T f + \widehat{u_0}.$$

Thus, up to a constant, the error in the local solution for a local load f is

$$\begin{aligned} e \quad &:= \quad u - A\widehat{u} \\ &= \quad K^\dagger f - A\,\color{red}{\widehat{K}^\dagger}A^T f \\ &= \quad \left(K^\dagger - A\color{red}{\widehat{K}^\dagger}A^T\right) f. \end{aligned}$$

We want to choose $\color{red}{\widehat{K}}$ such that e is small.

"†" denotes the Moore-Penrose pseudoinverse.

A Brief Digression – Pseudoinverses

- Also called generalized inverses
- Studied by Fredholm, Hilbert, and many others for integral and differential operators.
- Introduced by E. H. Moore for matrices in 1920 using projections. Trivia: E. H. Moore was R. L. Moore's advisor (no relation).
- Rediscovered by Roger Penrose in 1955 using an "axiomatic" approach.

Hence we have many ways of defining/introducing pseudoinverses.

- Via least squares type minimization problems (more intuitive)
- Via an axiomatic approach (Penrose equations)

Moore-Penrose pseudoinverse

- exist for singular and rectangular matrices, and
- reduce to regular inverses for invertible matrices.

Moore-Penrose Pseudoinverse – Definitions

We can introduce Moore-Penrose pseudoinverse by least-squares problems. Let $Y \in \mathbb{R}^{M\times N}$ and $X \in \mathbb{R}^{N\times M}$. Then

$$Y^\dagger = \operatorname{argmin} \left|\left| \underset{X}{\operatorname{argmin}} ||YX - I_M||_F^2 \right|\right|_F$$

There are simpler formulas for full rank rectangular matrices.

Books on Linear Algebra typically define $Y^\dagger$ using the Singular Value Decomposition (SVD) of Y. Let $U\Sigma V^T$ be the SVD of Y. Then

$$Y^\dagger = V\Sigma^\dagger U^T$$

where

$$\Sigma^\dagger = \operatorname{diag}(1/\sigma_1, 1/\sigma_2, \ldots, 1/\sigma_r, 0, \ldots, 0)$$

and r is the rank of Y.

Later we will see two different methods for computing Moore-Penrose pseudoinverse that exploit sparsity.

Homogenization – Error as a Number

$$e(\widehat{K}) = \left(K^\dagger - A\widehat{K}^\dagger A^T\right) f$$

The problem of finding a unique $\widehat{K}$ by minimizing $e(\widehat{K})$, in any norm, is ill-posed simply because $\widehat{K}$ enters the equation by its action on a single vector $A^T f$. So we try "regularization".

For $\epsilon > 0$, $f \neq 0$, and $\widehat{K}^\dagger$ symmetric, $B \in \mathbb{R}^{N\times N}$ symmetric positive definite, let the error $\mathcal{E}$ to be minimized be defined as

$$\mathcal{E}(\widehat{K}^\dagger) := \frac{1}{2}\underbrace{\left|\left|(K^\dagger - A\widehat{K}^\dagger A^T)f\right|\right|_B^2}_{\substack{\text{Error in local solution}\\ \text{for a local load f}}} + \frac{\epsilon}{2}\underbrace{\left|\left|K^\dagger - A\widehat{K}^\dagger A^T\right|\right|_{F,B}^2}_{\substack{\text{Difference of local fine-scale and}\\ \text{interpolated "compliance" matrices}}} ||f||_2^2 .$$

Here $||X||_{F,B}^2 := \mathrm{trace}(X^T B X)$. This is a $B-$weighted Frobenius norm.

Note that e is a highly nonlinear function of $\widehat{K}$. $\mathcal{E}$, however, is a quadratic function of entries of $\widehat{K}^\dagger$.

