Fast algorithms and numerical methods for the solution of Boundary Element Methods

Session 1: Introduction and Boundary Integral Representation

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Specificities of Numerical methods for wave propagation

Domain methods (FEM, SEM, ...)	BEM
$\rightarrow$ Domain mesh	$\rightarrow$ Surface mesh (i.e. reduced dim.)
$\rightarrow$ Approx. radiation conditions	$\rightarrow$ Exact radiation conditions
$\rightarrow$ Sparse matrix	$\rightarrow$ Fully-populated matrix

Overview of Boundary Element Methods for waves

BEM adequate for large (unbounded) media with simple properties

Since we want to consider medium to high frequency problems (real-life configurations), the fully-populated BEM influence matrix is a severe limiting factor. Most of current research is devoted to this point

Solution of fully-populated systems

$$\mathbb{A}\mathbf{x} = \mathbf{b} \quad \text{matrix of size } N \times N$$

Memory requirements: $O(N^2)$ to store the fully-populated matrix

Direct solvers: direct approximation of the solution

- Gaussian elimination with full pivoting: too expensive
- Gaussian elimination with partial pivoting: problem of stability
- Convergence of direct solvers proven but it is difficult to estimate the accuracy of the result (depends on the choice of pivot)

$$\mathbb{A}\mathbf{x} \simeq \mathbb{A}\mathbf{x}' \nRightarrow \mathbf{x} \simeq \mathbf{x}'$$

Iterative solvers: sequence of solutions that tend to the true solution

- No *a priori* knowledge of the converge
- Study of the conditioning of the system matrix
- These methods are usually faster than direct solvers

Complexity in terms of CPU time: at least $O(N^2)$ (to perform a matrix-vector product) and up to $O(N^3)$ for Gaussian elimination

Computational limitations of standard BEMs

High memory cost: assembly of the system matrix $O(N^2)$

Limited geometric complexity: mesh size depends on the details

Limited (piecewise) heterogeneity: the BEM is defined for homogeneous domains.

- BE-BE coupling for piecewise heterogeneous domains
- Coupling with other methods for locally heterogeneous media

Limited frequency range

- The mesh size depends on the wavenumber k
- We are interested in high frequency problems (seismology: the domain is hundreds of wavelengths long; radar: waves of 10 cm)

Main goal: How can we reduce the complexity of the system solution in terms of memory requirements and CPU time?

Towards real-life applications: Principle of Fast BEMs

It is not possible to speed-up solution of initial fully-populated system

But it is possible for an approximate system

$$\mathbb{A} := \begin{bmatrix} -2 & 4 & 6 & -3 \\ 4 & -8 & -12 & 6 \\ -6 & 12 & 18 & -9 \\ -8 & 16 & 24 & -12 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \\ 3 \\ 4 \end{bmatrix} \begin{bmatrix} -2 & 4 & 6 & -3 \end{bmatrix}$$

The BEM system is not low-rank but it can be approximated by a low-rank system: reduction of storage and solution time.

Main tools used in modern fast BEMs

- $\mathcal{H}-$ matrices and low-rank approximations
- Fast Multipole Method

Outline of the sessions

I will introduce BEMs and modern fast BEMs ... but a large fraction of the time will be devoted to practice (in Matlab, Python, Fortran, ...)

- 15/09 Introduction / Fundamental solutions and Boundary Integral Representation - TP0 (report 2 pages for 22/09)
- 22/09 TP on Boundary Integral Representation (5 pages for 29/09)
- 29/09 Boundary Integral Equations / TP on BIE (5 pages for 06/10)
- 06/10 Fast algebraic BEMs / TP on low rank approximations
- 09/10 TP on low rank approximations (2 pages for 03/11)
- 03/11 TP on Hierarchical Matrices - clustering (2 pages for 10/11)
- 06/11 TP on Hierarchical Matrices - admissibility condition (2 pages for 10/11)
- 10/11 TP on Hierarchical Matrices - matrix-vector product (5 pages for 17/11)
- 17/11 Presentation of Fast Multipole Method and TP
- 20/11 Link between fast BEMs and GNN. Written Exam

Grading: Projects (by pair) and a Written exam (1h)

Digression on algorithms

Why do we need to study algorithms?

