NSF Workshop on the
Emerging Applications and Future Directions of the BEM

Fast Boundary Element Methods: A Mathematical View

Olaf Steinbach

Institute of Computational Mathematics, TU Graz, Austria

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This lecture is based on joint work with

- W. L. Wendland (Stuttgart), U. Langer (Linz), S. Rjasanow (Saarbrücken)
- G. Of; S. Engleder, G. Unger, P. Urthaler, M. Windisch, ...

Boundary element methods

- Direct vs. indirect formulation
- Weakly singular vs. hypersingular boundary integral equation
- 1st kind vs. 2nd kind boundary integral equation
- Collocation vs. Galerkin discretization
- pw constant vs. pw linear basis functions (hp BEM)
- Interpolation vs. projection of given boundary data
- Adaptive vs. uniform refinement
- Direct vs. preconditioned iterative solution (construction of preconditioners)
- Acceleration
  (Panel Clustering, Fast Multipole, Adaptive Cross Approximation, . . .)
- parallelization and domain decomposition methods
- . . .

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  (Panel Clustering, Fast Multipole, Adaptive Cross Approximation, ...)
- parallelization and domain decomposition methods
- ...

While all of these topics are related to each other, we aim to end up with a most efficient, stable and accurate procedure to solve todays challenging problems from particular applications.

Model problem

$$-\Delta u(x) = 0 \quad \text{for } x \in \Omega \subset \mathbb{R}^3, \quad u(x) = g(x) \quad \text{for } x \in \Gamma = \partial\Omega$$

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Indirect approach for $x \in \Omega$

$$u(x) = \frac{1}{4\pi} \int_\Gamma \frac{1}{|x-y|} w(y) ds_y, \quad u(x) = \frac{1}{4\pi} \int_\Gamma \frac{(n_y, y-x)}{|x-y|^3} v(y) ds_y$$

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Boundary integral equations for $x \in \Gamma$

$$\frac{1}{4\pi} \int_\Gamma \frac{1}{|x-y|} w(y) ds_y = g(x), \quad \frac{1}{2} v(x) + \frac{1}{4\pi} \int_\Gamma \frac{(n_y, y-x)}{|x-y|^3} v(y) ds_y = g(x)$$

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Representation formula for $x \in \Omega$ (direct approach)

$$u(x) = \frac{1}{4\pi} \int_\Gamma \frac{1}{|x-y|} \frac{\partial}{\partial n_y} u(y) ds_y + \frac{1}{4\pi} \int_\Gamma \frac{(n_y, y-x)}{|x-y|^3} u(y) ds_y$$

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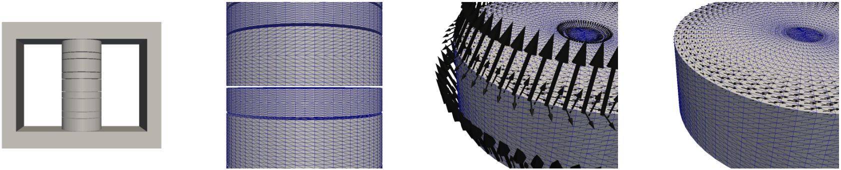
Boundary integral equation for $x \in \Gamma$

$$\frac{1}{4\pi} \int_\Gamma \frac{1}{|x-y|} t(y) ds_y = \frac{1}{2} g(x) - \frac{1}{4\pi} \int_\Gamma \frac{(n_y, y-x)}{|x-y|^3} g(y) ds_y$$

Example: Controllable reactor [Z. Andjelic, G. Of, OS, P. Urthaler 2010]

- results in potential equation with piecewise constant material parameters
- indirect single layer potential approach
  2nd kind boundary integral equation, simple, easy to solve
- direct domain decomposition approach (Steklov–Poincaré operator)
  more advanced formulation
- on the continuous level both formulations are equivalent



indirect direct

- difference in regularity of solutions → different approximation properties
- 122880 boundary elements → Adaptive Cross Approximation

