

Méthode d'éléments de frontière

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Outline

1. Review of boundary integral equation formulations

Electrostatics

Laplace

Elastostatics

Frequency-domain wave equations

2. Review of classical BEM concepts

3. The GMRES iterative solver

4. The fast multipole method (FMM) for the Laplace equation

Multipole expansion of $1/r$

The single-level fast multipole method

The multi-level fast multipole method

5. The fast multipole method (FMM) for elastostatics

6. The fast multipole method for elastodynamics

7. Other acceleration methods

Exponential representation of $1/r$

FMM using equivalent sources

Clustering and low-rank approximations

Kernel-independent acceleration via kernel interpolation

Adaptive cross approximation

8. Preconditioning

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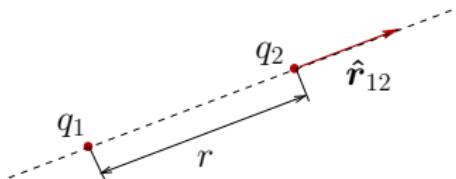
Electrostatics

- ▶ Well-known, and simple, physical setting
- ▶ Allows to introduce important concepts of integral equation formulations with a clear physical meaning
- ▶ Said concepts will generalize to other settings (elasticity, electromagnetics...)
- ▶ Also helpful later for a physical understanding of the fast multipole method (FMM)

Electrostatics: discrete charged particles

- ▶ Coulomb interaction force:

$$\mathbf{F}_{12} = \frac{q_1 q_2}{4\pi\epsilon} \frac{1}{r^2} \hat{\mathbf{r}}_{12}$$



- ▶ Electrostatic field:

$$\mathbf{F}_{12} = q_2 \mathbf{E}_{12}, \quad \mathbf{E}_{12} = \frac{q_1}{4\pi\epsilon} \frac{1}{r^2} \hat{\mathbf{r}}_{12}$$

- ▶ Electrostatic potential:

$$\mathbf{E}_{12} = -\nabla_2 V, \quad V = \frac{q_1}{4\pi\epsilon} \frac{1}{r}$$

(with ϵ : **permittivity** of the medium (material constant))

Electrostatics: continuous charge distributions

- Continuous charge distribution: $dq = \rho dV$:

$$\mathbf{E}(\mathbf{x}) = \frac{1}{4\pi\epsilon} \int_V \frac{\rho(\xi)}{r^2} \hat{\mathbf{r}} dV_\xi \quad \mathbf{r} = \xi - \mathbf{x}, \quad r = \|\mathbf{r}\|, \quad \hat{\mathbf{r}} = \mathbf{r}/r$$

- Gauss theorem:

$$\operatorname{div} \mathbf{E} = \frac{\rho}{\epsilon}$$

- Poisson equation (Gauss theorem with $\mathbf{E} = -\nabla V$):

$$\Delta V + \frac{\rho}{\epsilon} = 0$$

Electrostatics: continuous charge distributions

Proof of Gauss theorem:

$$\begin{aligned}\int_V \operatorname{div} \mathbf{E} dV &= \int_{\partial V} \mathbf{E} \cdot \mathbf{n} dS \\ &= \frac{1}{4\pi\varepsilon} \int_V \left\{ \int_{\partial V} \frac{1}{r^2} (\hat{\mathbf{r}} \cdot \mathbf{n}(\mathbf{x})) dS_x \right\} \varrho(\xi) dV_\xi \\ &= \frac{1}{4\pi\varepsilon} \int_V \Theta(\xi) \varrho(\xi) dV_\xi\end{aligned}$$

where $\Theta(\xi)$ is the **solid angle** of the (closed) surface ∂V from origin ξ :

$$\Theta(\xi) = 4\pi \quad (\xi \in V), \quad \Theta(\xi) = 0 \quad (\xi \in \mathbb{R}^3 \setminus \bar{V})$$

Hence:

$$\int_V \operatorname{div} \mathbf{E} dV = \int_V \frac{\varrho}{\varepsilon} dV$$

Since this is true for any domain V , one has $\operatorname{div} \mathbf{E} = \varrho/\varepsilon$, i.e. the Gauss theorem holds.

Electrostatic volume potential

The electrostatic volume potential results from the superposition of electric fields generated by elementary charges $\varrho \, dV$ distributed in a volume V :

$$\mathcal{V}[\varrho, V](\mathbf{x}) = \frac{1}{4\pi\epsilon} \int_V \frac{\varrho(\xi)}{r} \, dV_\xi$$

As already seen, $\mathcal{V}[\varrho, V]$ satisfies the Poisson equation:

$$\Delta \mathcal{V}[\varrho, V] + \frac{\varrho}{\epsilon} = 0 \quad (\mathbf{x} \in V), \quad \Delta \mathcal{V}[\varrho, V] = 0 \quad (\mathbf{x} \in \mathbb{R}^3 \setminus \bar{V})$$

Properties of electrostatic volume potentials

- The volume integral is weakly singular (i.e. singular, but integrable) for $\mathbf{x} \in V$, so that $\mathcal{V}[\varrho, V]$ is well-defined inside the charged domain V : one has

$$dV_x = r^2 dr d\Theta = O(r^2)$$

- $\mathcal{V}[\varrho, V]$ is continuous everywhere, and in particular across the boundary ∂V .

Electrostatic single-layer potential

The electrostatic single-layer potential results from the superposition of electric fields generated by elementary charges ϱdS distributed on a surface S :

$$\mathcal{S}[\varrho, S](\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \int_S \frac{\varrho(\xi)}{r} dS_\xi$$

$\mathcal{S}[\varrho, S]$ is harmonic outside of S :

$$\Delta \mathcal{S}[\varrho, S] = 0 \quad (\mathbf{x} \in \mathbb{R}^3 \setminus S)$$

Properties of electrostatic single-layer potentials

- The surface integral is weakly singular (i.e. singular, but integrable) for $\mathbf{x} \in S$, so that $\mathcal{S}[\varrho, S]$ is well-defined on the charged surface V : one has

$$dS_x = r dr d\theta = O(r)$$

- $\mathcal{S}[\varrho, S]$ is continuous everywhere, and in particular across S .

Electrostatic double-layer potential

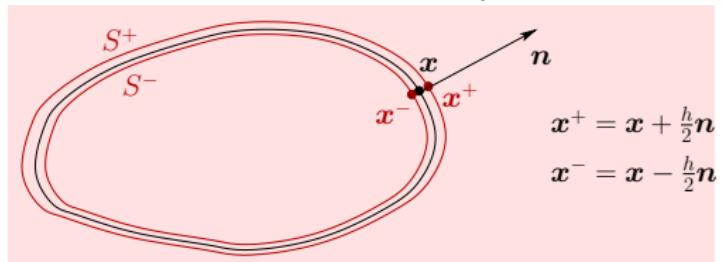
The electrostatic double-layer potential is the limiting case of the superposition of two single-layer potentials of (i) arbitrary close supports S^\pm , (ii) opposite charge density, (iii) finite dipolar moment q :

$$\mathcal{D}[q, S](\mathbf{x}) = \lim_{h \rightarrow 0} \mathcal{S}[\varrho_h, S^+](\mathbf{x}) + \mathcal{S}[-\varrho_h, S^-](\mathbf{x})$$

with

$$\lim_{h \rightarrow 0} [h\varrho_h](\mathbf{x}) = q(\mathbf{x})$$

(note: q is analogous to a concentrated moment)



Performing the limit $h \rightarrow 0$, one finds:

$$\mathcal{D}[q, S](\mathbf{x}) = -\frac{1}{4\pi\epsilon} \int_S \frac{1}{r^2} \hat{\mathbf{r}} \cdot \mathbf{n}(\xi) q(\xi) dS_\xi$$

Electrostatic double-layer potential

$$\mathcal{D}[q, S](\mathbf{x}) = -\frac{1}{4\pi\varepsilon} \int_S \frac{1}{r^2} \hat{\mathbf{r}} \cdot \mathbf{n}(\xi) q(\xi) dS_\xi$$

Properties of electrostatic double-layer potentials

- $\mathcal{D}[q, S]$ is harmonic outside of S :

$$\Delta \mathcal{D}[q, S] = 0 \quad (\mathbf{x} \in \mathbb{R}^3 \setminus S)$$

- The surface integral is weakly singular (i.e. singular, but integrable) for $\mathbf{x} \in S$, so that $\mathcal{D}[q, S]$ is well-defined on the charged surface V .

This is not obvious and stems from

$$dS_x = r dr d\theta = O(r) \quad \text{and} \quad \frac{1}{r^2} \hat{\mathbf{r}} \cdot \mathbf{n} = O\left(\frac{1}{r}\right)$$

- $\mathcal{D}[q, S]$ is **discontinuous** across S , with

$$\mathcal{D}[q, S](\mathbf{x}^+) - \mathcal{D}[q, S](\mathbf{x}^-) = q(\mathbf{x})$$

Electrostatic potentials: comments

- (a) Electrostatic potentials have a clear physical meaning as the potential fields associated with volume, surface or dipolar charge distributions.
- (b) Electrostatic potentials, as mathematical constructs, define harmonic fields for arbitrary choices of supports V, S and densities ϱ, q .
- (c) As we will shortly see, **any** harmonic function can be expressed in terms of such potentials.

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Physical problems governed by the Laplace or Poisson equation

Poisson equation:

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

(Laplace equation if $b=0$)

- ▶ Electrostatics (u : electrostatic potential);
- ▶ Potential fluid flow (u : velocity potential);
- ▶ Thermal equilibrium (u : temperature);
- ▶ Torsion (u : warping function defined on 2-D section of shaft)

...

Reciprocity identity and integral representation

$$\Delta u + b = 0 \quad (\text{in } \Omega) \quad + \text{unspecified well-posed BCs}$$

Integral representation of u based on two ingredients:

(i) Reciprocity identity:

$$\int_{\Omega} (u \Delta v - v \Delta u) \, dV = \int_{\partial\Omega} (uv_{,n} - vu_{,n}) \, dV \quad (u_{,n} \equiv \nabla u \cdot \mathbf{n})$$

(ii) Fundamental solution:

$$\Delta G(\mathbf{x}, \cdot) + \delta(\cdot - \mathbf{x}) = 0 \quad (\text{in } \mathcal{O} \supset \Omega)$$

Choosing $v = G(\mathbf{x}, \cdot)$ in (i) yields the **integral representation formula**:

$$u(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}, \xi) b(\xi) \, dV_{\xi} + \int_{\partial\Omega} (G(\mathbf{x}, \xi) u_{,n}(\xi) - G_{,n}(\mathbf{x}, \xi) u(\xi)) \, dS_{\xi} \quad (\mathbf{x} \in \Omega)$$

Full-space fundamental solution ($\mathcal{O} = \mathbb{R}^3$):

$$G(\mathbf{x}, \xi) = \frac{1}{4\pi r} \quad (r = \|\xi - \mathbf{x}\|)$$

Volume and single-layer potentials

- The **single-layer potential** \mathcal{S} solves the Laplace equation in $\mathbb{R}^3 \setminus \partial\Omega$, where

$$\mathcal{S}[\varphi, \partial\Omega](\mathbf{x}) := \int_{\partial\Omega} G(\mathbf{x}, \xi) \varphi(\xi) dS_\xi$$

The **volume potential** \mathcal{V} solves the Poisson equation, where

$$\mathcal{V}[b, \Omega](\mathbf{x}) := \int_{\Omega} G(\mathbf{x}, \xi) b(\xi) dV_\xi$$

- Continuity across $\partial\Omega$ (with $\llbracket f \rrbracket := f^+ - f^-$):

$$\llbracket \mathcal{V}(\mathbf{x}) \rrbracket = 0, \quad \llbracket \mathcal{S}(\mathbf{x}) \rrbracket = 0, \quad (\mathbf{x} \in \partial\Omega)$$

Double-layer potentials

- The following potential solve the Laplace equation in $\mathbb{R}^3 \setminus \partial\Omega$:

$$\mathcal{D}[\psi, \partial\Omega](\mathbf{x}) := \int_{\partial\Omega} G_n(\mathbf{x}, \xi) \psi(\xi) dS_\xi \quad (\text{double-layer potential})$$

- Jump relation:

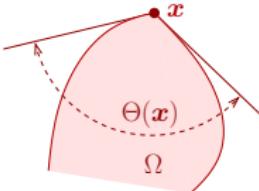
$$[\![\mathcal{D}(\mathbf{x})]\!] = \psi(\mathbf{x}) \quad (\mathbf{x} \in \partial\Omega)$$

- Boundary traces of double-layer potential:

$$\begin{aligned}\mathcal{D}[\psi, \partial\Omega](\mathbf{x}^-) &= (c(\mathbf{x}) - 1)\psi(\mathbf{x}) + \mathcal{D}[\psi, \partial\Omega](\mathbf{x}), \\ \mathcal{D}[\psi, \partial\Omega](\mathbf{x}^+) &= \mathcal{D}[\psi, \partial\Omega](\mathbf{x}^-) + \psi(\mathbf{x})\end{aligned}$$

with the definitions ($\Theta(\mathbf{x})$: solid angle of Ω seen from $\mathbf{x} \in \partial\Omega$):

$$\mathcal{D}[\psi, \partial\Omega](\mathbf{x}) := \int_{\partial\Omega} G_n(\mathbf{x}, \xi) \psi(\xi) dS_\xi, \quad c(\mathbf{x}) = \Theta(\mathbf{x})/(4\pi) \quad (\mathbf{x} \in \partial\Omega)$$



When $\partial\Omega$ is smooth at \mathbf{x} (the usual case), $\Theta(\mathbf{x}) = 2\pi$ and $c(\mathbf{x}) = 1/2$

Integral representation as sum of potentials

Expressing the integral representation formula in terms of potentials yields

$$u(\mathbf{x}) = \mathcal{V}[b, \Omega](\mathbf{x}) + \mathcal{S}[u_n, \partial\Omega](\mathbf{x}) - \mathcal{D}[u, \partial\Omega](\mathbf{x})$$

Any harmonic function is representable as a single-layer, or a double-layer potential, or a linear combination of both.

Any solution of the Poisson equation is representable as a sum of the volume potential of density b and arbitrary surface potentials.

Singular integral equations

Boundary integral equations are obtained as the limiting situation when $\mathbf{z} \in \Omega \rightarrow \mathbf{z} \in \partial\Omega$ of integral representations:

$$\begin{aligned} u(\mathbf{x}) &= \lim_{\mathbf{z} \rightarrow \mathbf{x}} u(\mathbf{z}) \\ &= \lim_{\mathbf{z} \rightarrow \mathbf{x}} \left[\mathcal{V}[b, \Omega](\mathbf{z}) + \mathcal{S}[u, n, \partial\Omega](\mathbf{z}) - \mathcal{D}[u, \partial\Omega](\mathbf{z}) \right] \\ &= \mathcal{V}[b, \Omega](\mathbf{x}) + \mathcal{S}[u, n, \partial\Omega](\mathbf{x}) - \mathcal{D}[u, \partial\Omega](\mathbf{x}) + (1 - c(\mathbf{x}))u(\mathbf{x}) \end{aligned}$$

to obtain:

$$c(\mathbf{x})u(\mathbf{x}) + \mathcal{D}[u, \partial\Omega](\mathbf{x}) - \mathcal{S}[u, n, \partial\Omega](\mathbf{x}) = \mathcal{V}[b, \Omega](\mathbf{x}) \quad (\mathbf{x} \in \partial\Omega)$$

i.e. (in expanded form)

$$c(\mathbf{x})u(\mathbf{x}) + \int_{\partial\Omega} (G_{,n}(\mathbf{x}, \xi)u(\xi) - G(\mathbf{x}, \xi)u_n(\xi)) dS_\xi = \int_{\Omega} G(\mathbf{x}, \xi)b(\xi) dV_\xi \quad (\mathbf{x} \in \partial\Omega)$$

Outline of the boundary integral equation method

$$c(\mathbf{x})u(\mathbf{x}) + \mathcal{D}[u, \partial\Omega](\mathbf{x}) - \mathcal{S}[u_{,n}, \partial\Omega](\mathbf{x}) = \mathcal{V}[b, \Omega](\mathbf{x}) \quad (\mathbf{x} \in \partial\Omega)$$

1. Insert given boundary data;
Solve for the remaining boundary unknown
2. Then, invoke integral representation for evaluation of \mathbf{u} (and related quantities, e.g. $\nabla \mathbf{u}$) at interior points

Example ($\partial\Omega = S_u \cup S_q$, with $\mathbf{u} = \mathbf{u}^D$ on S_u and $u_{,n} = q^D$ on S_q):

1. Solve for $u|_{S_q}$ and $u_{,n}|_{S_u}$ the integral equation system

$$\begin{aligned} & c(\mathbf{x})u(\mathbf{x}) + \mathcal{D}[u, S_q](\mathbf{x}) - \mathcal{S}[u_{,n}, S_u](\mathbf{x}) \\ &= -\mathcal{D}[u^D, S_u](\mathbf{x}) + \mathcal{S}[q^D, S_q](\mathbf{x}) + \mathcal{V}[b, \Omega](\mathbf{x}) \quad (\mathbf{x} \in S_q) \\ & \mathcal{D}[u, S_q](\mathbf{x}) - \mathcal{S}[u_{,n}, S_u](\mathbf{x}) \\ &= -c(\mathbf{x})u^D(\mathbf{x}) - \mathcal{D}[u^D, S_u](\mathbf{x}) + \mathcal{S}[q^D, S_q](\mathbf{x}) + \mathcal{V}[b, \Omega](\mathbf{x}) \quad (\mathbf{x} \in S_u) \end{aligned}$$

2. Integral representation:

$$u(\mathbf{x}) = \mathcal{V}[b, \Omega](\mathbf{x}) + \mathcal{S}[u_{,n}, \partial\Omega](\mathbf{x}) - \mathcal{D}[u, \partial\Omega](\mathbf{x})$$

Fundamental solution, Green's function

$$\Delta u + b = 0 \quad (\text{in } \Omega) \quad u = u^D \quad (\text{on } S_u), \quad u_{,n} = q^D \quad (\text{on } S_q)$$

- ▶ Fundamental solution (again):

$$\Delta G(\mathbf{x}, \cdot) + \delta(\cdot - \mathbf{x}) = 0 \quad (\text{in } \mathcal{O} \supset \Omega)$$

i.e. **any** field induced in Ω by a unit point source placed at $\mathbf{x} \in \Omega$

- ▶ Green's function: fundamental solution with homogeneous BCs on $\partial\Omega$:

$$\Delta_\xi \mathcal{G}(\mathbf{x}, \cdot) + \delta(\cdot - \mathbf{x}) = 0 \quad (\text{in } \Omega)$$

$$\mathcal{H}(\mathbf{x}, \cdot) := \nabla \mathcal{G}(\mathbf{x}, \cdot) \cdot \mathbf{n}(\cdot) = 0 \quad (\text{on } S_q),$$

$$\mathcal{G}(\mathbf{x}, \cdot) = 0 \quad (\text{on } S_u)$$

- ▶ Fundamental solution → boundary unknowns u (on S_q) and $u_{,n}$ (on S_u) (boundary integral equation needed)
- ▶ Green's function → **explicit** integral representation formula (boundary integral equation **not** needed)

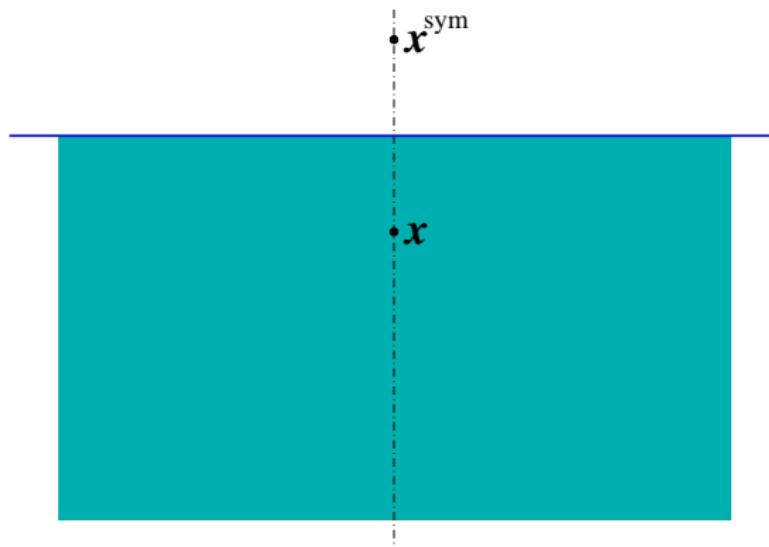
$$u(\mathbf{x}) = \int_{\Omega} \mathcal{G}(\mathbf{x}, \boldsymbol{\xi}) b(\boldsymbol{\xi}) dV_{\boldsymbol{\xi}} + \int_{S_q} \mathcal{G}(\mathbf{x}, \boldsymbol{\xi}) q^D(\boldsymbol{\xi}) dS_{\boldsymbol{\xi}} - \int_{S_u} \mathcal{H}(\mathbf{x}, \boldsymbol{\xi}) u^D(\boldsymbol{\xi}) dS_{\boldsymbol{\xi}} \quad (\mathbf{x} \in \Omega)$$

Green's functions (Laplace): half-space

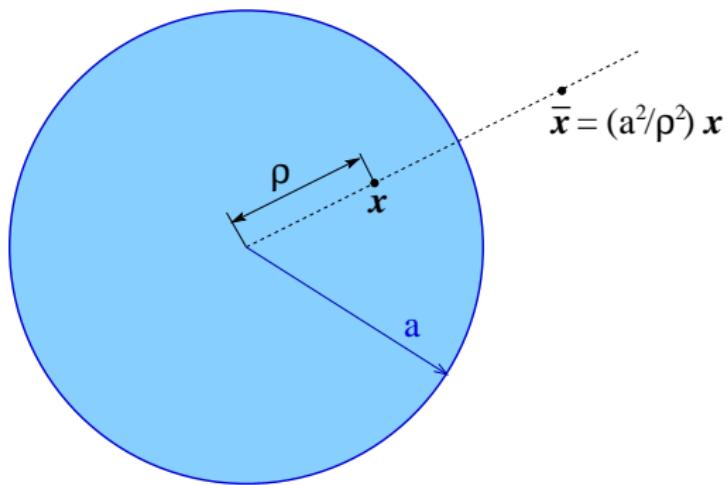
"Method of images":

$$\mathcal{G}(\mathbf{x}, \xi) = G(\mathbf{x}, \xi) + G(\mathbf{x}^{\text{sym}}, \xi) \quad \text{Neumann BC on free surface}$$

$$\mathcal{G}(\mathbf{x}, \xi) = G(\mathbf{x}, \xi) - G(\mathbf{x}^{\text{sym}}, \xi) \quad \text{Dirichlet BC on free surface}$$



Green's functions (Laplace): sphere



$$\mathcal{G}(x, \xi) = \frac{1}{4\pi} \left(\frac{1}{r} - \frac{a}{\rho} \frac{1}{\bar{r}} \right) \quad (\text{Dirichlet BC on surface})$$

Indirect boundary integral equations:

- ▶ Seek solutions of Laplace equation using potentials:

$$u(\mathbf{x}) = \mathcal{S}[\varphi, \partial\Omega](\mathbf{x}) + \mathcal{D}[\psi, \partial\Omega](\mathbf{x}) \quad (\mathbf{x} \in \Omega)$$

Dirichlet problem ($u = u^D$ on $\partial\Omega$) using double-layer potential:

$$-c(\mathbf{x})\psi(\mathbf{x}) + \mathcal{D}[\psi, \partial\Omega](\mathbf{x}) = u^D(\mathbf{x}) \quad (\mathbf{x} \in \partial\Omega)$$

Neumann problem ($u_{,n} = p^D$ on $\partial\Omega$) using single-layer potential:

$$c(\mathbf{x})\varphi(\mathbf{x}) - \partial_{n(\mathbf{x})}\mathcal{S}[\varphi, \partial\Omega](\mathbf{x}) = p^D(\mathbf{x}) \quad (\mathbf{x} \in \partial\Omega)$$

- ▶ Seek solutions of Poisson equation using potentials:

$$u(\mathbf{x}) = \mathcal{V}[b, \partial\Omega](\mathbf{x}) + \mathcal{S}[\varphi, \partial\Omega](\mathbf{x}) + \mathcal{D}[\psi, \partial\Omega](\mathbf{x}) \quad (\mathbf{x} \in \Omega)$$

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Reciprocity identity and integral representation

- Additive decomposition of strain into elastic and initial (e.g. thermal, plastic, visco-plastic) parts (assuming infinitesimal strain):

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^E + \boldsymbol{\varepsilon}^I \quad \text{where} \quad \boldsymbol{\sigma} = \mathcal{C} : \boldsymbol{\varepsilon}^E$$

- Constitutive equation (\mathcal{C} : fourth-order tensor of elastic moduli):

$$\boldsymbol{\sigma} = \mathcal{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^I)$$

- For isotropic elasticity (μ : shear modulus, ν : Poisson ratio):

$$\mathcal{C}_{ijkl} = \mu \left[\frac{2\nu}{1-2\nu} \delta_{ij}\delta_{kl} + (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \right]$$

- Governing field equation for unknown displacement field $\mathbf{u}(\xi)$:

$$\mathcal{C}_{ijab}(u_{a,bj} - \varepsilon_{ab,j}^I) + b_i = 0 \quad (\xi \in \Omega)$$

Elastostatic fundamental solution

Kelvin fundamental solution: unit point force applied at $\mathbf{x} \in \mathbb{R}^3$ along k -direction in unbounded elastic medium, i.e.:

$$C_{ijab} U_{a,bj}^k + \delta(\cdot - \mathbf{x}) \delta_{ik} = 0 \quad (\xi \in \mathbb{R}^3)$$

$$U_i^k(\mathbf{x}, \xi) = \frac{1}{16\pi\mu(1-\nu)} \frac{1}{r} [\hat{r}_i \hat{r}_k + (3 - 4\nu) \delta_{ik}]$$

$$\Sigma_{ij}^k(\mathbf{x}, \xi) = -\frac{1}{8\pi(1-\nu)} \frac{1}{r^2} [3\hat{r}_i \hat{r}_k \hat{r}_j + (1 - 2\nu)(\delta_{ik} \hat{r}_j + \delta_{jk} \hat{r}_i - \delta_{ij} \hat{r}_k)] \quad \mathbf{x}, \xi \in \mathbb{R}^3$$

$$T_i^k(\mathbf{x}, \xi) = \Sigma_{ij}^k(\mathbf{x}, \xi) n_j(\xi)$$

$$(r = |\xi - \mathbf{x}|, \quad \hat{r}_i = (\xi_i - x_i)/r)$$

Reciprocity identity and integral representation

Governing field equation for unknown displacement field $\mathbf{u}(\xi)$:

$$\int_{\Omega} \left\{ C_{ijab} (u_{a,bj} - \varepsilon^l_{ab,j}) + b_i \right\} \times U_i^k(\mathbf{x}, \xi) dV_\xi = 0 \quad (1)$$