- Computing time and resources are a bounded resource
- We want to use the simplest method to implement

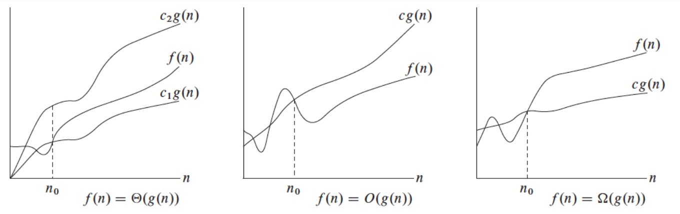
Especially true for BEM since the matrices are fully-populated

Analyzing algorithms

- Predicting resources that the algorithm requires
  - Computational time, memory, communications
- Define the costs of the instructions
  - Arithmetic, data movement, control
- Finding the worst-case running time

Cormen, Leiserson, Rivest, Stein. *Introduction to algorithms*, MIT Press, 2009.

Order of growth of the running time



Estimation of complexity

- The order of growth is used to compare the relative performance of alternative algorithms
- Complexity is $O(N^\alpha) \rightarrow$ the worst-case running time is $O(N^\alpha)$
- Only leading terms (others are insignificant for large values of N)

Remark: Due to constant factors and lower order terms, for small N an algorithm with a higher order complexity might take less time

Boundary Integral Representation: an overview

1 Boundary Integral Representation: an overview

Principle of derivation of Boundary Integral Representation

Boundary-value problem over Ω : $\begin{cases} \mathcal{L}u + f = 0 & \text{in } \Omega, \\ u = g_1 & \text{on } \partial\Omega_D, \\ T^n(u) = g_2 & \text{on } \partial\Omega_N. \end{cases}$

where u: unknown; g_1, g_2 and source f given. T^n: first-order partial differential operator, linear with respect to n. $\mathcal{L}$ linear second-order partial differential operator

- $\mathcal{L}$ and T^n assumed to satisfy the reciprocity identity

$$\int_\Omega (\mathcal{L}u.v - \mathcal{L}v.u) dV = \int_{\partial\Omega} (T^n(u).v - T^n(v).u) dS$$

- G: fundamental solution (point source f applied at x $\notin \partial\Omega$)

$$\mathcal{L}G(\boldsymbol{x}, \boldsymbol{y}) + \delta(\boldsymbol{y} - \boldsymbol{x}) = 0 \quad \text{in } \Omega$$

- Property of the Dirac distribution

$$\int_\Omega \delta(\boldsymbol{y} - \boldsymbol{x}) u(\boldsymbol{y}) dV_y = \kappa u(\boldsymbol{x}) \quad (\kappa = 1 \; if \; \boldsymbol{x} \in \Omega, \quad \kappa = 0 \; if \; \boldsymbol{x} \notin \Omega)$$

- Integral Representation formula: $x \notin \partial\Omega$

$$\kappa u(\boldsymbol{x}) = \int_\Omega f(\boldsymbol{y}) G(\boldsymbol{x}, \boldsymbol{y}) dV_y + \int_{\partial\Omega} (u(\boldsymbol{y}) T^n G(\boldsymbol{x}, \boldsymbol{y}) - T^n u(\boldsymbol{y}) G(\boldsymbol{x}, \boldsymbol{y})) dS_y$$

Integral Representation for Poisson equation

$$\Delta u + b = 0 \text{ on } \Omega \quad + \text{(unspecified well-posed B.C.)}$$

i.e., $\mathcal{L} = \Delta$ and $T^n = \nabla.n$ (normal der.)

