Numerical homogenization of geometric network models

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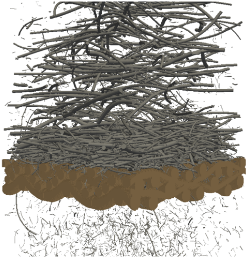
Motivation: Numerical simulation of paper

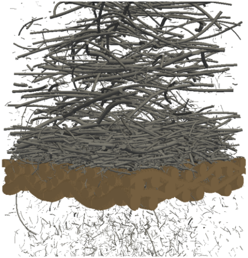


▷ fluid-structure interaction

▷ elastic network model

- Optimize paper making (dimensions, distribution, fabric)
- Optimize material properties (tensile, bending, avoid defects)
- Numerical simulation is not used extencively

Motivation: Numerical simulation of paper



▷ fluid-structure interaction

▷ elastic network model

- Sweden export: €8B/year (paper and cardboard)
- Fraunhofer Chalmers Centre
- Stora Enso and Albany International
- Gustav Kettil, PhD 2014-2019, (Chalmers/FCC)
- Morgan Görtz, PhD 2019- (Chalmers/FCC, SSF)

Motivation: Numerical simulation of paper

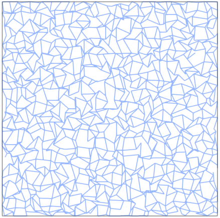
Aim:

- Large (A4) scale simulation (periodically expand 9mm $\times$ 9mm)
- Tensile and bending strength, crack propagation
- Virtual lab
- Offline-online setting

We have support to develop a multiscale approach.

Outline

A geometric network model



- Nodes $\{x_i\}_{i=1}^n \in \bar{\Omega}$ and edges $\{e_{ij}\}$.
- $V = \{v \in \mathbb{R}^n : v(x_i) = 0 \text{ for all } x_i \in \partial\Omega\}$
- $F \in V$
- $K : \mathbb{R}^n \to \mathbb{R}^n, \quad K = \sum_{i=1}^n K_i, \quad K_i \quad$ SP(semi-)D

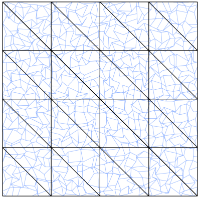
Find $u \in V$ such that

$$(v, Ku) = (v, F), \quad \forall v \in V$$

where $(v, w) = v^\top w$.

- We assume (v, Kv) to be coercive on V, i.e. we have a unique solution $u \in V$.
- For inhomogeneous bc let $u = u_0 + g$, $u_0 \in V$.

FE discretization



- $\mathcal{T}_H = \{T\}$, $H = \max \operatorname{diam}(T)$, quasi-uniform, shape regular $\frac{\operatorname{diam} B_T}{\operatorname{diam}(T)} \geq \rho$
- $P1$-FEM space $S_H = \operatorname{span}(\{\varphi_j\}_{j=1}^{m})$, $\varphi_j(y_i) = \delta_{ij}$
- $S_{H,0} = \{v \in S_H : v|_{\partial\Omega} = 0\} = \operatorname{span}(\{\varphi_j\}_{j=1}^{m_0})$

We interpolate φ_j onto the network to construct

$$\phi_j(x_i) = \varphi_j(x_i), \quad 1 \leq j \leq m,\ 1 \leq i \leq n$$

and let $V_H = \operatorname{span}(\{\phi_j\}_{j=1}^{m_0}) \subset V$.

To each network node x_i we associate one element T, $x_i \in T$, and define

$$(v, w)_T = \sum_{x_i \in T} v(x_i) w(x_i).$$

Interpolation and decomposition

Scott-Zhang type interpolation operator $\mathcal{I}_H : V \to V_H$

$$\mathcal{I}_H v = \sum_{j=1}^{m_0} (\psi_j, v)_{T_j} \phi_j.$$

with $(\psi_j, \phi_i)_{T_j} = \delta_{ij}$ being the dual basis defined on an element T_j adjacent to j.

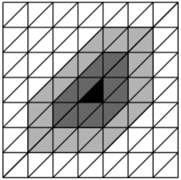
$$W = \ker(\mathcal{I}_H) \qquad V_H^{\text{ms}} = \{v \in V : (w, Kv) = 0 \ \forall w \in W\}.$$

By defining $Q : V \to W$ fulfilling

$$(w, KQv) = (w, Kv), \quad \forall w \in W$$

we can write $V_H^{\text{ms}} = (1 - Q)V_H$ and $V = V_H^{\text{ms}} \oplus W$.