Governing field equation for fundamental solution:

$$\int_{\Omega} \left\{ C_{ijab} U_{a,bj}^k + \delta(\xi - \mathbf{x}) \delta_{ik} \right\} \times u_i(\xi) dV_\xi = 0 \quad (2)$$

Performing (1)-(2) and invoking the divergence identity, one obtains the **integral representation formula** of the displacement:

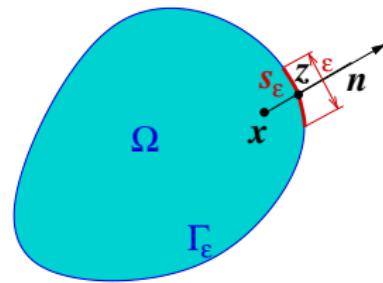
$$\boxed{u_k(\mathbf{x}) = \int_{\partial\Omega} \left\{ U_i^k(\mathbf{x}, \xi) t_i(\xi) - T_i^k(\mathbf{x}, \xi) u_i(\xi) \right\} dS_\xi + \int_{\Omega} \left\{ U_i^k(\mathbf{x}, \xi) b_i(\xi) + \Sigma_{ij}^k(\mathbf{x}, \xi) \varepsilon_{ij}^l(\xi) \right\} dV_\xi}$$

- ▶ **Partially unknown** contribution of $\partial\Omega$ (BC + unknown trace)
- ▶ **Known** contribution of Ω (if ε^l is known beforehand)

Displacement boundary integral equation

Limiting process as $\mathbf{x} \in \Omega \longrightarrow \mathbf{z} \in \partial\Omega$ in integral representation:

$$\begin{aligned} u_k(\mathbf{x}) = & \int_{\partial\Omega} \left\{ U_i^k(\mathbf{x}, \xi) t_i(\xi) - T_i^k(\mathbf{x}, \xi) u_i(\xi) \right\} dS_\xi \\ & + \int_{\Omega} \left\{ U_i^k(\mathbf{x}, \xi) b_i(\xi) + \Sigma_{ij}^k(\mathbf{x}, \xi) \varepsilon_{ij}^l(\xi) \right\} dV_\xi \end{aligned}$$



Non-integrable singularity of $\mathbf{T}^k(\mathbf{x}, \xi)$:

- ▶ Limit to the boundary approach
- ▶ Direct approach using exclusion neighbourhood of \mathbf{z}
- ▶ Indirect regularization approach

Displacement boundary integral equation

Integral equation, singular form:

$$\begin{aligned} \frac{1}{2} u_k(\mathbf{x}) + \text{P.V.} \int_{\partial\Omega} T_i^k(\mathbf{x}, \xi) u_i(\xi) dS_\xi - \int_{\partial\Omega} U_i^k(\mathbf{x}, \xi) t_i(\xi) dS_\xi \\ = \int_{\Omega} \left\{ U_i^k(\mathbf{x}, \xi) b_i(\xi) + \Sigma_{ij}^k(\mathbf{x}, \xi) \varepsilon_{ij}^l(\xi) \right\} dV_\xi \end{aligned}$$

Integral equation, regularized form:

$$\begin{aligned} \int_{\partial\Omega} \left\{ T_i^k(\mathbf{x}, \xi) [u_i(\xi) - u_i(\mathbf{x})] - U_i^k(\mathbf{x}, \xi) t_i(\xi) \right\} dS_\xi \\ = \int_{\Omega} \left\{ U_i^k(\mathbf{x}, \xi) b_i(\xi) + \Sigma_{ij}^k(\mathbf{x}, \xi) \varepsilon_{ij}^l(\xi) \right\} dV_\xi \end{aligned}$$

- ▶ Both forms require $\mathbf{u} \in C^{0,\alpha}$ (otherwise process $\mathbf{x} \in \Omega \rightarrow \mathbf{z} \in \partial\Omega$ breaks down)
- ▶ Numerical implementation based on (well-documented) singular element integration methods.
- ▶ Boundary-only formulations in the absence of body forces and initial strains.
- ▶ Treatments (double / multiple reciprocity methods) sometimes allow to convert domain integrals with $\mathbf{b}, \boldsymbol{\varepsilon}^l$ into boundary integrals.

Volume, single-layer and double-layer elastic potentials

- ▶ Volume potential (prescribed body forces):

$$\mathcal{V}_k^b[\mathbf{b}, \Omega](\mathbf{x}) = \int_{\Omega} U_i^k(\mathbf{x}, \xi) b_i(\xi) dV_\xi$$

(displacement field created in \mathbb{R}^3 by \mathbf{b} given on Ω)

- ▶ Volume potential (prescribed initial strains):

$$\mathcal{V}_k^\varepsilon[\varepsilon^!, \Omega](\mathbf{x}) = \int_{\Omega} \Sigma_{ij}^k(\mathbf{x}, \xi) \varepsilon_{ij}^!(\xi) dV_\xi$$

(displacement field created in \mathbb{R}^3 by $\varepsilon^!$ given on Ω)

- ▶ Single-layer elastic potential:

$$\mathcal{S}[\varphi, \partial\Omega]_k(\mathbf{x}) = \int_{\partial\Omega} U_i^k(\mathbf{x}, \xi) \varphi_i(\xi) dS_x$$

- ▶ Double-layer elastic potential:

$$\mathcal{D}[\psi, \partial\Omega]_k(\mathbf{x}) = \int_{\partial\Omega} T_i^k(\mathbf{x}, \xi) \psi_i(\xi) dS_x$$

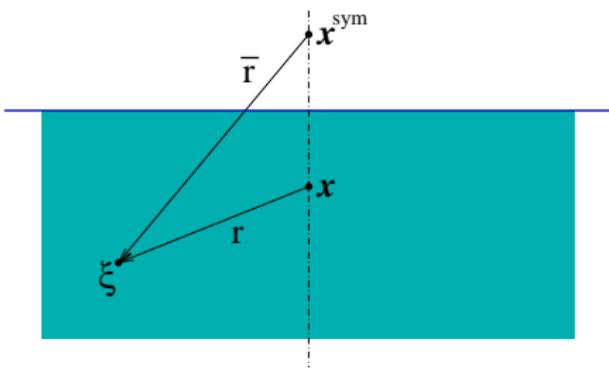
Green's tensor (elasticity): half-space (Mindlin solution)

$$U_i^k(\mathbf{x}, \xi) = \frac{1}{16\pi\mu(1-\nu)} \left\{ \frac{\kappa}{r} \delta_{ik} + \frac{1}{\bar{r}} \delta_{ik} + \frac{r_{,i} r_{,k}}{r} + \kappa \frac{\bar{r}_{,i} \bar{r}_{,k}}{\bar{r}} + \frac{2x_3 y_3}{\bar{r}^3} [\delta_{ik} - 3\bar{r}_{,i} \bar{r}_{,k}] \right. \\ \left. + \frac{\chi}{\bar{r}(1+\bar{r}_{,3})} \left[\delta_{ik} - \frac{\bar{r}_{,i} \bar{r}_{,k}}{1+\bar{r}_{,3}} \right] \right\}$$

$$U_3^k(\mathbf{x}, \xi) = \frac{1}{16\pi\mu(1-\nu)} \left\{ \frac{r_{,3} r_{,k}}{r} + \kappa \frac{\bar{r}_{,k}}{\bar{r}} \left[\bar{r}_{,3} - \frac{2x_3}{\bar{r}} \right] - \frac{6x_3 y_3}{\bar{r}^3} \bar{r}_{,3} \bar{r}_{,k} + \chi \frac{\bar{r}_{,k}}{\bar{r}(1+\bar{r}_{,3})} \right\}$$

$$U_i^3(\mathbf{x}, \xi) = \frac{1}{16\pi\mu(1-\nu)} \left\{ \frac{r_{,i} r_{,3}}{r} + \kappa \frac{\bar{r}_{,k}}{\bar{r}} \left[\bar{r}_{,3} - \frac{2x_3}{\bar{r}} \right] + \frac{6x_3 y_3}{\bar{r}^3} \bar{r}_{,i} \bar{r}_{,3} - \chi \frac{\bar{r}_{,i}}{\bar{r}(1+\bar{r}_{,3})} \right\}$$

$$U_3^3(\mathbf{x}, \xi) = \frac{1}{16\pi\mu(1-\nu)} \left\{ \frac{\kappa}{r} + \frac{1+\chi}{\bar{r}} + \frac{r_{,3}^2}{r} + \kappa \frac{\bar{r}_3 \bar{r}_3}{\bar{r}} - \frac{2x_3 y_3}{\bar{r}^3} [1 - 3\bar{r}_{,3} \bar{r}_{,3}] \right\}$$



$$(\kappa = 3 - 4\nu, \chi = 4(1 - \nu)(1 - 2\nu))$$

Green's tensors (elasticity)

- ▶ Full-space (Kelvin):
exact solutions (within full-space idealization):
→ Response to arbitrary eigenstrain distribution:

$$u_k(\mathbf{x}) = \int_{\Omega} \Sigma_{ij}^k(\mathbf{x}, \boldsymbol{\xi}) \varepsilon_{ij}^l(\boldsymbol{\xi}) \, dV_{\boldsymbol{\xi}}$$

- Elastic ellipsoidal inhomogeneity (Eshelby problem), using equivalent-inclusion approach
- ▶ Half-space with free surface (Mindlin, 1936), Boussinesq as special case:
exact solutions (within half-space idealization):
 - Soil mechanics and geotechnics;
 - Contact mechanics (Hertz solution, Galin formulae)
- ▶ Two perfectly-bonded half spaces (Rongved, 1955) – closed form
- ▶ Elastic layer between two parallel planar free surfaces (Benitez and Rosakis 1987) – integral transform

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Reciprocity identity and integral representation

$$\Delta u + k^2 u = 0 \quad (\text{in } \Omega) \quad + \text{unspecified well-posed BCs}$$

Time-harmonic problems ($u(\xi, t) = \operatorname{Re}[u(\xi)e^{-i\omega t}]$); wavenumber $k = \omega/c$.
e.g. linear acoustics (u : pressure, $(i\rho\omega)^{-1}\nabla u$: velocity)

- ▶ Reciprocity identity:

$$\int_{\Omega} (u \Delta v - v \Delta u) \, dV = \int_{\partial\Omega} (uv_{,n} - vu_{,n}) \, dV \quad (u_{,n} \equiv \nabla u \cdot \mathbf{n})$$

- ▶ Fundamental solution (full space):

$$\Delta G(\mathbf{x}, \cdot) + k^2 G(\mathbf{x}, \cdot) + \delta(\cdot - \mathbf{x}) = 0 \quad (\text{in } \mathcal{O} \supset \Omega)$$

$$G(\mathbf{x}, \xi) = \frac{e^{ik\|\xi - \mathbf{x}\|}}{4\pi\|\xi - \mathbf{x}\|} \quad (\mathcal{O} = \mathbb{R}^3)$$

Integral representation:

$$u(\mathbf{x}) = \int_{\partial\Omega} \left\{ G(\mathbf{x}, \xi) u_{,n}(\xi) - G_{,n}(\mathbf{x}, \xi) u(\xi) \right\} dS_{\xi} \quad (\mathbf{x} \in \Omega)$$

Singular integral equation

- Dynamic (Helmholtz) and static (Laplace) fundamental solutions have same singularity:

$$G(\mathbf{x}, \boldsymbol{\xi}) = \frac{e^{ik\|\boldsymbol{\xi}-\mathbf{x}\|}}{4\pi\|\boldsymbol{\xi}-\mathbf{x}\|} = \frac{1}{4\pi\|\boldsymbol{\xi}-\mathbf{x}\|} + O(1) \quad (\boldsymbol{\xi} \rightarrow \mathbf{x})$$

- Limit to the boundary (or other) approach yields the same free term $c(\mathbf{x})$ as with Laplace problems
- **Singular integral equation:**

$$c(\mathbf{x})u(\mathbf{x}) + \int_{\partial\Omega} \left\{ G_{,n}(\mathbf{x}, \boldsymbol{\xi})u(\boldsymbol{\xi}) - G(\mathbf{x}, \boldsymbol{\xi})u_{,n}(\boldsymbol{\xi}) \right\} dS_{\boldsymbol{\xi}} = 0 \quad (\mathbf{x} \in \partial\Omega)$$

- Singular integrals: invoke methods for handling **static** singular kernels:

$$\begin{aligned} \int_{\partial\Omega} G_{,n}(\mathbf{x}, \boldsymbol{\xi})u(\boldsymbol{\xi}) dS_{\boldsymbol{\xi}} &= \int_{\partial\Omega} \left\{ G_{,n}(\mathbf{x}, \boldsymbol{\xi}) - G_{,n}(\mathbf{x}, \boldsymbol{\xi}; \omega = 0) \right\} u(\boldsymbol{\xi}) dS_{\boldsymbol{\xi}} \\ &\quad + \int_{\partial\Omega} G_{,n}(\mathbf{x}, \boldsymbol{\xi}; \omega = 0)u(\boldsymbol{\xi}) dS_{\boldsymbol{\xi}} \end{aligned}$$

Half-space problems

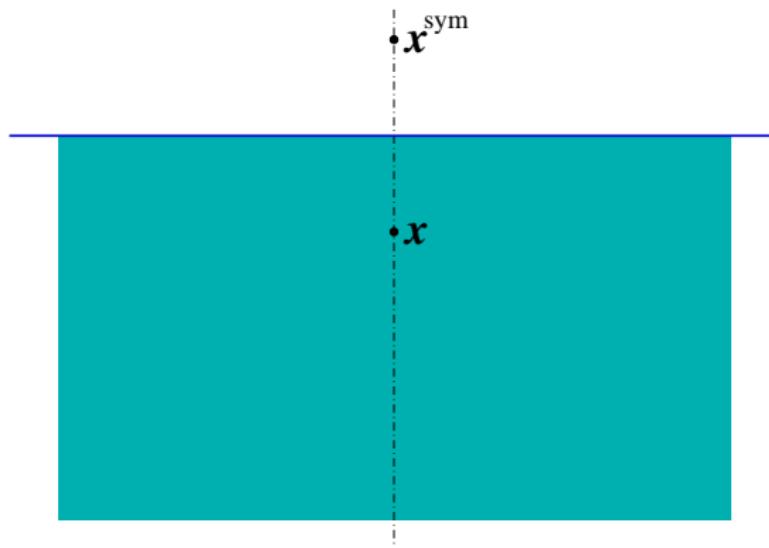
Method of images still applicable:

$$\mathcal{G}(\mathbf{x}, \xi) = G(\mathbf{x}, \xi) + G(\mathbf{x}^{\text{sym}}, \xi)$$

Neumann BC on free surface

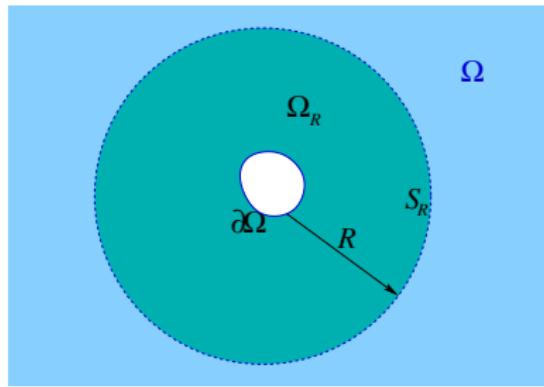
$$\mathcal{G}(\mathbf{x}, \xi) = G(\mathbf{x}, \xi) - G(\mathbf{x}^{\text{sym}}, \xi)$$

Dirichlet BC on free surface



Unbounded media

Wave equations (scalar, elastic, Maxwell...) frequently employed for media idealized as **unbounded**



Limiting case as $R \rightarrow \infty$ of

$$c(\mathbf{x})u(\mathbf{x}) + \left\{ \int_{S_R} + \int_{\partial\Omega} \right\} (G_{,n}(\mathbf{x}, \xi)u(\xi) - G(\mathbf{x}, \xi)u_{,n}(\xi)) dS_\xi = 0 \quad (\mathbf{x} \in \partial\Omega)$$

Unbounded media, radiation conditions

Integral equation

$$c(\mathbf{x})u(\mathbf{x}) + \int_{\partial\Omega} (G_{,n}(\mathbf{x}, \xi)u(\xi) - G(\mathbf{x}, \xi)u_{,n}(\xi)) dS_\xi = 0 \quad (\mathbf{x} \in \partial\Omega)$$

valid if \mathbf{u} satisfies a **radiation condition** at infinity:

- ▶ Integral form:

$$\lim_{R \rightarrow \infty} \int_{S_R} (G_{,n}(\mathbf{x}, \xi)u(\xi) - G(\mathbf{x}, \xi)u_{,n}(\xi)) dS_\xi = 0$$

- ▶ Local form, sufficient, known as Sommerfeld condition:

$$\nabla u \cdot \hat{\mathbf{x}} - iku = o(\|\mathbf{x}\|^{-1}) \quad \|\mathbf{x}\| \rightarrow \infty$$

(Sommerfeld is known to imply $\mathbf{u} = o(1)$, i.e. decay of \mathbf{u} at infinity)

The radiation condition is satisfied by $G(\mathbf{x}, \cdot)$, and consequently also by

- The fundamental solution
- Volume, single-layer, double-layer potentials
- Integral representation formula

Scattering of incident waves by hard obstacles

- Governing equations (hard obstacle[s])

$$\Delta u + k^2 u = 0 \quad \text{in } \Omega$$

$$\nabla u \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega \quad (\text{no normal velocity, i.e. hard obstacle})$$

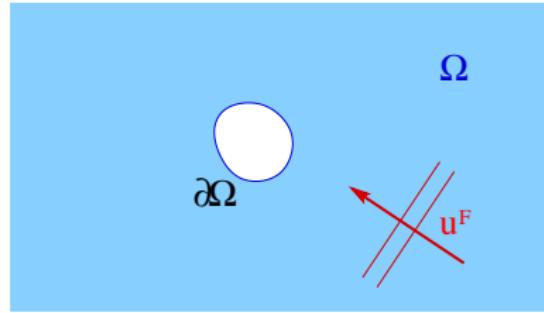
- Known** incident wave (or 'free-field') u^F ; radiation conditions not assumed (e.g. plane wave):

$$\Delta u^F + k^2 u^F = 0 \quad (\text{in } \mathbb{R}^3)$$

- Decomposition:**

$u = u^F + v = \text{incident} + \text{scattered},$

+ radiation conditions for v



Scattering of incident waves by hard obstacles

- ▶ Scattered field verifies integral equation (by virtue of radiation cnnds):

$$c(\mathbf{x})v(\mathbf{x}) + \int_{\partial\Omega} \left\{ G_{,n}(\mathbf{x}, \xi)v(\xi) - G(\mathbf{x}, \xi)v_{,n}(\xi) \right\} dS_\xi = 0 \quad (\text{a})$$

- ▶ Free-field verifies **integral equation for interior of scatterer**:

$$[c(\mathbf{x}) - 1]u^F(\mathbf{x}) + \int_{\partial\Omega} \left\{ G_{,n}(\mathbf{x}, \xi)u^F(\xi) - G(\mathbf{x}, \xi)u_{,n}^F(\xi) \right\} dS_\xi = 0 \quad (\text{b})$$

- ▶ **Simplified** integral equation formulation (a)+(b) in terms of total field:

$$c(\mathbf{x})u(\mathbf{x}) + \int_{\partial\Omega} G_{,n}(\mathbf{x}, \xi)u(\xi) dS_\xi = u^F(\mathbf{x})$$

Fictitious eigenfrequencies

BIE formulations for **exterior** problems break down when ω is an eigenfrequency for a certain **interior** problem.

Example:

- Direct BIE formulation for exterior Neumann problem (scattering by rigid obstacle):

$$c(\mathbf{x})u(\mathbf{x}) + \int_{\partial\Omega} G_{,n}(\mathbf{x}, \xi)u(\xi) dS_\xi = u^F(\mathbf{x}) \quad (\text{a})$$

- Indirect BIE formulation (using a double-layer potential representation) for interior homogeneous Dirichlet problem (using same normal as (a)):

$$c(\mathbf{x})\psi(\mathbf{x}) + \int_{\partial\Omega} G_{,n}(\mathbf{x}, \xi)\psi(\xi) dS_\xi = 0 \quad (\text{b})$$

- (b) has non-trivial solutions if ω is a Dirichlet eigenvalue.
- Therefore, so does (a) as the governing integral operator is the same

Remedies include:

- (i) enforcing an extra set of integral identities at interior points;
- (ii) combining (with complex coefficients) two BIE formulations having different eigenvalues (see treatment in Pyl, Clouteau, Degrande 2004)

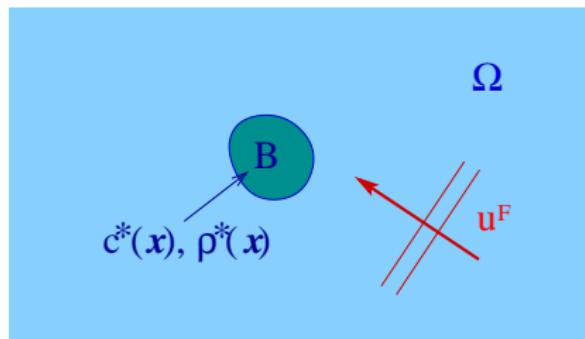
Scattering of incident waves by penetrable obstacles

- ▶ **Penetrable** inclusion ($\rho^*(\xi), c^*(\xi)$ and with definitions $\beta = \rho/\rho^*$, $\gamma = c/c^*$):

$$\begin{aligned} (\Delta + k^2)u &= 0 \quad (\text{in } \Omega \setminus \bar{B}) & (\Delta + \gamma^2 k^2)u^* &= 0 \quad (\text{in } B) \\ u &= u^*, \quad u_{,n} = \beta u_{,n}^* \quad (\text{on } \partial B) \end{aligned}$$

- ▶ Domain integral equation of Lippman-Schwinger type (proof: combine reciprocity identities written on B for u^* and on $\mathbb{R}^3 \setminus B$ for $u - u^F$):

$$u(\mathbf{x}) + \int_B [(\beta - 1) \nabla G(\mathbf{x}, \xi) \nabla u(\xi) + (1 - \beta \gamma^2) k^2 G(\mathbf{x}, \xi) u(\xi)] dV_\xi = u^F(\mathbf{x})$$



Linear elastodynamics

Governing field equation:

$$\operatorname{div}(\mathcal{C} : \boldsymbol{\varepsilon}[\mathbf{u}]) + \rho\omega^2\mathbf{u} + \mathbf{b} = 0 \quad (\text{in } \Omega)$$

Fundamental solution (full space):

$$U_i^k(\mathbf{x}, \boldsymbol{\xi}) = \frac{1}{k_s^2 \mu} \left[(\delta_{qs} \delta_{ik} - \delta_{qk} \delta_{is}) \frac{\partial}{\partial x_q} \frac{\partial}{\partial \xi_s} G(\|\mathbf{x} - \boldsymbol{\xi}\|; k_s) + \frac{\partial}{\partial x_i} \frac{\partial}{\partial \xi_k} G(\|\mathbf{x} - \boldsymbol{\xi}\|; k_p) \right]$$

$$G(z; k) = \frac{e^{ikz}}{4\pi z}, \quad k_s^2 = \frac{\rho\omega^2}{\mu}, \quad k_p^2 = \frac{1-2\nu}{2(1-\nu)} k_s^2$$

Radiation conditions for unbounded media, local form:

$$\left. \begin{aligned} \sigma[\mathbf{u}^p] \cdot \hat{\mathbf{x}} - i\rho\omega c_p &= o(\|\mathbf{x}\|^{-1}) \\ \sigma[\mathbf{u}^s] \cdot \hat{\mathbf{x}} - i\rho\omega c_s &= o(\|\mathbf{x}\|^{-1}) \end{aligned} \right\} \quad \|\mathbf{x}\| \rightarrow \infty$$

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Interpolation

- Partition $\partial\Omega$ into elements (possibly curvilinear and with curvilinear edges):

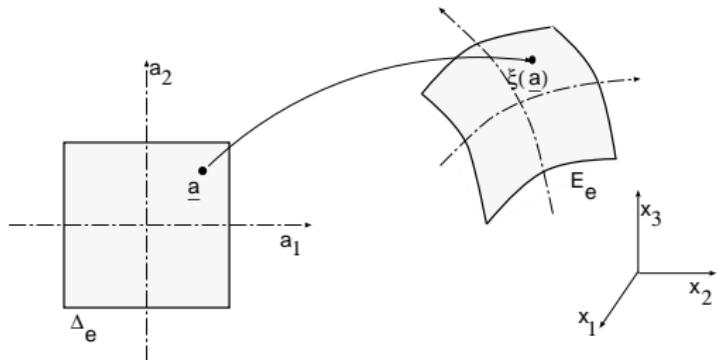
$$\partial\Omega = \bigcup_{e=1}^{N_e} E_e$$

- Isoparametric representation (most commonly used) of $\partial\Omega$ and unknown ϕ :

$$\mathbf{x} = \sum_{q=1}^{n(e)} N_q(\mathbf{a}) \mathbf{x}^q$$

$$\phi(\mathbf{x}) = \sum_{q=1}^{n(e)} N_q(\mathbf{a}) \phi^q$$

$$(\mathbf{a} = (a_1, a_2) \in \Delta_e)$$



- Connectivity table:

$Q(e, q)$ global number of q -th node of E_e ($1 \leq e \leq N_e, 1 \leq q \leq n(e)$)

- Isoparametric interpolation: $N = N_N$ (for scalar problems).