Derivation of reciprocity identity: u^1, u^2 sol. of eq. and $q(\boldsymbol{y}) = \nabla u(\boldsymbol{y}).n(\boldsymbol{y})$

$$\int_{\partial\Omega} q^1 u^2 dS + \int_{\Omega} (b^1 u^2 - \nabla u^1.\nabla u^2) dV = 0$$

$$\int_{\partial\Omega} q^2 u^1 dS + \int_{\Omega} (b^2 u^1 - \nabla u^1.\nabla u^2) dV = 0$$

$$\int_{\partial\Omega} (q^1 u^2 - q^2 u^1) dS = \int_{\Omega} (b^2 u^1 - b^1 u^2) dV$$

Fundamental sol.:

$$\Delta G(\boldsymbol{x}, \boldsymbol{y}) + \delta(\boldsymbol{y} - \boldsymbol{x}) = 0,\ G(\boldsymbol{x}, \boldsymbol{y}) = \tfrac{1}{4\pi||x-y||} \text{ (full-space)}$$

Boundary Integral Representation

$$\kappa u(\boldsymbol{x}) = \int_{\Omega} b(\boldsymbol{y}) G(\boldsymbol{x}, \boldsymbol{y}) dV_y + \int_{\partial\Omega} (u_{,n}(\boldsymbol{y}) G(\boldsymbol{x}, \boldsymbol{y}) - u(\boldsymbol{y}) G_{,n}(\boldsymbol{x}, \boldsymbol{y})) dS_y \quad (x \notin \partial\Omega)$$

Single and Double-layer potentials for Laplace equation

The single-layer potential solves the Laplace equation in $\mathbb{R}^3 \backslash \partial\Omega$

$$\mathcal{S}\phi(\boldsymbol{x}) := \int_{\partial\Omega} G(\boldsymbol{x}, \boldsymbol{y})\phi(\boldsymbol{y}) dS_y$$

The double-layer potential solves the Laplace equation in $\mathbb{R}^3 \backslash \partial\Omega$

$$\mathcal{D}\psi(\boldsymbol{x}) := \int_{\partial\Omega} G_{,n}(\boldsymbol{x}, \boldsymbol{y})\psi(\boldsymbol{y}) dS_y$$

Boundary Integral Representation

$$u(\boldsymbol{x}) = \int_{\Omega} b(\boldsymbol{y}) G(\boldsymbol{x}, \boldsymbol{y}) dV_y + \mathcal{S}u_{,n}(\boldsymbol{x}) - \mathcal{D}u(\boldsymbol{x})$$

Fundamental solution for Helmholtz equation

By definition

$$\Delta G + \omega^2 G = -\delta_0 \ \text{ in } \ \mathbb{R}^3$$

with $\delta_0 = \delta$: Dirac distribution at the origin

Rigorously it is true for distributions in $\mathcal{D}'(\mathbb{R}^3)$:

$$\forall v \in \mathcal{D}(\mathbb{R}^3), \ \ < \Delta G + \omega^2 G, v >= - < \delta, v >= -v(0)$$

How to derive it?

First appraoch. With Fourier since $\widehat{\delta} = 1$

$$(-|\xi|^2 + \omega^2)\widehat{G} = -1 \Rightarrow \widehat{G} = \frac{-1}{\omega^2 - |\xi|^2}$$

$$G(x) = \mathcal{F}_\xi^{-1}\left(\frac{-1}{\omega^2 - |\xi|^2}\right)$$

Second approach. We look for $G(x) = G(r)$.

Evaluation of fundamental solution for 3D Helmholtz

$G(x) = G(r)$ such that

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dG}{dr}) + \omega^2 G = \delta$$

With $z = \omega r$ and $G(r) = \frac{u(z)}{z}$, we obtain

$$\frac{d^2u(z)}{dz^2} + u(z) = 0$$

Such that $\quad G(r) = A\frac{e^{i\omega r}}{r} + B\frac{e^{-i\omega r}}{r}$

If $\omega \in \mathbb{C}^+$ we need B=0 to avoid the exponential growth at infinity.