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Hypersingular boundary integral equation for $x \in \Gamma$

$$t(x) = \frac{1}{2}t(x) - \frac{1}{4\pi}\int_\Gamma \frac{(n_x, x-y)}{|x-y|^3}t(y)ds_y + \frac{1}{4\pi}\frac{\partial}{\partial n_x}\int_\Gamma \frac{(n_y, y-x)}{|x-y|^3}u(y)ds_y$$

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System of boundary integral equations (Calderon projector)

$$\begin{pmatrix} u \\ t \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K' \end{pmatrix}\begin{pmatrix} u \\ t \end{pmatrix}$$

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Consequences

$$VK' = KV, \quad VD = \frac{1}{4}I - K^2$$

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- single layer potential symmetrizes the double layer potential [Plemelj 1911]
- single layer potential is a preconditioner for the hypersingular boundary integral operator, and vice versa [OS 1996; OS, Wendland 1998]

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Dirichlet to Neumann map (Steklov–Poincaré operator)

$$t = Su$$

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$$t = Su = V^{-1}(\frac{1}{2}I + K)u = [D + (\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K)]u = \dots$$

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2nd kind boundary integral equation [OS, Wendland 2001]

$$(\frac{1}{2}I - K)v = g$$

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2nd kind boundary integral equation [OS, Wendland 2001]

$$(\frac{1}{2}I - K)v = g, \quad v = \sum_{\ell=0}^{\infty}(\frac{1}{2}I + K)^{\ell}g, \quad \|(\frac{1}{2}I + K)v\|_{V^{-1}} \le c_K\|v\|_{V^{-1}}, \quad c_K < 1$$

Boundary value problem

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Representation formula for $x \in \Omega$

$$u(x) = \frac{1}{4\pi}\int_\Gamma \frac{1}{|x-y|} t(y) ds_y + \frac{1}{4\pi}\int_\Gamma \frac{(n_y, y-x)}{|x-y|^3} g(y) ds_y$$

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For an arbitrary boundary element solution t_h we define

$$\widetilde{u}(x) = \frac{1}{4\pi} \int_\Gamma \frac{1}{|x-y|} t_h(y) ds_y + \frac{1}{4\pi} \int_\Gamma \frac{(n_y, y-x)}{|x-y|^3} g(y) ds_y$$

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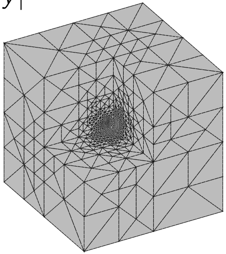
Error equation for $x \in \Gamma$ [H. Schulz, OS 2000]

$$(\frac{1}{2}I - K')[t - t_h](x) = \widetilde{t}(x) - t_h(x)$$



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Boundary integral equation for $x \in \Gamma$

$$(Vt)(x) = \frac{1}{2} g(x) + (Kg)(x)$$

Approximation

$$t_h(x) = \sum_{k=1}^{N} t_k \psi_k(x), \quad g_h(x) = \sum_{i=1}^{M} g_i \varphi_i(x)$$

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Galerkin discretization

$$\sum_{k=1}^{N} t_k \int_\Gamma (V\psi_k)(x)\psi_\ell(x) ds_x = \sum_{i=1}^{M} g_i \int_\Gamma (\frac{1}{2} I + K)\varphi_i(x)\psi_\ell(x) ds_x \quad \text{for } \ell = 1, \ldots, N$$

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Algebraic system of linear equations

$$V_h \underline{t} = (\frac{1}{2} M_h + K_h)\underline{g}, \quad \underline{t} = V_h^{-1}(\frac{1}{2} M_h + K_h)\underline{g}$$

Discretization of Dirichlet to Neumann map (Steklov–Poincaré operator)

$$\int_\Gamma (Sg_h)(x)\varphi_j(x)ds_x = \int_\Gamma t_h(x)\varphi_j(x)ds_x = \sum_{k=1}^{N} t_k \int_\Gamma \psi_k(x)\varphi_j(x)ds_x$$

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Boundary element approximation

$$S_h\underline{g} = M_h^\top \underline{t} = M_h^\top V_h^{-1}(\frac{1}{2}M_h + K_h)\underline{g}, \quad S_h = M_h^\top V_h^{-1}(\frac{1}{2}M_h + K_h)$$