(with N_N : number of nodes and N : number of unknown nodal DOFs)

Collocation BEM

Sample integral equation (Laplace + Dirichlet, direct or single-layer formulation):

$$\int_{\partial\Omega} G(\mathbf{x}, \boldsymbol{\xi}) \varphi(\boldsymbol{\xi}) dS_{\xi} = b(\mathbf{x}) \quad (\mathbf{x} \in \partial\Omega)$$

- ▶ Principle: enforce integral equation at the N_N nodes $\mathbf{x} = \mathbf{x}^1, \dots, \mathbf{x}^{N_N}$.
- ▶ Leads to linear system of equations

$$\boxed{\mathbf{A}\varphi = \mathbf{b}} \quad (\mathbf{A} \in \mathbb{R}^{N \times N}, \mathbf{b} \in \mathbb{R}^N)$$

where

$$A_{PQ} = \sum_{e \in I(Q)} \int_{\Delta_e} G(\mathbf{x}^P, \boldsymbol{\xi}(\mathbf{a})) N_Q(\mathbf{a}) J(\mathbf{a}) d\mathbf{a} \quad (1 \leq P, Q \leq N)$$

$$b_P = b(\mathbf{x}^P)$$

- ▶ Matrix **A square, fully-populated, invertible, non-symmetric** obtained by assembly of element matrices

$$\mathbf{A}^e(\mathbf{x}^P) \in \mathbb{R}^{1, n(e)} = \left[\int_{\Delta_e} G(\mathbf{x}^P, \boldsymbol{\xi}(\mathbf{a})) N_q(\mathbf{a}) J(\mathbf{a}) d\mathbf{a} \right]_{1 \leq q \leq n(e)}$$

Evaluation of element integrals

$$\mathbf{A}^e(\mathbf{x}^P) \in \mathbb{R}^{1,n(e)} = \left[\int_{\Delta_e} G(\mathbf{x}^P, \xi(\mathbf{a})) N_q(\mathbf{a}) J(\mathbf{a}) \, d\mathbf{a} \right]_{1 \leq q \leq n(e)}$$

- If $\mathbf{x}^P \notin E_e$ (nonsingular element integral): Gaussian quadrature

$$\mathbf{A}^e(\mathbf{x}^P) \approx \sum_{g=1}^G w_g G(\mathbf{x}^P, \xi(\mathbf{a}_g)) N_q(\mathbf{a}_g) J(\mathbf{a}_g)$$

- If $\mathbf{x}^P \in E_e$ (singular element integral): specialized treatment:
 - Weakly singular integrals ($O(r^{-1})$ kernel in 3-D) removed by suitable transformation of parametric coordinates \mathbf{a}
 - Strongly singular integrals ($O(r^{-2})$ in 3-D) either
 - (i) recast into weakly singular integrals using regularization techniques
 - (ii) evaluated directly as Cauchy principal values
 - For simple element shapes and interpolations (e.g. 3-noded isoparametric triangle), analytic singular integration available

Galerkin BEM

Example (simplest): solve Dirichlet problem for Laplace equation using single-layer potential

$$\forall \tilde{\varphi} \in H^{-1/2}(\partial\Omega), \quad \text{find } \varphi \in H^{-1/2}(\partial\Omega), \quad \mathcal{B}(\varphi, \tilde{\varphi}) = \langle b, \tilde{\varphi} \rangle_{\partial\Omega}$$

with $\mathcal{B}(\varphi, \tilde{\varphi}) = \int_{\partial\Omega} \int_{\partial\Omega} \varphi(\xi) G(\mathbf{x}, \xi) \tilde{\varphi}(\mathbf{x}) dS_\xi dS_x$

- ▶ Leads to linear system of equations

$$\boxed{\mathbf{A}\varphi = \mathbf{b}} \quad (\mathbf{A} \in \mathbb{R}^{N \times N}, \mathbf{b} \in \mathbb{R}^N)$$

where

$$A_{PQ} = \sum_{e' \in I(P)} \sum_{e \in I(Q)} \int_{\Delta_{e'}} N_P(\mathbf{a}') \left\{ \int_{\Delta_e} G(\mathbf{x}(\mathbf{a}'), \xi(\mathbf{a})) N_Q(\mathbf{a}) J(\mathbf{a}) d\mathbf{a} \right\} J(\mathbf{a}') d\mathbf{a}'$$

$$b_P = \sum_{e' \in I(P)} \int_{\Delta_{e'}} N_P(\mathbf{a}') b(\mathbf{x}(\mathbf{a}')) J(\mathbf{a}') d\mathbf{a}'$$

- ▶ Matrix **A** square, fully-populated, invertible, symmetric

Limitations of “traditional” BEM

CPU for the main steps of traditional BEMs:

- (a) Set-up of \mathbf{A} : CPU = $O(N^2)$;
- (b) Solution using direct solver (usually LU factorization): CPU = (N^3) ;
- (c) Evaluation of integral representations at M points: CPU = $O(N \times M)$.

Besides:

- (d) $O(N^2)$ memory needed for storing \mathbf{A} .
 \implies Problem size N at most $O(10^4)$

Reasons for (a)-(d):

- ▶ $G(\mathbf{x}, \xi)$ non-zero for all (\mathbf{x}, ξ) ;
- ▶ Element matrices $\mathbf{A}^e(\mathbf{x}^P)$ recomputed for each new collocation point \mathbf{x}^P .

Overcoming the limitations of “traditional” BEM

Two issues:

1. To accelerate the BEM (i.e. to reduce its $O(N^3)$ complexity)
2. To increase permitted problem sizes.

Main ideas:

- (i) Iterative solution of BEM matrix equation
 $\implies \text{CPU} = O(N^2 \times N_l)$, with usually $N_l/N \rightarrow 0$;
- (ii) Acceleration of matrix-vector product $\mathbf{A}\varphi$ for given density φ .
 \implies complexity lower than $O(N^2)$.

Several strategies available for developing fast BEMs

The Fast Multipole Method (FMM) is the most developed to date.

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The GMRES algorithm

- Linear system

$$\mathbf{A}\mathbf{u} = \mathbf{b} \quad \begin{cases} \mathbf{A} \in \mathbb{R}^{N \times N} \text{ or } \mathbb{C}^{N \times N}, \mathbf{A} \text{ invertible} \\ \mathbf{u} \in \mathbb{R}^N \text{ ou } \mathbb{C}^N, \\ \mathbf{b} \in \mathbb{R}^N \text{ ou } \mathbb{C}^N \end{cases}$$

- Generalized Minimal RESiduals (GMRES): principle

$$\mathbf{u}^{(k)} = \arg \min_{u \in u^{(0)} + V_k} \|\mathbf{b} - \mathbf{A}\mathbf{u}\|^2, \quad V_k = \text{Vect}\{\mathbf{v}_1, \dots, \mathbf{v}_k\} \text{ to be specified}$$

Explicit form of minimisation:

$$\mathbf{u}^{(k)} = \mathbf{u}^{(0)} + \sum_{j=1}^k \alpha_j^{(k)} \mathbf{v}_j$$

$$\text{with } \boldsymbol{\alpha}^{(k)} \equiv (\alpha_1^{(k)}, \dots, \alpha_k^{(k)}) = \arg \min_{\alpha_1, \dots, \alpha_k} \left\| \mathbf{r}^{(0)} - \sum_{j=1}^k \alpha_j \mathbf{A}\mathbf{v}_j \right\|^2$$

- Iteration k : basis $(\mathbf{v}_1, \dots, \mathbf{v}_{k-1})$ augmented with a new vector \mathbf{v}_k , hence

$$V_{k-1} \subset V_k.$$

Minimization problem size increases with k : **restart** when $k > m$, GMRES(m)

The GMRES algorithm

- If $k = N$, one must have $\mathbf{u}^{(N)} = \mathbf{u}$ (hence convergence within $\leq N$ iterations)
- In practice: (i) $N_{\text{iter}} \ll N$ is desired, (ii) exact convergence not necessary.

$$r^{(k)} \equiv \|\mathbf{b} - \mathbf{A}\mathbf{u}^{(k)}\| \leq \epsilon r^{(0)} \quad (\epsilon: \text{tolerance})$$

- Construction of subspace $V_k = \text{Vect}\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ using *Krylov vectors*:

$$V_k = \text{Vect}\{\mathbf{w}_1, \mathbf{w}_2 = \mathbf{A}\mathbf{w}_1, \dots, \mathbf{w}_k = \mathbf{A}\mathbf{w}_{k-1}\} \quad \text{with } \mathbf{w}_1 = \mathbf{r}^{(0)}$$

- Sequence $(\mathbf{v}_1, \dots, \mathbf{v}_k)$ constructed using **orthonormalization** of Krylov vectors $(\mathbf{w}_1, \dots, \mathbf{w}_k)$:

$$\mathbf{v}_\ell^\top \mathbf{v}_k = 0$$

$$\|\mathbf{v}_k\| = 1 \quad \text{for all } k \geq 1$$

$$\text{Vect}\{\mathbf{w}_1, \dots, \mathbf{w}_k\} = \text{Vect}\{\mathbf{v}_1, \dots, \mathbf{v}_k\} = V_k$$

Main contribution to computational cost: evaluation of matrix-vector products \mathbf{Aw} for given \mathbf{w} .

Preconditioning

- ▶ *Left preconditioning:*

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{u} = \mathbf{M}^{-1}\mathbf{b}$$

Improved convergence (i.e. less iterations) if $\mathbf{M}^{-1}\mathbf{A}$ better conditioned than \mathbf{A}

- ▶ Krylov sequence associated with matrix $\mathbf{M}^{-1}\mathbf{A}$:

$$\mathbf{r}^{(0)} = \mathbf{M}^{-1}\mathbf{b} - \mathbf{M}^{-1}\mathbf{A}\mathbf{u}^{(0)} = \mathbf{w}_1 \quad \text{i.e. } \mathbf{M}\mathbf{w}_1 = \mathbf{b} - \mathbf{A}\mathbf{u}^{(0)}$$

$$\mathbf{w}_{k+1} = \mathbf{M}^{-1}\mathbf{A}\mathbf{w}_k \quad \text{i.e. } \mathbf{M}\mathbf{w}_{k+1} = \mathbf{A}\mathbf{w}_k \quad (k \geq 0)$$

- ▶ Modified convergence criterion:

$$\|\mathbf{M}^{-1}\mathbf{b} - \mathbf{M}^{-1}\mathbf{A}\mathbf{u}^{(k)}\| \leq \epsilon \|\mathbf{M}^{-1}\mathbf{b}\|$$

- ▶ Many approaches available for defining preconditioning matrices \mathbf{M} :
 - Diagonal preconditioner $M_{ij} = A_{ij}\delta_{ij}$;
 - Incomplete LU factorization of \mathbf{A} ;
 - Sparse approximate inverses;
 - Multigrid approaches;
 - Preconditioners exploiting specific features of the problems, e.g. single-inclusion case for many-inclusion problems.

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Elastostatics

Frequency-domain wave equations

2. Review of classical BEM concepts

3. The GMRES iterative solver

4. The fast multipole method (FMM) for the Laplace equation

Multipole expansion of $1/r$

The single-level fast multipole method

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Exponential representation of $1/r$

FMM using equivalent sources

Clustering and low-rank approximations

Kernel-independent acceleration via kernel interpolation

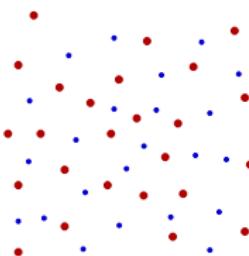
Adaptive cross approximation

8. Preconditioning

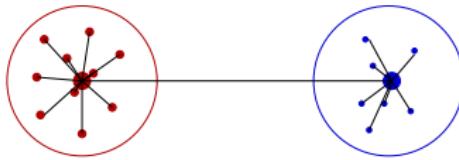
Origins of the FMM: fast computation of potentials

$$\Phi(\mathbf{x}_i) = C \sum_{j=1}^{N_\xi} \frac{q_j}{\|\boldsymbol{\xi}_j - \mathbf{x}_i\|} \quad (1 \leq i \leq N_x)$$

$C = (4\pi\epsilon_0)^{-1}$, electric charges q_j (electrostatic); $C = \mathcal{G}$, masses q_j (gravitation)



- ▶ Straightforward computation: $\text{CPU} = O(N_x N_\xi)$;
- ▶ Reason: influence coefficient $\|\boldsymbol{\xi}_j - \mathbf{x}_i\|^{-1}$ depends on both \mathbf{x}_i and $\boldsymbol{\xi}_j$;
- ▶ **Fast summation** (Greengard, 1985): $\text{CPU} = O(N_x + N_\xi)$



Iterative solution of integral equation

Model problem:

$$\text{find } \varphi, \quad \int_{\partial\Omega} G(\mathbf{x}, \xi) \varphi(\xi) dS_\xi = b(\mathbf{x}), \quad \text{i.e. } \mathcal{S}[\varphi, \partial\Omega](\mathbf{x}) = b(\mathbf{x}) \quad (\mathbf{x} \in \partial\Omega)$$

Krylov vector: $\mathbf{A}\varphi$ discretized version of

$$\mathcal{S}[\varphi, \partial\Omega](\mathbf{x}) := \int_{\partial\Omega} G(\mathbf{x}, \xi) \varphi(\xi) dS_\xi$$

Integral operator \mathcal{S} : a generalization to infinite-dimensional function spaces (here $H^{-1/2}(\partial\Omega)$) of the concept of matrix.

- ▶ Using traditional BEM: $\text{CPU} = O(N^2)$ for each evaluation of $\mathbf{A}\varphi$;
- ▶ **Aim of the Fast Multipole Method:** evaluation of $\mathbf{A}\varphi$ at CPU cost **lower than $O(N^2)$** .

FMM: main ideas

$$\mathcal{S}[\varphi, \partial\Omega](\mathbf{x}) := \int_{\partial\Omega} G(\mathbf{x}, \boldsymbol{\xi}) \varphi(\boldsymbol{\xi}) dS_{\boldsymbol{\xi}}$$

- ▶ **Main idea:** seek to **reuse** element integrations (w.r.t. $\boldsymbol{\xi}$) when collocation point \mathbf{x} is changed;
- ▶ **Method:** express the fundamental solution as a **series of products**:

$$G(\mathbf{x}, \boldsymbol{\xi}) = \sum_{n=0}^{\infty} g_n(\mathbf{x}) h_n(\boldsymbol{\xi})$$

and truncate the series at suitable level p :

$$G(\mathbf{x}, \boldsymbol{\xi}) = \sum_{n=0}^p g_n(\mathbf{x}) h_n(\boldsymbol{\xi}) + \epsilon_G(p)$$

- ▶ **Consequence:**

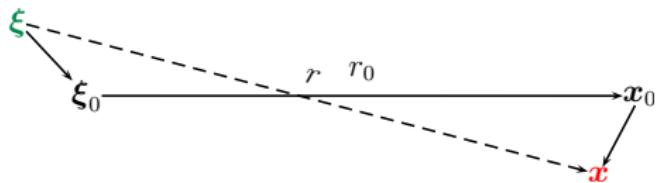
$$\mathcal{S}[\varphi, \partial\Omega](\mathbf{x}) = \sum_{n=0}^p g_n(\mathbf{x}) \int_{\partial\Omega} h_n(\boldsymbol{\xi}) \varphi(\boldsymbol{\xi}) dS_{\boldsymbol{\xi}} + \epsilon(p)$$

The p integrations are independent on \mathbf{x} and are reusable as \mathbf{x} is changed.

FMM: main ideas

How to express $G(\mathbf{x}, \xi)$ as a sum (series) of products? Taylor expansion about origins \mathbf{x}_0 and ξ_0 :

$$\begin{aligned} G(\mathbf{x}, \xi) &= \sum_{m \geq 0} \frac{1}{m!} [\partial_\xi^m G](\mathbf{x}, \xi_0) (\xi - \xi_0)^m \\ &= \sum_{n \geq 0} \sum_{m \geq 0} \frac{1}{m! n!} [\partial_x^n \partial_\xi^m G](\mathbf{x}_0, \xi_0) (\mathbf{x} - \mathbf{x}_0)^n (\xi - \xi_0)^m \end{aligned}$$



For Laplace kernel $1/r$: sophisticated version of Taylor expansion leads to **multipole expansion** (see next).

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Multipole expansion of $1/r$

The Multipole expansion of $1/r$ is given (see proof later) by:

$$\frac{1}{\|\xi - \mathbf{x}\|} = \sum_{n=0}^{+\infty} \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0) \sum_{n'=0}^{+\infty} \sum_{m'=-n'}^{n'} (-1)^n \overline{S_{n+n', m+m'}(\xi_0 - \mathbf{x}_0)} R_{n', m'}(\xi - \xi_0)$$

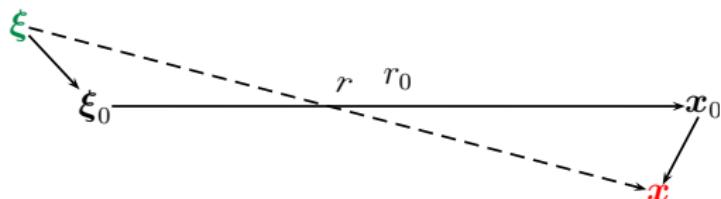
$$R_{n,m}(\mathbf{z}) = \frac{1}{(n+m)!} P_n^m(\cos \alpha) e^{im\beta} \rho^n$$

$$S_{n,m}(\mathbf{z}) = (n-m)! P_n^m(\cos \alpha) e^{im\beta} \frac{1}{\rho^{n+1}}$$

$$\text{with } \mathbf{z} = \rho [\sin \alpha (\cos \beta \mathbf{e}_1 + \sin \beta \mathbf{e}_2) + \cos \alpha \mathbf{e}_3]$$

Conditions for convergence of the multipole expansion:

$$\|\mathbf{x} - \mathbf{x}_0\| < \|\xi - \mathbf{x}_0\| \quad \text{and} \quad \|\xi - \xi_0\| < \|\mathbf{x} - \xi_0\|$$



Multipole expansion of $1/r$: computation of solid harmonics $R_{n,m}$, $S_{n,m}$

Solid harmonics $R_{n,m}$ and $S_{n,m}$ evaluated **using Cartesian coordinates** using recursion formulae derived from those for Legendre polynomials:

- The $R_{n,m}(z)$ are computed recursively by setting $R_{0,0}(z) = 1$ and using

$$R_{n+1,n+1}(z) = \frac{z_1 + iz_2}{2(n+1)} R_{n,n}(z)$$

$$((n+1)^2 - m^2) R_{n+1,m}(z) - (2n+1) z_3 R_{n,m}(z) + |z|^2 R_{n-1,m}(z) = 0 \quad (n \geq m)$$

- The $S_{n,m}(z)$ are computed recursively by setting $S_{0,0}(z) = 1/|z|$ and using

$$S_{n+1,n+1}(z) = \frac{(2n+1)(z_1 + iz_2)}{|z|^2} R_{n,n}(z)$$

$$|z|^2 S_{n+1,m}(z) - (2n+1) z_3 S_{n,m}(z) + (n^2 - m^2) S_{n-1,m}(z) = 0 \quad (n \geq m)$$

- Finally, $R_{n,m}(z)$ and $S_{n,m}(z)$ for negative values of m are computed via the identities

$$R_{n,-m}(z) = (-1)^m \overline{R_{n,m}(z)} \quad S_{n,-m}(z) = (-1)^m \overline{S_{n,m}(z)}$$

Multipole expansion of $1/r$: computation of solid harmonics $R_{n,m}$, $S_{n,m}$

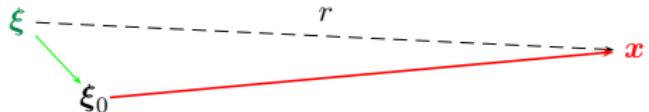
Derivatives of the $R_{n,m}$:

$$\frac{\partial}{\partial z_1} R_{n,m}(z) = \frac{1}{2} (R_{n-1,m-1} - R_{n-1,m+1})(z)$$

$$\frac{\partial}{\partial z_2} R_{n,m}(z) = \frac{i}{2} (R_{n-1,m-1} + R_{n-1,m+1})(z)$$

$$\frac{\partial}{\partial z_3} R_{n,m}(z) = R_{n-1,m}$$

Multipole expansion of $1/r$: proof (1/4)



$$G(\mathbf{x}, \boldsymbol{\xi}) = \frac{1}{4\pi \|\boldsymbol{\xi} - \mathbf{x}\|}$$

$$\boldsymbol{\xi} - \mathbf{x} = (\boldsymbol{\xi} - \boldsymbol{\xi}_0) - (\mathbf{x} - \boldsymbol{\xi}_0)$$

Spherical coordinates:

$$(\boldsymbol{\xi} - \boldsymbol{\xi}_0) = \rho [\sin\alpha (\cos\beta \mathbf{e}_1 + \sin\beta \mathbf{e}_2) + \cos\alpha \mathbf{e}_3]$$

$$(\mathbf{x} - \boldsymbol{\xi}_0) = R [\sin\theta (\cos\varphi \mathbf{e}_1 + \sin\varphi \mathbf{e}_2) + \cos\theta \mathbf{e}_3]$$

$$\boxed{\frac{1}{\|\boldsymbol{\xi} - \mathbf{x}\|} = (R^2 - 2\rho R \cos\Phi + \rho^2)^{-1/2}}$$

$$\cos\Phi = \frac{1}{\rho R} (\boldsymbol{\xi} - \boldsymbol{\xi}_0) \cdot (\mathbf{x} - \boldsymbol{\xi}_0) = \sin\alpha \sin\theta \cos(\beta - \varphi) + \cos\alpha \cos\theta$$

Multipole expansion of $1/r$: proof (2/4)

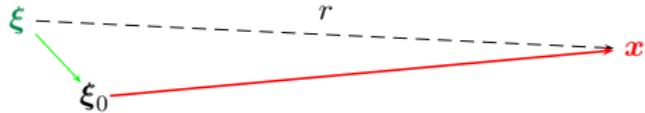
$$\begin{aligned}\frac{1}{\|\xi - \mathbf{x}\|} &= (R^2 - 2\rho R \cos \Phi + \rho^2)^{-1/2} \\ &= \frac{1}{R}(1 - 2zt + t^2)^{-1/2} \quad \left(z = \cos \Phi, \quad t = \frac{\rho}{R} \right)\end{aligned}$$

Since $(1 - 2zt + t^2)^{-1/2}$ is the generating function of the Legendre polynomials,
i.e.:

$$(1 - 2zt + t^2)^{-1/2} = \sum_{n \geq 0} P_n(z) t^n \quad (t < 1)$$

one has:

$$\boxed{\frac{1}{\|\xi - \mathbf{x}\|} = \sum_{n=0}^{+\infty} \frac{P_n(\cos \Phi)}{R^{n+1}} \rho^n} \quad (\rho < R)$$



Multipole expansion of $1/r$: proof (3/4)

$$\frac{1}{\|\xi - \mathbf{x}\|} = \sum_{n=0}^{+\infty} \frac{P_n(\cos \Phi)}{R^{n+1}} \rho^n \quad (\rho < R)$$

To recast as a series of products $g(\rho, \alpha, \beta)h(R, \theta, \varphi)$: addition theorem for Legendre polynomials:

$$P_n(\cos \Phi) = \sum_{m=-n}^n \frac{(n-m)!}{(n+m)!} \left(P_n^m(\cos \alpha) e^{im\beta} \right) \left(P_n^m(\cos \theta) e^{-im\varphi} \right)$$

$$\frac{1}{\|\xi - \mathbf{x}\|} = \sum_{n=0}^{+\infty} \sum_{m=-n}^n R_{n,m}(\xi - \xi_0) \overline{S_{n,m}(\mathbf{x} - \xi_0)}$$

$$R_{n,m}(\mathbf{z}) = \frac{1}{(n+m)!} P_n^m(\cos \alpha) e^{im\beta} \rho^n$$

$$S_{n,m}(\mathbf{z}) = (n-m)! P_n^m(\cos \theta) e^{im\varphi} \frac{1}{R^{n+1}}$$

The series is convergent if $\|\xi - \xi_0\| < \|\mathbf{x} - \xi_0\|$.