A is obtained by evaluating

$$\forall v \in \mathcal{D}(\mathbb{R}^3), \;\; < \Delta G + \omega^2 G, v >= - < \delta, v >= -v(0)$$

Expression in 3D. $G(r) = \dfrac{1}{4\pi r}e^{i\omega r}$ with $r = |\mathbf{x} - \mathbf{y}|$

Expression in 2D. $G(r) = \dfrac{i}{4}H_0^{(1)}(\omega r)$ avec $r = |\mathbf{x} - \mathbf{y}|$

Integral Representation for Helmholtz equation

Scattering problen in Ω_ℓ ($\ell = e$ or $\ell = i$): $u \in H^1(\Omega_1)$

$$\Delta u + \omega^2 u = 0 \text{ in } \Omega_\ell$$

Rigorously we could only assume $u \in H^1(\Delta; \Omega_1)$ and use duality parings $< ., . >_{H^{-1/2}, H^{1/2}}$ instead of integrals on Γ

Notations: n normal from Ω_i to Ω_e. f^i/f^i interior/exterior traces

$$[f]_\Gamma = f^i - f^e$$

We know that

$$\Delta G(\mathbf{y}, \mathbf{x}) + \omega^2 G(\mathbf{y}, \mathbf{x}) = -\delta_x(y) \quad G(\mathbf{y}, \mathbf{x}) = G(r) = \frac{1}{4\pi r} e^{i\omega r} \text{ with } r = |x - y|$$

Derivation of Boundary Integral Representations

We want to apply the Green's formula

$$\int_\Omega (\Delta w + \omega^2 w) v d\Omega = -\int_\Omega \nabla w . \nabla v d\Omega + \omega^2 \int_\Omega w v d\Omega - \int_{\partial\Omega} \frac{\partial w}{\partial n} v d\gamma$$

with $w = u$, $v = G(\mathbf{x}, .)$ then $w = G(., \mathbf{x})$, $v = u$

But rigorously we cannot write

" $\int_\Omega (\Delta G(\mathbf{x}, .) + \omega^2 G(\mathbf{x}, .)) v d\Omega = \int_\Omega \delta_x v d\Omega$" since $\delta_x \notin L^2$

Approach: we avoid the singularity in $\mathbf{y} = \mathbf{x}$. $\forall v \in \mathcal{D}(\mathbb{R}^3)$

$$< \Delta G(\mathbf{x}, .) + \omega^2 G(\mathbf{x}, .), v >= -v(\mathbf{x})$$

$\forall D_x$ that does not include x, $\forall v \in \mathcal{D}(D_x)$

$$< \Delta G(\mathbf{x}, .) + \omega^2 G(\mathbf{x}, .), v >= 0$$

Such that

$$\Delta G(\mathbf{x}, .) + \omega^2 G(\mathbf{x}, .) = 0 \quad \text{in} \quad D_x$$

...Derivation of Boundary Integral Representations

First case: $\mathbf{x} \in \Omega^e$ such that $D_x = \Omega_i$,

$$\Delta G(\mathbf{x},\mathbf{y}) + \omega^2 G(\mathbf{x},\mathbf{y}) = 0 \quad \forall \mathbf{y} \in \Omega_i$$

and we can write

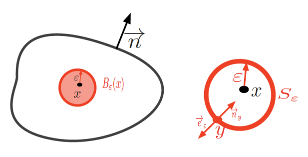
$$\int_{\Omega_i} \underbrace{(\Delta u + \omega^2 u)(\mathbf{y})}_{=0} G(r) d\Omega_y = -\int_{\Omega_i} \nabla u(\mathbf{y}).\nabla_y G(r) d\Omega_y + \omega^2 \int_{\Omega} u(\mathbf{y}) G(r) d\Omega_y - \int_{\Gamma} \frac{\partial u}{\partial n}(\mathbf{y}))^i G(r) d\gamma$$

