Numerical simulation of spatial network models

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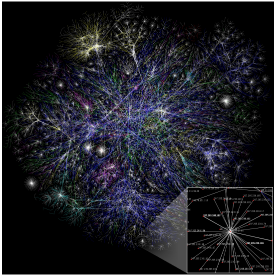
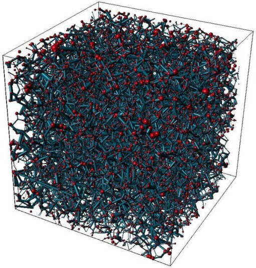
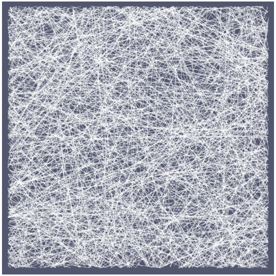
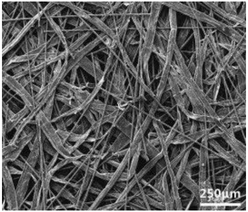
Spatial network models

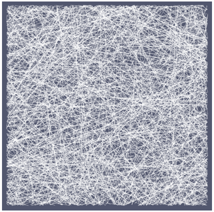






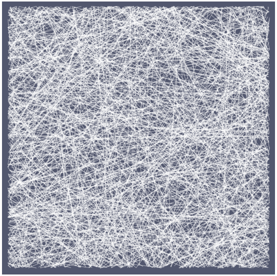
Fibre based materials





- Fraunhofer Chalmers Centre, Stora Enso, Albany International
- Paper forming, network model (Gustav Kettil, 2014-2019)
- Mechanical properties, solvers (Morgan Görtz, 2019-)
- Development (fiber dimensions, distribution, virtual lab)
- Evaluation (tensile, bending, defects)
- Numerical simulation is not used extensively in paper industry

Numerical simulation of spatial network models



- Efficient solver for

$$Ku = F$$

  a simplified network model of an elliptic PDE
- K is SPD but ill-conditioned (FCC uses direct solver)
- Multiscale problem (similar to rapidly varying diffusion)

Outline

Graph Laplacian

- Let $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ be a graph of nodes and edges
- Notation: $i \sim j$ if x_i and x_j are connected by an edge
- Let D be the degree and A be the adjacency matrix
- The graph Laplacian $L^g := D - A$ is SP(semi-)D, $L^g 1 = 0$
- Let $\hat{V} : \mathcal{N} \to \mathbb{R}$ be scalar functions on $\mathcal{N}$. For $v, w \in \hat{V}$

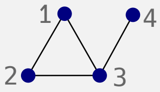
$$(v, w) = \sum_j v(x_j) w(x_j)$$

$$(L^g v, v) = \sum_{(i,j) \in \mathcal{E}} (v(x_i) - v(x_j))^2$$

$$L^g = \sum_i L_i^g$$

$$(L_i^g v, v) = \frac{1}{2} \sum_{j \sim i} (v(x_i) - v(x_j))^2$$

Example:



$$L^g = \begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 3 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}$$

Weighted graph Laplacian

- A weighted graph Laplacian and diagonal mass matrix

$$(L_i v, v) = \frac{1}{2}\sum_{j\sim i} \frac{(v(x_i) - v(x_j))^2}{|x_i - x_j|}, \quad L = \sum L_i$$

$$(M_i v, v) := \frac{1}{2} v(x_i)^2 \sum_{j\sim i} |x_i - x_j|, \quad M = \sum M_i$$

- Consider the 1D mesh $0 = x_0 < x_1 < \cdots < x_n = 1$.

$$(Lv, v) := \sum_{(i,j)\in\mathcal{E}} \frac{(v(x_i) - v(x_j))^2}{|x_i - x_j|}$$

- L is the P1-FEM stiffness matrix $(-\Delta)$
- $Lu = Mf$ corresponds to P1-FEM with lumped mass matrix

Spatial network vs. PDE

Spatial network notation		Continuous analogue
(Lu, v)	$\leftrightarrow$	$\int_\Omega \nabla u \cdot \nabla v$
$(L_\omega u, v) := \sum_{x_i \in \omega} (L_i u, v)$	$\leftrightarrow$	$\int_\omega \nabla u \cdot \nabla v$
(Mu, v)	$\leftrightarrow$	$\int_\Omega u\, v$
$(M_\omega u, v) := \sum_{x_i \in \omega} (M_i u, v)$	$\leftrightarrow$	$\int_\omega u\, v$
$\|v\|_L := (Lv, v)^{1/2}$	$\leftrightarrow$	$\|\nabla v\|_{L^2(\Omega)}$
$\|v\|_{L,\omega} := (L_\omega v, v)^{1/2}$	$\leftrightarrow$	$\|\nabla v\|_{L^2(\omega)}$
$\|v\|_M := (Mv, v)^{1/2}$	$\leftrightarrow$	$\|v\|_{L^2(\Omega)}$
$\|v\|_{M,\omega} := (M_\omega v, v)^{1/2}$	$\leftrightarrow$	$\|v\|_{L^2(\omega)}$