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Stability (2D, ψ_k pw constant, ϖ_j pw linear)

$$M_h^\top = \frac{1}{2}h \begin{pmatrix} 1 & & \cdots & & 1 \\ 1 & 1 & & & \vdots \\ & 1 & \ddots & & \vdots \\ & & \ddots & 1 & \\ & & & 1 & 1 \end{pmatrix}$$

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Discretization of Dirichlet to Neumann map (Steklov–Poincaré operator)

$$\int_\Gamma (Sg_h)(x)\varphi_j(x)ds_x = \int_\Gamma t_h(x)\varphi_j(x)ds_x = \sum_{k=1}^N t_k \int_\Gamma \psi_k(x)\varphi_j(x)ds_x$$

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Symmetric boundary element approximation

$$S_h = D_h + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}(\frac{1}{2}M_h + K_h)$$

Boundary value problem

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Variational formulation to find u, $u(x) = g(x)$ for $x \in \Gamma$:

$$\int_\Omega \nabla u(x) \cdot \nabla v(x) dx = 0 \quad \text{for all } v, v(x) = 0, x \in \Gamma$$

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Finite element formulation for $\ell = 1, \ldots, M_\Omega$

$$\sum_{k=1}^{M_\Omega} u_k \int_\Omega \nabla \varphi_k(x) \cdot \nabla \varphi_\ell(x) dx + \sum_{i=M_\Omega+1}^{M} g_i \int_\Omega \nabla \varphi_i(x) \cdot \nabla \varphi_\ell(x) dx = 0$$

Linear system of algebraic equations

$$K_{II} \underline{u}_I + K_{CI} \underline{g} = \underline{0}$$

Boundary value problem

$$-\Delta u(x) = 0 \quad \text{for } x \in \Omega, \qquad u(x) = g(x) \quad \text{for } x \in \Gamma$$

Variational formulation to find u, $u(x) = g(x)$ for $x \in \Gamma$:

$$\int_\Omega \nabla u(x) \cdot \nabla v(x) dx = 0 \quad \text{for all } v, v(x) = 0, x \in \Gamma$$

Finite element formulation for $\ell = 1, \ldots, M_\Omega$

$$\sum_{k=1}^{M_\Omega} u_k \int_\Omega \nabla \varphi_k(x) \cdot \nabla \varphi_\ell(x) dx + \sum_{i=M_\Omega+1}^{M} g_i \int_\Omega \nabla \varphi_i(x) \cdot \nabla \varphi_\ell(x) dx = 0$$

Linear system of algebraic equations

$$K_{II} \underline{u}_I + K_{CI} \underline{g} = \underline{0}, \qquad \underline{u}_I = -K_{II}^{-1} K_{CI} \underline{g}$$

Dirichlet to Neumann map (Steklov–Poincaré operator)

$$\int_\Gamma (Sg)(x)v(x)ds_x = \int_\Gamma \frac{\partial}{\partial n_x} u(x)v(x)ds_x$$

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Discretization for $j = M_\Omega + 1, \ldots, M$

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Discrete Steklov–Poincaré operators

$$S_h^{\text{BEM}} = D_h + (\frac{1}{2} M_h^\top + K_h^\top) V_h^{-1} (\frac{1}{2} M_h + K_h), \quad S_h^{\text{FEM}} = K_C - K_{IC} K_{II}^{-1} K_{CI}$$

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- different FE/BE approximations of the Steklov–Poincaré operator
- coupling of FEM/BEM via domain decomposition methods

Model problem in 1D

$$-u''(x) = f(x) \quad \text{for } x \in (0,1), \quad u(0) = u(1) = 0$$

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$$h = \frac{1}{n}, \quad x_k = kh, \quad -u''(x_k) \approx \frac{-u_{k-1} + 2u_k - u_{k+1}}{h^2} \quad \text{for } k = 1, \ldots, n-1$$

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Linear system of algebraic equations

$$\frac{1}{h^2} \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{pmatrix}$$

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- FDM/FEM stiffness matrix is sparse
- What do we know about its inverse?