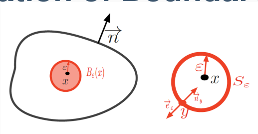
$$\int_{\Omega_i} \underbrace{(\Delta G + \omega^2 G)(r)}_{=0} u(\mathbf{y}) d\Omega_y = -\int_{\Omega_i} \nabla u(\mathbf{y}).\nabla_y G(r) d\Omega_y + \omega^2 \int_{\Omega} u(\mathbf{y}) G(r) d\Omega_y - \int_{\Gamma} \frac{\partial G}{\partial n_y}(r) u^i(\mathbf{y}) d\gamma$$

such that

$$0 = \int_{\Gamma} (\frac{\partial G}{\partial n_y}(\mathbf{x},\mathbf{y}) u^i(\mathbf{y}) - G(\mathbf{x},\mathbf{y})(\frac{\partial u}{\partial n})^i(\mathbf{y})) d\gamma_y, \quad \mathbf{x} \in \Omega_e$$

Second case $\mathbf{x} \in \Omega^i$. We remove the singularity with $D_x^\varepsilon := \Omega_i \backslash B_\varepsilon(\mathbf{x})$





$$0=\int_{\partial D_x^\varepsilon}\Big(\frac{\partial G}{\partial n_y}(x,y)u(\mathbf{y})-G(\mathbf{x},\mathbf{y})\big(\frac{\partial u}{\partial n}\big)(\mathbf{y})\Big)d\gamma_y$$

$$0=\int_{\partial\Gamma}\Big(\frac{\partial G}{\partial n_y}(\mathbf{x},\mathbf{y})u^i(\mathbf{y})-G(\mathbf{x},\mathbf{y})\big(\frac{\partial u}{\partial n}\big)^i(\mathbf{y})\Big)d\gamma_y+\int_{S_\varepsilon}\Big(\frac{\partial G}{\partial n_y}(\mathbf{x},\mathbf{y})u(\mathbf{y})-G(\mathbf{x},\mathbf{y})\big(\frac{\partial u}{\partial n}\big)(\mathbf{y})\Big)d\gamma_y$$

If $\mathbf{y}\in S_\varepsilon$, $\varepsilon=|\mathbf{y}-\mathbf{x}|$ and $-\boldsymbol{n}_y=\frac{\mathbf{y}-\mathbf{x}}{|\mathbf{y}-\mathbf{x}|}$ such that

$$G(\mathbf{x},\mathbf{y})=\frac{1}{4\pi\varepsilon}e^{i\omega\varepsilon}\quad\text{and}\quad\frac{\partial G}{\partial n_y}(\mathbf{x},\mathbf{y})=\frac{1}{4\pi\varepsilon}\big(\frac{1}{\varepsilon}-i\omega\big)e^{i\omega\varepsilon}$$

u is regular for every D that do not touch Γ: $u(\mathbf{y})=u(\mathbf{x})+O(\varepsilon)$

$$\int_{S_\varepsilon}\frac{\partial G}{\partial n_y}(\mathbf{x},\mathbf{y})u(\mathbf{y})d\gamma_y=\int_{\theta=0}^{2\pi}\int_{\varphi=0}^{\pi}\frac{1}{4\pi\varepsilon}\big(\frac{1}{\varepsilon}-i\omega\big)e^{i\omega\varepsilon}(u(\mathbf{x})+O(\varepsilon))\varepsilon^2\sin\varphi d\theta d\varphi$$

$$=\frac{1}{4\pi}u(\mathbf{x})e^{i\omega\varepsilon}\int_{\theta=0}^{2\pi}\int_{\varphi=0}^{\pi}\varepsilon^2\sin\varphi d\theta d\varphi+O(\varepsilon)\longrightarrow u(\mathbf{x})$$

$$\Big|\int_{S_\varepsilon}\frac{\partial u}{\partial n_y}(\mathbf{y})G(\mathbf{x},\mathbf{y})d\gamma_y\Big|\longrightarrow 0$$

Representation Theorem

(a) If u is solution in Ω_i then

$$\int_\Gamma \left(G(x,y) \left(\frac{\partial u}{\partial n}\right)^i (y) - \frac{\partial G}{\partial n_y}(x,y) u^i(y) \right) d\gamma_y = \begin{cases} u(x) \text{ if } x \in \Omega_i \\ 0 \text{ if } x \in \Omega_e \end{cases}$$