Model problem

Let $u \in V := \{v \in \hat{V} : v(x_i) = 0 \text{ for } x_i \in \Gamma_D\}$ solve

$$Ku = Mf \quad \Longleftrightarrow \quad (Ku, v) = (Mf, v), \quad v \in V.$$

We assume K to be symmetric, invertable and

$$\alpha(Lv, v) \leq (Kv, v) \leq \beta(Lv, v), \quad \forall v \in V.$$

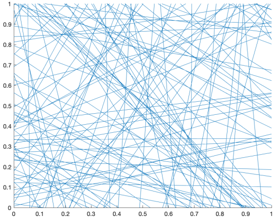
Example:

- Weighted graph Laplacian

$$(Kv, v) = \sum_{(i,j)\in\mathcal{E}} \gamma_{ij} \frac{(v(x_i) - v(x_j))^2}{|x_i - x_j|}, \quad \alpha \leq \gamma_{ij} \leq \beta$$

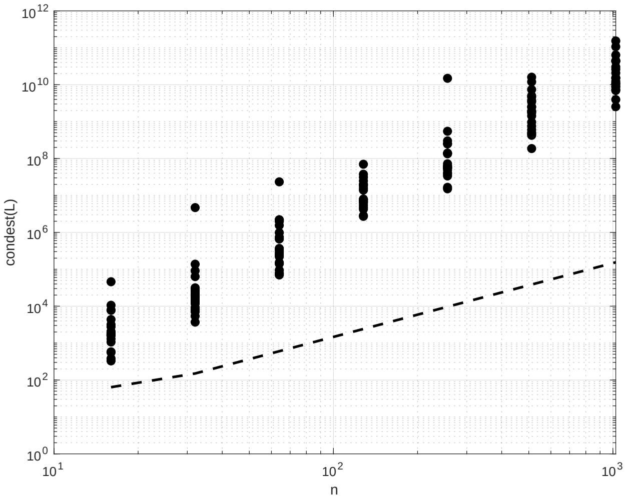
- Elasticity model for a fibre network.

Example: random infinite lines



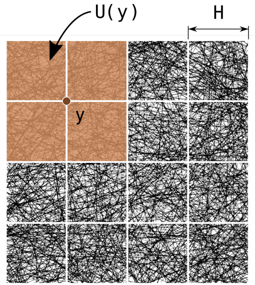
- Poisson line process
- Given random points (θ, r), perpendicular chords are constructed in a circle
- Unit square is cut out, principal component kept
- Intersections are nodes, two nodes are connected by an edge
- Dirichlet nodes on the boundary

Condition number



Outline

Multilevel solver: coarse scale representation



- $\mathcal{T}_H$ is a mesh of squares
- $\hat{V}_H$ is Q1-FEM with basis $\{\varphi_y\}_y$ [1]
- $V_H \subset \hat{V}_H$ satisfy the boundary conditions
- Clément type interpolation operator

$$\mathcal{I}_H v = \sum_{\text{free DoFs } y} \frac{(M_{U(y)} 1, v)}{(M_{U(y)} 1, 1)} \varphi_y \in V_H$$

Lemma (Stability and approximability of $\mathcal{I}_H$)

Under assumptions on network and mesh, for all $v \in V$, $T \in \mathcal{T}_H$, and for sufficiently large H,

$$H^{-1} |v - \mathcal{I}_H v|_M + |\mathcal{I}_H v|_L \leq C |v|_L.$$

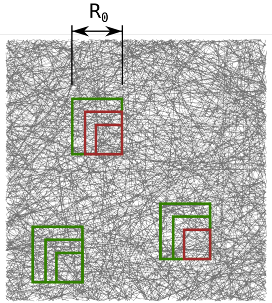
[1] M. & Peterseim, Numer. Math., 2015

Network homogeneity assumption

1. All edges are shorter than $R_0 > 0$ (length scale)
2. For any square $B_R(x)$, centered at x with side length $2R$, with $R \geq R_0$,

$$\rho \leq (2R)^{-d} |1|^2_{M,B_R} \leq \sigma\rho$$

where $\sigma \geq 1$ and $\rho > 0$ are uniformity and density constants.