Homogenization – A QP Formulation

We denote $\widehat{K}^\dagger$ by X now. Given $K \in \mathbb{R}^{N\times N}$, K symmetric, $A \in \mathbb{R}^{N\times M}$, $B \in \mathbb{S}^N_{++}$, $f \in \mathbb{R}^N - \{0\}$, and $\epsilon > 0$, solve the linear equality constrained convex quadratic problem

$$\min_{X=X^T} \mathcal{E}(X).$$

Using a Lagrange multiplier matrix Λ to impose the symmetry we get

$$\begin{aligned} UXV - W &= \Lambda^T - \Lambda, \quad \text{where} \\ \left.\begin{aligned} U &:= A^T B A \\ V &:= A^T(ff^T + \epsilon\,||f||_2^2\, I)A \\ W &:= A^T B K^\dagger(ff^T + \epsilon\,||f||_2^2\, I)A \\ C &:= V^{-1}U \\ D &:= V^{-1}(W + W^T)V^{-1}. \end{aligned}\right\} &\in \mathbb{R}^{M\times M} \end{aligned}$$

Eliminating Λ and using $X = X^T$ shows that X solves the **Lyapunov equation**

$$\boxed{CX + XC^T = D.}$$

Homogenization – Other QP Formulations

Let $E := (K^\dagger - AXA^T)$. We had defined the **regularization** form of error as

$$\mathcal{E}(X) := \frac{1}{2}\,||Ef||_B^2 \;+\; \frac{\epsilon}{2}\,||E||_{F,B}^2\,||f||_2^2\,.$$

Using this will give the same X as the **penalty** formulation

$$\min_{X=X^T} \mathcal{E}_P(X) := \frac{\mathcal{E}(X)}{\epsilon} \text{ where } \frac{\mathcal{E}(X)}{\epsilon} = \frac{1}{2\epsilon}\,||Ef||_B^2 \;+\; \frac{1}{2}\,||E||_{F,B}^2\,||f||_2^2\,.$$

The penalty formulation above imposes (one of the) constraints approximately. Imposing that constraint exactly, we get

$$\min \mathcal{E}_S(X) := \frac{1}{2}\,||E||_{F,B}^2 \quad \text{such that} \quad X = X^T \quad \text{and} \quad A^T B E f = 0.$$

This gets rid of the parameter ϵ, but leads to a **saddle-point** problem with Kronecker product structure and more unknowns (the Lagrange multipliers). We will work with the regularization/penalty formulation.

Homogenization – A Special Case

If $f \equiv 0$, or it is unknown, or we want to treat all loads equally, the definition of the error $\mathcal{E}$ should be

$$\mathcal{E}(X) := \frac{1}{2} \left|\left| K^\dagger - AXA^T \right|\right|_{F,B}^2 .$$

For $B =$ Identity, it can be proved that $\mathcal{E}$ is minimum at

$$X = A^\dagger K^\dagger (A^T)^\dagger .$$

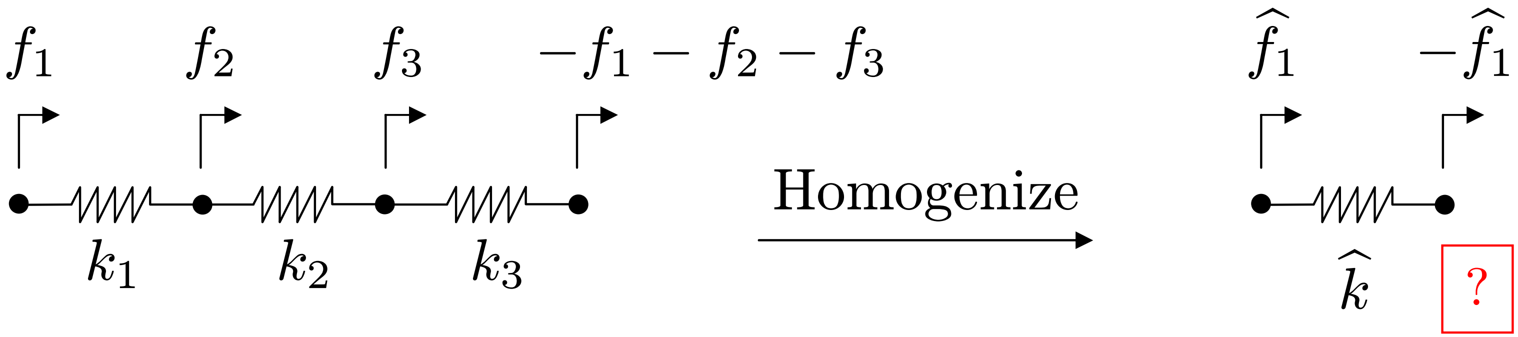
Thus

$$\boxed{\widehat{K} = X^\dagger = \left(A^\dagger K^\dagger (A^T)^\dagger \right)^\dagger .}$$