Localized Orthogonal Decomposition



- $U(\omega)$ is the union of elements that intersect ω
- $U^k(T) = U(U^{k-1}(T))$ with $U^1(T) = U(T)$
- $N(\omega) = \{i \in 1, \dots, n : x_i \in \omega\}$
- $W(U^k(T)) = \{w \in W : w(x_i) = 0 \; i \in N(U^k(T))^c\}$

Let $K_T = \sum_{x_i \in T} K_i$. Find $Q_T^k v \in W(U^k(T))$ such that

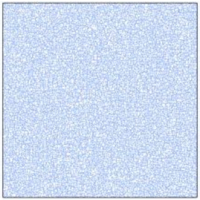
$$(w, KQ_T^k v) = (w, K_T v), \quad \forall w \in W(U^k(T))$$

We let $Q^k = \sum_{T \in \mathcal{T}_H} Q_T^k$ and define $V_{H,k}^{\text{ms}} := (1 - Q^k) V_H$.

The LOD formulation reads: find $u_{H,k}^{\text{ms}} \in V_{H,k}^{\text{ms}}$ such that

$$(v, K u_{H,k}^{\text{ms}}) = (v, F), \quad \forall v \in V_{H,k}^{\text{ms}}$$

Example: A weighted graph Laplacian

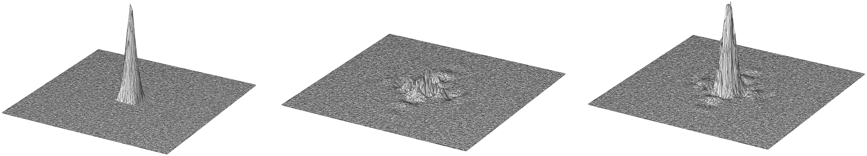


- Material parameter $\gamma_e > 0$, $K = \sum_e K_e$
- $K_{e_{ij}}([i,j],[i,j]) = K_{e_{ij}}([i,j],[i,j]) + \frac{\gamma_{e_{ij}}}{|e_{ij}|^2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$
- $K = \sum_{i=1}^{n} K_i, \quad K_i = \frac{1}{2} \sum_{j:e_{ij} \neq \emptyset} K_{e_{ij}}$

K_i are symmetric positive semi-definite and $c \in \ker(K_i)$ (constants).

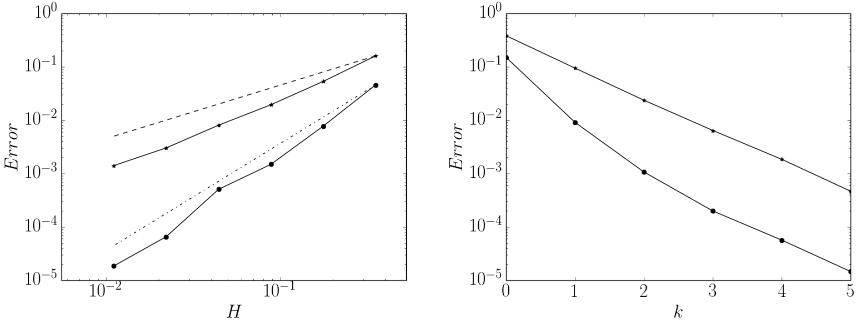
If $\gamma_{e_{ij}} = |e_{ij}|^2$, $K = D - A$, D (degree) and A (adjacency) matrices.

K is invertable on $V_{H,k}^{\text{ms}} \subset V$ and on $W(U^k(T)) \subset V$.



Example: A weighted graph Laplacian

We let $F = 1$, $\gamma_e \in [0.1, 1]$, and Dirichlet bc., quads $\mathcal{T}_H$, $16k$ dofs.



Left: $k = \lceil \log(H^{-1}) \rceil$

Right: $H = 2^{-5}$

Relative errors in $\| \cdot \| = (\cdot, \cdot)^{1/2}$ and $||| \cdot ||| = (\cdot, K\cdot)^{1/2}$.