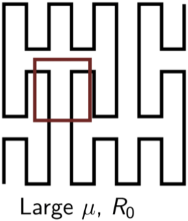
- For a certain pair (σ, ρ), the boxes must be at least R_0 large to satisfy the conditions.
- R_0 is a length scale at which the material is homogeneous.

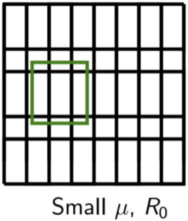
Network connectivity assumption

Existence of a Poincaré and Friedrich-type constants

There is a $\mu < \infty$, such that for all $x \in \Omega$, and $H > R_0$

$$
\begin{aligned}
|v - \bar{v}|_{M,B_H(x)} &\leq \mu H |v|_{L,B_{H+R_0}(x)}, \quad \forall v \in \hat{V} \\
|v|_{M,B_H(x)} &\leq \mu H |v|_{L,B_{H+R_0}(x)}, \quad \forall v \in V
\end{aligned}
$$





Large μ, R_0 Small μ, R_0

Network connectivity assumption

If there exists a connected subgraph $\mathcal{G}' = (\mathcal{N}', \mathcal{E}') \subset \mathcal{G}$ so that

- all nodes in $B_H(x)$ are included
- no nodes in $B_{H+R_0}(x)$ are included

Then

$$|v - \bar{v}|_{M,B_H(x)} \leq |v - \bar{v}|_{M,\mathcal{N}'} \leq \lambda_2^{-1/2}|v|_{L,\mathcal{N}'} \leq \lambda_2^{-1/2}|v|_{L,B_{H+R_0}(x)}$$

where $\lambda_2 = \inf_{(M'1,v)=0} \frac{(L'v,v)}{(M'v,v)}$ measure connectivity[1].

If $\mathcal{G}'$ is isoperimetric[2] $|\delta(X)| \geq c_d \text{vol}(X)^{(d-1)/d}$, $|X| \leq |\mathcal{N}' \setminus X|$

$$\text{isoperimetric} \implies \lambda_2 \geq CH^2 \implies |v - \bar{v}|_{M,B_H(x)} \leq \mu H |v|_{L,B_{H+R_0}(x)}$$

[1] Cheeger 1970, Fiedler 1973

[2] F. Chung, Spectral graph theory, AMS, 1997

Interpolation error bound and product rule

Homogeneity and connectivity allow us to prove

Lemma (Stability and approximability of $\mathcal{I}_H$)

For $H > R_0$ it holds

$$H^{-1}|v - \mathcal{I}_H v|_M + |\mathcal{I}_H v|_L \le C_{\mu,\sigma}|v|_L, \quad \forall v \in V$$

Local Poincaré and Friedrich inequalities are used.

$$|v\varphi|^2_{L,\omega} = (L_\omega(v\varphi), v\varphi) = \frac{1}{2}\sum_{x_i\in\omega}\sum_{i\sim j}\frac{(v(x_i)\varphi(x_i) - v(x_j)\varphi(x_j))^2}{|x_i - x_j|}$$

$$= \frac{1}{2}\sum_{x_i\in\omega}\sum_{i\sim j}\frac{(v(x_i)(\varphi(x_i) - \varphi(x_j)) + (v(x_i) - v(x_j))\varphi(x_j))^2}{|x_i - x_j|}$$

$$\le \sum_{x_i\in\omega}\sum_{i\sim j}\frac{v(x_i)^2|x_i - x_j|^2H^{-2} + (v(x_i) - v(x_j))^2}{|x_i - x_j|} = 2\left(H^{-2}|v|^2_{M,\omega} + |v|^2_{L,\omega}\right)$$

Outline

1. Graph Laplacian and model problem
2. Network assumptions
3. **Semi-iterative solver**
4. Numerical examples
5. Multiscale solver
6. Ongoing projects and future directions

Subspace decomposition preconditioner[3]

Let

$$V_0 = V_H, \quad V_j = V(U(y_j)), \quad j = 1, \dots, m,$$

and let $P_j : V \to V_j$ to be orthogonal projections fulfilling

$$(KP_j v, v_j) = (Kv, v_j), \quad \forall v_j \in V_j.$$

The existence and uniqueness follows since $V_j \subset V$. We let

$$P = P_0 + P_1 + \cdots + P_m.$$

- $P = BK$ will be used as a preconditioner: $BKu = BMf$.
- Involves direct solution of decoupled problems (semi-iterative).