$n = 9$

$$K_9 = 81 \begin{pmatrix} 2 & -1 & & & & & & \\ -1 & 2 & -1 & & & & & \\ & -1 & 2 & -1 & & & & \\ & & -1 & 2 & -1 & & & \\ & & & -1 & 2 & -1 & & \\ & & & & -1 & 2 & -1 & \\ & & & & & -1 & 2 & -1 \\ & & & & & & -1 & 2 \end{pmatrix}$$

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$$K_9^{-1} = \frac{1}{81} \cdot \frac{1}{9} \begin{pmatrix} 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 7 & 14 & 12 & 10 & 8 & 6 & 4 & 2 \\ 6 & 12 & 18 & 15 & 12 & 9 & 6 & 3 \\ 5 & 10 & 15 & 20 & 16 & 12 & 8 & 4 \\ 4 & 8 & 12 & 16 & 20 & 15 & 10 & 5 \\ 3 & 6 & 9 & 12 & 15 & 18 & 12 & 6 \\ 2 & 4 & 6 & 8 & 10 & 12 & 14 & 7 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{pmatrix}$$

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- inverse FDM/FEM stiffness matrix is dense, but data sparse!

$$K_9^{-1} = \frac{1}{729}\begin{pmatrix} \begin{matrix} \begin{pmatrix}8&7\\7&14\end{pmatrix} & \begin{pmatrix}1\\2\end{pmatrix}\begin{pmatrix}6&5\end{pmatrix} \\ \begin{pmatrix}6\\5\end{pmatrix}\begin{pmatrix}1&2\end{pmatrix} & \begin{pmatrix}18&15\\15&20\end{pmatrix}\end{matrix} & \begin{pmatrix}1\\2\\3\\4\end{pmatrix}\begin{pmatrix}4&3&2&1\end{pmatrix} \\ \begin{pmatrix}4\\3\\2\\1\end{pmatrix}\begin{pmatrix}1&2&3&4\end{pmatrix} & \begin{matrix} \begin{pmatrix}20&15\\15&18\end{pmatrix} & \begin{pmatrix}5\\6\end{pmatrix}\begin{pmatrix}2&1\end{pmatrix} \\ \begin{pmatrix}2\\1\end{pmatrix}\begin{pmatrix}5&6\end{pmatrix} & \begin{pmatrix}14&7\\7&8\end{pmatrix}\end{matrix}\end{pmatrix}.$$

$$
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\left(
\begin{array}{cc}
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&
\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \begin{pmatrix} 4 & 3 & 2 & 1 \end{pmatrix}
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$$

Storage requirement for off diagonal block

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\left(\frac{n-1}{2}\right)^2 = \frac{1}{4}(n-1)^2 \quad \to \quad 2\,\frac{n-1}{2} = n-1
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Stiffness matrix

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$\rightarrow$ Rank 1 representation of matrix block

Low rank approximation of matrices

$$A \in \mathbb{R}^{m \times n}, \quad \mu = \operatorname{rank} A \leq \min\{m, n\}$$

with

$$A^\top A \in \mathbb{R}^{n \times n}, \quad \lambda_1(A^\top A) \geq \lambda_2(A^\top A) \geq \ldots \geq \lambda_n(A^\top A) \geq 0$$

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Singular values

$$\sigma_k := \sqrt{\lambda_k(A^\top A)} \geq 0 \quad \text{for } k = 1, \ldots, \mu$$

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Singular value decomposition

$$D := \operatorname{diag}(\lambda_k(A)) = V^\top A^\top A V, \quad A^\top A \underline{v}_k = \lambda_k \underline{v}_k$$

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$$A = U \Sigma V^\top = \sum_{k=1}^{\mu} \sigma_k(A) \underline{u}_k \underline{v}_k^\top$$

Approximation

$$A_r = \sum_{k=1}^{r} \sigma_k(A) \underline{u}_k \underline{v}_k^\top, \quad \|A - A_r\|_2 = \sigma_{r+1}(A)$$