Multipole expansion of $1/r$: proof (4/4)

$$\frac{1}{\|\xi - \mathbf{x}\|} = \sum_{n=0}^{+\infty} \sum_{m=-n}^n R_{n,m}(\xi - \xi_0) \overline{S_{n,m}(\mathbf{x} - \xi_0)}$$

Application to evaluation of potentials:

$$\Phi(\mathbf{x}_i) = C \sum_{j=1}^{N_\xi} \frac{q_j}{\|\xi_j - \mathbf{x}_i\|} = C \sum_{n=0}^{+\infty} \sum_{m=-n}^n M_{n,m}(\xi_0) \overline{S_{n,m}(\mathbf{x}_i - \xi_0)}$$

with **multipole moments** defined by

$$M_{n,m}(\xi_0) = \sum_{j=1}^{N_\xi} q_j R_{n,m}(\xi_j - \xi_0)$$

Truncation of series to $n < p$ (with error control available, see later):

- ▶ Evaluation of $N_\xi N_x$ influence coefficients $\|\xi_j - \mathbf{x}_i\|^{-1}$ replaced with evaluation of $p^2 N_x$ products $M_{n,m}(\xi_0) \overline{S_{n,m}(\mathbf{x}_i - \xi_0)}$

Multipole expansion of $1/r$: proof

Insertion of local origin \mathbf{x}_0 into $\mathbf{x}_i - \boldsymbol{\xi}_0$:

- ▶ Note identity

$$S_{n,m}(\mathbf{z}) = (-1)^n \left(\frac{\partial}{\partial z_1} + i \frac{\partial}{\partial z_2} \right)^m \frac{\partial^{n-m}}{\partial z_3^{n-m}} \frac{1}{\|\mathbf{z}\|} \quad (m > 0) \quad (\text{a})$$

$$= (-1)^{n+m} \left(\frac{\partial}{\partial z_1} - i \frac{\partial}{\partial z_2} \right)^{-m} \frac{\partial^{n+m}}{\partial z_3^{n+m}} \frac{1}{\|\mathbf{z}\|} \quad (m < 0) \quad (\text{b})$$

- ▶ Invoke multipole expansion of $1/\|\mathbf{z}\|$ with $\mathbf{z} = (\mathbf{x}_i - \mathbf{x}_0) - (\boldsymbol{\xi}_0 - \mathbf{x}_0)$:

$$\frac{1}{\|\mathbf{x}_i - \boldsymbol{\xi}_0\|} = \sum_{n'=0}^{+\infty} \sum_{m'=-n'}^n R_{n',m'}(\mathbf{x}_i - \mathbf{x}_0) \overline{S_{n',m'}(\boldsymbol{\xi}_0 - \mathbf{x}_0)}$$

- ▶ Use representation (a,b) for $S_{n',m'}(\boldsymbol{\xi}_0 - \mathbf{x}_0)$;
- ▶ Exploit harmonicity of $1/\|\boldsymbol{\xi}_0 - \mathbf{x}_0\|$ via

$$\left(\frac{\partial}{\partial \xi_1^0} + i \frac{\partial}{\partial \xi_2^0} \right) \left(\frac{\partial}{\partial \xi_1^0} - i \frac{\partial}{\partial \xi_2^0} \right) \frac{1}{\|\boldsymbol{\xi}_0 - \mathbf{x}_0\|} + \frac{\partial^2}{\partial \xi_3^0 \partial \xi_3^0} \frac{1}{\|\boldsymbol{\xi}_0 - \mathbf{x}_0\|} = 0$$

- ▶ Reorder and reorganize resulting formula

$$S_{n,m}(\mathbf{x}_i - \boldsymbol{\xi}_0) = \sum_{n'=0}^{+\infty} \sum_{m'=-n'}^n \overline{R_{n',m'}(\mathbf{x}_i - \mathbf{x}_0)} S_{n+n',m+m'}(\boldsymbol{\xi}_0 - \mathbf{x}_0)$$

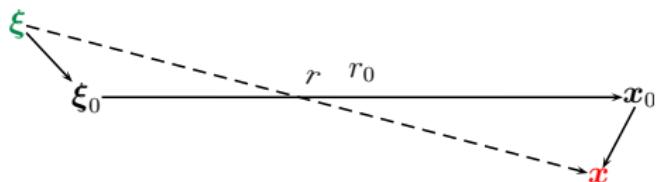
Multipole expansion: truncation error

Assume one can find $R > 0$ and $\chi > 1$ such that

$$(\|\mathbf{x} - \mathbf{x}_0\| < R \text{ et } \|\boldsymbol{\xi} - \mathbf{x}_0\| > \chi R) \quad \text{et} \quad (\|\boldsymbol{\xi} - \boldsymbol{\xi}_0\| < R \text{ et } \|\mathbf{x} - \boldsymbol{\xi}_0\| > \chi R)$$

An upper bound of the error arising from truncating the multipole expansion at order p is:

$$\left| \frac{1}{\|\boldsymbol{\xi} - \mathbf{x}\|} - \sum_{n=0}^p \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0) \right. \\ \left. - \sum_{n'=0}^p \sum_{m'=-n'}^{n'} (-1)^n S_{n+n', m+m'}(\boldsymbol{\xi}_0 - \mathbf{x}_0) R_{n', m'}(\boldsymbol{\xi} - \boldsymbol{\xi}_0) \right| \leq \frac{1}{R(\chi - 1)\chi^{p+1}}$$

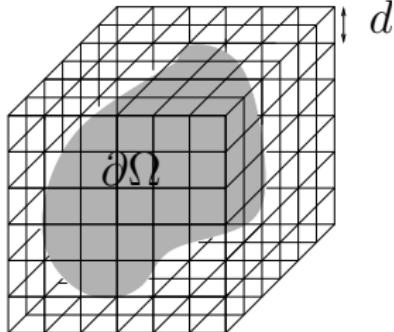


The truncation error is scale-independent

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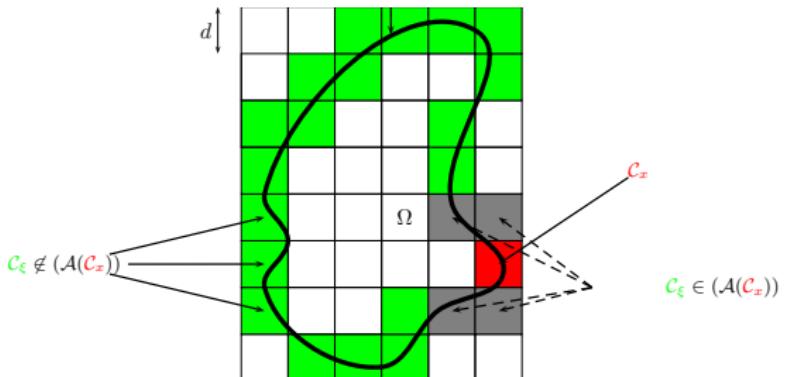
Single-level fast multipole method

Boundary of interest enclosed in
a cubic grid



Convergence of multipole
expansion guaranteed if x and ξ
lie in non-adjacent cells, with

$$\chi \geq \sqrt{3}$$



Single-level FMM

- Matrix-vector product ← integral operator evaluation

$$\mathcal{S}[\varphi, \partial\Omega](\textcolor{red}{x}) = \int_{\partial\Omega} G(\textcolor{red}{x}, \xi) \varphi(\xi) dS_\xi$$

- Split into **near** and **far** contributions:

$$\int_{\partial\Omega} = \sum_{C_\xi \in \mathcal{A}(C_x)} \int_{\partial\Omega \cap C_\xi} + \sum_{C_\xi \notin \mathcal{A}(C_x)} \int_{\partial\Omega \cap C_\xi}$$

$$\mathcal{S}[\varphi, \partial\Omega](\textcolor{red}{x}) = \mathcal{S}[\varphi, \partial\Omega]^{\text{near}}(\textcolor{red}{x}) + \mathcal{S}[\varphi, \partial\Omega]^{\text{far}}(\textcolor{red}{x})$$

Single-level FMM

Far contribution $\mathcal{S}[\varphi, \partial\Omega]^{\text{far}}(\mathbf{x})$:

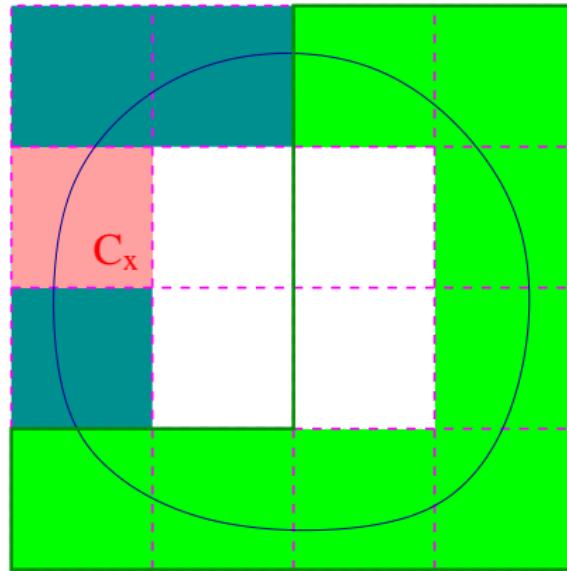
$$\mathcal{S}[\varphi, \partial\Omega]^{\text{far}}(\mathbf{x}) = \sum_{\mathcal{C}_\xi \notin \mathcal{A}(\mathcal{C}_x)} \int_{\partial\Omega \cap \mathcal{C}_\xi} G(\mathbf{x}, \boldsymbol{\xi}) \varphi(\boldsymbol{\xi}) dS_\xi \quad (\mathbf{x} \in \mathcal{C}_x)$$

Introduce (truncated) multipole expansion of $G(\mathbf{x}, \boldsymbol{\xi})$, with $\boldsymbol{\xi}_0$ and \mathbf{x}_0 chosen as centres of cells \mathcal{C}_ξ and \mathcal{C}_x :

$$\begin{aligned} \mathcal{S}[\varphi, \partial\Omega]^{\text{far}}(\mathbf{x}) &\approx \sum_{\mathcal{C}_\xi \notin \mathcal{A}(\mathcal{C}_x)} \frac{1}{4\pi} \sum_{n=0}^p \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0) \sum_{n'=0}^p \sum_{m'=-n'}^{n'} (-1)^n \overline{S_{n+n', m+m'}}(\boldsymbol{\xi}_0 - \mathbf{x}_0) \\ &\quad \times \int_{\partial\Omega \cap \mathcal{C}_\xi} R_{n', m'}(\boldsymbol{\xi} - \boldsymbol{\xi}_0) \varphi(\boldsymbol{\xi}) dS_\xi \end{aligned}$$

$$\begin{aligned} &= \frac{1}{4\pi} \sum_{n=0}^p \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0) \\ &\quad \sum_{\mathcal{C}_\xi \notin \mathcal{A}(\mathcal{C}_x)} \sum_{n'=0}^p \sum_{m'=-n'}^{n'} (-1)^n \overline{S_{n+n', m+m'}}(\boldsymbol{\xi}_0 - \mathbf{x}_0) M_{n', m'}(\mathcal{C}_\xi) \end{aligned}$$

Single-level FMM



Single-level FMM: complexity

- Compute and store multipole moments $M_{n,m}(\mathcal{C}_\xi)$ for each integration cell:

$$\text{CPU} = O(p^2 \times N_B \times (N/N_B)) = O(p^2 \times N).$$

- For each collocation cell \mathcal{C}_x :

- (a) Compute local coefficients $L_{n,m}(\mathcal{C}_x, \mathcal{C}_\xi)$ (M2L):

$$\text{CPU} = O(p^2 \times p^2 \times N_B) = O(p^4 \times N_B);$$

$$L_{n,m}(\mathcal{C}_x) = \sum_{\mathcal{C}_\xi \notin \mathcal{A}(\mathcal{C}_x)} \sum_{n'=0}^p \sum_{m'=-n'}^{n'} (-1)^{n'} \overline{S_{n+n', m+m'}(\xi_0 - \mathbf{x}_0)} M_{n', m'}(\mathcal{C}_\xi)$$

- (b) Far contribution $S[\varphi, \partial\Omega]^{\text{far}}(\mathbf{x})$ to integral operator, for all $\mathbf{x} \in \mathcal{C}_x$:

$$\text{CPU} = O(p^2 \times (N/N_B))$$

$$S[\varphi, \partial\Omega]^{\text{far}}(\mathbf{x}) = \sum_{n=0}^{+\infty} \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0) L_{n,m}(\mathcal{C}_x)$$

- (c) Near contribution $S[\varphi, \partial\Omega]^{\text{near}}(\mathbf{x})$ to integral operator, using standard BEM procedures: $\text{CPU} = O(|\mathcal{A}(\mathcal{C}_x)| \times (N/N_B) \times (N/N_B)) = O(|\mathcal{A}(\mathcal{C}_x)| \times N^2/N_B^2)$

Single-level FMM: optimal complexity

Total CPU time for one evaluation of $\mathcal{S}[\varphi, \partial\Omega]$:

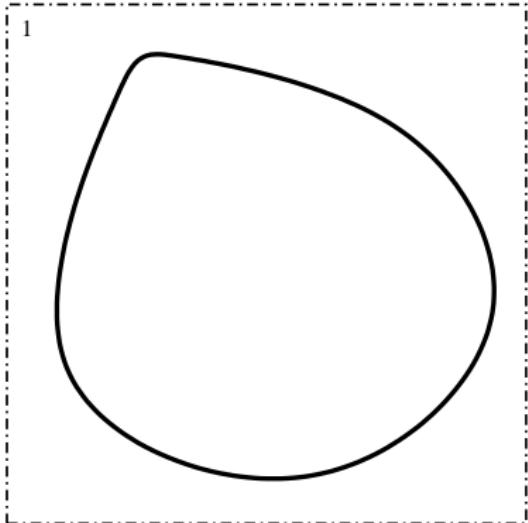
$$\begin{aligned}\text{CPU} &= Ap^2N + N_B \left(Bp^4N_B + Cp^2(N/N_B) + D |\mathcal{A}(C_x)| N^2/N_B^2 \right) \\ &= (A + C)p^2N + Bp^4N_B^2 + DN^2/N_B\end{aligned}$$

Optimal choice: $N_B = O(N^{2/3})$, yielding CPU / GMRES iteration = $O(N^{4/3})$

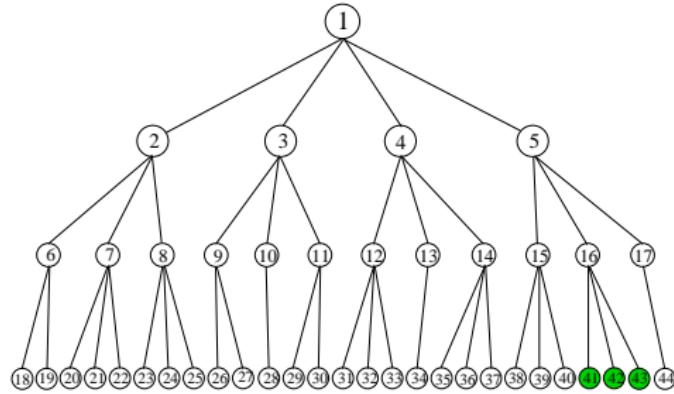
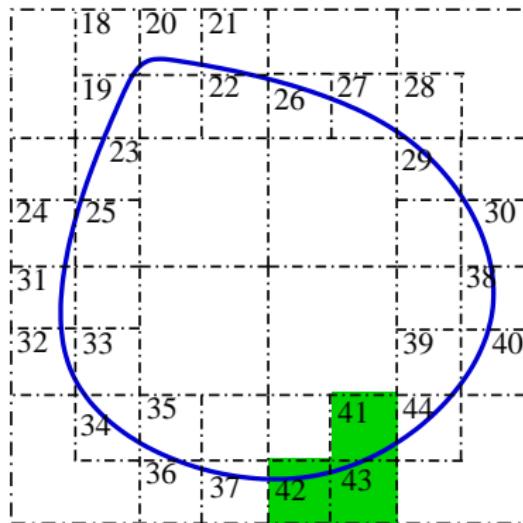
- ▶ Single-level FMM (Laplace and other elliptic PDEs): $\text{CPU} = O(N^{4/3})$;
- ▶ To further improve complexity: **multi-level FMM**

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Multi-level FMM

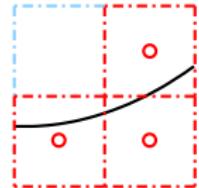


Multi-level FMM: initialization of multipole moments

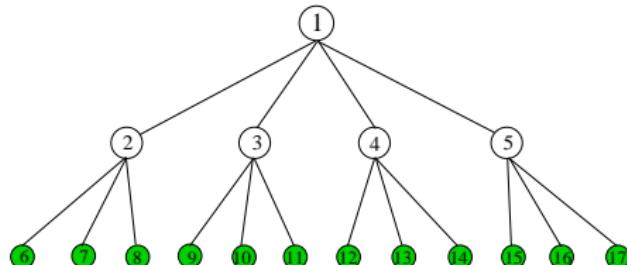
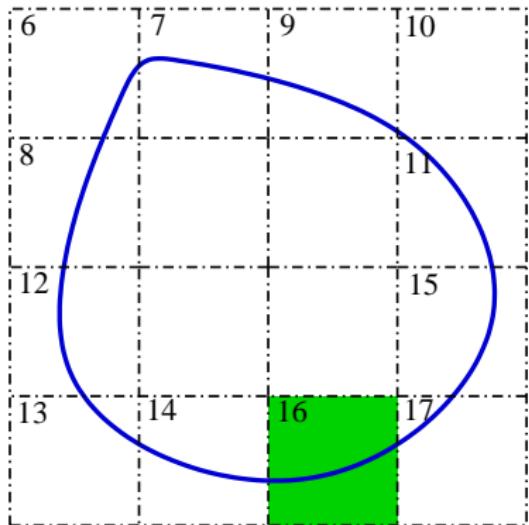


Computation of multipole moments, leaf level cells ($\ell = \bar{\ell} = 3$ here):

$$M_{n,m}(\mathcal{C}_\xi^{(\bar{\ell})}; \xi_0^{(\bar{\ell})}) = \int_{\partial\Omega \cap \mathcal{C}_\xi^{(\bar{\ell})}} R_{n,m}(\xi - \xi_0^{(\bar{\ell})}) \varphi(\xi) dS_\xi$$



Multi-level FMM: upward pass

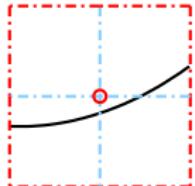


Computation of multipole moments, parent cells ($\ell = 3 \rightarrow \ell = 2$ here):

$$M_{n,m}(\mathcal{C}_\xi^{(\ell-1)}; \xi_0^{(\ell-1)}) = \sum_{\mathcal{C}_\xi^{(\ell)} \in \text{Children}(\mathcal{C}_\xi^{(\ell-1)})} M_{n,m}(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell-1)}) \quad (\text{M2M})$$

Upward pass needs translation of origin $\xi_0^{(\ell)} \rightarrow \xi_0^{(\ell-1)}$ in

$$M_{n,m}(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell)})$$



Multi-level FMM: M2M translation formula for upward pass

$$M_{n,m}(\mathcal{C}_\xi^{(\ell-1)}; \xi_0^{(\ell-1)}) = \sum_{\mathcal{C}_\xi^{(\ell)} \in \text{Children}(\mathcal{C}_\xi^{(\ell-1)})} \int_{\partial\Omega \cap \mathcal{C}_\xi^{(\ell)}} R_{n,m}(\xi - \xi_0^{(\ell-1)}) \varphi(\xi) dS_\xi$$

M2M translation identity:

$$R_{n,m}(\xi - \xi_0^{(\ell-1)}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} R_{n',m'}(\xi_0^{(\ell)} - \xi_0^{(\ell-1)}) R_{n-n', m-m'}(\xi - \xi_0^{(\ell)})$$

$$M_{n,m}(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell-1)}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} R_{n',m'}(\xi_0^{(\ell)} - \xi_0^{(\ell-1)}) M_{n-n', m-m'}(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell)})$$

Multi-level FMM: M2M translation formula for upward pass

Proof:

- ▶ write $\|\mathbf{x} - \boldsymbol{\xi}\|^{-1}$ in two ways (inserting either $\boldsymbol{\xi}_0^{(\ell-1)}$ or $\boldsymbol{\xi}_0^{(\ell)}$ as pole):

$$\frac{1}{\|\mathbf{x} - \boldsymbol{\xi}\|} = \sum_{n=0}^{+\infty} \sum_{m=-n}^n R_{n,m}(\boldsymbol{\xi} - \boldsymbol{\xi}_0^{(\ell)}) \overline{S_{n,m}(\mathbf{x} - \boldsymbol{\xi}_0^{(\ell)})} \quad (\text{a})$$

$$= \sum_{n=0}^{+\infty} \sum_{m=-n}^n R_{n,m}(\boldsymbol{\xi} - \boldsymbol{\xi}_0^{(\ell-1)}) \overline{S_{n,m}(\mathbf{x} - \boldsymbol{\xi}_0^{(\ell-1)})} \quad (\text{b})$$

- ▶ Invoke identity

$$S_{n,m}(\mathbf{x} - \boldsymbol{\xi}_0^{(\ell-1)}) = (-1)^n \sum_{n'=0}^{+\infty} \sum_{m'=-n'}^n \overline{R_{n',m'}(\boldsymbol{\xi}_0^{(\ell-1)} - \boldsymbol{\xi}_0^{(\ell)})} S_{n+n',m+m'}(\mathbf{x} - \boldsymbol{\xi}_0^{(\ell)})$$

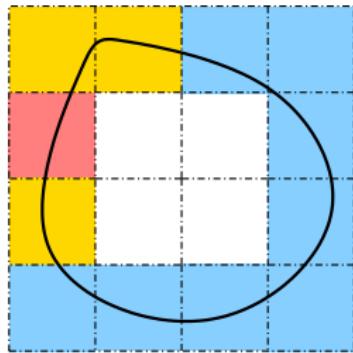
- ▶ Redefine summation indices ($(n, m) \leftarrow (n+n', m+m')$), reorder summations
- ▶ Identify cofactors of $S_{n,m}(\mathbf{x} - \boldsymbol{\xi}_0^{(\ell-1)})$ in (a) and (b)

$$R_{n,m}(\boldsymbol{\xi} - \boldsymbol{\xi}_0^{(\ell-1)}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} R_{n',m'}(\boldsymbol{\xi}_0^{(\ell)} - \boldsymbol{\xi}_0^{(\ell-1)}) R_{n-n',m-m'}(\boldsymbol{\xi} - \boldsymbol{\xi}_0^{(\ell)})$$

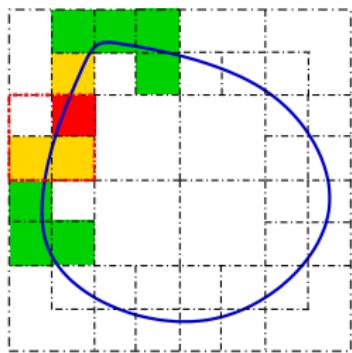
Multi-level FMM: definition of interaction list

Definition of interaction list $\mathcal{I}(\mathcal{C})$:

$$\mathcal{C}' \in \mathcal{I}(\mathcal{C}) \iff \mathcal{C}' \notin \mathcal{A}(\mathcal{C}) \text{ but } \text{Father}(\mathcal{C}') \in \mathcal{A}(\text{Father}(\mathcal{C}))$$



$$\begin{aligned}\mathcal{C}' &\in \mathcal{I}(\mathcal{C}) \\ \mathcal{C}'' &\in \mathcal{A}(\mathcal{C})\end{aligned}$$

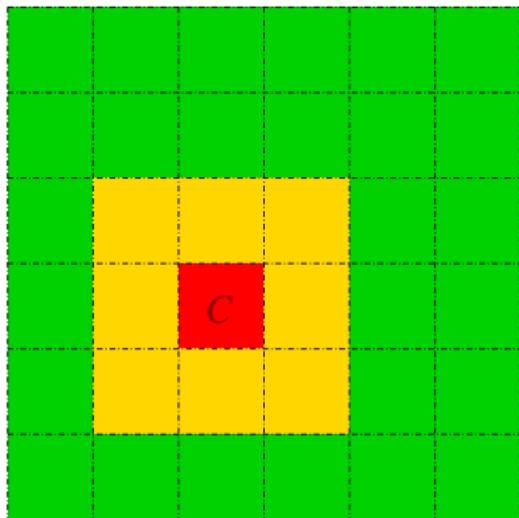


Note: $\mathcal{C}' \in \mathcal{I}(\mathcal{C}) \iff \mathcal{C}' \notin \mathcal{A}(\mathcal{C})$ for level $\ell = 2$.

$$\ell = 3$$

Multi-level FMM: definition of interaction list

General case, for generic cell \mathcal{C} :



$$\mathcal{C}' \in \mathcal{I}(\mathcal{C})$$

$$\mathcal{C}'' \in \mathcal{A}(\mathcal{C})$$

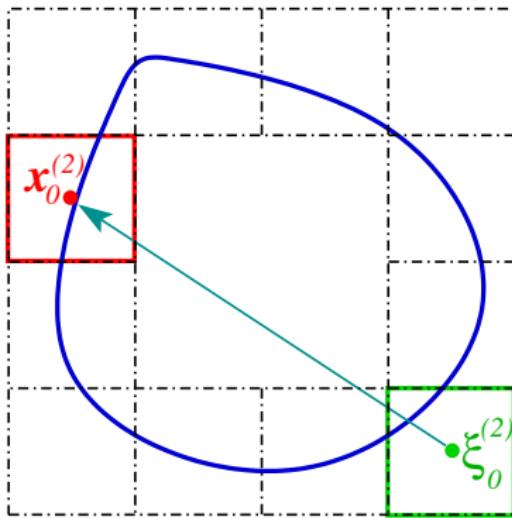
$\mathcal{I}(\mathcal{C})$ contains up to

- ▶ $6^3 - 3^3 = 189$ cells (3-D);
- ▶ $6^2 - 3^2 = 27$ cells (2-D)

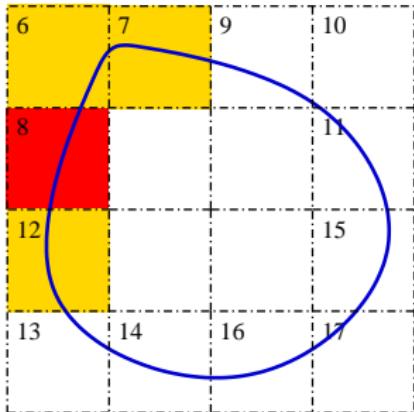
Multi-level FMM: M2L translation, upper level $\ell=2$

M2L translation formula between **disjoint** same-level cells:

$$L_{n,m}(\mathcal{C}_x^{(\ell)}) = \sum_{\xi \notin \mathcal{A}(\mathcal{C}_x^{(\ell)})} \sum_{n'=0}^p \sum_{m'=-n'}^{n'} (-1)^n \overline{S_{n+n', m+m'}(\xi_0^{(\ell)} - x_0^{(\ell)})} M_{n', m'}(\mathcal{C}_\xi^{(\ell)})$$



Multi-level FMM: M2L translation, upper level $\ell=2$

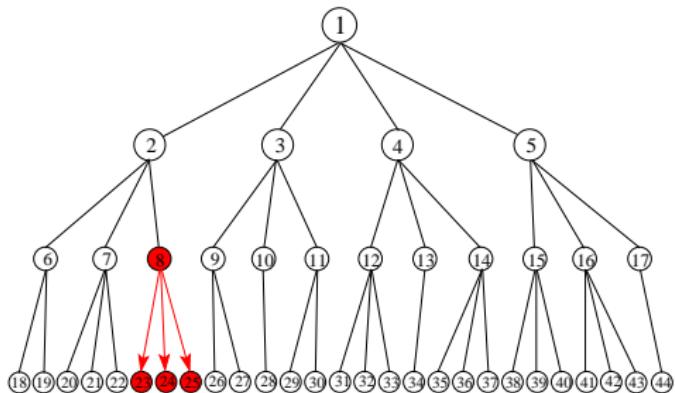
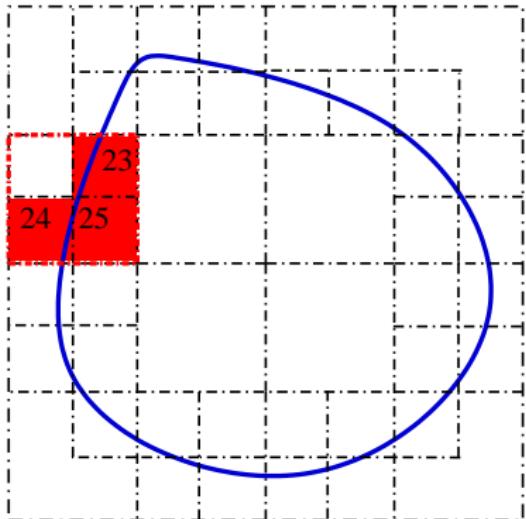


- ▶ Collocation cell $C_x^{(0)}$: no action taken
- ▶ Collocation cell $C_x^{(1)}$: no action taken
- ▶ Collocation cell $C_x^{(2)}$: **initialize M2L**

$$L_{n,m}(C_x^{(2)}) = \sum_{\substack{C_\xi^{(2)} \notin \mathcal{A}(C_x^{(2)})}}^p \sum_{n'=0}^{n'} \sum_{m'=-n'}^{n'} (-1)^n \overline{S_{n+n', m+m'}(\xi_0^{(2)} - x_0^{(2)})} M_{n', m'}(C_\xi^{(2)})$$