$$(Ku, Pv) = \sum_{j=0}^{m} (Ku, P_j v) = \sum_{j=0}^{m} (KP_j u, P_j v) = \sum_{j=0}^{m} (KP_j u, v) = (KPu, v)$$

[3] Kornhuber & Yserentant, MMS, 2016

Spectral bound of P

Lemma

Under the network and operator assumptions and for $H \geq R_0$ there is a decomposition $v = \sum_{j=0}^{m} v_j$ that satisfies

$$\sum_{j=0}^{m} |v_j|_K^2 \leq C_1 |v|_K^2.$$

Moreover, every decomposition $v = \sum_{j=0}^{m} v_j$ with $v_j \in V_j$ satisfies

$$|v|_K^2 \leq C_2 \sum_{j=0}^{m} |v_j|_K^2.$$

$C_1 = C_d \beta \alpha^{-1} \sigma \mu^2$, $C_2 = C_d \beta \alpha^{-1}$, *$C_d$ only depends on d.*

Spectral bound of P

Sketch of proof:

We start in L-norm:

$$|v|_L^2 \leq 2|v_0|_L^2 + 2|\sum_{j=1}^{m} v_j|_L^2.$$

Pick $T \in \mathcal{T}_H$. Since $v_j \in V(U(y_j))$ and $L_T v = 0$ for $v \in V(\Omega \setminus U_2(y_j))$, $L_T v_j$ can be non-zero for at most C_d meshnodes j. We get

$$|\sum_{j=1}^{m} v_j|_{L,T}^2 \leq C_d \sum_{j=1}^{m} |v_j|_{L,T}^2.$$

Summing over $T \in \mathcal{T}_H$ proves the inequality in L-norm and therefore also in K with $C_2 = C_d \beta \alpha^{-1}$.

Spectral bound of P

Sketch of proof:

$$\sum_{j=1}^{m} |v_j|_L^2 := \sum_{j=1}^{m} |\varphi_j(v - \mathcal{I}_H v)|_L^2$$

$$\leq 2 \sum_{j=1}^{m} \sum_{T \in U_2(y_j)} \left(H^{-2} |v - \mathcal{I}_H v|_{M,T}^2 + |v - \mathcal{I}_H v|_{L,T}^2 \right)$$

$$\leq C_d \left(H^{-2} |v - \mathcal{I}_H v|_M^2 + |v - \mathcal{I}_H v|_L^2 \right) \leq C_d \sigma \mu^2 |v|_L^2.$$

Furthermore $|v_0|_L = |\mathcal{I}_H v|_L \leq C_d \sigma^{1/2} \mu |v|_L$. All together we have

$$\sum_{j=0}^{m} |v_j|_L^2 \leq C_d \sigma \mu^2 |v|_L^2.$$

Equivalence of L- and K-norms gives $C_1 = C_d \beta \alpha^{-1} \sigma \mu^2$.

Spectral bound of P

We get the following spectral bound for P[4].

Lemma

Under the same assumptions

$$C_1^{-1}|v|_K^2 \leq (KPv, v) \leq C_2|v|_K^2.$$

and for any polynomial p it holds

$$|p(P)| := \sup_{v \in V} \frac{|p(P)v|_K}{|v|_K} \leq \max_{\lambda \in [C_1^{-1}, C_2]} |p(\lambda)|.$$

[4] Kornhuber & Yserentant, MMS, 2016

Preconditioned conjugate gradient

We use $P = BK$ as a preconditioner for CG:

$$BKu = BMf.$$

For some polynomial p_ℓ of degree ℓ fulfilling $p_\ell(0) = 1$

$$u - u^{(\ell)} = p_\ell(P)(u - u^{(0)}),$$

CG minimizes $|u - u^{(\ell)}|_K$ over (Krylov) span$(\{s, Ps, P^2 s, \ldots, P^{\ell-1} s\})$:

$$|u - u^{(\ell)}|_K \leq \min_{\substack{\deg(p) \leq \ell \\ p(0)=1}} |p(P)||u - u^{(0)}|_K \leq \min_{\substack{\deg(p) \leq \ell \\ p(0)=1}} \max_{\lambda \in [C_1^{-1}, C_2]} |p(\lambda)||u - u^{(0)}|_K$$