Compare this with the $\widehat{K}$ that is obtained without resolving the fine scales. There

$$\widehat{K} = A^T K A.$$

Homogenization – A Sanity Check



If we load only on the end-points, use $B = I$, and $\epsilon \to 0$, we get

$$\widehat{k} = \frac{10\, k_1 k_2 k_3}{9\, k_1 k_2 + 12\, k_1 k_3 + 9\, k_2 k_3}.$$

Classical effective spring constant is

$$k = \frac{k_1 k_2 k_3}{k_1 k_2 + k_1 k_3 + k_2 k_3}.$$

The discrepancy exists because the displacements of the inner points are ignored in the classical case. It is possible to match the classical value by choosing a B that uses only the end-points.

Homogenization – Computational Aspects

- Solution of Lyapunov Equation on the coarse scale
  - Bartels-Stewart algorithm using real Schur decomposition of C
  - Implemented in SLICOT – a LAPACK-like systems and control library

$$CX + XC^T = D$$

- Computation of Moore-Penrose pseudoinverse
  - Of a large sparse fine-scale element stiffness matrices K
    - SVD very expensive
    - Use Tikhonov regularization and a sparse direct solver for symmetric matrices (we use CHOLMOD)
    - Or use the knowledge of the null-space of K to transform the problem to a linear non-singular "practically sparse" system of equations

$$\left(A^\dagger \overset{\downarrow}{K^\dagger} (A^T)^\dagger\right)^\dagger$$

  - Of a dense full-rank rectangular interpolation matrix A
    - Use QR decomposition on normal equations

$$\left(\overset{\downarrow}{A^\dagger} K^\dagger \overset{\downarrow}{(A^T)^\dagger}\right)^\dagger$$

  - For recovering the dense element stiffness matrix after solving the Lyapunov Equation for X
    - Cleanup spurious non-zero singular values and use SVD

$$\left(A^\dagger K^\dagger (A^T)^\dagger\right)^{\overset{\downarrow}{\dagger}}$$

Moore-Penrose Pseudoinverse – No SVD – 1

For a given vector f and a sparse Y that is **known** to be not full-rank, we want to compute $Y^\dagger f$ without computing the SVD of Y.

If we regularize a least squares problem, it can be proved that

$$Y^\dagger = \lim_{\delta \to 0} (Y^T Y + \delta I)^{-1} Y^T = \lim_{\delta \to 0} Y^T (Y Y^T + \delta I)^{-1}.$$

The limit definitions work well if even if δ is finite but small enough, like $\mathbf{10^{-7}} \, ||Y||^2$. We can then compute $x = Y^\dagger f$ by solving

$$(Y^T Y + \delta I) x = Y^T f$$

for x using a sparse direct solver. The relative error in $\left|\left|Y^\dagger f\right|\right|_2$ is of order $\mathbf{10^{-7}}$.

Moore-Penrose Pseudoinverse – No SVD – 2

When a matrix comes from physical problems, we typically know its null-space *a priori*. For example, rigid body motion in elasticity.

This knowledge can be used to avoid the SVD and reduce computation of pseudoinverse to solving a linear system of algebraic equations (by direct or iterative methods).

Let $Y \in \mathbb{R}^{N \times N}$ be a symmetric matrix with a rank deficiency p $(0 < p \leq n)$. Let $R \in \mathbb{R}^{n \times p}$ be an orthonormal basis for the null-space of Y. We have

$$Y^\dagger = (I - RR^T)(Y + RR^T)^{-1} = (Y + RR^T)^{-1}(I - RR^T).$$

Thus, computing $x = Y^\dagger f$ means solving

$$(Y + RR^T)x = (I - RR^T)f$$

for x. If Y is sparse, this can be done by iterative methods for sparse symmetric matrices without forming the dense $Y + RR^T$.