To apply M2L to $\mathcal{A}(C_x^{(2)})$: **subdivision**

Multi-level FMM: M2L translation, downward pass



$$\begin{aligned}
 L_{n,m}(\mathcal{C}_x^{(\ell)}; \mathbf{x}_0^{(\ell)}) &= L_{n,m}(\mathcal{C}_x^{(\ell-1)}; \mathbf{x}_0^{(\ell)}) \\
 &+ \sum_{\mathcal{C}_\xi^{(\ell)} \in \mathcal{I}(\mathcal{C}_x^{(\ell)})} \sum_{n'=0}^p \sum_{m'=-n'}^{n'} (-1)^n \overline{S_{n+n', m+m'}(\boldsymbol{\xi}_0^{(\ell)} - \mathbf{x}_0^{(\ell)})} M_{n', m'}(\mathcal{C}_\xi^{(\ell)})
 \end{aligned}$$

Downward pass entails translation of origin $\mathbf{x}_0^{(\ell-1)} \rightarrow \mathbf{x}_0^{(\ell)}$

Multi-level FMM: M2L translation formula for downward pass

$$L_{n,m}(\mathcal{C}_x^{(\ell-1)}; \mathbf{x}_0^{(\ell)}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} R_{n'-n, m'-m}(\mathbf{x}_0^{(\ell)} - \mathbf{x}_0^{(\ell-1)}) L_{n', m'}(\mathcal{C}_x^{(\ell-1)}; \mathbf{x}_0^{(\ell-1)})$$

Proof: one must have

$$\sum_{n=0}^{\infty} \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0^{(\ell)}) L_{n,m}(\mathcal{C}_x^{(\ell-1)}; \mathbf{x}_0^{(\ell)}) \quad (a)$$

$$= \sum_{n=0}^{\infty} \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0^{(\ell-1)}) L_{n,m}(\mathcal{C}_x^{(\ell-1)}; \mathbf{x}_0^{(\ell-1)}) \quad (b)$$

Then, insert identity

$$R_{n,m}(\mathbf{x} - \mathbf{x}_0^{(\ell-1)}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} R_{n', m'}(\mathbf{x} - \mathbf{x}_0^{(\ell)}) R_{n-n', m-m'}(\mathbf{x}_0^{(\ell)} - \mathbf{x}_0^{(\ell-1)})$$

into (b) and identify cofactors of $R_{n,m}(\mathbf{x} - \mathbf{x}_0^{(\ell)})$ in (a) and (b)

Multi-level FMM: overall complexity

Fixed number M of DOFs per leaf cell

$$\implies \bar{\ell} = O(\log N) \text{ and } O(N/M) \text{ leaf cells;}$$

Each non-empty level- ℓ cell has (on average) 4 non-empty children cells

$$\implies \text{on average, } N^{(\ell)} = O(4^{-\ell}N) \text{ DOFs per level-}\ell\text{ cell}$$

(i) Evaluation of multipole moments in leaf cells:

$$\text{CPU} = O(p^2 \times M \times (N/M)) = O(p^2 N)$$

(ii) Upward pass (M2M):

$$\text{CPU} = O(p^4 \times (N/M)[1 + 4^{-1} \dots + 4^{3-\bar{\ell}}]) = O(p^4 N/M)$$

(iii) Transfer (M2L) at each level $2 \leq \ell \leq \bar{\ell}$ from interaction list of each cell:

$$\text{CPU} = O(p^4 \times (N/M)[1 + 4^{-1} \dots + 4^{2-\bar{\ell}}]) = O(p^4 N/M);$$

(iv) Downward pass (L2L) at each level:

$$\text{CPU} = O(p^4 \times (N/M)[1 + 4^{-1} \dots + 4^{3-\bar{\ell}}]) = O(p^4 N/M)$$

(v) Evaluation of local expansions at leaf cells:

$$\text{CPU} = O(p^2 N/M)$$

(vi) Evaluation of near contributions $\mathcal{S}[\varphi, \partial\Omega]^{\text{near}}(\textcolor{red}{x})$ using standard BEM techniques:

$$\text{CPU} = O((N/M) \times M \times |\mathcal{A}(\mathcal{C})|M) = O(|\mathcal{A}(\mathcal{C}_x)|MN)$$

Overall complexity:

$\text{CPU} = O(N)$

1. Review of boundary integral equation formulations

Electrostatics

Laplace

Elastostatics

Frequency-domain wave equations

2. Review of classical BEM concepts

3. The GMRES iterative solver

4. The fast multipole method (FMM) for the Laplace equation

Multipole expansion of $1/r$

The single-level fast multipole method

The multi-level fast multipole method

5. The fast multipole method (FMM) for elastostatics

6. The fast multipole method for elastodynamics

7. Other acceleration methods

Exponential representation of $1/r$

FMM using equivalent sources

Clustering and low-rank approximations

Kernel-independent acceleration via kernel interpolation

Adaptive cross approximation

8. Preconditioning

Elastostatics

Reformulation of Kelvin solution in terms of $1/r$:

$$U_i^k(\mathbf{x}, \boldsymbol{\xi}) = \frac{1}{16\pi\mu(1-\nu)} \left\{ (3-4\nu)\delta_{ik} \frac{1}{r} + (\xi_i - x_i) \frac{\partial}{\partial x_k} \frac{1}{r} \right\} \quad (a)$$

$$\begin{aligned} T_i^k(\mathbf{x}, \boldsymbol{\xi}) = & -\frac{1}{8\pi\mu(1-\nu)} \left\{ (1-2\nu) \left[n_k(\boldsymbol{\xi}) \frac{\partial}{\partial x_i} \frac{1}{r} - n_i(\boldsymbol{\xi}) \frac{\partial}{\partial x_k} \frac{1}{r} \right] \right. \\ & \left. + 2(1-\nu)\delta_{ik} n_j(\boldsymbol{\xi}) \frac{\partial}{\partial x_j} \frac{1}{r} + (\xi_j - x_j) n_j(\boldsymbol{\xi}) \frac{\partial^2}{\partial x_i \partial x_k} \frac{1}{r} \right\} \quad (b) \end{aligned}$$

Substitute multipole expansion of $1/r$ into (a) and (b):

$$\frac{1}{\|\boldsymbol{\xi} - \mathbf{x}\|} = \sum_{n=0}^{+\infty} \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0) \sum_{n'=0}^{+\infty} \sum_{m'=-n'}^{n'} (-1)^n \overline{S_{n+n', m+m'}(\boldsymbol{\xi}_0 - \mathbf{x}_0)} R_{n', m'}(\boldsymbol{\xi} - \boldsymbol{\xi}_0) \quad (\text{again})$$

Elastostatics: multipole expansion of Kelvin solution

$$U_i^k(\mathbf{x}, \boldsymbol{\xi}) = \frac{1}{16\pi\mu(1-\nu)} \sum_{n'=0}^{+\infty} \sum_{m'=-n'}^{n'} \left\{ F_{ki}^{n',m'}(\mathbf{x}-\boldsymbol{\xi}_0) R_{n',m'}(\boldsymbol{\xi}-\boldsymbol{\xi}_0) + G_k^{n',m'}(\mathbf{x}-\boldsymbol{\xi}_0)(\xi_i - \xi_{i0}) R_{n',m'}(\boldsymbol{\xi}-\boldsymbol{\xi}_0) \right\}$$

$$F_{ki}^{n',m'}(\mathbf{x}-\boldsymbol{\xi}_0) = \sum_{n=0}^{+\infty} \sum_{m=-n}^n (-1)^n \overline{S_{n+n',m+m'}(\boldsymbol{\xi}_0 - \mathbf{x}_0)} \left[(3-4\nu)\delta_{ik} R_{n,m}(\mathbf{x}-\mathbf{x}_0) + (\xi_{i0} - x_{i0} - x_i - x_{i0}) \frac{\partial}{\partial x_k} R_{n,m}(\mathbf{x}-\mathbf{x}_0) \right]$$

$$G_k^{n',m'}(\mathbf{x}-\boldsymbol{\xi}_0) = \sum_{n=0}^{+\infty} \sum_{m=-n}^n (-1)^n \overline{S_{n+n',m+m'}(\boldsymbol{\xi}_0 - \mathbf{x}_0)} \frac{\partial}{\partial x_k} R_{n,m}(\mathbf{x}-\mathbf{x}_0)$$

A similar formula (not shown) can be established for the multipole representation of $T_i^k(\mathbf{x}, \boldsymbol{\xi})$

Elastostatics: multipole moments

$$M_{n',m';i}^t(\mathcal{C}_\xi; \boldsymbol{\xi}_0) = \int_{\partial\Omega \cup \mathcal{C}_\xi} R_{n',m'}(\boldsymbol{\xi} - \boldsymbol{\xi}_0) t_i(\boldsymbol{\xi}) dS_\xi$$

$$M_{n',m'}^t(\mathcal{C}_\xi; \boldsymbol{\xi}_0) = \int_{\partial\Omega \cup \mathcal{C}_\xi} R_{n',m'}(\boldsymbol{\xi} - \boldsymbol{\xi}_0) (\xi_i - \xi_{i0}) t_i(\boldsymbol{\xi}) dS_\xi$$

$$M_{n',m';ki}^u(\mathcal{C}_\xi; \boldsymbol{\xi}_0) = \int_{\partial\Omega \cup \mathcal{C}_\xi} R_{n',m'}(\boldsymbol{\xi} - \boldsymbol{\xi}_0) n_k(\boldsymbol{\xi}) u_i(\boldsymbol{\xi}) dS_\xi$$

$$M_{n',m';k}^u(\mathcal{C}_\xi; \boldsymbol{\xi}_0) = \int_{\partial\Omega \cup \mathcal{C}_\xi} R_{n',m'}(\boldsymbol{\xi} - \boldsymbol{\xi}_0) n_k(\boldsymbol{\xi}) (\xi_i - \xi_{i0}) u_i(\boldsymbol{\xi}) dS_\xi$$

M2M, M2L and L2L formulae

M2M, M2L and L2L formulae are derived using those for $1/r$. For example, the elastostatic M2M formulae are:

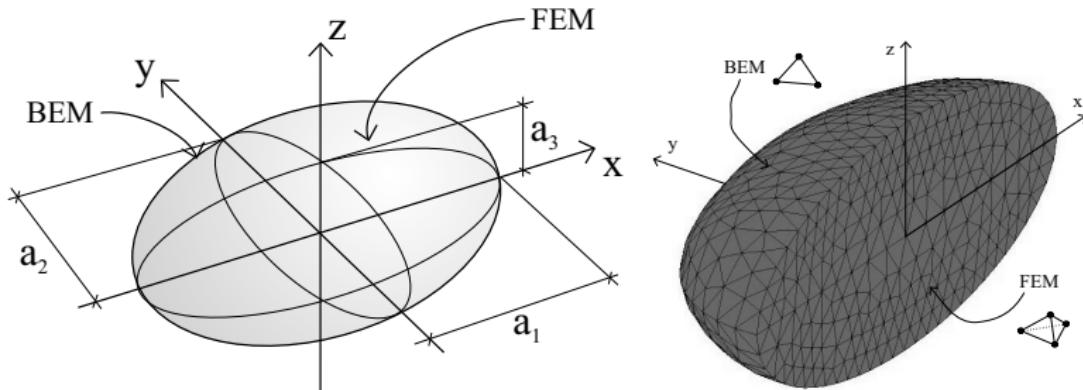
$$M_{n,m;i}^t(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell-1)}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} R_{n',m'}(\xi_0^{(\ell)} - \xi_0^{(\ell-1)}) M_{n-n',m-m';i}^t(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell)})$$

$$\begin{aligned} M_{n,m}^t(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell-1)}) &= \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} \left\{ R_{n',m'}(\xi_0^{(\ell)} - \xi_0^{(\ell-1)}) M_{n-n',m-m'}(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell)}) \right. \\ &\quad \left. + (\xi_{i0}^{(\ell)} - \xi_{i0}^{(\ell-1)}) M_{n-n',m-m';i}^t(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell)}) \right\} \end{aligned}$$

$$M_{n,m;ki}^u(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell-1)}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} R_{n',m'}(\xi_0^{(\ell)} - \xi_0^{(\ell-1)}) M_{n-n',m-m';ki}(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell)})$$

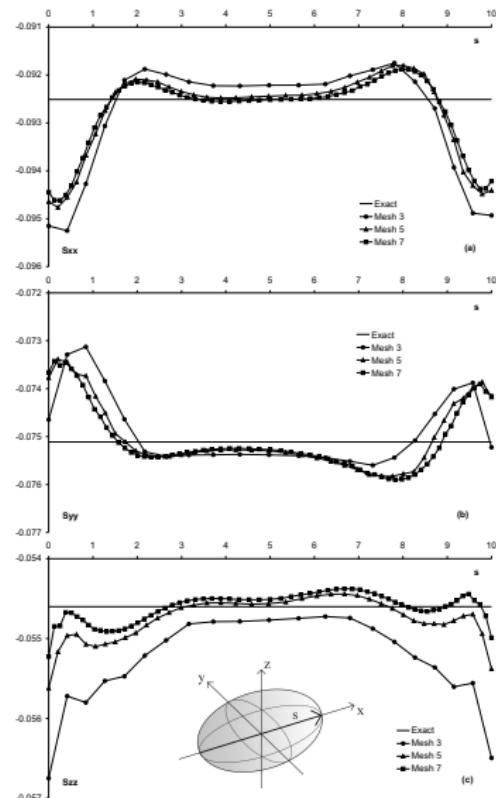
$$\begin{aligned} M_{n,m;k}^u(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell-1)}) &= \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} \left\{ R_{n',m'}(\xi_0^{(\ell)} - \xi_0^{(\ell-1)}) M_{n-n',m-m';k}(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell)}) \right. \\ &\quad \left. + (\xi_{i0}^{(\ell)} - \xi_{i0}^{(\ell-1)}) M_{n-n',m-m';ki}^t(\mathcal{C}_\xi^{(\ell)}; \xi_0^{(\ell)}) \right\} \end{aligned}$$

Numerical example: uniform thermal strain in ellipsoidal region

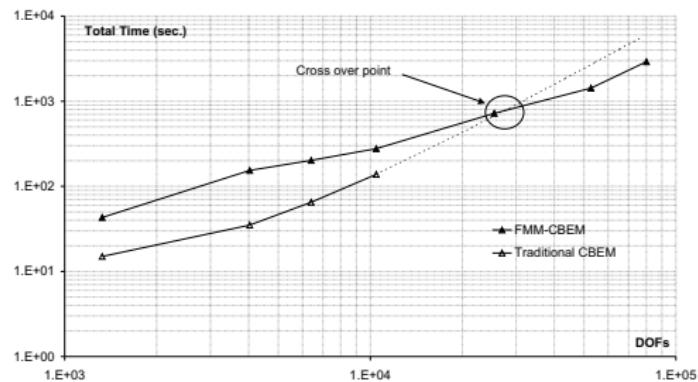


Mesh	Nodes	Elements		Oct-tree		DOFs		
		BEM	FEM	Max level	Leaves	N_{BEM}	N_F	$N_{\text{BEM}} + N_F$
1	267	346	979	3	42	1050	276	1326
2	822	1038	3153	3	100	3126	903	4029
3	1362	1540	5563	3	103	4632	1770	6402
4	2274	2418	9626	4	301	7266	3189	10455
5	5881	5200	26602	4	422	15612	9837	25449
6	12868	9402	61770	5	1175	28218	24495	52713
7	20258	12842	100200	6	1403	38538	41505	80043

Numerical example: uniform thermal strain in ellipsoidal region



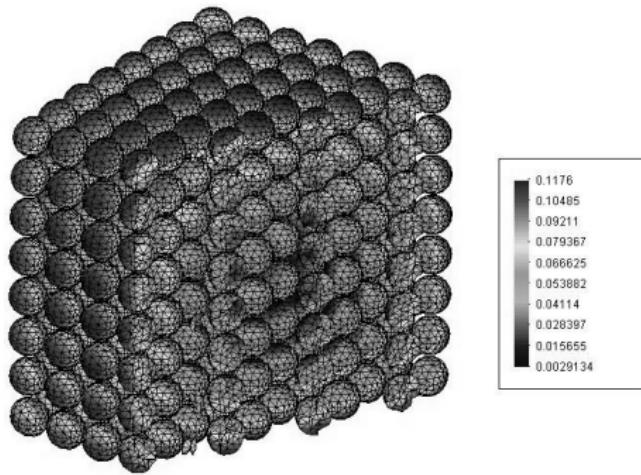
Mesh	Precond. (s)	FMM (s/iter)	Iters n	Total time (s)
BEM	FEM			
1	10	<1	1	43
2	36	<1	2	154
3	50	<1	3	202
4	64	3	6	277
5	169	18	11	721
6	349	101	19	1425
7	512	279	42	2913



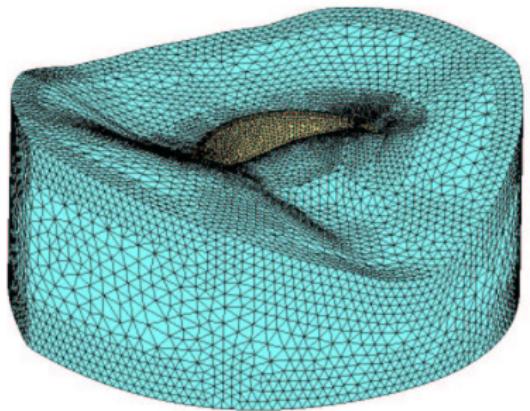
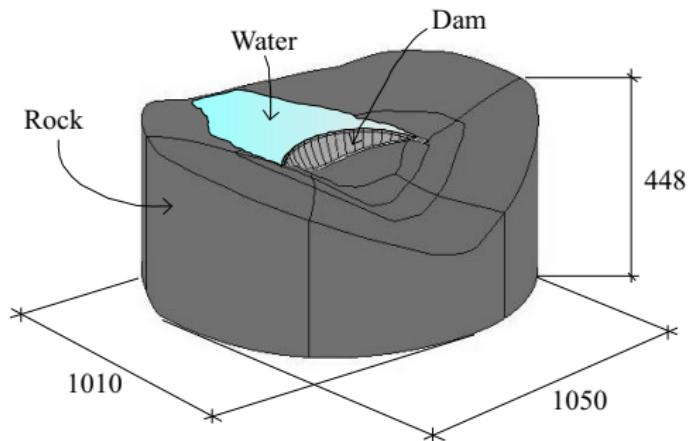
Numerical example: many-inclusion problem

Nodes	Elements		Oct-tree		DOFs		
	BEM	FEM	Max. level	Leaves	N_{BEM}	N_{F}	$N_{\text{BEM}} + N_{\text{F}}$
93227	122880	326493	5	7176	374784	92289	467073

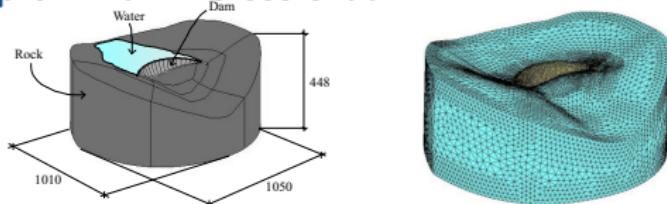
Precond. (s)		Time (s)				Iters	Total time
BEM	FEM	Upw.	Downw.	Direct	Cycle	n	(s)
6609	19	47	48	84	180	147	39656



Numerical example: Pian Telessio dam



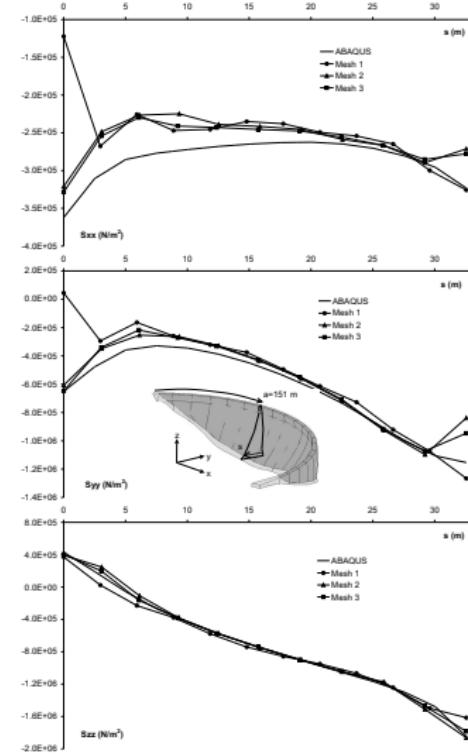
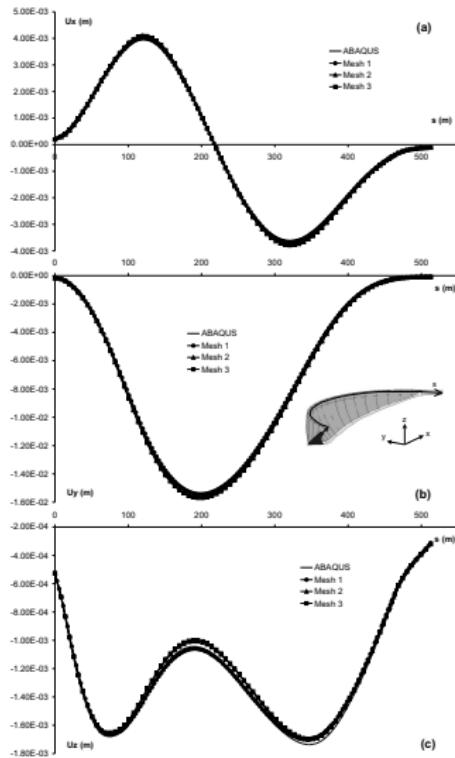
Numerical example: Pian Telessio dam



Mesh	Nodes	Elements		Oct-tree		DOFs		
		BEM	FEM	Levels	Leaves	N_{BEM}	N_F	Total
1	25443	21684 (T3)	73569 (T4)	9	8953	38118	43797	81915
2	23433	7726 (T6)	10307 (T10)	8	3548	50490	46773	97263
3	51978	15296 (T6)	14462 (T10)	8	6786	96636	64152	160788
A	406035	—	279742	—	—	—	—	1218105

Mesh	Precond. (s)		Time (s)					Iters n	Total time (s)
	BEs	FEs	Upw.	Down.	Direct	Cycle			
1	186	26	23	27	24	76	83	7916	
2	328	114	11	21	23	57	82	5818	
3	1215	223	23	36	102	165	85	17775	
A	—	—	—	—	—	—	—	3749	

Numerical example: Pian Telessio dam



Exemple, calcul d'amortissements dans les MEMS

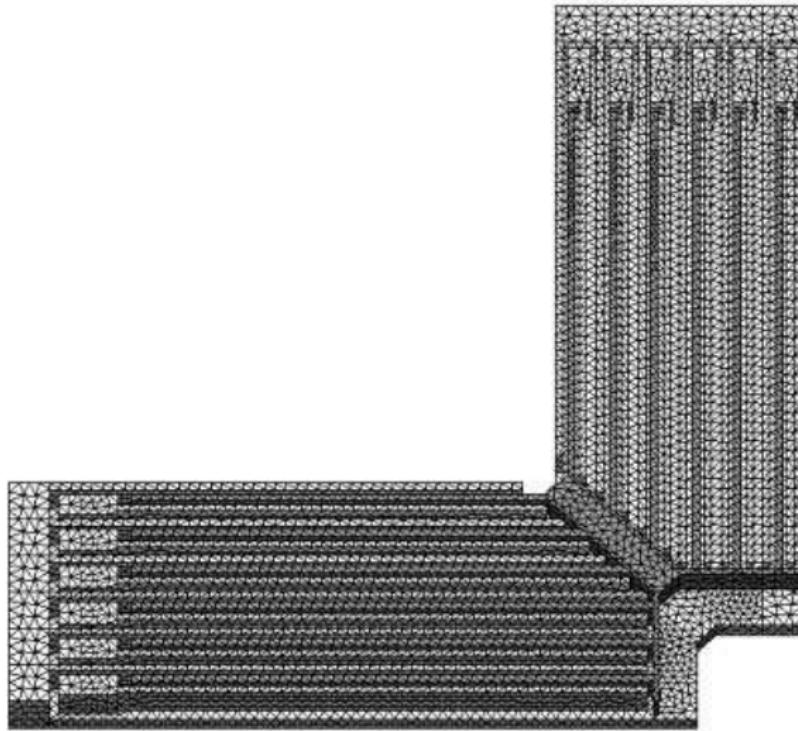


Figure 5. More realistic model of one-fourth of the MEMS: geometry and mesh.

Frangi A., Spinola G., Vigna B., IJNME **68**:1031–1051

Exemple, calcul d'amortissements dans les MEMS

Table II. Comparison between meshes of increasing refinement.

Mesh employed	Mesh 1	Mesh 2	Mesh 3
Number of unknowns	125 058	272 364	548 388
Global force (N)	1.80×10^{-4}	2.01×10^{-4}	2.12×10^{-4}

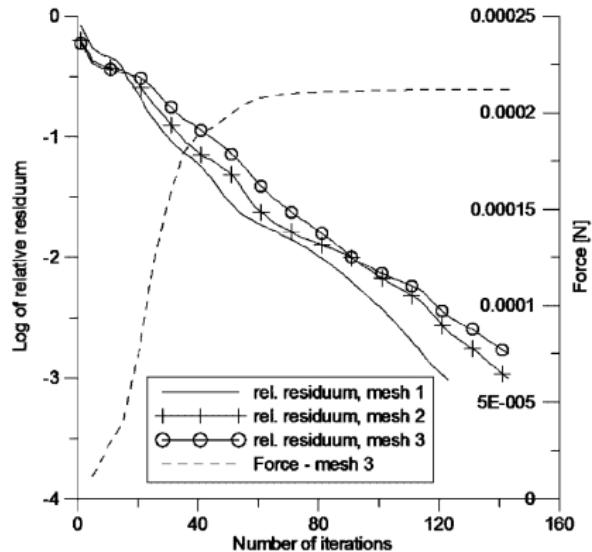


Figure 6. Convergence of the GMRES solver and of the force computed.

