Parallel Time-Domain Boundary Element Method for 3-Dimensional Wave Equation

Space-Time Methods for PDEs, RICAM Linz, November 10, 2016

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Parallel Time-Domain Boundary Element Method for 3-Dimensional Wave Equation

Outline

- Parallel fast BEM and applications
- Boundary integral formulation of sound-hard scattering
- Time-domain boundary element method
- Parallelization, preconditioning, numerical experiments
- Conclusion, outlook, references
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Parallel fast BEM and applications

Laplace equation in an unbounded domain

\[ \Omega \subset \mathbb{R}^3 \text{ lipschitz domain} \]

\[
\begin{cases}
-\Delta u(\tilde{x}) = 0, & \tilde{x} \in \Omega^e := \mathbb{R}^3 \setminus \overline{\Omega} \\
\gamma_N u(x) := \frac{du}{dn}(x) = g(x), & x \in \Gamma := \partial\Omega \\
|u(\tilde{x})| = O(1/|\tilde{x}|), & |\tilde{x}| \to \infty.
\end{cases}
\]

Representation formula

\[
\forall \tilde{x} \in \Omega : \quad u(\tilde{x}) = -\int_{\Gamma} \gamma_N u(y) G(\tilde{x}, y) \, dS(y) + \int_{\Gamma} u(y) \gamma_{N,y} G(\tilde{x}, y) \, dS(y),
\]

where \( G(\tilde{x}, y) := \frac{1}{4\pi|\tilde{x} - y|} \).

An indirect method

Find an auxiliary double-layer density \( \phi : \Gamma \to \mathbb{R} \) such that

\[
\gamma_N \int_{\Gamma} \phi(y) \gamma_{N,y} G(x, y) \, dS(y) = g(x), \quad x \in \Gamma \quad \leadsto \quad u(\tilde{x}) = \int_{\Gamma} \phi(y) \gamma_{N,y} G(\tilde{x}, y) \, dS(y), \quad \tilde{x} \in \Omega^e.
\]
Parallel fast BEM and applications

Shape optimization of a DC electromagnet, FEM-BEM coupling

L., Postava, Životský: J Magn Magn Mater ’10, Math Comput Simulat ’12
Parallel fast BEM and applications

Acoustics of a railway wheel $\rightsquigarrow$ $\mathcal{H}$-matrices, ACA/FMM
Parallel fast BEM and applications

Parallel fast BEM using cyclic graph decompositions

Solution to the system of 2.7M DOFs on 273 cores in 16 minutes.

L., Kovář, Kovářová, Merta: Numer Alg ’15
Parallel fast BEM and applications

Elmg. forming of plates with Fraunhofer IWU Chemnitz, FEM-BEM
Parallel fast BEM and applications

Structural health monitoring of aircrafts with Honeywell Int.

using 3d anisotropic mixed elements (TD-NNS) by [Pechstein (Sinwel), Schöberl ’12].
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Boundary integral formulation of sound-hard scattering

Sound-hard scattering

Given the scatterer $\Omega$ and the causal incident wave $u^{\text{inc}}$ (satisfying $\ddot{u} - \nabla^2 u = 0$), we look for the scattered field $u$:

\[
\begin{align*}
\ddot{u} - \nabla^2 u &= 0 \text{ in } \Omega^e \times [0, T], \\
u(., 0) &= \dot{u}(., 0) = 0 \text{ in } \Omega^e, \\
\frac{\partial u}{\partial n} &= -\frac{\partial u^{\text{inc}}}{\partial n} \text{ on } \Gamma \times [0, T].
\end{align*}
\]
Boundary integral formulation of sound-hard scattering

Double-layer indirect boundary integral method

We search for $u$ in the form of the retarded double-layer potential

$$u(x, t) = -\frac{1}{4\pi} \int_{\Gamma} n(y) \cdot (x - y) \left( \frac{\phi(y, t - \|x - y\|)}{\|x - y\|^2} + \frac{\dot{\phi}(y, t - \|x - y\|)}{\|x - y\|} \right) dS(y),$$

which satisfies the wave equation and the initial conditions. It remains to fulfill the Neumann boundary condition

$$\lim_{\Omega \ni \tilde{x} \to x \in \Gamma} n(x) \cdot \nabla_{\tilde{x}} u(\tilde{x}, t) = g(x, t) \text{ on } \Gamma \times [0, T],$$

where $g := -\frac{\partial u^{\text{inc}}}{\partial n}$. 
Boundary integral formulation of sound-hard scattering