Goal-oriented *hp*-adaptivity

$$\begin{array}{llcll}
\text{Exact primal} & \text{Find } u^{EX} \in u_D + V & : \mathcal{B}(u^{EX}, v) & = & \mathcal{L}(v) & \forall v \in V \\
\text{Approx. primal} & \text{Find } u^{hp} \in u_D + V^{hp} & : \mathcal{B}(u^{hp}, v^{hp}) & = & \mathcal{L}(v^{hp}) & \forall v^{hp} \in V^{hp} \\
\text{Exact adjoint} & \text{Find } w^{EX} \in V & : \mathcal{B}(e, w^{EX}) & = & \mathcal{G}(e) & \forall e \in V \\
\text{Approx. adjoint} & \text{Find } w^{hp} \in V^{hp} & : \mathcal{B}(e^{hp}, w^{hp}) & = & \mathcal{G}(e^{hp}) & \forall e^{hp} \in V^{hp}
\end{array}$$

Then, error in goal $\mathcal{G}(u^{EX}) - \mathcal{G}(u^{hp}) = \mathcal{B}(u^{EX} - u^{hp}, w^{EX} - w^{hp})$.

For mesh adaptivity, we use two grids – a coarse (c) and a fine (f) – with a projection-based interpolation operator Π^c from fine to coarse[1,2]. The element-wise estimates of error in energy and goal are

$$\left|\left|u^f - \Pi^c u^f\right|\right|_{\mathcal{B}}^2 = \sum_{\text{elements } j} \left|\left|u^f - \Pi^c u^f\right|\right|_{\mathcal{B}_j}^2 \quad \text{and}$$

$$\left|\mathcal{G}(u^f) - \mathcal{G}(u^c)\right| \lesssim \sum_{\text{elements } j} \left|\left|u^f - \Pi^c u^f\right|\right|_{\mathcal{B}_j} \left|\left|w^f - \Pi^c w^f\right|\right|_{\mathcal{B}_j}.$$

1. L. Demkowicz, Computing with hp-ADAPTIVE FINITE ELEMENTS: Volume I: One and Two Dimensional Elliptic and Maxwell Problems, 2006.
2. L. Demkowicz et al., Computing with hp-ADAPTIVE FINITE ELEMENTS: Volume II Frontiers: Three Dimensional Elliptic and Maxwell Problems with Applications, 2007.

Homogenization – Goal-oriented Adaptivity

For the load $\mathcal{L}$ and goal $\mathcal{G}$ defined on the fine scale, define the restricted load and goal as

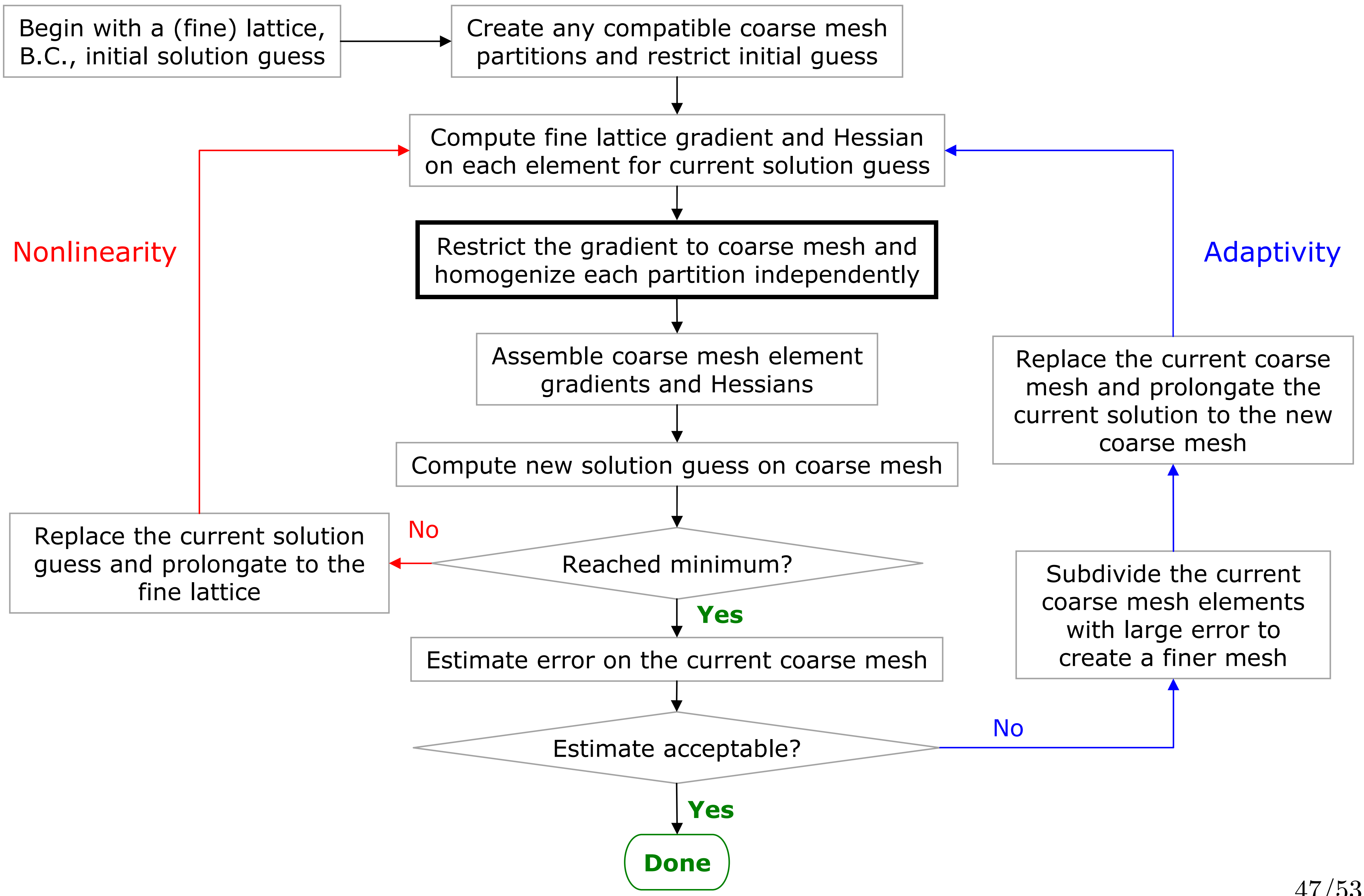
$$\begin{aligned}
\widehat{\mathcal{L}}(\widehat{v}) &:= \mathcal{L}(A\widehat{v}) \quad \forall \quad \widehat{v} \in \widehat{V} \\
\widehat{\mathcal{G}}(\widehat{v}) &:= \mathcal{G}(A\widehat{v}) \quad \forall \quad \widehat{v} \in \widehat{V}.
\end{aligned}$$