Exemple, homogénéisation numérique

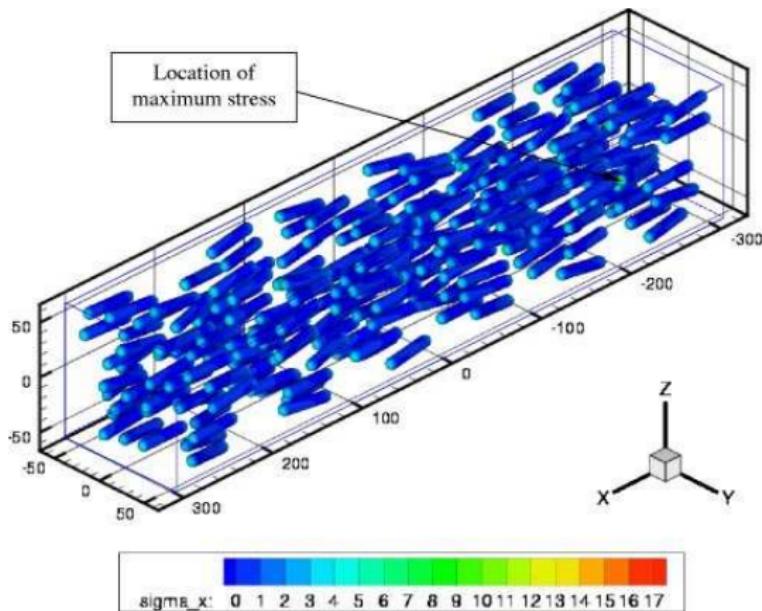


Fig. 10 Contour plot of surface stresses ($\times \sigma^*$) for a model with 216 "randomly" distributed and oriented short fibers

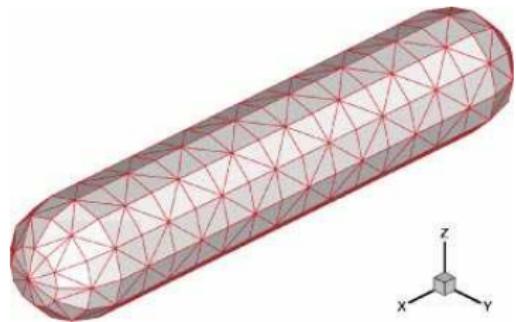


Fig. 9 A BEM mesh used for the short fiber inclusion (with 456 elements)

Liu Y.J., Nishimura N. et al., ASME J. Appl. Mech. 72:115–128 (2005)

Exemple, homogénéisation numérique

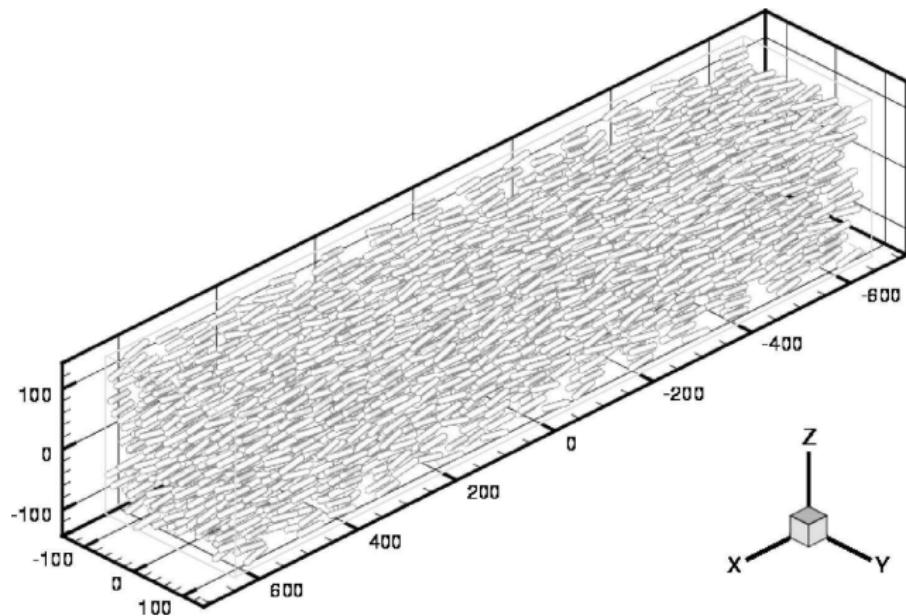


Fig. 11 A RVE containing 2197 short fibers with the total DOF=3 018 678

Liu Y.J., Nishimura N. et al., ASME J. Appl. Mech. 72:115–128 (2005)

Exemple, homogénéisation numérique

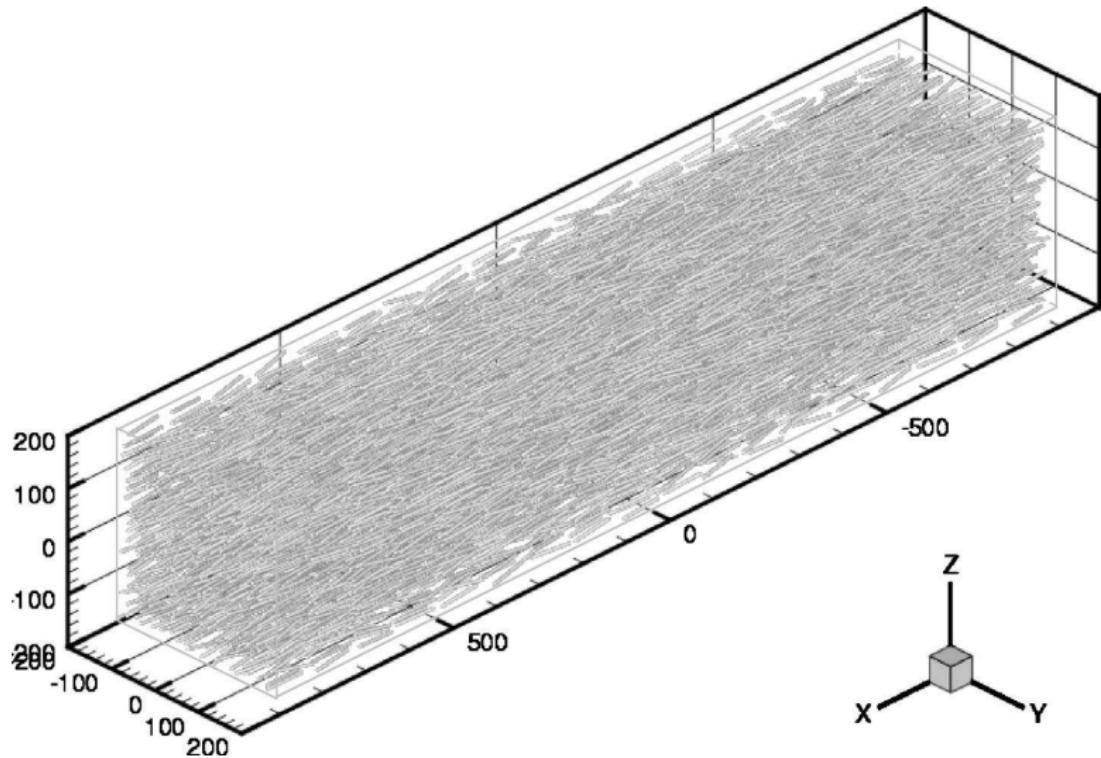


Fig. 14 A RVE containing 5832 long fibers with the total DOF=10 532 592

Liu Y.J., Nishimura N. et al., ASME J. Appl. Mech. 72:115–128 (2005)

Exemple, homogénéisation numérique

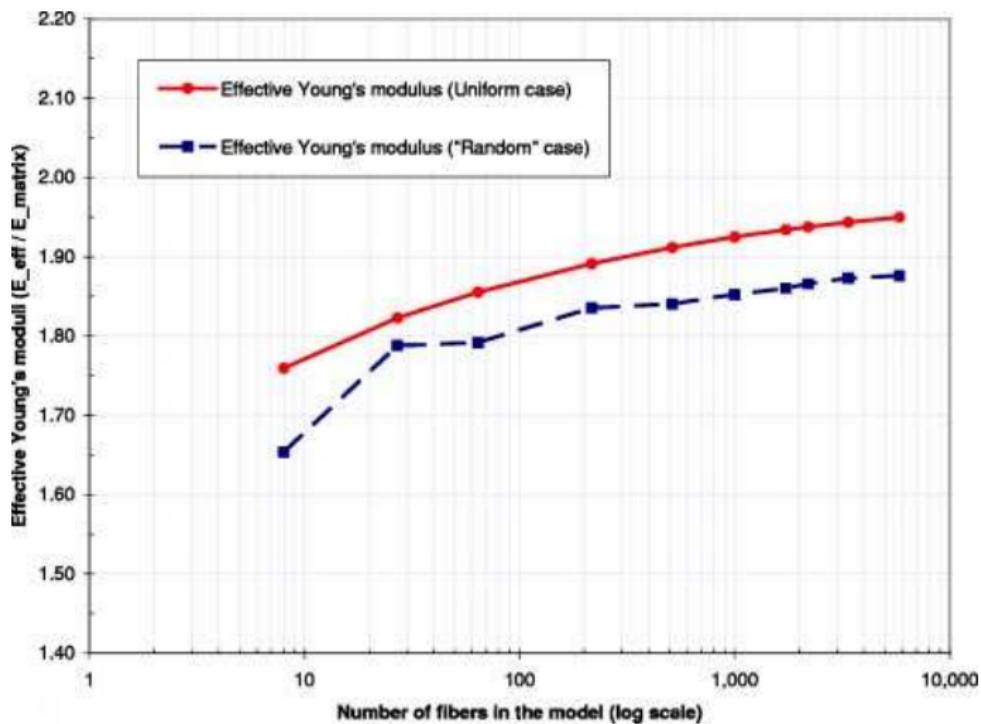


Fig. 15 Estimated effective Young's moduli in the x -direction for the composite model with up to 5832 long rigid fibers (fiber volume fraction=3.85%)

Liu Y.J., Nishimura N. et al., ASME J. Appl. Mech. 72:115–128 (2005)

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The multi-level fast multipole method

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6. The fast multipole method for elastodynamics

7. Other acceleration methods

Exponential representation of $1/r$

FMM using equivalent sources

Clustering and low-rank approximations

Kernel-independent acceleration via kernel interpolation

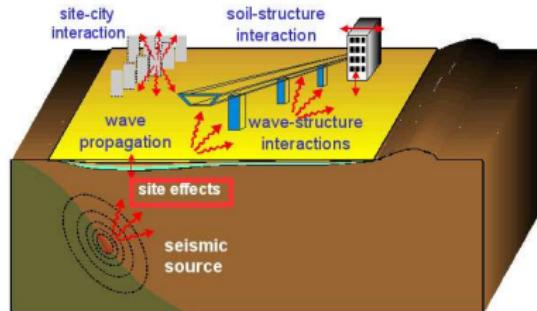
Adaptive cross approximation

8. Preconditioning

Avec: Jean-François Semblat (Civil Engineering Research Lab [LCPC], Paris)
Nicolas Nemitz (doctoral thesis, 2002-2006)
Stéphanie Chaillat (doctoral thesis, 2005–)
Eva Grasso (doctoral thesis, 2008–)
Tekoing Lim (doctoral thesis, Atomic Energy Commission [CEA], 2007–)

Motivation

Modelling of elastic wave propagation in large/unbounded domains



- ▶ Soil-structure interaction
- ▶ Site effects
- ▶ Computational forward solution method for inverse problems

Pros and cons of BEMs for elastic waves

FEM, FDM, DG...

BEM

- | | |
|--------------------------------|--|
| → Domain mesh | → Surface mesh (i.e. reduced dimensionality) |
| → Approx. radiation conditions | → Exact radiation conditions |
| → Sparse matrix | → Fully-populated matrix |

BEM adequate for large (unbounded) media with simple (linear) properties.
Fully-populated BEM influence matrix is a priori a severe limiting factor

Standard BEM (3-D elastodynamics, frequency domain)

Governing integral equation for boundary displacements and tractions

$$c_{ik}(\mathbf{x}) u_i(\mathbf{x}) = \int_{\partial\Omega} [t_i(\mathbf{x}) U_i^k(\mathbf{x}, \boldsymbol{\xi}; \omega) - u_i(\mathbf{x}) T_i^k(\mathbf{x}, \boldsymbol{\xi}; \omega)] dS_\xi \quad (\mathbf{x} \in \partial\Omega)$$

Full-space elastodynamic fundamental solutions

$$U_i^k(\mathbf{x}, \boldsymbol{\xi}; \omega) = \frac{1}{4\pi k_S^2 \mu} ((\delta_{qs} \delta_{ik} - \delta_{qk} \delta_{is}) \frac{\partial}{\partial x_q} \frac{\partial}{\partial y_s} G_S(\|\mathbf{x} - \boldsymbol{\xi}\|) + \frac{\partial}{\partial x_i} \frac{\partial}{\partial y_k} G_P(\|\mathbf{x} - \boldsymbol{\xi}\|))$$

$$T_i^k(\mathbf{x}, \boldsymbol{\xi}; \omega) = C_{ijh\ell} \frac{\partial}{\partial y_\ell} U_h^k(\mathbf{x}, \boldsymbol{\xi}; \omega) n_j(\boldsymbol{\xi})$$

$$G_\alpha(z) = \frac{\exp(ik_\alpha z)}{z} \text{ (fund. sol. Helmholtz eqn., } \alpha = P, S)$$

BEM discretization \implies fully-populated system of linear equations.

Computational limitations of standard BEM

Solution of fully-populated matrix equation

- ▶ Direct solvers (LU factorisation, ...) :
 - ▶ Pros: robust, accurate;
 - ▶ Cons: $O(N^2)$ memory and $O(N^3)$ CPU
- ▶ Iterative solvers (GMRES, ...) :
 - ▶ Pros: $O(N_{iter} \times N^2)$ CPU;
 - ▶ Cons: $O(N^2)$ memory; N_{iter} may be large

(N : number of BE DOFs)

Limitations of standard BEM

- ▶ High memory cost
 - problem size limit $N = O(10^4)$ (PC, single-proc.)
- ▶ Limited geometric complexity, (piecewise) heterogeneity, frequency range

Fast multipole accelerated BEM

Fast Multipole Method (FMM):

- ▶ Based on **iterative** linear equation solvers (GMRES)
- ▶ Fast method for evaluating matrix-vector products, i.e. discretized versions of e.g.

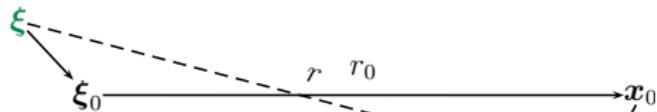
$$\int_{\partial\Omega} t_i(\mathbf{x}) U_i^k(\mathbf{x}, \boldsymbol{\xi}; \omega) dS_\xi \quad (\text{for given solution candidate } \mathbf{t})$$

A few milestones

- ▶ Laplace: Rokhlin (1985)
- ▶ Electrostat.: Greengard (1988)
- ▶ Electromag.: Chew (1994), Darve (2000), Sylvand (2002)...
- ▶ Elastodyn. freq. domain: Fujiwara (2000)
- ▶ Elastodyn., time domain: Nishimura (2002)
- ▶ BEM-FEM : Margonari, Bonnet (2004), Gaul et al...
- ▶ Effective prop. of composite mater.: Nishimura, Liu (2005)

Decomposition of Helmholtz fundamental solution

Multipole expansion formula (“diagonal form”, Epton and Dembart 1995)



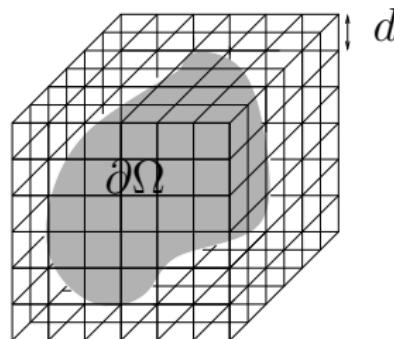
$$\frac{\exp(ik\|\xi - \mathbf{x}\|)}{\|\xi - \mathbf{x}\|} = \frac{ik}{4\pi} \lim_{L \rightarrow +\infty} \int_{\hat{s} \in S} e^{ik\hat{s} \cdot \xi} \mathcal{G}_L(\hat{s}; \mathbf{r}_0; k) e^{-ik\hat{s} \cdot \mathbf{x}} d\hat{s}$$

Transfer function

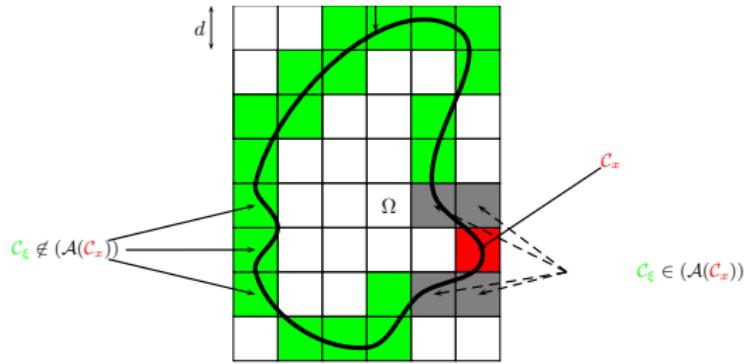
$$\mathcal{G}_L(\hat{s}; \mathbf{r}_0; k) = \sum_{p=0}^L (2p+1) i^p h_p^{(1)}(k\|\mathbf{r}_0\|) P_p(\cos(\hat{s}, \mathbf{r}_0))$$

Single-level FMM

Boundary of interest enclosed in cubic grid



Convergence of multipole expansion assured if \mathbf{x} and ξ lie in non-adjacent cells



Single-level FMM

Matrix-vector product \leftarrow evaluation of integral operator

- Must compute e.g.:

$$[\mathcal{K}\{t\}](\mathbf{x}) := \int_{\partial\Omega} t_i(\mathbf{x}) U_i^k(\mathbf{x}, \xi; \omega) dS_\xi \quad (\text{for given solution candidate } \mathbf{t})$$

- Split integrals into near and FM contributions:

$$\int_{\partial\Omega} = \sum_{C_\xi \in \mathcal{A}(C_x)} \int_{\partial\Omega \cap C_\xi} + \sum_{C_\xi \notin \mathcal{A}(C_x)} \int_{\partial\Omega \cap C_\xi}$$

$$[\mathcal{K}\{t\}](\mathbf{x}) = [\mathcal{K}\{t\}]^{\text{near}}(\mathbf{x}) + [\mathcal{K}\{t\}]^{\text{far}}(\mathbf{x})$$

Single-level FMM algorithm: principle



$$\int_{\partial\Omega} t_i(\mathbf{x}) U_i^k(\mathbf{x}, \boldsymbol{\xi}; \omega) dS_\xi \quad (\text{for given solution candidate } \mathbf{t})$$

$$\frac{\exp(ik\|\boldsymbol{\xi} - \mathbf{x}\|)}{\|\boldsymbol{\xi} - \mathbf{x}\|} = \frac{ik}{4\pi} \lim_{L \rightarrow +\infty} \int_{\hat{\mathbf{s}} \in S} e^{iks \cdot \boldsymbol{\xi}} \mathcal{G}_L(\hat{\mathbf{s}}; \mathbf{r}_0; k) e^{-ik\hat{\mathbf{s}} \cdot \mathbf{x}} d\hat{\mathbf{s}}$$

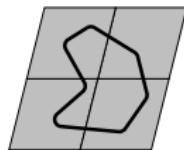
- ▶ compute multipole moments for each cell \mathcal{C}_ξ and quadrature point
- ▶ Transfer (M2L) from \mathcal{C}_ξ to non-adjacent \mathcal{C}_x
- ▶ Evaluate FM contribution to matrix-vector product
- ▶ Add near contribution to matrix-vector product (computed using standard BEM techniques)

Complexity of single-level elastodynamic FMM: $O(N^{3/2})$ per GMRES iteration

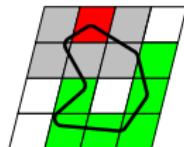
Multi-level FMM



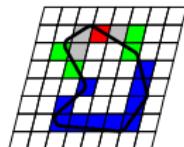
level $\ell = 0$



level $\ell = 1$



level $\ell = 2$



level $\ell = 3$

→ highest level for which FMM is applicable.

⋮

level $\ell = \bar{\ell}$ (leaf)

computation organization based on recursive subdivision (oc-tree)

Complexity of multi-level elastodynamic FMM: $O(N \log_2 N)$

Computational issues: truncation of transfer function

Transfer function

$$\mathcal{G}_L(\hat{\mathbf{s}}; \mathbf{r}_0; k) = \sum_{p=0}^L (2p+1)i^p h_p^{(1)}(k\|\mathbf{r}_0\|) P_p(\cos(\hat{\mathbf{s}}, \mathbf{r}_0))$$

Choice of truncation parameter:

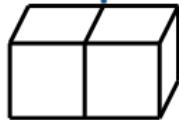
- ▶ L too small: convergence not reached for $\mathcal{G}_L(\hat{\mathbf{s}}; \mathbf{r}_0; k)$;
- ▶ L too large: divergence of $h_p^{(1)}$

Empirical formula used

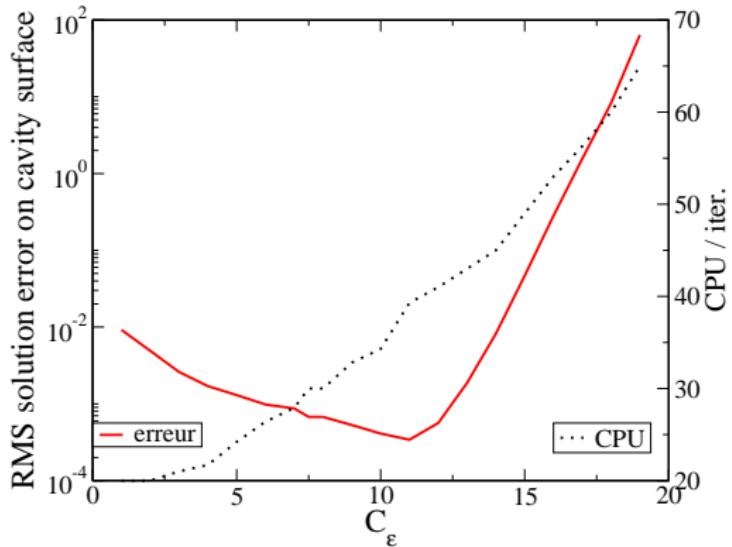
$$L = \sqrt{3}k_S d + C_\epsilon \log_{10}(\sqrt{3}k_S d + \pi)$$

(see Darve 2000 and Sylvand 2002 for Maxwell eqns)

Computational issues: adjustment of constant C_ϵ



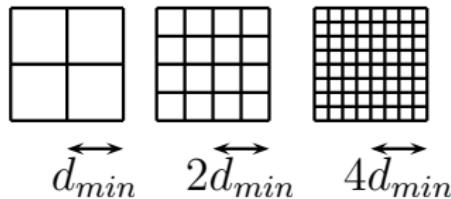
$$L = \sqrt{3}k_S d + C_\epsilon \log_{10}(\sqrt{3}k_S d + \pi)$$



→ $C_\epsilon = 7.5$

(consistent with Sylvand 2002, Maxwell eqns)

Computational issues: number of levels



$$L = \sqrt{3}k_S d + C_\epsilon \log_{10}(\sqrt{3}k_S d + \pi)$$

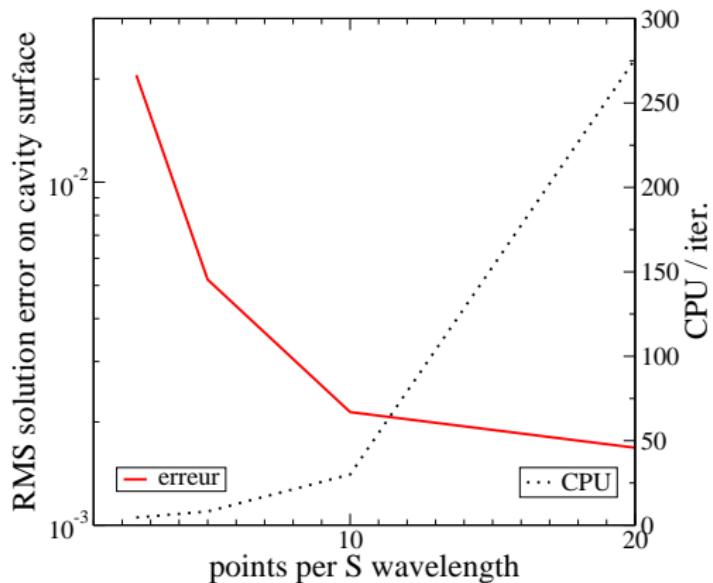
# of levels	$d_{min} \times k_S / 2\pi$	rel. err. / BEM	CPU / iter (s)
4	1.32	$1.1 \cdot 10^{-5}$	367
5	0.66	$4.7 \cdot 10^{-4}$	134
6	0.33	$3.7 \cdot 10^{-3}$	104
7	0.17	$5.1 \cdot 10^{-2}$	200
8	0.083	$1.7 \cdot 10^{-1}$	380

Choice of leaf cell size (\Leftrightarrow choice of # of levels):

- ▶ influence on CPU
- ▶ influence on accuracy

$$\rightarrow d_{min} \geq 0.3 \times \lambda_S$$

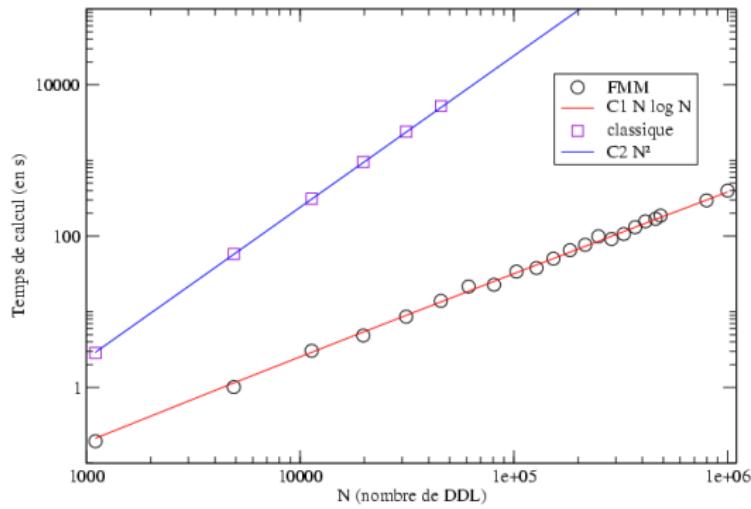
Computational issues: discretization relative to wavelength