Outline

Error analysis (weighted graph Laplacian)

Local and global norms:

$$\|v\|_T^2 = (v,v)_T = \sum_{x_i \in T} v(x_i)^2 \qquad \|v\|^2 = \sum_{T \in \mathcal{T}_H} \|v\|_T^2$$

$$|||v|||_T^2 = (v, K_T v) = \sum_{x_i \in T} (v, K_i v) \qquad |||v|||^2 = \sum_{T \in \mathcal{T}_H} |||v|||_T^2$$

We assume (related to the Fiedler eigenvalue)

$$\mu_T := \inf_{c \notin v \in V(U^2(T))} \frac{(v, Kv)}{(v,v)} \geq CH^{-2}$$

Lemma

It holds for any $v \in V$ and $j = 1, \ldots, m$

$$H^{-1}\|v - \mathcal{I}_H v\|_T + |||\mathcal{I}_H v|||_T \leq C|||v|||_{U^2(T)}$$

$$|||diag(\phi_j)(v - \mathcal{I}_H v)|||_T \leq C|||v - \mathcal{I}_H v|||_{U^2(T)}$$

Sketch of proof of first part (interior element)

We use that $\|\mathcal{I}_H c - c\|_T = 0$ to conclude

$$\begin{aligned}\|v - \mathcal{I}_H v\|_T &\leq \inf_{c\in\mathbb{R}} \|(v-c) - \mathcal{I}_H(v-c)\|_T \\ &\leq \inf_{c\in\mathbb{R}} \left(\|v-c\|_T + \|\mathcal{I}_H(v-c)\|_T\right)\end{aligned}$$

$$\inf_{c\in\mathbb{R}} \|\mathcal{I}_H(v-c)\|_T \leq \sum_{j:y_j\in\bar{T}} |(v-c,\psi_j)|\,\|\phi_j\|_T \leq \sum_{j:y_j\in\bar{T}} \|\psi_j\|_{U(T)}\|\phi_j\|_T\|v-c\|_{U(T)}$$

$$\begin{aligned}\|v-\mathcal{I}_H v\|_T &\leq \left(1 + \sum_{j:y_j\in\bar{T}} \|\psi_j\|_{U(T)}\|\phi_j\|_T\right) \inf_{c\in\mathbb{R}} \|v-c\|_{U(T)} \\ &\leq (1+C)\inf_{c\in\mathbb{R}} \|v-c\|_{U^2(T)} \leq C\mu_T^{-1/2}|||v|||_{U^2(T)} \leq CH|||v|||_{U^2(T)}.\end{aligned}$$

Here $\sum_{j:y_j\in\bar{T}} \|\psi_j\|_{U(T)}\|\phi_j\|_T \leq C$ holds if $\frac{\max_{y\in\Omega} \#\{i:x_i\in B(y,\rho H_{\min}/(d+2))\}}{\min_{y\in\Omega} \#\{i:x_i\in B(y,\rho H_{\min}/(d+2))\}} \leq C$.

Error in ideal method

Theorem

Under the assumptions above

$$|||u - u_H^{ms}||| \leq CH\|F\|.$$

Proof.

Let $u = u_H^{\mathrm{ms}} + u_w$ where $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ and $u_w \in W$. We get

$$\begin{aligned} |||u_w|||^2 &= (u_w, Ku_w) = (u, Ku_w) = (F, u_w) \leq \|F\|\,\|u_w - \mathcal{I}_H u_w\| \\ &\leq CH\|F\|\,|||u_w|||. \end{aligned}$$

□

To bound $u_H^{\mathrm{ms}} - u_{H,k}^{\mathrm{ms}}$ we first show that $Q_T v$ decays exponentially.

Kornhuber-Peterseim-Yserentant approach[3]

Let $U(y_j) = \{T \in \mathcal{T}_H : y_j \in \bar{T}\}$ and $N_j = \{i \in 1, \dots, n : x_i \in U(y_j)\}$.

$$V_j = V(N_j) \qquad W_j = (1 - \mathcal{I}_H)V_j \subset W.$$

Any $w \in W$ can be written as

$$w = \sum_{j=1}^{m} (1 - \mathcal{I}_H)(\mathrm{diag}(\phi_j) w) := \sum_{j=1}^{m} w_j,$$

with $w_j \in W_j$. We now let $P_j : V \to W_j$ solve

$$(w, KP_j v) = (w, Kv). \quad \forall w \in W_j.$$

and define $P = \sum_{j=1}^{m} P_j$.

P spreads non-zeros within a radius of $2H$ in each iteration.

[3]Kornhuber et. al. SIAM MMS (2016), Kornhuber et. al., Math. Comp. (2018)

DD approach to approximate Q

We define $Q_{\mathrm{dd}}^k : V \to W$ using the preconditioned modified Richardson iteration

$$Q_{\mathrm{dd}}^k v = Q_{\mathrm{dd}}^{k-1} v + \omega P(v - Q_{\mathrm{dd}}^{k-1} v). \quad k \geq 1.$$

We get

$$(Q - Q_{\mathrm{dd}}^k)v = (1 - \omega P)(Q - Q_{\mathrm{dd}}^{k-1})v = (1 - \omega P)^k Q v$$

since $Pv = PQv$. If we can show for some ω that

$$|||1 - \omega P||| = \sup_{w \in W} \frac{|||w - \omega P w|||}{|||w|||} \leq \delta < 1$$

we have exponential decay in the error $Q - Q_{\mathrm{dd}}^k$.