Weak boundary integral formulation [Bamberger, HaDuong ’86]

Find $\phi \in V$ such that

$$a(\xi, \phi) = b(\xi) \quad \forall \xi \in V,$$

where

$$a(\xi, \phi) := \int_0^T \int_{\Gamma} \int_{\Gamma} \left\{ \frac{n(x) \cdot n(y)}{4\pi \|x - y\|} \frac{\dot{\xi}(x, t) \ddot{\phi}(y, t - \|x - y\|)}{4\pi \|x - y\|} \right\} dS(y) dS(x) dt,$$

and

$$b(\xi) := \int_0^T \int_{\Gamma} g(x, t) \dot{\xi}(x, t) dS(x) dt.$$

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Time-domain boundary element method

Discrete ansatz

Replace $V$ by a finite-dimensional subspace $V_h^{\Delta t}$ spanned by the tensor-product of $N$ temporal and $M$ spatial basis functions:

$$\phi_h^{\Delta t}(x, t) := \sum_{l=1}^{N} \sum_{j=1}^{M} \alpha_j^l \varphi_j(x) b_l(t).$$

We arrive at the $(N \times M) \times (N \times M)$ block linear system

$$\begin{pmatrix}
A_{1,1} & \cdots & A_{1,N} \\
\vdots & \ddots & \vdots \\
A_{N,1} & \cdots & A_{N,N}
\end{pmatrix}
\begin{pmatrix}
\alpha_1 \\
\vdots \\
\alpha_N
\end{pmatrix}
=
\begin{pmatrix}
b_1 \\
\vdots \\
b_N
\end{pmatrix},$$

where

$$(A_{k,l})_{i,j} := a(\varphi_i(x) b_k(t), \varphi_j(y) b_l(t)), \quad (b_k)_i := b(\varphi_i(x) b_k(t)), \quad (\alpha_l)_j := \alpha_l^j.$$
Time-domain boundary element method

Matrix: a deeper look

\[(A_{k,l})_{i,j} = \int_{\text{supp } \varphi_i} \int_{\text{supp } \varphi_j} \frac{n(x) \cdot n(y)}{4\pi \|x - y\|} \varphi_i(x) \varphi_j(y) \left( \int_0^T \dot{b}_k(t) \dot{b}_l(t - \|x - y\|) \, dt \right) \, dS(y) \, dS(x) \]

\[+ \int_{\text{supp } \varphi_i} \int_{\text{supp } \varphi_j} \frac{\text{curl}_\Gamma \varphi_i(x) \cdot \text{curl}_\Gamma \varphi_j(y)}{4\pi \|x - y\|} \left( \int_0^T \dot{b}_k(t) \dot{b}_l(t - \|x - y\|) \, dt \right) \, dS(y) \, dS(x), \]

\[=: \Psi_{k,l}(\|x-y\|) \]

Piecewise smooth time-ansatz \(\sim\) expensive quadrature
due to nontrivial intersection of the light cone

\[\text{supp } \Psi_{k,l}, \quad \text{supp } \tilde{\Psi}_{k,l} \]

with

\[\text{supp } \varphi_i \times \text{supp } \varphi_j.\]

[El Gharib '99], [Stephan, Maischak, Ostermann '08]
Time-domain boundary element method

$C^\infty$-smooth (partition of unity) temporal basis [Sauter, Veit ’12, ’14]

- allows for Sauter-Schwab quadrature over $\text{supp} \varphi_i \times \text{supp} \varphi_j$
- and for higher-order approximation in time.

\[
\begin{align*}
\mathbf{A}_{k,l}^{i,j} &= \int_{\text{supp} \varphi_i} \int_{\text{supp} \varphi_j} \frac{n(x) \cdot n(y)}{4\pi \|x - y\|} \varphi_i(x) \varphi_j(y) \left( \int_0^T \dot{b_k}(t) \dot{b_l}(t - \|x - y\|) \, dt \right) \, dS(y) \, dS(x) \\
&\quad + \int_{\text{supp} \varphi_i} \int_{\text{supp} \varphi_j} \frac{\text{curl}_\Gamma \varphi_i(x) \cdot \text{curl}_\Gamma \varphi_j(y)}{4\pi \|x - y\|} \left( \int_0^T \dot{b_k}(t) \dot{b_l}(t - \|x - y\|) \, dt \right) \, dS(y) \, dS(x),
\end{align*}
\]