→ 10 points per S wavelength

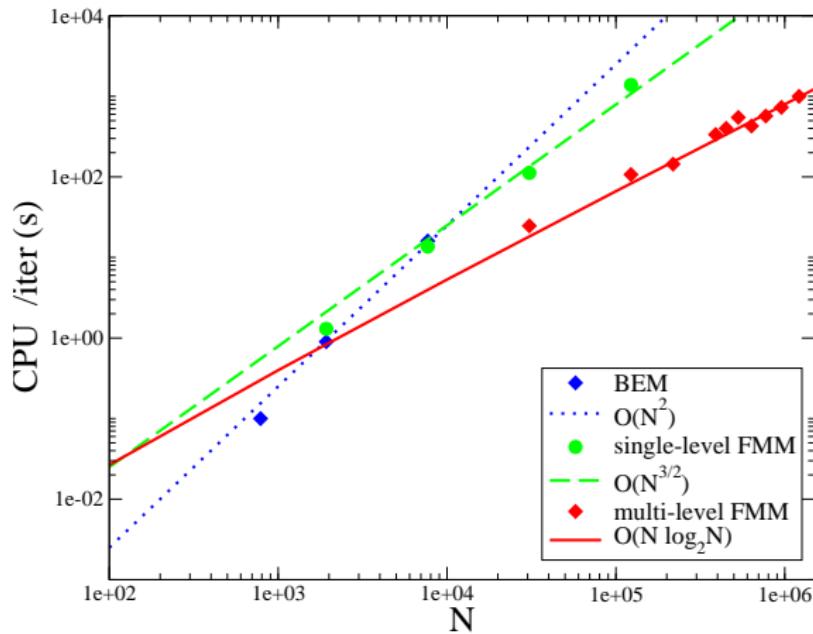
Numerical verification of theoretical complexity (CPU), Helmholtz

Example: sphere under uniform normal velocity. Mesh refinement, mesh density / wavelength kept fixed



N. Nemitz, M. Bonnet, *Eng. Anal. Bound. Elem* (2008)

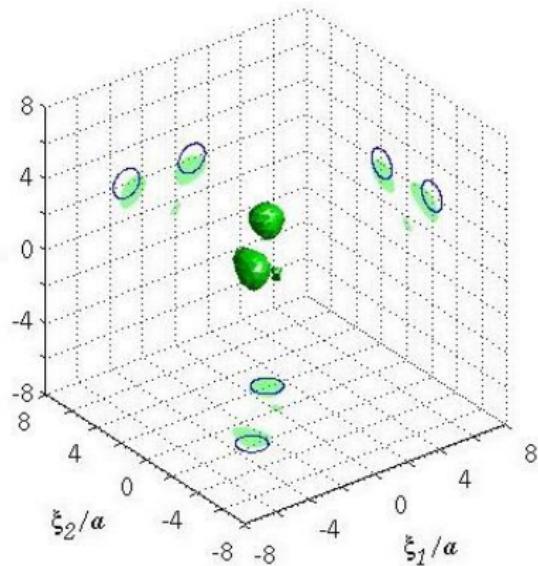
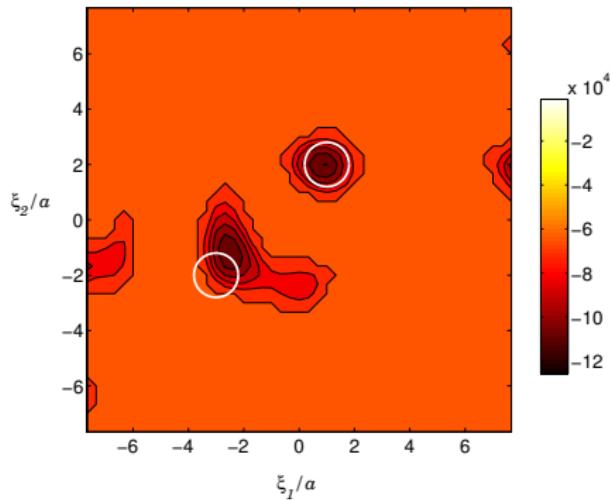
Numerical verification of theoretical complexity (CPU), elastodynamics



Chaillat S., Bonnet M., Semblat J.F., *Comp. Meth. Appl. Mech. Engng.* (2008)

Example (Helmholtz)

Identification of a dual hard scatterer



N. Nemitz, M. Bonnet, *Eng. Anal. Bound. Elem* (2008).

Example (Helmholtz)

FMM: numerical parameters

Element and DOF count (FM-BEM):

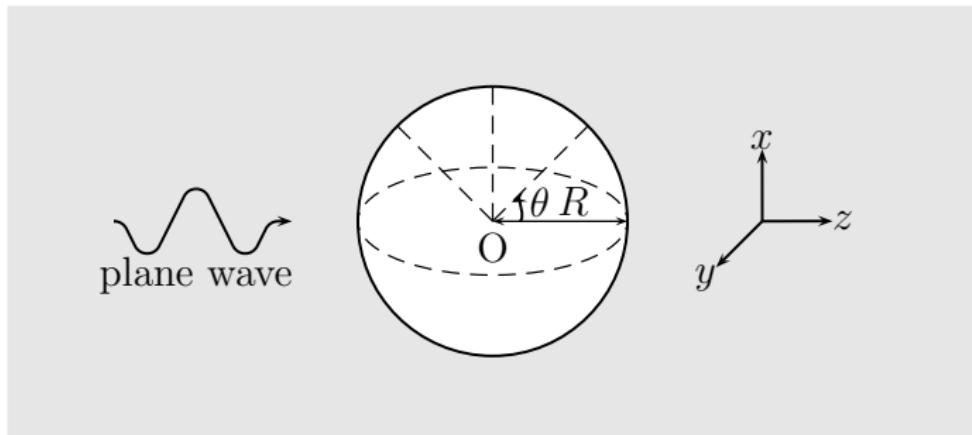
Cube size	Cube		Obstacle		Total		\mathcal{G}
	Elements	DDLs	Elements	DDLs	Elements	DDLs	
16a	76800	38402	336	170	77136	38572	100^3
32a	307200	153602	336	170	307536	153772	150^3

CPU timing (single-CPU PC) and GMRES iteration count

Cube size	u_{true} on $S \cup \Gamma_{\text{true}}$	u on S	\hat{u} on S	\mathcal{T} on \mathcal{G}
16a	1444s ($N_{\text{iter}} = 435$)	969s ($N_{\text{iter}} = 282$)	1163s ($N_{\text{iter}} = 342$)	852s
32a	6461s ($N_{\text{iter}} = 439$)	5615s ($N_{\text{iter}} = 388$)	6818s ($N_{\text{iter}} = 476$)	1860s

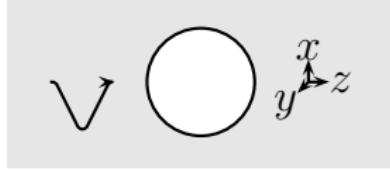
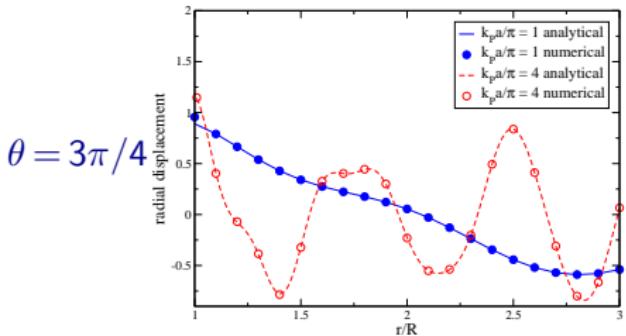
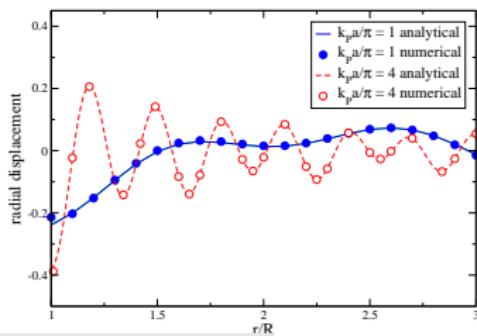
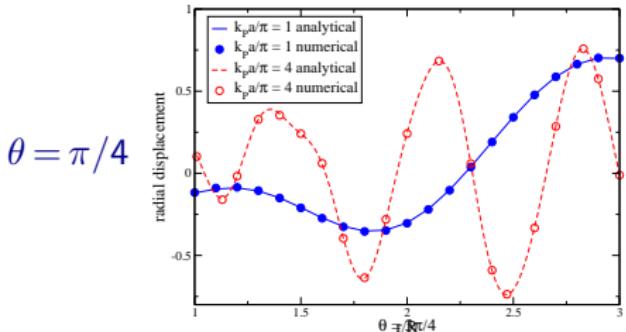
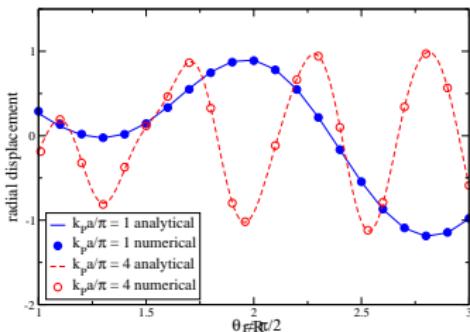
N. Nemitz, M. Bonnet, *Eng. Anal. Bound. Elem.* (2008).

Example: scattering of a plane P wave by a spherical cavity



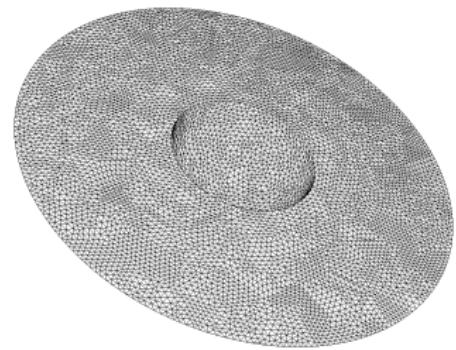
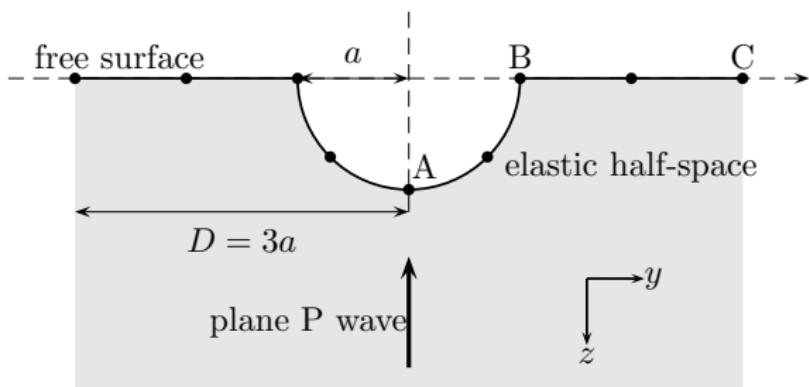
Chaillat S., Bonnet M., Semblat J.F., *Comp. Meth. Appl. Mech. Engng.* (2008)

Example: scattering of a plane P wave by a spherical cavity



$N = 122,886$

Example: scattering of a plane P wave by a hemispheric canyon

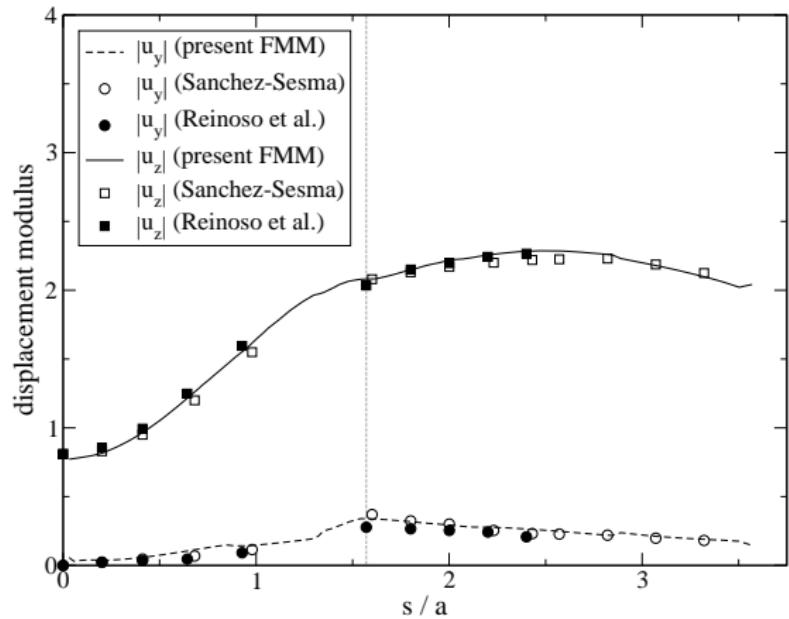
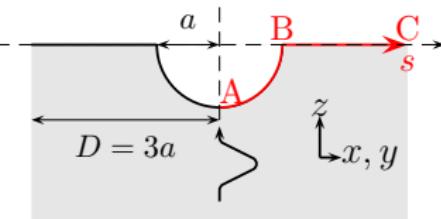


- ▶ Simplified configuration for topographic site effect
- ▶ Low frequency: comparison with other published results
- ▶ Higher frequency: FMM

Chaillat S., Bonnet M., Semblat J.F., *Comp. Meth. Appl. Mech. Engng.* (2008)

Example: scattering of a plane P wave by a hemispheric canyon

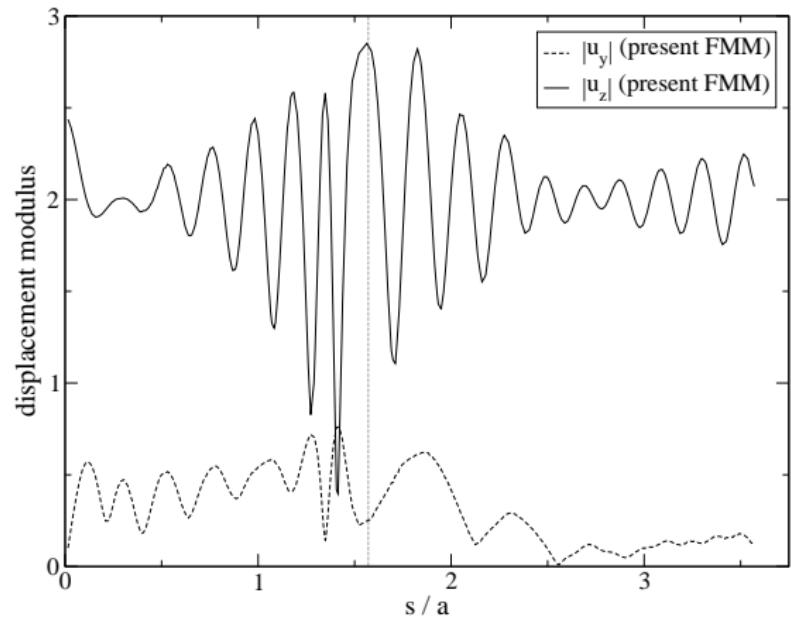
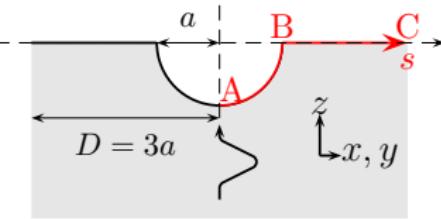
Comparaison with earlier results, $k_P a = 0.25$ (low frequency)



Example: scattering of a plane P wave by a hemispheric canyon

Results for higher frequency $k_p a = 5$

$N = 287\,946$ (86 iter., 210 s / iter, single-proc. 3 GHz PC)

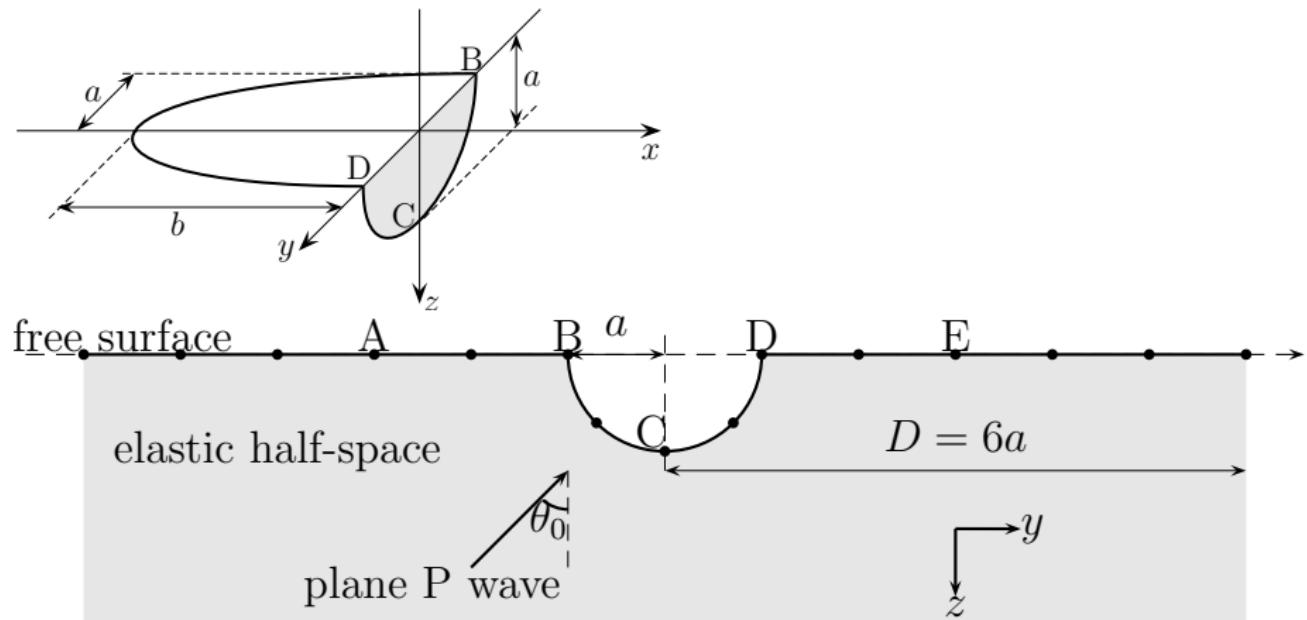


Example: scattering of a plane P wave by a hemispheric canyon

Study of convergence of GMRES

	$kPa = 0.25$	$kPa = 0.5$	$kPa = 0.75$	$kPa = 1.5$	$kPa = 5$	$kPa = 10$
$D = 3a$	7 (23382)	10 (23382)	12 (23382)	19 (23382)	86 (287946)	> 280 (114570)
$D = 5a$	7 (61875)	10 (61875)	15 (61875)	28 (61875)	159 (774180)	
$D = 7a$	8 (77565)	13 (77565)	17 (77565)	43 (77565)		
$D = 20a$	14 (98844)	39 (98844)	43 (98844)			

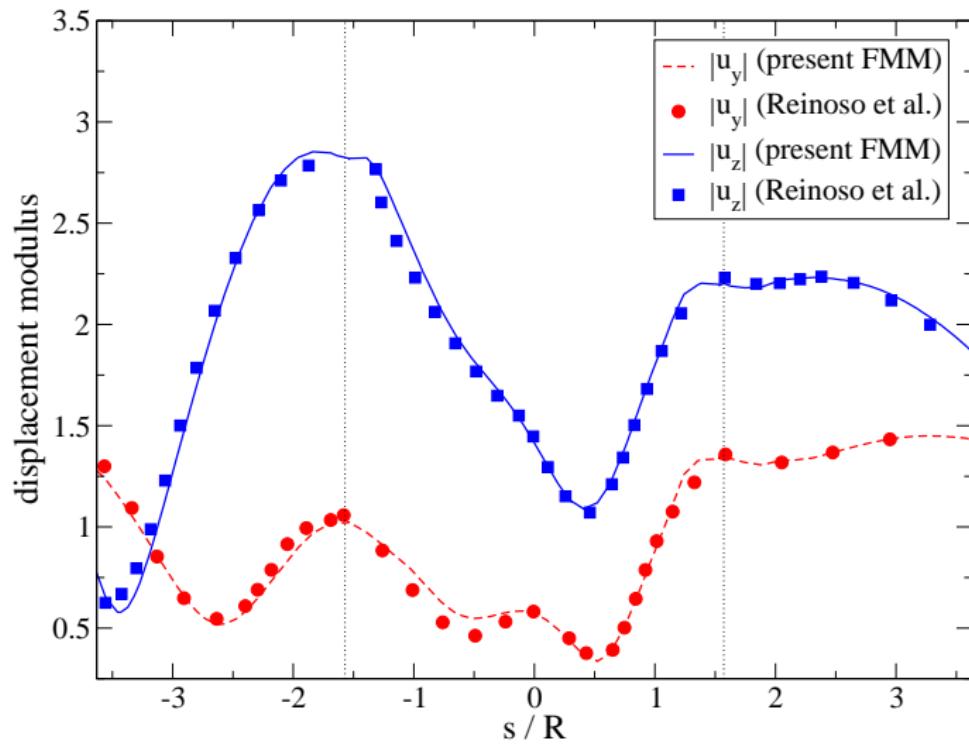
Example: scattering of a plane P wave by a semi-elliptical canyon



- ▶ Simplified configuration for topographic site effect
- ▶ Low frequency: comparison with other published results
- ▶ Higher frequency: FMM

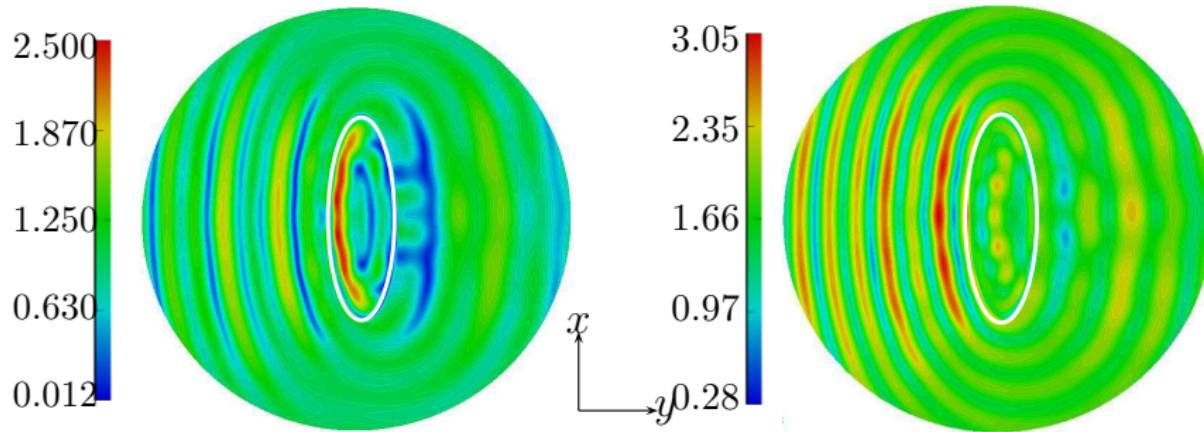
Example: scattering of a plane P wave by a semi-elliptical canyon

Comparaison with earlier results, $k_s a = 0.5$ (low frequency), $N = 25\,788$



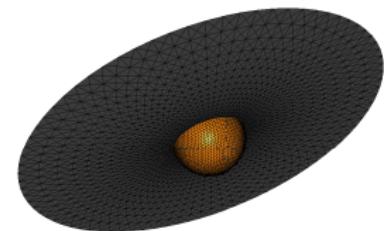
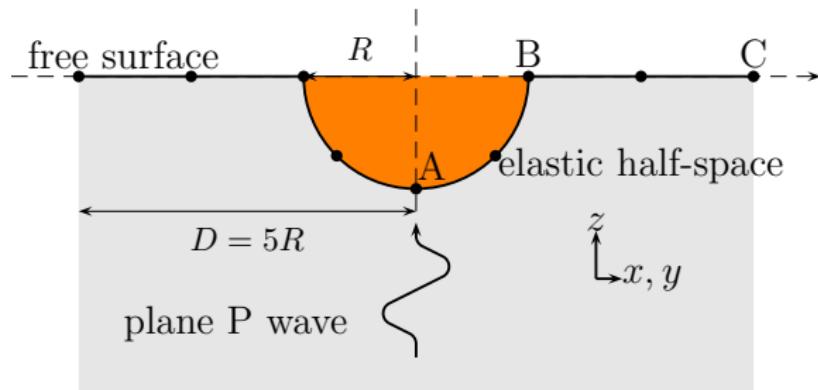
Example: scattering of a plane P wave by a semi-elliptical canyon

Results for higher frequency $k_s a = 2$



$N = 353\,232$ (32 iter., 140 s / iter, single-proc. 3 GHz PC)

Example: scattering of a plane P wave by an alluvial hemispheric valley



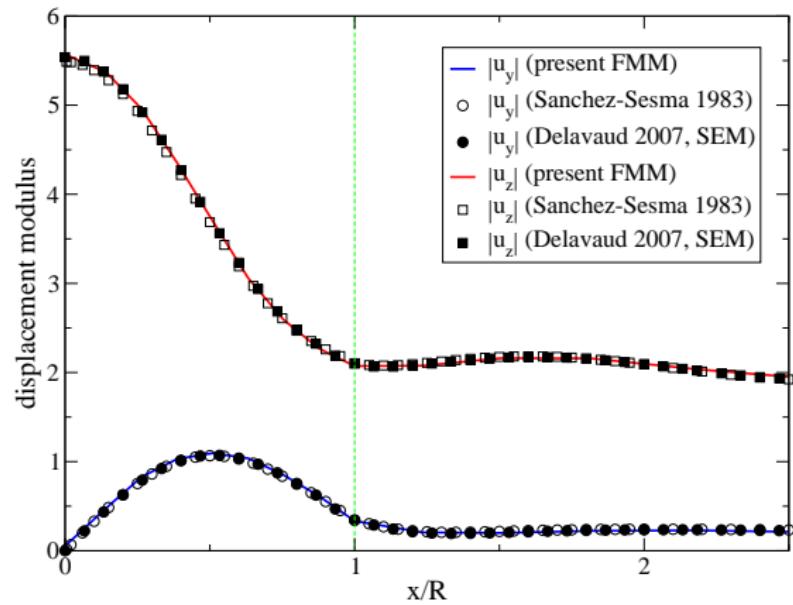
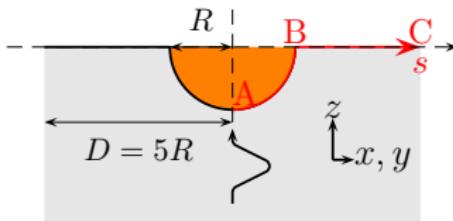
($N = 17409$)

- ▶ $\mu_2 = 0.3\mu_1$, $\rho_2 = 0.6\rho_1$, $\nu_1 = 0.25$, $\nu_2 = 0.3$
- ▶ Low frequency: comparison with Sanchez-Sesma (1983) and Delavaud (2007)
- ▶ Higher frequency: FMM

