Iterative solution of spatial network models by subspace decomposition

Axel Målqvist

Morgan Görtz and Fredrik Hellman

Department of Mathematical Sciences
Chalmers University of Technology and University of Gothenburg
Fraunhofer Chalmers Centre

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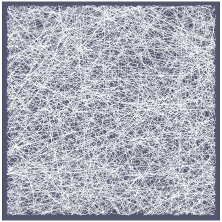
Simulation of spatial network models at FCC



- We consider

$$Ku = f$$

a simplified network model of an elliptic PDE (K is SPD)

- K is ill-conditioned (geometry and material data variation), only direct solver works
- The goal is to develop an iterative solver[1]

[1] Görtz-Hellman-M., Iterative solution of spatial network models by subspace decomposition, arXiv:2207.07488

Outline

1. **Graph Laplacian and model problem**
2. Network assumptions
3. Convergence of a semi-iterative solver
4. Numerical examples
5. Future work

Graph Laplacian

- Let $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ be a graph of nodes and edges, $x \in \Omega \subset \mathbb{R}^d$
- The graph Laplacian L^g is SP(semi-)D, $L^g 1 = 0$
- Let $\hat{V} : \mathcal{N} \to \mathbb{R}$ be scalar functions on $\mathcal{N}$. For $v, w \in \hat{V}$

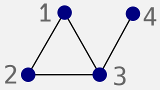
$$(v, w) = \sum_x v(x)w(x)$$

$$(L^g v, v) = \sum_{(x,y)\in\mathcal{E}} (v(x) - v(y))^2$$

$$L^g = \sum_x L^g_x$$

$$(L^g_x v, v) = \frac{1}{2} \sum_{y\sim x} (v(x) - v(y))^2$$

Example:



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

$x \sim y$ denotes that x and y are connected by an edge

Weighted graph Laplacian

- A weighted graph Laplacian and diagonal mass matrix

$$(L_x v, v) = \frac{1}{2}\sum_{y\sim x}\frac{(v(x)-v(y))^2}{|x-y|}, \quad L = \sum L_x$$

$$(M_x v, v) := \frac{1}{2}v(x)^2\sum_{y\sim x}|x-y|, \quad M = \sum M_x$$

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

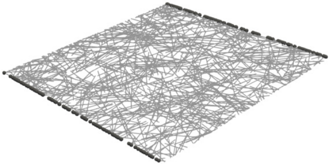
$$(Lv, v) := \sum_{i=1}^{n}\frac{(v(x_i)-v(x_{i-1}))^2}{|x_i - x_{i-1}|}$$

- L is the P1-FEM stiffness matrix $(-\Delta)$ and M is the lumped mass matrix

Model problem

Find $u \in V := \{v \in \hat{V} : v(x) = 0 \text{ for } x \in \Gamma_D\}$:

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



Assume: $(K\cdot,\cdot)$ is scalar product on V and

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

Example:

- $$(Kv, v) = \sum_{(x,y)\in\mathcal{E}} \gamma_{xy} \frac{(v(x) - v(y))^2}{|x - y|}, \quad \alpha \leq \gamma_{xy} \leq \beta$$
- P1-FEM for 1D diffusion-reaction model on network with continuity and Kirchhoff flux constraint in junctions
- Structural model of a fibre network.

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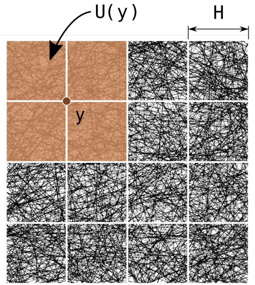
Multilevel solver: coarse scale representation



- $\mathcal{T}_H$ is a mesh of squares
- $\hat{V}_H$ is Q1-FEM with basis $\{\varphi_y\}_y$
- $V_H \subset \hat{V}_H$ 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 $\mathcal{I}_H$)

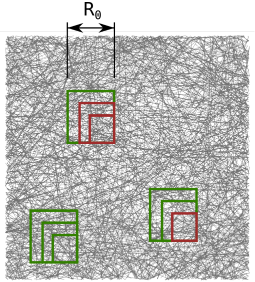
Under assumptions on the network (below) and for $H > 2R_0$,

$$H^{-1}|v - \mathcal{I}_H v|_M + |\mathcal{I}_H v|_L \leq C|v|_L, \quad \forall v \in V,$$

where $|\cdot|_M^2 = (M\cdot,\cdot)$, $|\cdot|_L^2 = (L\cdot,\cdot)$ *and* $C = C_d \mu \sqrt{\sigma}$.