Exponential decay

Lemma

For any $w = \sum_{j=1}^m w_j$ *with* $w_j \in W_j$: $|||w|||^2 \leq C_2 \sum_{j=1}^m |||w_j|||^2$.

With $w_j = (1 - \mathcal{I}_H)(diag(\phi_j)w)$: $\sum_{j=1}^m |||w_j|||^2 \leq C_1 |||w|||^2$

Proof.

It holds $|||w|||_T^2 \leq C_2 \sum_{j=1}^m |||w_j|||_T^2$ where C_2 is the number of subdomains $U^2(T')$ overlapping T. Sum over T yields the result.

$$\sum_{j=1}^m |||w_j|||^2 \leq C \sum_{j=1}^m |||\text{diag}(\phi_j)w|||^2 = C \sum_{j=1}^m \sum_{T \in \mathcal{T}_H} |||\text{diag}(\phi_j)w|||_T^2$$
$$\leq C' \sum_{T \in \mathcal{T}_H} |||w|||_{U^2(T)}^2 := C_1 |||w|||^2.$$

□

Exponential decay

Lemma

With $\omega = (C_2 + C_1^{-1})^{-1}$ *it holds*

$$|||1 - \omega P||| = \sup_{w \in W} \frac{|||w - \omega Pw|||}{|||w|||} \leq \delta := \frac{C_2}{C_2 + C_1^{-1}} < 1$$

Kornhuber et. al., *Numerical homogenization of elliptic multiscale problems by subspace decomposition,* SIAM MMS 2016

Theorem

For any $w \in W$ *it holds*

$$|||Qw - Q_{dd}^k w||| \leq exp(-k(2C_1 C_2)^{-1})|||w|||$$

If w has support on T, Q_{dd}^k has support within radius $2Hk$, therefore Qw decays exponentially.

A priori error bound for the full method

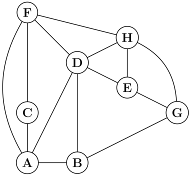
Theorem

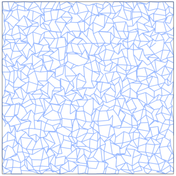
For the weighted graph Laplacian K the error fulfills

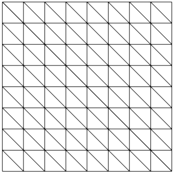
$$|||u - u^{ms}_{H,k}||| \leq C(H + exp(-k(4C_1C_2)^{-1}))||F||$$

- The constants depend on the contrast in γ_e.
- Balls with a fix radius on the scale of H include a similar number of nodes in the sense $\max / \min \leq C$.
- The result holds in a regime $H \geq H_0$.
- The "Fiedler eigenvalue" μ_T can be difficult to bound analytically but it can be estimated numerically.
- The result will be generalized to a large class of K including FEM, FD, fibre network model, ...

Structure needed for LOD







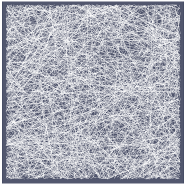
▷ algebraic network ▷ geometric network ▷ discretized PDE

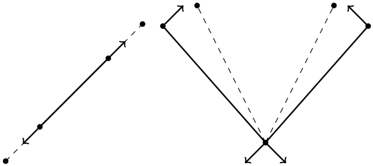
- functionals defining W and scalar product $v^T K w$ defining V_H^{ms}, $V = V_H^{\text{ms}} \oplus W$.
- FE like space V_H (interpolated to network), $V_H^{\text{ms}} = (1 - Q)V_H$, geometric patches, uniformly distributed nodes (H scale).
- Conforming coarse space $V_H \subset V_h$, $W = \ker(\mathcal{I}_H)$, FE error analysis.

We are in the setting of a geometric network model.