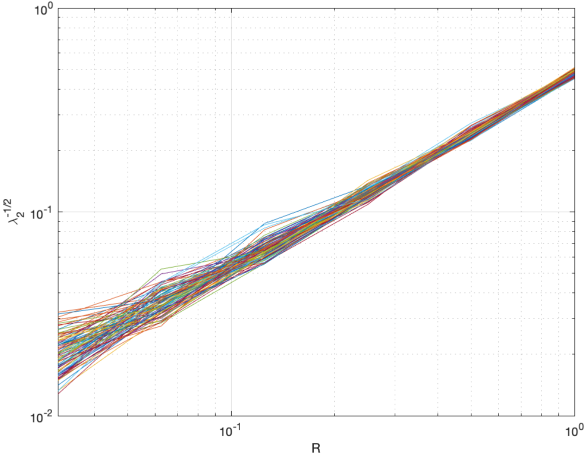
realized by a shifted and scaled Chebyshev polynomial:

$$|u - u^{(\ell)}|_K \leq 2\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^\ell |u - u^{(0)}|_K, \qquad \sqrt{\kappa} = C_d \alpha^{-1} \beta \mu \sqrt{\sigma}.$$

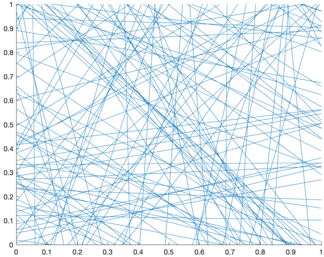
Outline

Example: connectivity $\lambda_2^{-1/2} \approx \mu R$

- Generate $n = 256$ lines on smallest circle enclosing $[0, 1]^2$.
- Cut a square $[0, R]^2$, $R = 2^{-r}$, $r = 0, 1, \ldots, 5$, 100 samples.

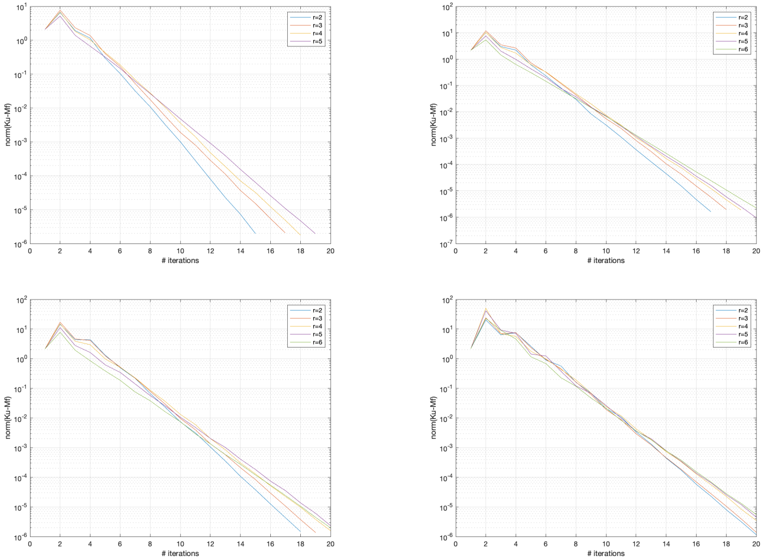


Example: weighted graph Laplacian



- Poisson line process $n = 256, 512, 1024, 2048$ lines (at most around $800k$ dofs)
- No material data $\gamma = 1$ i.e. we solve $Lu = Mf$
- Right hand side $f = 1$ and homogeneous Dirichlet boundary conditions.
- Coarse mesh size $H = 2^{-r}$, $r = 2, 3, 4, 5, 6$

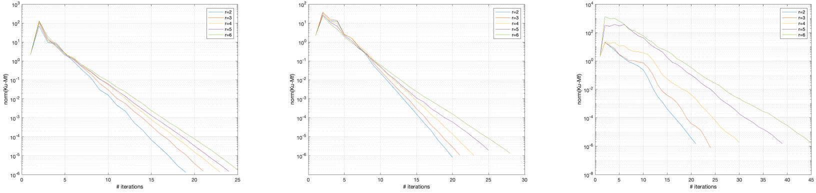
Example: weighted graph Laplacian



Example: weighted graph Laplacian

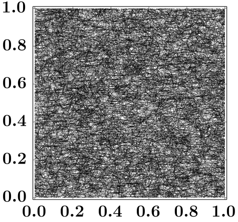
Right hand side $f = 1$, homogeneous Dirichlet bc, $n = 1024$.