Fine primal	Find $u \in u_D + V$	$: \mathcal{B}(u, v)$	$=$	$\mathcal{L}(v)$	$\forall v \in V$
Fine adjoint	Find $w \in V$	$: \mathcal{B}(e, w)$	$=$	$\mathcal{G}(e)$	$\forall e \in V$
Homogenized primal	Find $\widehat{u} \in u_D + \widehat{V}$	$: \widehat{\mathcal{B}}(\widehat{u}, \widehat{v})$	$=$	$\widehat{\mathcal{L}}(\widehat{v})$	$\forall \widehat{v} \in \widehat{V}$
Homogenized adjoint	Find $\widehat{w} \in \widehat{V}$	$: \widehat{\mathcal{B}}(\widehat{e}, \widehat{w})$	$=$	$\widehat{\mathcal{G}}(\widehat{e})$	$\forall \widehat{e} \in \widehat{V}$

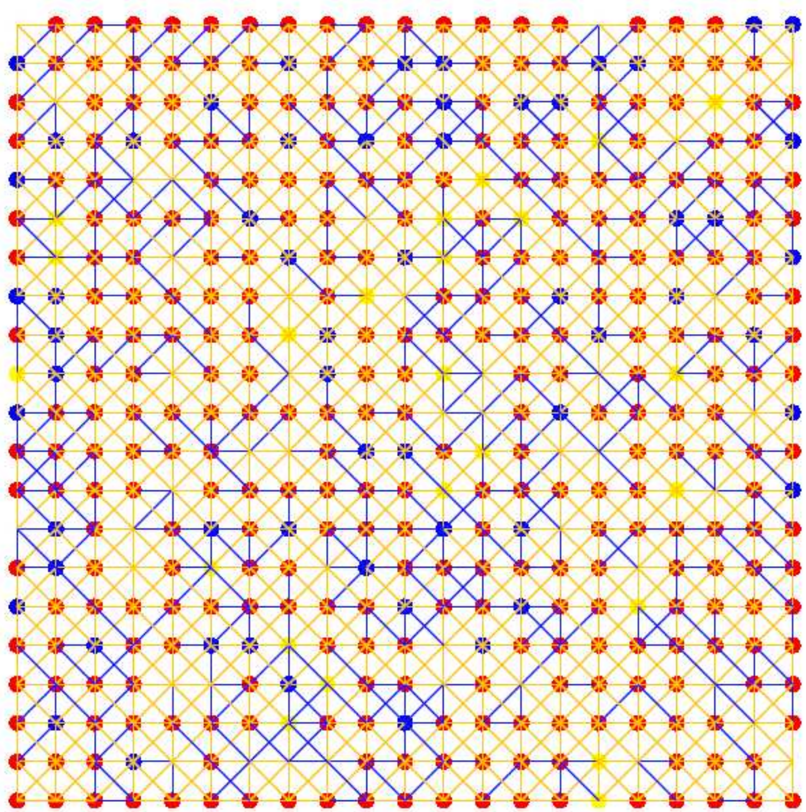
It can be shown that $\mathcal{B}(u, A\widehat{w}) = \widehat{\mathcal{B}}(\widehat{u}, \widehat{w})$. Using this, the error in the goal $\mathcal{G}(u) - \widehat{\mathcal{G}}(\widehat{u})$, is