Outline

A fibre network model[4]



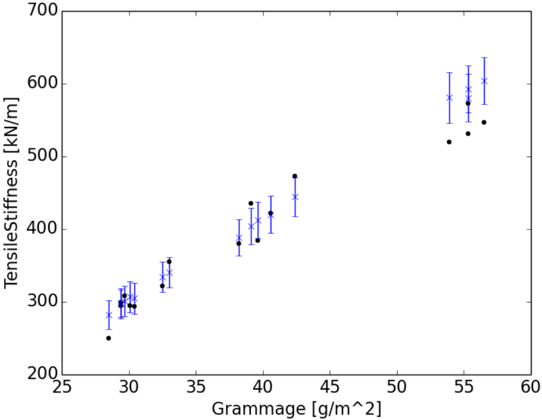


- Fibers are made of line segments in 3D, close lines are connected with bonds, the solution is the displacement
- Length 0.5 – 4mm, width 0.021 – 0.03mm, cross section $200(\mu\text{m})^2$
- Young's module of elasticity $E = 25$GPa.
- Two forces in the model: edge extension and angular deviation
- Edge pairs still allow $K = \sum_{i=1}^{n} K^i$, translations is in $\ker(K)$

[4]Kettil et. al. BIT 2020

Validation with experiments

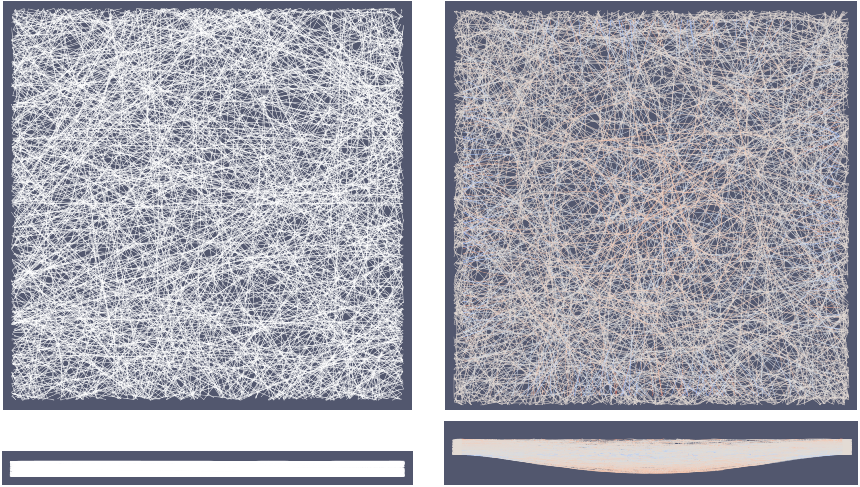
Clamped and pulled, randomly generated fibre configurations, mean and standard deviation.



Stiffness vs area density.

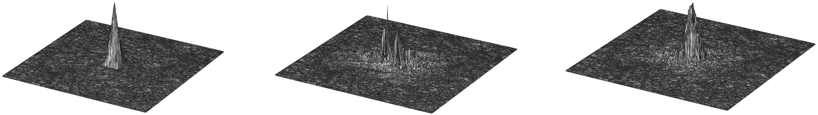
Example: LOD for fibre network model

Fixed boundary, constant force applied in all nodes.



Example: LOD for fibre network model

Similar localization as in LOD for linear elasticity[5].



[5] Henning et. al. CMAME 2016

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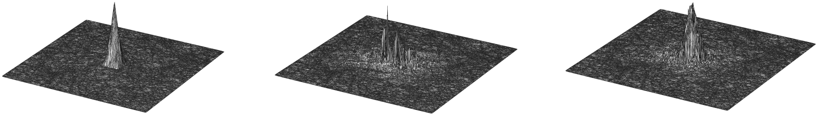
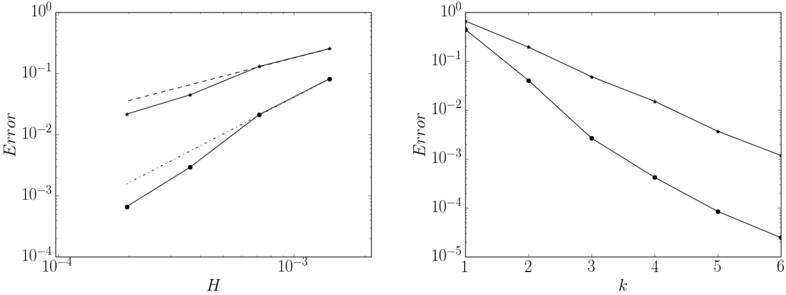


Relative errors ($\|\cdot\|$, $|||\cdot|||$). Left: $k = \lceil 1.5 \log(H^{-1}) \rceil$. Right: $H = 2^{-5}$.



[5]Henning et. al. CMAME 2016

Outline

Future work

- Error analysis for full problem
- Periodic code using symmetry to scale up siumulation
- Defects and cracks, reuse of basis locally
- Elastic wave propagation
- Algebraic LOD

Kettil et. al. *Numerical upscaling of discrete network models,* BIT (2020)

Thank you!