Approximation

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Storage requirement

$$nm \quad \text{vs} \quad r(n+m)$$

Matrix by vector multiplication

$$A_r \underline{w} = \sum_{k=1}^{r} \sigma_k(A) \underline{u}_k \underline{v}_k^\top \underline{w} = \sum_{k=1}^{r} \sigma_k(A) (\underline{v}_k^\top \underline{w}) \underline{u}_k, \quad r(n+m)$$

- low rank matrix is singular
- block decomposition due to some admissibility condition
- low rank approximation of blocks

Model problem

$$-\Delta u(x) = 0 \quad \text{for } x \in \Omega, \qquad u(x) = g(x) \quad \text{for } x \in \Gamma$$

Boundary integral equation for $x \in \Gamma$

$$\int_\Gamma U^*(x,y)t(y)ds_y = \frac{1}{2}g(x) + \int_\Gamma \frac{\partial}{\partial n_y}U^*(x,y)g(y)ds_y = f(x)$$

Ansatz (piecewise constant)

$$t(x) \sim t_h(x) = \sum_{k=1}^{N} t_k \psi_k(x), \quad \psi_k(x) = \begin{cases} 1 & \text{for } x \in \tau_k \\ 0 & \text{elsewhere} \end{cases}$$

Collocation

$$\sum_{k=1}^{N} t_k \frac{\Delta_\ell}{4\pi} \int_{\tau_k} \frac{1}{|x_\ell^* - y|} ds_y \;=\; \Delta_\ell f(x_\ell^*) \quad \text{for } \ell = 1, \ldots, N$$

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Galerkin

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$$\begin{aligned} s_0(x,y) &= 0, \quad r_0(x,y) = k(x,y), \\ s_k(x,y) &= s_{k-1}(x,y) + \frac{r_{k-1}(x,y_k)r_{k-1}(x_k,y)}{r_{k-1}(x_k,y_k)} \\ r_k(x,y) &= r_{k-1}(x,y) - \frac{r_{k-1}(x,y_k)r_{k-1}(x_k,y)}{r_{k-1}(x_k,y_k)} \end{aligned}$$

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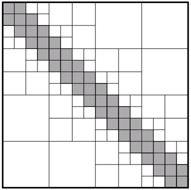


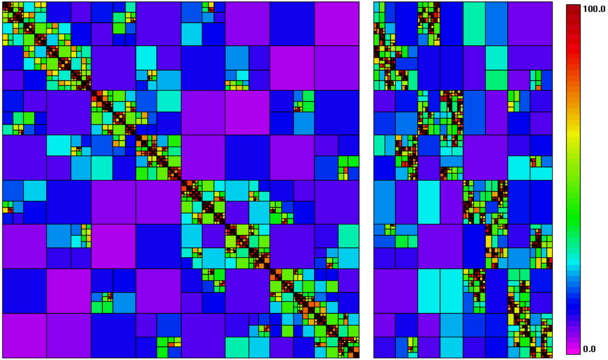
- Low rank approximation
- hierarchical clustering
- admissibility condition

$$\text{dist}(\omega_i^\kappa, \omega_j^\kappa) \geq \eta \max \left\{ \text{diam } \omega_i^\kappa, \text{diam } \omega_j^\kappa \right\}$$

- complexity

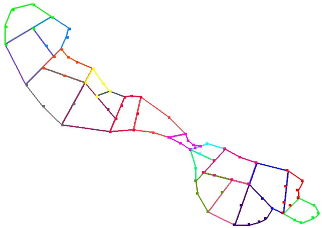
$$\mathcal{O}(N \log^2 N)$$

Adaptive Cross Approximation: Single and double layer potential



non–overlapping domain decomposition

$$-\mathrm{div}[\alpha(x)\nabla u(x)] = 0 \quad \text{for } x \in \Omega, \quad \overline{\Omega} = \bigcup_{i=1}^{p} \overline{\Omega}_i$$