Network locality, homogeneity and connectivity

1. All edges are shorter than $R_0 > 0$ (length scale)
2. Let $B_R(x)$ be a box at x of side length $2R$, with $H \geq R_0$,



$$1 \leq \frac{\max_x |1|^2_{M,B_H(x)}}{\min_x |1|^2_{M,B_H(x)}} \leq \sigma(R_0)$$

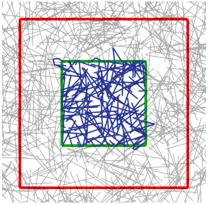
3. For all $x \in \Omega$ and $H > R_0$ there is a (uniform) $\mu(R_0) < \infty$ and $c_x \in \mathbb{R}$, such that the Poincaré-type inequality holds

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

Poincaré constant

Let $\mathcal{G}' = (\mathcal{N}', \mathcal{E}') \subset \mathcal{G}$ be connected and

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



With L', M' defined on $\mathcal{G}'$ we have

$$\lambda_1 = \inf \frac{(L'z, z)}{(M'z, z)} = \frac{(L'1, 1)}{(M'1, 1)} = 0, \quad \lambda_2 = \inf_{(M'1,z)=0} \frac{(L'z, z)}{(M'z, z)} > 0.$$

With $c_x = \frac{(M'1,v)}{(M'1,1)}$ we have $(M'1, v - c_x) = 0$ so

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

λ_2: measure connectivity[2] $\sim CH^{-2}$ if isoperimetric[3] dim d.

[2] Cheeger 1970, Fiedler 1973

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

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

Finite length fibers $r = 0.05$ and $|1|_M^2 = 1000$, $\Omega = [0, 1]^2$

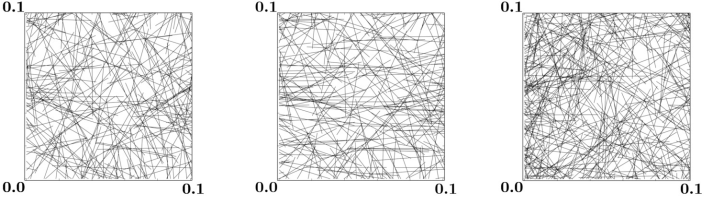


Table: (σ, μ) for different R

$R^{-1} = 4$	$R^{-1} = 8$	$R^{-1} = 16$	$R^{-1} = 32$	$R^{-1} = 64$
(1.04,0.49)	(1.08,0.53)	(1.27,0.57)	(1.85,0.675)	(3.42,1.53)
(1.04,0.59)	(1.08,0.61)	(1.27,0.69)	(1.87,0.83)	(2.93,1.35)
(1.04,0.53)	(1.57,0.54)	(2.13,0.58)	(3.1,0.76)	(6.86,1.45)

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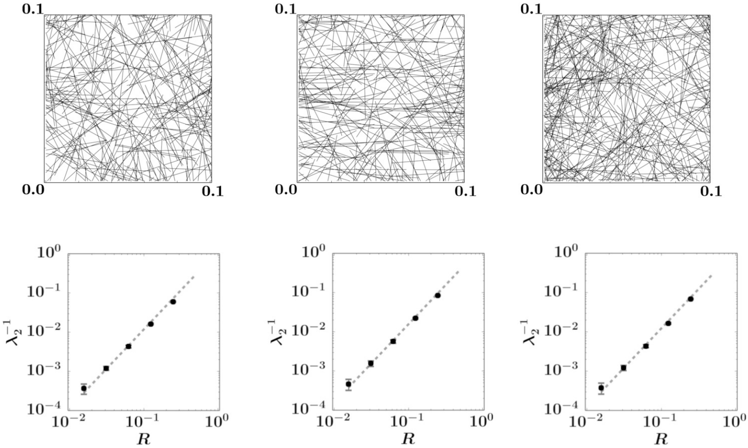

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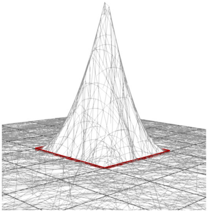
Subspace decomposition preconditioner[4]

Let $V_0 = V_H$. and

$$V_j = V(U(y_j)), \quad j = 1, \ldots, m.$$



Define projections $P_j : V \to V_j$ by

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

We add the projections to form

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

- $P = BK$ is used as a preconditioner: $BKu = Bf$.
- We use the preconditioned conjugate gradient method.
- Involves direct solution of decoupled problems (semi-iterative).