(b) If u is solution in Ω_e then (with the normal still from Ω_i to Ω_e)

$$\int_\Gamma \left(-G(x,y) \left(\frac{\partial u}{\partial n}\right)^e (y) + \frac{\partial G}{\partial n_y}(x,y) u^e(y) \right) d\gamma_y = \begin{cases} 0 \text{ if } x \in \Omega_i \\ u(x) \text{ if } x \in \Omega_e \end{cases}$$

(c) If u is solution in $\Omega_i \cup \Omega_e$ then

$$\forall x \in \Omega_i \cup \Omega_e,\ u(x) = \int_\Gamma \left(G(x,y) \left[\frac{\partial u}{\partial n}\right]_\Gamma (y) - \frac{\partial G}{\partial n_y}(x,y) [u]_\Gamma(y) \right) d\gamma_y$$

What is next?

For exterior problems, we have

$$u(\mathbf{x}) = \int_\Gamma \left(-G(\mathbf{x},\mathbf{y}) \left(\frac{\partial u}{\partial n} \right)^e (\mathbf{y}) + \frac{\partial G}{\partial n_y}(\mathbf{x},\mathbf{y}) u^e(\mathbf{y}) \right) d\gamma_y, \quad \forall \mathbf{x} \in \Omega_e, \mathbf{x} \notin \Gamma$$

☺ u in the domain is known only from values on boundary

☺ Reduction of computational costs and memory requirements

It is a Boundary Integral Representation (not an equation)

You need to obtain the traces of u on Γ (with an equation)

The Boundary Element Method is a two steps methods

1. Resolution of a boundary integral equation to obtain traces (TP2)
2. Application of the boundary integral representation to obtain solution in the domain (TP1)

Philosophie des TPs

But des trois TPs: mettre en oeuvre un solveur BEM rapide pour l'équation de Hemholtz 2D

Diffraction d'une onde incidente plane par un disque de rayon a centré en $\mathbf{0}$ et de frontière Γ

- $u^{inc} = e^{-i\mathbf{k}.\mathbf{x}}$
- $\mathbf{k}$: est le vecteur qui permet de déterminer l'angle d'incidence de l'onde (prendre un angle nul)
- Nombre d'onde: $k = |\mathbf{k}|$
- Domaine extérieur est noté Ω^+

Solution analytique pour le problème de Dirichlet: $u^+ + u^{inc} = 0$ sur Γ

$$e^{-ikr\cos\theta} = \sum_{n\in\mathbb{Z}} (-i)^n J_n(kr) e^{in\theta}$$

$$u^+(r,\theta) = \sum_{n\in\mathbb{Z}} A_n H_n^{(1)}(kr) e^{in\theta}, \quad r \geq a$$

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$$e^{-ikr\cos\theta} = \sum_{n\in\mathbb{Z}} (-i)^n J_n(kr) e^{in\theta}$$

$$u^+(r,\theta) = -\sum_{n\in\mathbb{Z}} (-i)^n \frac{J_n(ka)}{H_n^{(1)}(ka)} H_n^{(1)}(kr) e^{in\theta}, \quad r \geq a$$

TP0: Solution analytique - Génération du maillage

Générer un maillage du bord du disque: d’abord les noeuds du maillage puis les extrémités de chaque segment.

Quel est le nombre de segments (en fonction du nombre de noeuds du maillage)?

Etape 2: Trace de p analytique

$$p = -\partial_{\mathbf{n}} u^{+} - \partial_{\mathbf{n}} u^{inc}$$

- Déterminer la trace de p sur Γ
- La coder

Dans la réalité cette trace est obtenue en résolvant une équation intégrale. Pour avancer progressivement dans le TP et comprendre les notions les unes après les autres, on considère un cas avec une solution de référence

Vous aurez besoin de la formule suivante:

$$\frac{d}{dr} H_n^{(1)}(kr) = \frac{k}{2}\left(H_{n-1}^{(1)}(kr) - H_{n+1}^{(1)}(kr)\right) \tag{1}$$