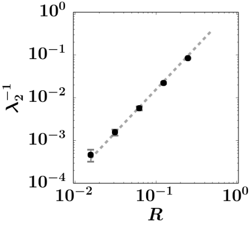
- (left) $\gamma_{ij} \in U([0.01, 1])$
- (center) $\gamma_{ij} = 0.01$ or $\gamma_{ij} = 1$ (1/16 lines)
- (right) $\gamma_{ij} = 10^{-6}$ or $\gamma_{ij} = 1$ (1/16 lines)

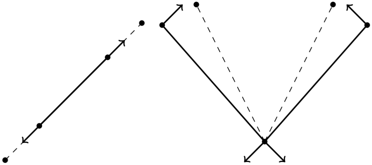


- Robust but high contrast may cause problems

Example: a fibre network model[5]



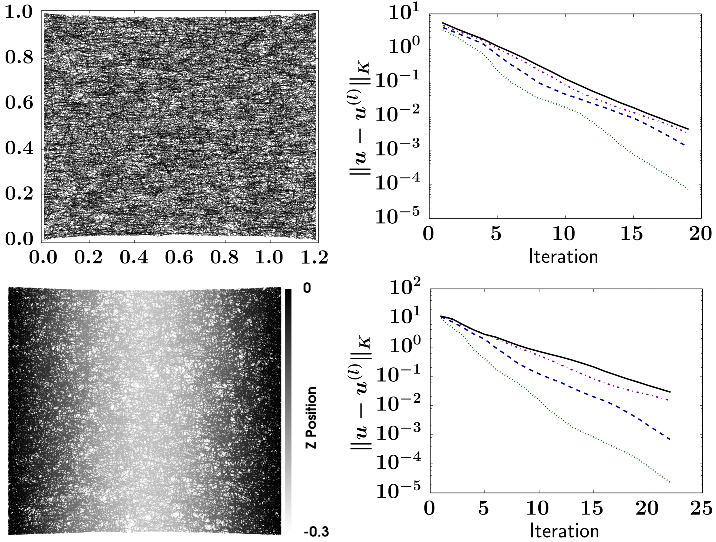




- $2 \cdot 10^4$ fibres, biased angle (x-axis), length 0.05, $3 \cdot 10^5$ nodes, $\alpha = 0.05$, $\beta = 500$.
- Two forces in the model: edge extension and angular deviation.
- Find displacement u: $Ku = Mf$ (tensile, distributed load)
- Theory extends to vector valued setting (Korn, $K \sim L$)
- DD with $H = 1/4, 1/8, 1/16, 1/32$.

[5] Kettil et. al. *Numerical upscaling of discrete network models*, BIT 2020

Example: A fibre network model



Outline

Interpolation and decomposition

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

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

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

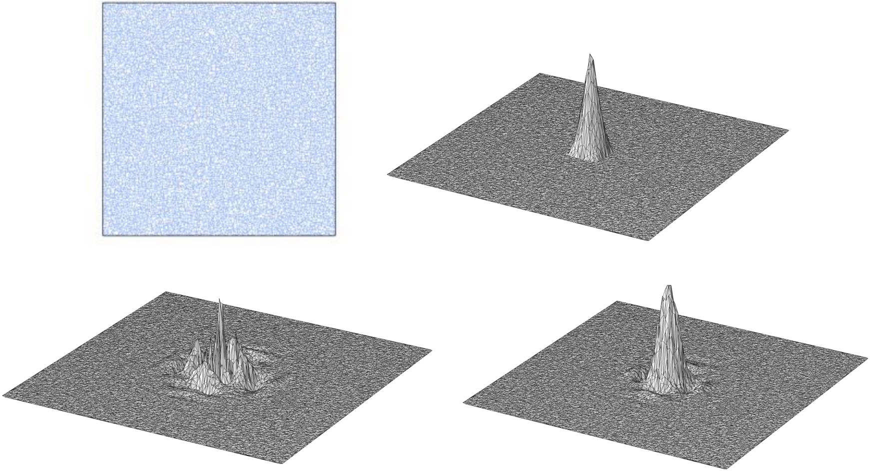
$$W = \ker(\mathcal{I}_H) \qquad V_H^{\text{ms}} = \{v \in V : (w, Kv) = 0 \ \forall w \in W\}.$$

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 $V = V_H^{\text{ms}} \oplus W$.