$$\underbrace{\mathcal{B}(u - A\widehat{u}, w - A\widehat{w})}_{\text{Standard characterization}} \quad + \quad \underbrace{\widehat{\mathcal{B}}(\widehat{u}, \widehat{w}) - \mathcal{B}(A\widehat{u}, A\widehat{w})}_{\text{Incompatible bilinear forms}} \quad .$$

Mesh-adaptive Homogenization – Overview

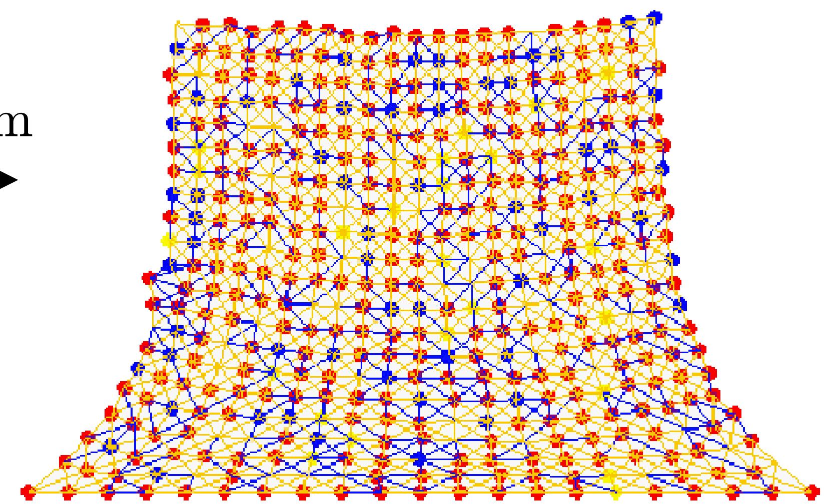


Homogenization – Numerical Results



20×20 lattice with fixed spacing on bottom (1.3)