[4]Kornhuber & Yserentant, MMS, 2016

Convergence analysis

Lemma (Spectral bound of P)

For $H > R_0$ it holds

$$C_1^{-1}|v|_K^2 \leq (KPv, v) \leq C_2|v|_K^2, \quad \forall v \in V,$$

where $C_1 = C_d\beta\alpha^{-1}\sigma\mu^2$ and $C_2 = C_d\beta\alpha^{-1}$.

Theorem (Convergence of PCG)

With $\sqrt{\kappa} = \sqrt{C_1 C_2} = C_d\beta\alpha^{-1}\mu\sqrt{\sigma}$ and $H > 2R_0$ it holds

$$|u - u^{(\ell)}|_K \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{\ell} |u - u^{(0)}|_K.$$

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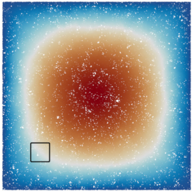
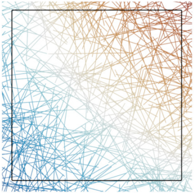
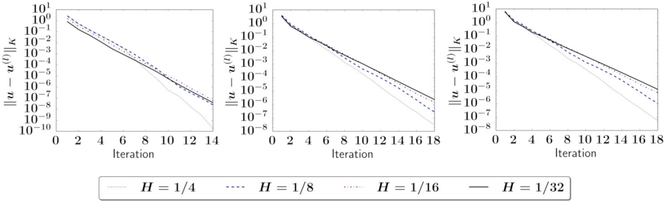
Example: Convergence graph Laplacian

Consider $Ku = M1$ with homogeneous Dirichlet bc $|1|_M^2 = 1000$.

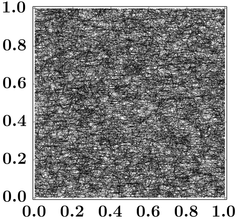


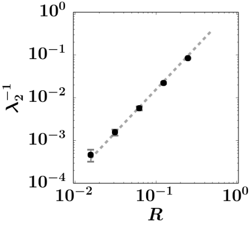


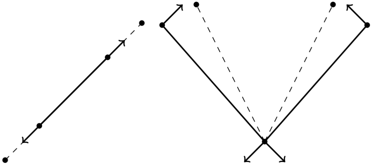
Grid $\gamma = 1$ (left), rand $\gamma = 1$ (center), rand $\gamma \in U([0.1, 1])$ (right)



Example: A fibre network model[5]



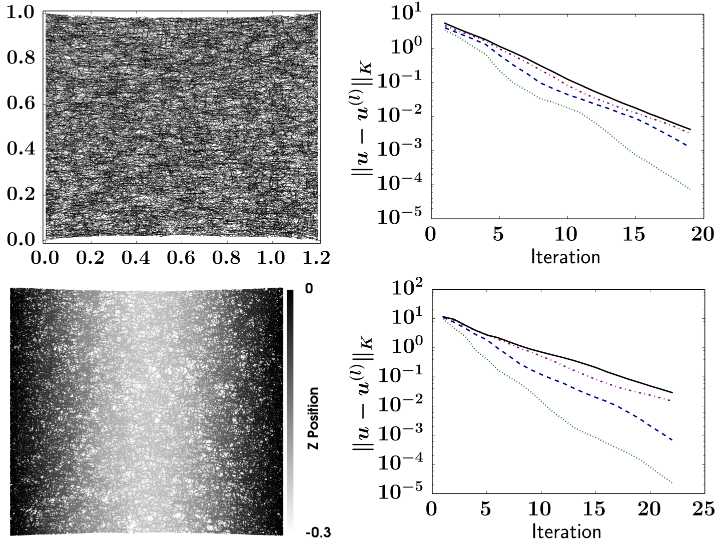




- $2 \cdot 10^4$ fibres, biased angle (x-axis), length 0.05, $3 \cdot 10^5$ nodes, $\alpha = 0.05, \beta = 500$.
- Two forces in the model: edge extension and angular deviation.
- Find displacement u: $Ku = f$ (tensile, distributed load)
- Theory extends to vector valued setting (Korn, $K \sim L$)
-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



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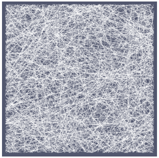

- Further investigation of (σ, μ)
- Mixed dim PDE (Hellman, Nilsson)
- LOD (Görtz, Kettil), SuperLOD (Hauck)
- Algebraic multilevel solver (Maier)
- Multilevel Monte Carlo
- Wave propagation (Ljung)
- Nonlinear fibre network model
- Pore network models