Example: weighted graph Laplacian



Localization

- $U^k(T) = U(U^{k-1}(T))$ with $U^1(T) = U(T)$
- $W(U^k(T)) = \{w \in W : w(x_i) = 0 \; x_i \notin U^k(T)\}$
- $K_T = \sum_{x_i \in T} K_i$

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

$$(v, Ku_{H,k}^{\text{ms}}) = (v, Mf), \quad \forall v \in V_{H,k}^{\text{ms}}$$

Error analysis

- Interpolation error bound under same network assumptions

$$H^{-1}|v - \mathcal{I}_H v|_M + |\mathcal{I}_H v|_L \leq C|v|_L$$

- Exponential decay of correctors established using fast convergences of iterative solvers in W. No V_0 space means finite spread of information in each iteration[6][7].

Theorem

If $k \sim |\log(H)|$ and $H > R_0$

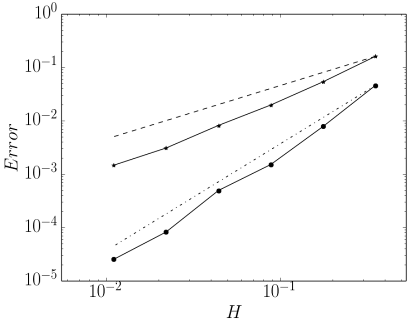
$$|u - u^{ms}_{H,k}|_K \leq CH|f|_M$$

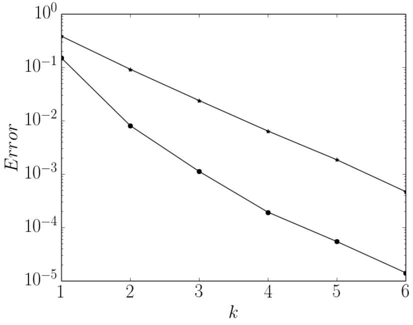
[6] Kornhuber Yserentant Peterseim, MMS 2016, MC 2018

[7] M. & Peterseim, Math. Comp. 2014, SIAM Spotlight 2020

Example: A weighted graph Laplacian

We let f const, $\gamma_{ij} \in [0.1, 1]$, and Dirichlet bc.





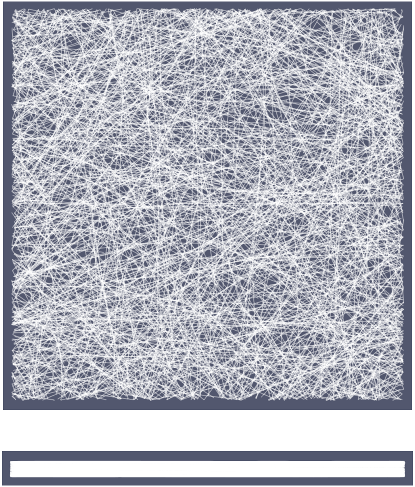
Left: $k = \lceil \log(H^{-1}) \rceil$

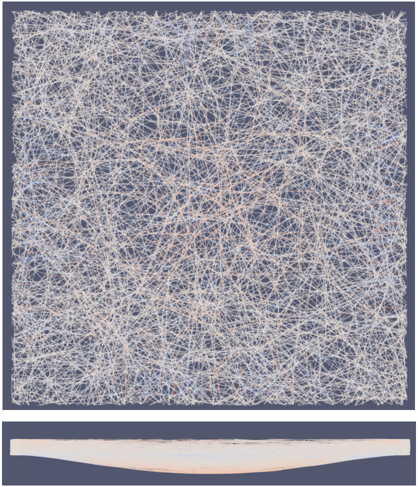
Right: $H = 2^{-5}$

Relative errors in $|\cdot|_M$ and $|\cdot|_K$.

Example: LOD for fibre network model

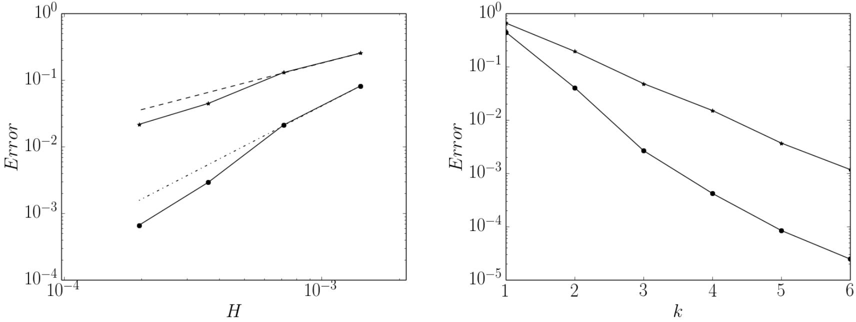
Fixed boundary, constant force applied in all nodes, 4mm $\times$ 4mm.