To accelerate the assembly, $\Psi$ and $\tilde{\Psi}$ are replaced by piecewise Chebyshev interpolants.
Time-domain boundary element method

Convergence of \( \| \phi^{h,\Delta t}(x,.) - \phi^{\text{analytical}}(x,.) \|_{L^2(0,T)} \) on the sphere [Veit ’12]

\( \Omega \) the unit sphere, \( \phi^{\text{analytical}} \) a spherical harmonic function, \( x \in \Gamma \)

1st-order time-basis functions

2nd-order time-basis functions
Matrix structure

The matrix is sparse and it has a block-Hessenberg structure.
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Parallelization, preconditioning, numerical experiments

Parallel implementation

- For equidistant time stepping only the blue parts have to be assembled.
- We employ a hybrid MPI-OpenMP model:
  - pairs of triangles corresponding to nonzero entries are evenly distributed to MPI nodes,
  - on each node the assembly (quadrature) is performed using OpenMP.
- We use up to 64 Intel Xeon E5 nodes (1024 cores) of the cluster Anselm, VŠB-TU Ostrava.
Parallelization, preconditioning, numerical experiments

Parallel implementation

We distribute blocks among MPI processes (nodes) as follows:

\[
\begin{bmatrix}
\tilde{A}_{1,1} & \tilde{A}_{1,2} & 0 & 0 & 0 & 0 & 0 & 0 \\
\tilde{A}_{2,1} & \tilde{A}_{2,2} & \tilde{A}_{2,3} & 0 & 0 & 0 & 0 & 0 \\
\tilde{A}_{3,1} & \tilde{A}_{3,2} & \tilde{A}_{3,3} & \tilde{A}_{3,4} & 0 & 0 & 0 & 0 \\
0 & \tilde{A}_{4,2} & \tilde{A}_{4,3} & \tilde{A}_{4,4} & \tilde{A}_{4,5} & 0 & 0 & 0 \\
0 & 0 & \tilde{A}_{5,3} & \tilde{A}_{5,4} & \tilde{A}_{5,5} & \tilde{A}_{5,6} & 0 & 0 \\
0 & 0 & 0 & \tilde{A}_{6,4} & \tilde{A}_{6,5} & \tilde{A}_{6,6} & \tilde{A}_{6,7} & 0 \\
0 & 0 & 0 & 0 & \tilde{A}_{7,5} & \tilde{A}_{7,6} & \tilde{A}_{7,7} & \tilde{A}_{7,8} \\
0 & 0 & 0 & 0 & 0 & \tilde{A}_{8,6} & \tilde{A}_{8,7} & \tilde{A}_{8,8}
\end{bmatrix}
\]

Each process does the following:

1. Precompute the sparsity pattern of the block.
2. Distribute pairs of elements among computational nodes using MPI.
3. On each computational node assemble its contribution to the block in a shared memory using OpenMP.
4. Gather the data on the MPI rank(s) owning the block.
Parallelization, preconditioning, numerical experiments

Weak parallel scalability of the assembly

Submarine surface decomposed into 5604 triangles, 40 time steps, 80 time DOFs
Parallelization, preconditioning, numerical experiments

Preconditioning

To accelerate FGMRES iterations we approximate the upper Hessenberg matrix by an algebraic multilevel preconditioner:

\[
A := \begin{pmatrix}
A_{I,I} & A_{I,II} \\
A_{II,I} & A_{II,II}
\end{pmatrix} \approx \begin{pmatrix}
A_{I,I} & 0 \\
A_{II,I} & A_{II,II}
\end{pmatrix}
\]

so that \(A_{I,I}^{-1}\) and \(A_{II,II}^{-1}\) are approximated by a small fixed number of FGMRES iterations eventually preconditioned the same again.
Parallelization, preconditioning, numerical experiments