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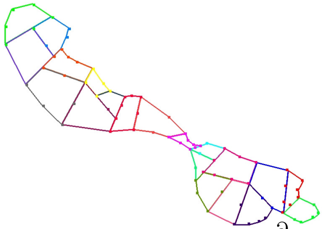

local boundary value problems

$$\begin{aligned} -\alpha_i \Delta u_i(x) &= 0 && \text{for } x \in \Omega_i, \\ u_i(x) &= g(x) && \text{for } x \in \Gamma_i \cap \Gamma \end{aligned}$$

transmission or coupling boundary conditions

$$u_i(x) = u_j(x), \quad \alpha_i \frac{\partial}{\partial n_i} u_i(x) + \alpha_j \frac{\partial}{\partial n_j} u_j(x) = 0 \quad \text{for } x \in \Gamma_i \cap \Gamma_j$$

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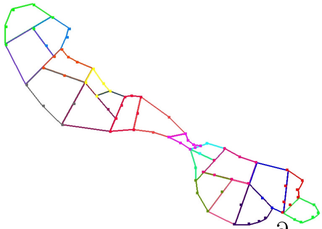

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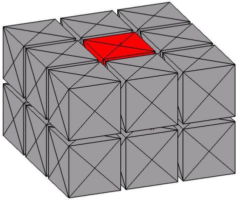
local Dirichlet to Neumann map

$$t_i(x) = \frac{\partial}{\partial n_i} u_i(x) = (S_i u_i)(x) \quad \text{for } x \in \Gamma_i$$

- Local FE/BE approximations of Steklov–Poincaré operators
- Tearing and interconnecting iterative solution procedures (FETI/BETI)

Example: Linear elasticity (steel/concrete)



18 subdomains

	BETI		all–floating	
L	t_2	It.	t_2	It.
0	31	19(21(10))	39	22(17(10))
1	217	28(33(14))	170	24(27(14))
2	2129	35(44(14))	1437	27(33(14))
3	14149	42(51(14))	9005	32(36(14))
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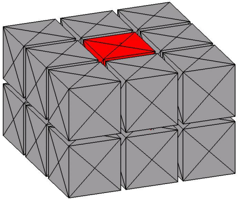

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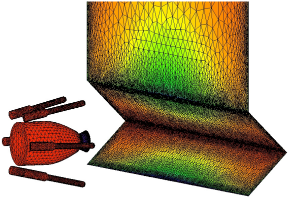
		Dirichlet DD		BETI		all–floating	
L	N_i	t_2	It.	t_2	It.	t_2	It.
0	24	7	53(10)	7	78	8	65
1	96	25	110(14)	19	100	19	82
2	384	181	130(14)	112	114	115	85
3	1536	986	148(14)	562	129	476	95
4	6144	6902	154(14)	4352	153	3119	105
5	24576	59264	166(16)	31645	172	23008	120

24576 boundary elements per subdomain $\approx$ 14 million tetrahedrons

Iterative solution of linear systems



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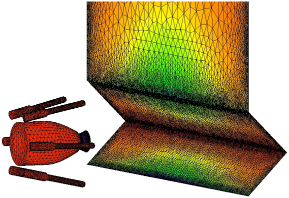
- scaling
- preconditioners for V_h, $S_h = D_h + K_h^\top V_h^{-1} K_h$



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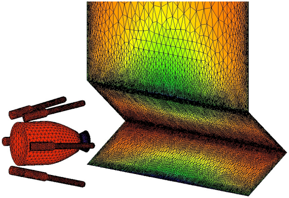
Preconditioners

- operators of opposite orders
- geometric and algebraic multilevel techniques



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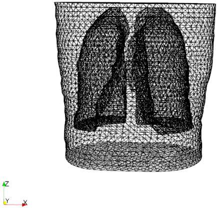

Acoustic and electromagnetic scattering problems

- Helmholtz, Maxwell
- combined boundary integral equations to avoid spurious modes
- domain decomposition methods, preconditioners

Optimization and inverse problems, eigenvalue problems, multiphysics, fluid structure interaction, FEM/BEM coupling, ...

Some Activities

- Söllerhaus Workshops on Fast Boundary Element Methods in Industrial Applications. Kleinwalsertal, Austria.
  September 30–October 3, 2010
  September 29–October 2, 2011
- IABEM Symposium, Brescia, Italy, September 5–8, 2011
- Annual GAMM Meeting, Graz, Austria, April 18–21, 2011

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