Example: LOD for fibre network model

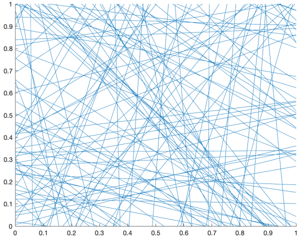
Left: $k = \lceil 1.5 \log(0.004/H) \rceil$. Right: $H = 0.004 \cdot 2^{-5}$.



- Relative errors in $|\cdot|_M$ and $|\cdot|_K$ norms.

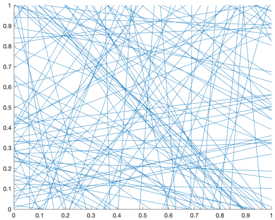
Outline

Isoperimetric dimension



- The edge boundary $|\delta(X)| \geq c_d \text{vol}(X)^{(d-1)/d}$ for all $|X| \leq |\mathcal{N}' \setminus X|$
- Can we say that c_d is above some threshold with high probability for PLP?
- Can it be generalized to finite length lines?
- What can we say in 3D (cylinders)?
- Initiated collaboration with probability theory group, Chalmers.

Bulk-interface model



$$
\begin{aligned}
-\Delta u_i^0 &= 0, \quad \text{in } \Omega_i^0, \\
u_i^0 &= g_i, \quad \text{in } \bar{\Omega}_i^0 \cap \partial\Omega, \\
-\text{div}_\tau A_j \nabla_\tau u_j^1 - \delta(u_i^0 - u_j^1) &= f_j, \quad \text{in } \partial\Omega_i^0 \cap \Omega_j^1, \\
u_j^1 &= g_j, \quad \text{on } \bar{\Omega}_j^1 \cap \partial\Omega,
\end{aligned}
$$

where u^1 is continuous. Weak coupling by Robin condition[8]

$$n \cdot \nabla u_i^0 + \delta(u_i^0 - u_j^1) = 0, \quad \text{on } \partial\Omega_i^0 \cap \Omega_j^1$$

[8]Boon, PhD thesis, 2018

Bulk-interface model

We introduce the Robin-to-Dirichlet operator $u_i^0|_{\partial\Omega_i^0} = \mathcal{R}u_j^1|_{\Omega_j^1}$ and get the interface equation (Schur compliment)

$$-\text{div}_\tau A\nabla_\tau u^1 + \delta u^1 - \delta\mathcal{R}u^1 = f, \quad \text{in } \Gamma.$$

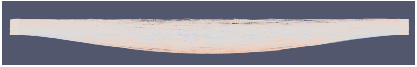
P1-FEM gives the network formulation

$$Ku^1 + \delta Bu^1 + \delta Ru^1 = Bf$$

$K \sim L$, $B \sim M$ (M is lumped) and R interacts over bulk regions.

- FEM (or possibly Boundary integral method) for RtD
- Prove $\alpha(Lv, v) \leq ((K + \delta B + \delta R)v, v) \leq \beta(Lv, v)$
- DD convergence when $\delta \gg 0$?
- What can be done in 3D?
- Malin Nilsson (2nd year PhD) works on this problem

Wave propagation on spatial network models



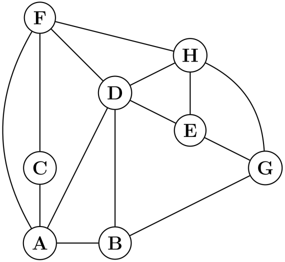
- Network-LOD for wave equation

$$M\ddot{u} + Ku = Mf.$$

- Re-use basis. Combine existing theoretical results[9].
- Assumptions on well prepared data.
- Elastic wave propagation with applications in fibre based materials. Interest from industry.
- Per Ljung (4th year PhD) and Morgan Görtz (3rd year PhD) works on this problem.

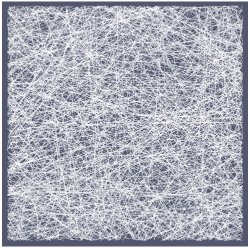
[9] Abdulle & Henning, 2017

Algebraic LOD/DD for network models



- How to construct a coarse scale representation?
- Patches will most likely depend on structure of K.
- Construct LOD space using functionals
  $W = \{v \in V : \ell_i(v) = 0\}$.
- Prove error bounds (isoperimetric dimension)?
- Initial discussions with Roland Maier and Fredrik Hellman.

Multilevel solvers for spatial networks



- Functional analysis in network setting[10]: Sobolev, Poincaré, Friedrich, Harnack, ...
- Multigrid, multi-level MC, Super-LOD, ...
- More applications

Thank you!

[10] Fan Chung, UCSD