Equilibrium →

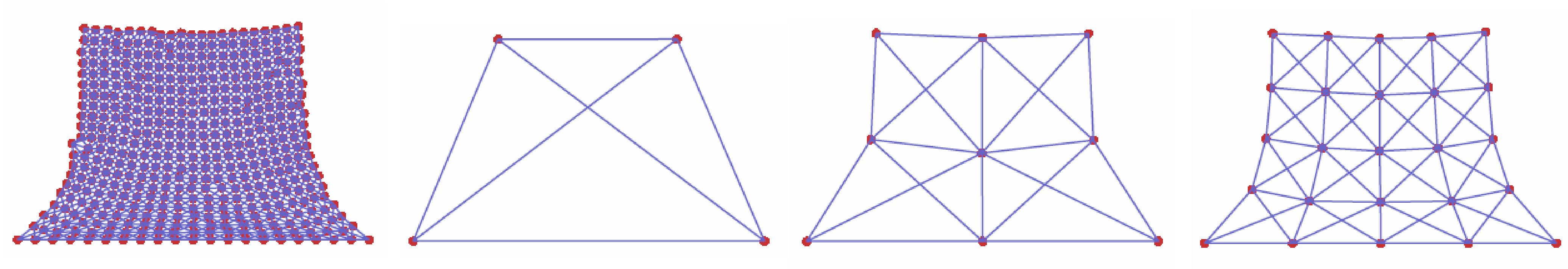


The fine-scale solution

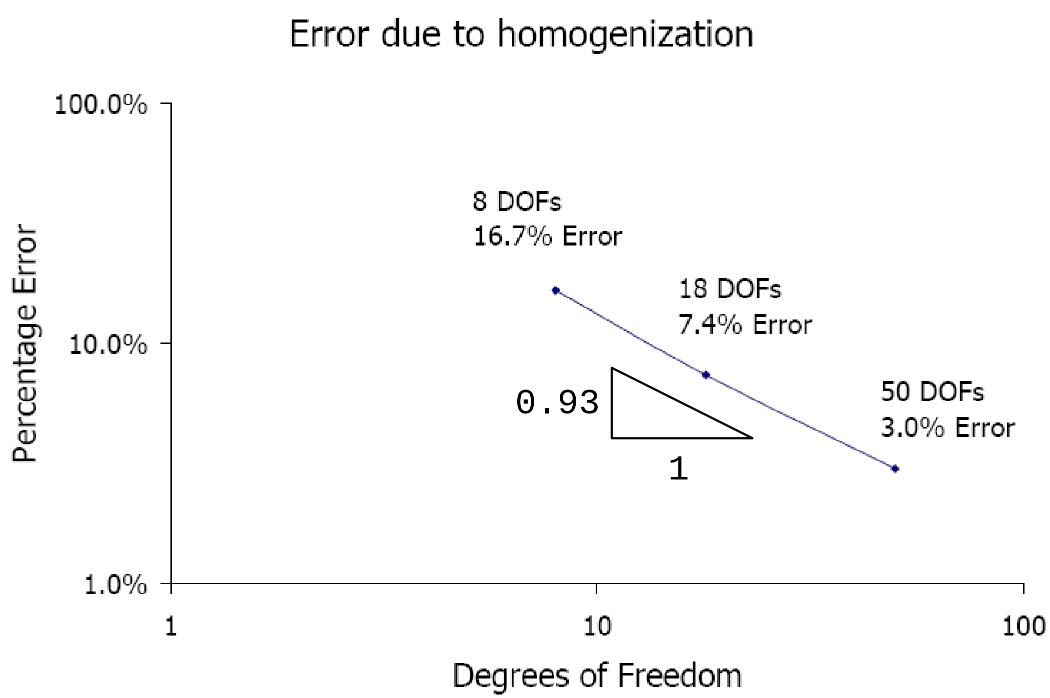
— bond stiffness 0.4, length 1.2

— bond stiffness 1.0, length 1.0

Homogenization – Error at Various Levels

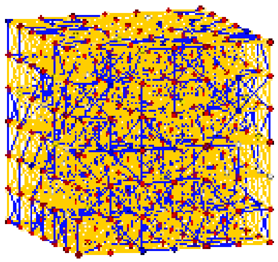


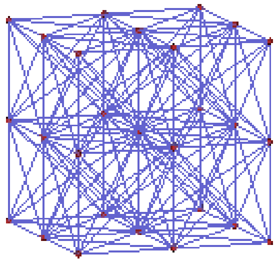
Original, 882 DOFs　　8 DOFs　　18 DOFs　　50 DOFs



Error in L^2 norm

Homogenization – Recent 3D Results





Software Packages Used

- BLAS, LAPACK, PETSc, TAO, and CHOLMOD
- hp[123]d
- SLICOT (Lyapunov equation solver)
- VTK (visualization), and
- Boost and MPICH.

Ongoing Work

- Integrate homogenization and mesh-adaptivity including error estimation
- Solve problems on representative SFIL lattices
- Use multiple realizations to compute statistical quantities
- Experiment with different optimization algorithms
- Compare the run-times of solving the base-model and the homogenized model
- Study technical aspects of homogenization
  - the choice of the norm for local homogenization
  - benefits of homogenizing for a given load when compared to homogenizing for arbitrary loads
  - program a suitable iterative solver to compute the Moore-Penrose pseudoinverse when the null-space is known
  - compare the run-times of iterative solver and sparse direct solver for computing the pseudoinverse.

Thank You!