Numerical experiments, ball, 162 nodes, 1st-order in time

<table>
<thead>
<tr>
<th>$N$</th>
<th>GMRES(50)</th>
<th>DGMRES(50, 4)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$# \text{ iterations}$</td>
<td>time [s]</td>
</tr>
<tr>
<td>5</td>
<td>595</td>
<td>1.6</td>
</tr>
<tr>
<td>10</td>
<td>2121</td>
<td>14.3</td>
</tr>
<tr>
<td>15</td>
<td>4021</td>
<td>44.5</td>
</tr>
<tr>
<td>20</td>
<td>5448</td>
<td>99.0</td>
</tr>
</tbody>
</table>

Table 1: Convergence of GMRES and DGMRES for $p = 1$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>FGMRES(50, 1(10))</th>
<th>FGMRES(50, 1(5))</th>
<th>FGMRES(50, 2(2, 10))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$# \text{ iterations}$</td>
<td>time [s]</td>
<td>$# \text{ iterations}$</td>
</tr>
<tr>
<td>5</td>
<td>24</td>
<td>0.7</td>
<td>45</td>
</tr>
<tr>
<td>10</td>
<td>43</td>
<td>3.1</td>
<td>126</td>
</tr>
<tr>
<td>15</td>
<td>51</td>
<td>7.3</td>
<td>205</td>
</tr>
<tr>
<td>20</td>
<td>48</td>
<td>9.7</td>
<td>341</td>
</tr>
</tbody>
</table>

Table 2: Convergence of FGMRES with recursive preconditioner for $p = 1$. 
Parallelization, preconditioning, numerical experiments

Numerical experiments, ball, 162 nodes, 2nd-order in time

<table>
<thead>
<tr>
<th>$N$</th>
<th>GMRES(50) # iterations</th>
<th>time [s]</th>
<th>DGMRES(50, 2) # iterations</th>
<th>time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1985</td>
<td>14.3</td>
<td>1434</td>
<td>11.6</td>
</tr>
<tr>
<td>10</td>
<td>5404</td>
<td>89.1</td>
<td>3834</td>
<td>67.9</td>
</tr>
<tr>
<td>15</td>
<td>4634</td>
<td>132.7</td>
<td>1491</td>
<td>52.1</td>
</tr>
<tr>
<td>20</td>
<td>6383</td>
<td>293.3</td>
<td>1269</td>
<td>68.1</td>
</tr>
</tbody>
</table>

**Table 3:** Convergence of GMRES and DGMRES for $p = 2$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>FGMRES(50, 1(10)) # iterations</th>
<th>time [s]</th>
<th>FGMRES(50, 1(5)) # iterations</th>
<th>time [s]</th>
<th>FGMRES(50, 2(2, 10)) # iterations</th>
<th>time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>83</td>
<td>5.5</td>
<td>210</td>
<td>8.9</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>10</td>
<td>257</td>
<td>44.3</td>
<td>627</td>
<td>77.3</td>
<td>94</td>
<td>26.6</td>
</tr>
<tr>
<td>15</td>
<td>148</td>
<td>48.3</td>
<td>363</td>
<td>82.2</td>
<td>56</td>
<td>24.8</td>
</tr>
<tr>
<td>20</td>
<td>91</td>
<td>45.9</td>
<td>399</td>
<td>139.4</td>
<td>63</td>
<td>40.4</td>
</tr>
</tbody>
</table>

**Table 4:** Convergence of FGMRES with recursive preconditioner for $p = 2$. 
Parallelization, preconditioning, numerical experiments

Numerical experiments, submarine

2804 nodes, 40 time steps, 1st-order in time.

\begin{align*}
\text{GMRES}(500): & \quad 9636 \text{ iters., } 1607 \text{ s} \\
\rightarrow \quad \text{FGMRES}(500,1(40)): & \quad 243 \text{ iters., } 962 \text{ s}
\end{align*}
Parallelization, preconditioning, numerical experiments

M. Merta, J. Zapletal et al.: BEM4I library
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Conclusion, outlook

✓ Time-domain BEM for 3d wave equation, adaptivity in time,
✓ parallely scalable assembly and postprocessing,
→ mapping properties of the operator, preconditioning,
→ adaptivity in time,
→ extension to the elastic wave equation.

References

• Analysis: Bamberger, Ha Duong, Math. Meth. Appl. Sci. ’86
• Numerics: Sauter, Veit, Numer. Math. ’14
• Parallel fast BEM: L., Kovář, Kovářová, Merta, Numer. Alg. ’15