Example: scattering of a plane P wave by an alluvial hemispheric valley

Comparaison with earlier results, $k_P R = 0.5$

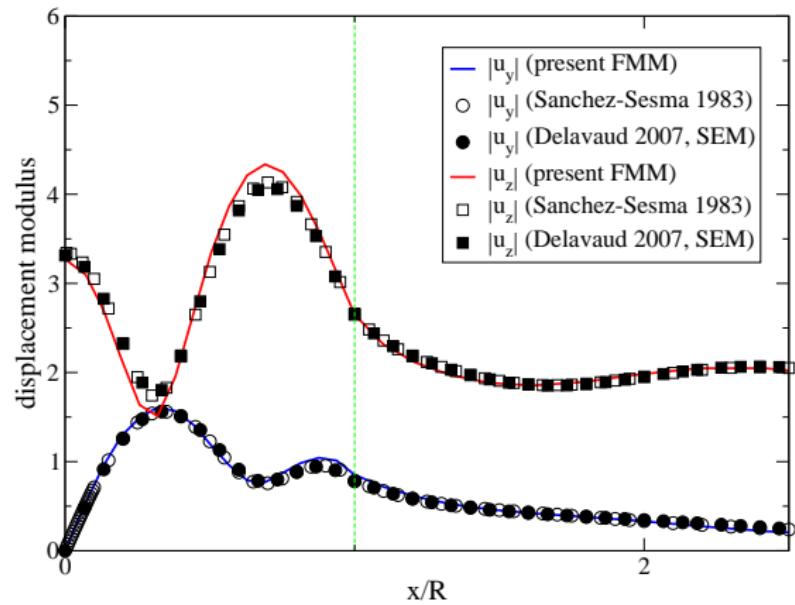
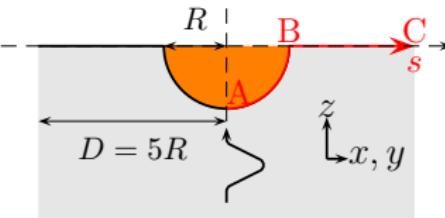
- ▶ Sanchez-Sesma, 1983 (semi-analytical)
- ▶ Delavaud, 2007 (spectral finite element method)



Example: scattering of a plane P wave by an alluvial hemispheric valley

Comparaison with earlier results, $k_P R = 0.7$:

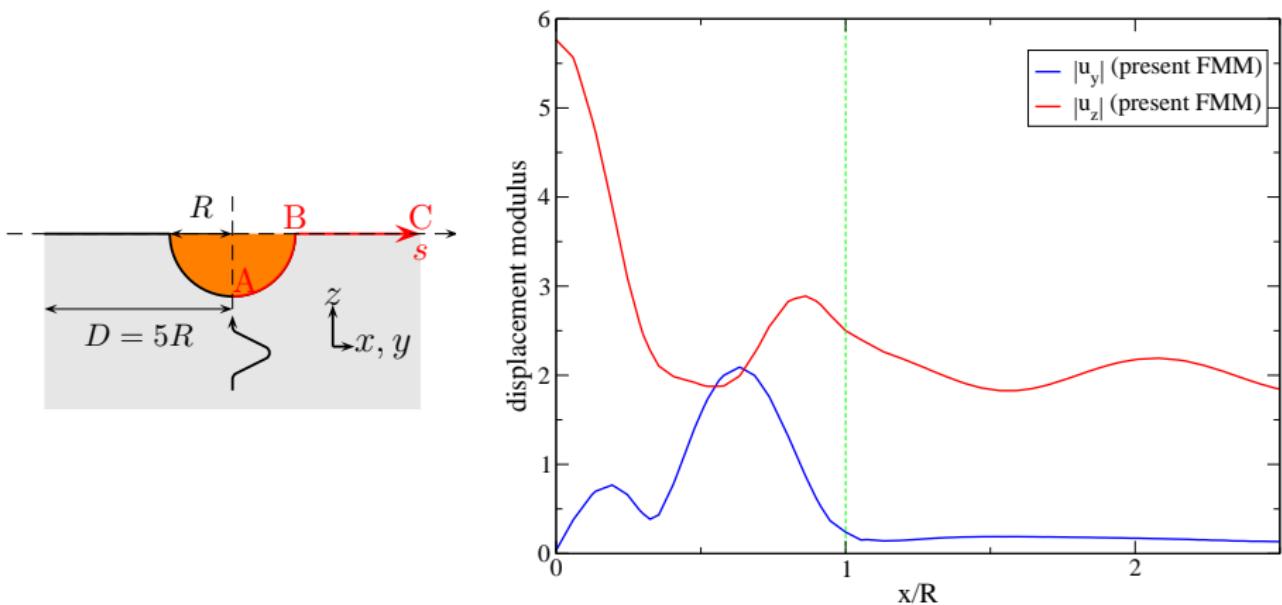
- ▶ Sanchez-Sesma, 1983 (semi-analytical)
- ▶ Delavaud, 2007 (spectral finite element method)



Example: scattering of a plane P wave by an alluvial hemispheric valley

Results for a higher frequency $k_P R = 1$

$N = 84\,882$ (76 iterations, single-proc. 3 GHz PC)



1. Review of boundary integral equation formulations

Electrostatics

Laplace

Elastostatics

Frequency-domain wave equations

2. Review of classical BEM concepts

3. The GMRES iterative solver

4. The fast multipole method (FMM) for the Laplace equation

Multipole expansion of $1/r$

The single-level fast multipole method

The multi-level fast multipole method

5. The fast multipole method (FMM) for elastostatics

6. The fast multipole method for elastodynamics

7. Other acceleration methods

Exponential representation of $1/r$

FMM using equivalent sources

Clustering and low-rank approximations

Kernel-independent acceleration via kernel interpolation

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Exponential representation of $1/r$

- ▶ Partial Fourier transform along (ξ_1, ξ_2) coordinates (η_1, η_2 transformed variable):

$$\Delta G(\mathbf{x}, \cdot) + \delta(\cdot - \mathbf{x}) = 0 \implies \hat{G}_{,33} - \eta^2 \hat{G} + \frac{e^{-i\eta \cdot \mathbf{x}}}{4\pi^2} \delta(\xi_3 - x_3) = 0$$

- ▶ Solve analytically for $\hat{G}(\eta_1, \eta_2, \xi_3; \mathbf{x})$ (case $(\xi_3 > x_3)$):

$$\hat{G}(\eta_1, \eta_2, \xi_3; \mathbf{x}) = \frac{1}{8\pi^2} \exp \left[-\eta(\xi_3 - x_3) + i(\eta_1(\xi_1 - x_1) + \eta_2(\xi_2 - x_2)) \right]$$

- ▶ Exponential representation of $1/r$ (case $\xi_3 > x_3$):

$$\boxed{\frac{1}{\|\xi - \mathbf{x}\|} = \frac{1}{2\pi} \int_0^{+\infty} \int_0^{2\pi} e^{-\eta [(\xi_3 - x_3) - i(\cos \alpha (\xi_1 - x_1) + \sin \alpha (\xi_2 - x_2))]} d\alpha d\eta}$$

- ▶ Similar (but distinct) formula available for the case $\xi_3 < x_3$.
- ▶ CHENG, H., GREENGARD, L., ROKHLIN, V. A fast adaptive multipole algorithm in three dimensions. *J. Comp. Phys.*, **155**:468–498 (1999).

Exponential representation of $1/r$

$$\frac{1}{\|\xi - \mathbf{x}\|} = \frac{1}{2\pi} \int_0^{+\infty} \int_0^{2\pi} e^{-\eta [(\xi_3 - x_3) - i(\cos \alpha (\xi_1 - x_1) + \sin \alpha (\xi_2 - x_2))]} d\alpha d\eta \quad (\xi_3 > x_3)$$

Division of interaction list into 6 (3-D) or 4 (2-D) sublists:

U	U	U	U	U	U
U	U	U	U	U	U
U	C				U
W					E
D					D
D	D	D	D	D	D

- ▶ Uplist (U)
- ▶ Downlist (D)
- ▶ Eastlist (E)
- ▶ Westlist (W)
- ▶ Northlist (N), for 3-D
- ▶ Southlist (S), for 3-D

Exponential representation of $1/r$: numerical quadrature

$$\left| \frac{1}{\|\xi - \mathbf{x}\|} - \sum_{k=1}^{s_\epsilon} \frac{w_k}{M_k} \sum_{j=1}^{M_k} e^{-\eta_k [(\xi_3 - x_3) - i(\cos \alpha_{j,k} (\xi_1 - x_1) + \sin \alpha_{j,k} (\xi_2 - x_2))]} \right| < \epsilon$$

- ▶ Outer numerical quadrature: points η_k and weights w_k given by Cheng, Rokhlin, Yarvin (1999);
- ▶ Inner numerical quadrature: M_k equally-spaced angles $\alpha_{j,k} = 2\pi j / M_k$, with M_k also given by Cheng, Rokhlin, Yarvin (1999).
- ▶ Comparison with "traditional" multipole expansion:

$$M_1 + \dots + M_{s_\epsilon} = O(p_\epsilon^2)$$

- ▶ CHENG, H., ROKHLIN, V., YARVIN, N. Nonlinear optimization, quadrature and interpolation. *SIAM J. Optim.*, 9:901–923 (1999).

Exponential representation of $1/r$ and diagonal translations

$$\left| \frac{1}{\|\xi - \mathbf{x}\|} - \sum_{k=1}^{s_\epsilon} \frac{w_k}{M_k} \sum_{j=1}^{M_k} e^{-\eta_k [(\xi_3 - x_3) - i(\cos \alpha_{j,k} (\xi_1 - x_1) + \sin \alpha_{j,k} (\xi_2 - x_2))]} \right| < \epsilon$$

Insert poles \mathbf{x}, ξ , define multipole moments and translation operations.

- ▶ Multipole moments:

$$M(k, j) = \int_{\partial\Omega \cup \mathcal{C}_\xi} e^{-\eta_k [(\xi_3 - \xi_{3,0}) - i(\cos \alpha_{j,k} (\xi_1 - \xi_{1,0}) + \sin \alpha_{j,k} (\xi_2 - \xi_{2,0}))]} \phi(\xi) dS_\xi$$

- ▶ M2M, M2L, L2L translations are diagonal, e.g.:

$$L(k, j) = M(k, j) e^{-\eta_k [(\xi_{3,0} - x_{3,0}) - i(\cos \alpha_{j,k} (\xi_{1,0} - x_{1,0}) + \sin \alpha_{j,k} (\xi_{2,0} - x_{2,0}))]}$$

Speeds up M2M, M2L, L2L operations

($O(p^2 N)$ instead of $O(p^4 N)$ using "traditional" FMM)

- ▶ Summation w.r.t. (k, i) performed on local expansions, at the very end (after upward, M2L and downward phases)
- ▶ Exponential expansions available for other kernels, e.g. Helmholtz
Useful for FMM for low-frequency wave problems

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FMM using equivalent sources

Clustering and low-rank approximations

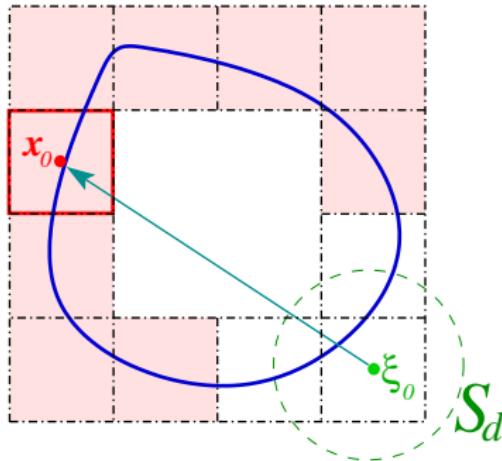
Kernel-independent acceleration via kernel interpolation

Adaptive cross approximation

FMM using equivalent sources

Main idea: express fields at remote points in terms of equivalent density, e.g.:

$$\int_{\partial\Omega \cap C_\xi} G_{,n}(x, \xi) u(\xi) dS_\xi = \int_{S_d} G(x, z) \phi(z) dS_z \quad \text{for some } \phi \quad (x \notin A(C_\xi))$$

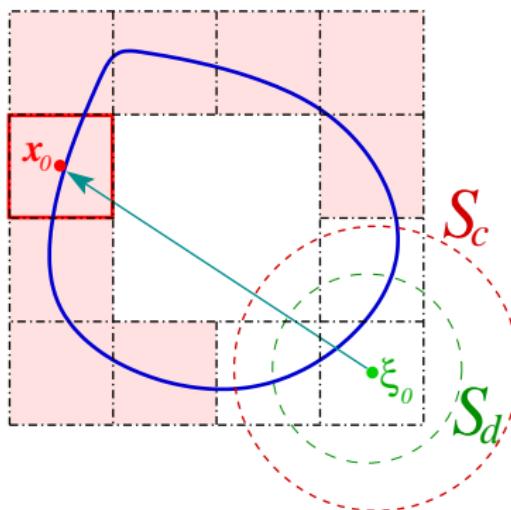


- YING, L., BIROS, G., ZORIN, D. A kernel-independent adaptive fast multipole in two and three dimensions. *J. Comp. Phys.*, **196**:591–626 (2004).

FMM using equivalent sources

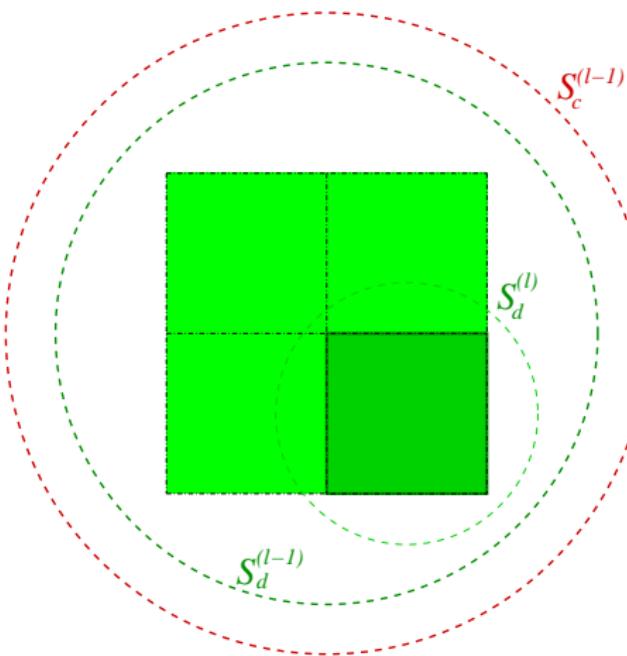
Main idea: express fields at remote points in terms of equivalent density, e.g.:

$$\int_{\partial\Omega \cap C_\xi} G_{,n}(\mathbf{x}, \boldsymbol{\xi}) u(\boldsymbol{\xi}) dS_\xi = \int_{S_d} G(\mathbf{x}, \mathbf{z}) \phi(\mathbf{z}) dS_z \quad \text{for some } \phi \quad (\mathbf{x} \in S_c)$$



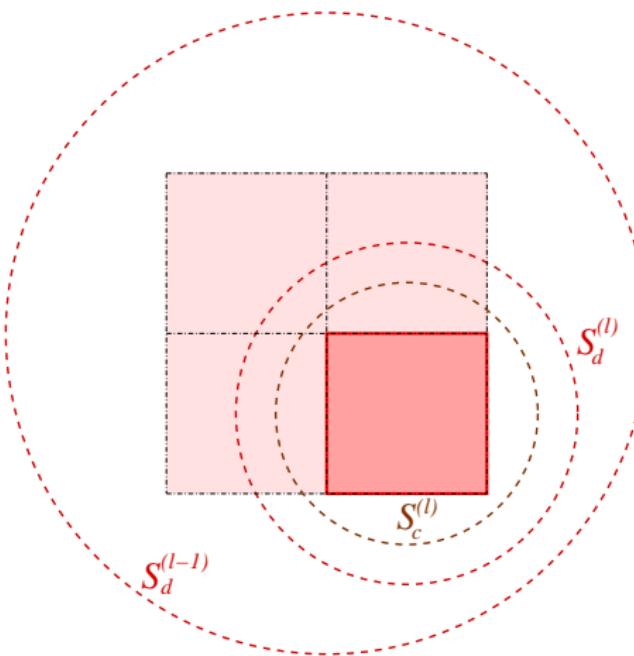
- ▶ Solve the above (Fredholm, 1st kind) integral equation for ϕ
- ▶ Truncation parameter = discretization of ϕ

FMM using equivalent sources: M2M translations



Find $\phi^{(\ell-1)}$, $\int_{S_d^{(\ell-1)}} G(\mathbf{x}, \mathbf{z}) \phi^{(\ell-1)}(\mathbf{z}) dS_z = \int_{S_d^{(\ell)}} G(\mathbf{x}, \mathbf{z}) \phi^{(\ell)}(\mathbf{z}) dS_z \quad (\mathbf{x} \in S_c^{(\ell-1)})$

FMM using equivalent sources: L2L translations



Find $\phi^{(\ell)}$, $\int_{S_d^{(\ell)}} G(\mathbf{x}, \mathbf{z}) \phi^{(\ell)}(\mathbf{z}) dS_z = \int_{S_d^{(\ell-1)}} G(\mathbf{x}, \mathbf{z}) \phi^{(\ell-1)}(\mathbf{z}) dS_z \quad (\mathbf{x} \in S_c^{(\ell)})$

FMM using equivalent sources

- ▶ Kernel-independent acceleration method;
- ▶ Truncation parameter p = discretization of ϕ (scale-independent for kernels associated with elliptic problems);
- ▶ Found by Ying, Biros, Zorin (2004) to have $O(p^2N)$ complexity / iteration;
- ▶ Requires solving 1st kind integral equations (ill-conditioned integral operator)

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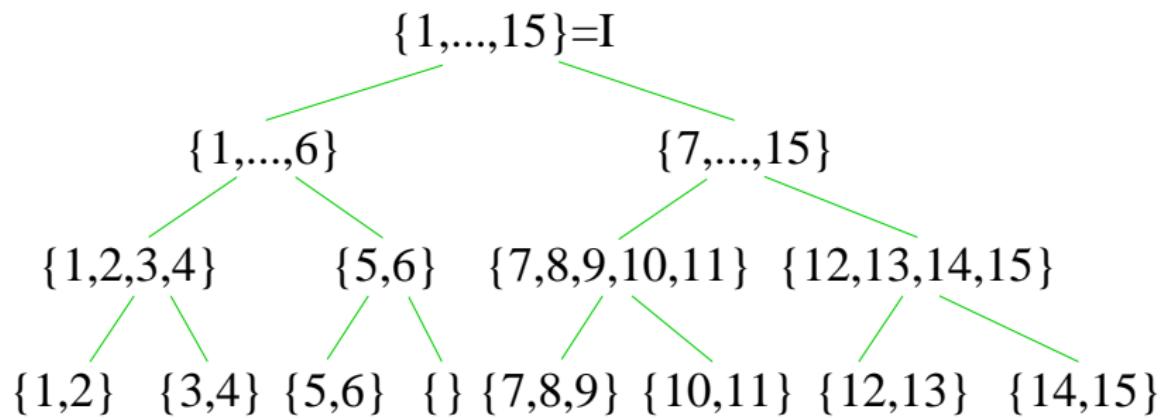
Kernel-independent acceleration via kernel interpolation

Adaptive cross approximation

DOF clustering

- ▶ Spatially local DOFs (e.g. nodal values on a BEM mesh);
- ▶ Recursive subdivision of set of DOFs into subsets, e.g. by bisection

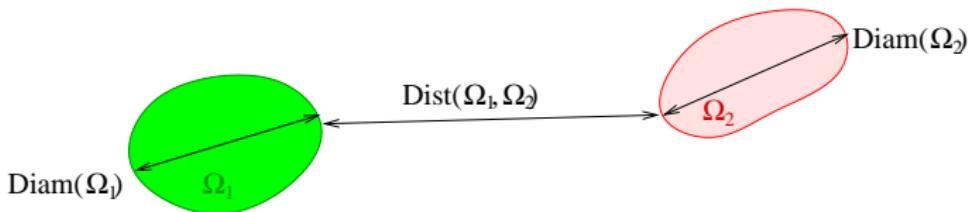
Example (1-D BE mesh, e.g for a 2-D crack problem):



Block clustering of influence matrix

- Let Ω_1, Ω_2 denote the geometrical support of two clusters (i.e. of two subsets of the DOF index list \mathcal{K}). For instances, Ω_1, Ω_2 are cubic cells.
 Ω_1, Ω_2 are **admissible** if

$$\text{Min}(\text{Diam}(\Omega_1), \text{Diam}(\Omega_2)) \leq \eta \text{Dist}(\Omega_1, \Omega_2)$$



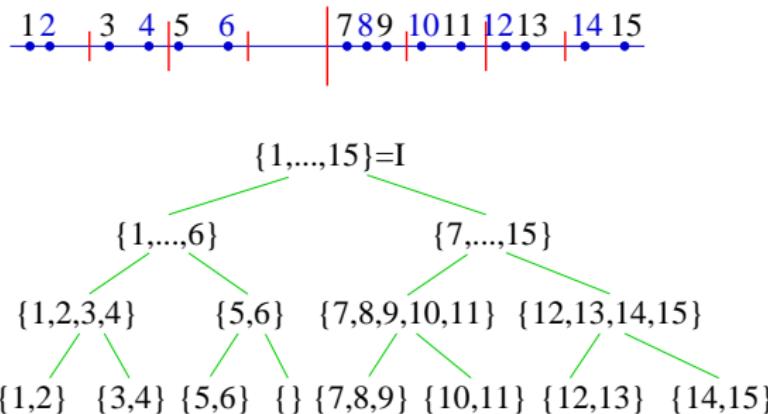
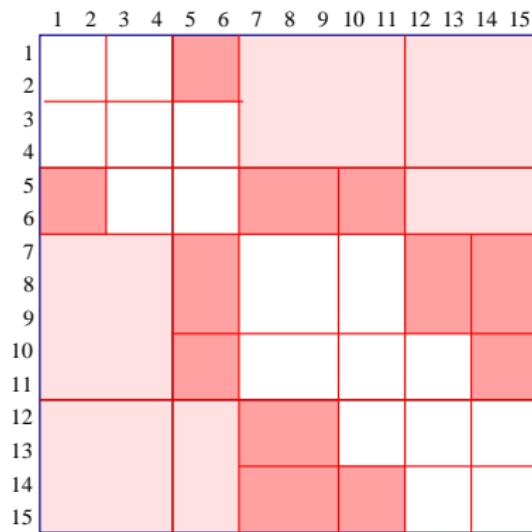
- Block clustering of (BEM) influence matrix into n blocks:

$$(I_1 \times J_1) \cup \dots \cup (I_n \times J_n) = \mathcal{K} \times \mathcal{K}, \quad I_k, J_k \text{ generated by DOF clustering of } \mathcal{K}$$

Such block clustering is not unique for a given index set \mathcal{K} .

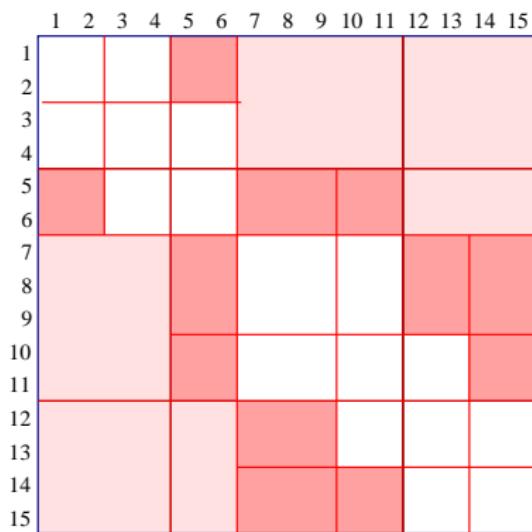
- Hierarchical, recursive** block clustering of (BEM) influence matrix into n blocks:
 - Block $\mathcal{K} \times \mathcal{K}$ is not admissible.
 - If block $(I \times J)$ is admissible, do nothing
 - Else, create sub-blocks of $(I \times J)$ using children sublists of (I, J)

Block clustering of influence matrix: example



Concept of panel clustering in the BEM (Hackbusch and Nowak, 1989)
 Concept of \mathcal{H} -matrices (Hackbusch, 1999)

Acceleration via low-rank approximation of blocks



Idea: use **low-rank approximations** of blocks:

$$\mathbf{A}(I, J) \approx \sum_{k=1}^r \mathbf{a}_k \mathbf{b}_k^T$$

Ideally, $r \ll |I|, |J|$

Matrix-vector product:

$$\mathbf{A}(I, J)\mathbf{u}(I) \approx \sum_{k=1}^r (\mathbf{b}_k^T \mathbf{u}(I)) \mathbf{a}_k$$

Block clustering + low-rank approximation of blocks = acceleration of matrix operations

SVD and block rank

- ▶ Any block $\mathbf{A}(I, J)$ of size $m \times n$ admits a **singular value decomposition** (SVD):

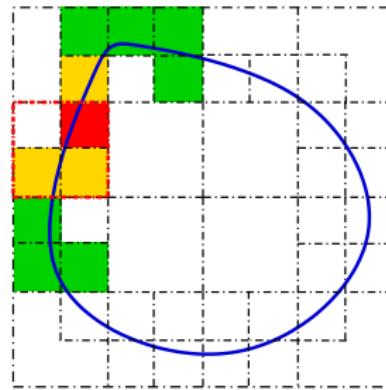
$$\mathbf{A}(I, J) = \mathbf{U}\mathbf{S}\mathbf{V}^T = \sum_{k=1}^R s_k \mathbf{u}_k \mathbf{v}_k^T \quad s_1 \geq s_2 \geq \dots s_R > 0, \quad \mathbf{u}_k^T \mathbf{u}_\ell = \mathbf{v}_k^T \mathbf{v}_\ell = \delta_{k\ell}$$

$R \leq \text{Min}(m, n)$ is the (numerical) **rank** of $\mathbf{A}(I, J)$

- ▶ $\mathbf{A}(I, J)$ has (approximate) low rank r if s_k is sufficiently small for $k > r$
- ▶ Computing complete SVD of $\mathbf{A}(I, J)$ needs $O(mn)$ memory + $O(mn^2)$ CPU
not acceptable; other strategies required
 - FMM (analytic decomposition of kernel required)
 - Kernel interpolation (analytic decomposition of kernel not required)
 - Algebraic treatment of matrix blocks: adaptive cross approximation
 - Wavelet transformation of basis functions (not addressed here)

FMM as block clustering with low-rank approximation of blocks

The multi-level Fast Multipole Method features **block clustering** (through hierarchical octree of cubic cells)



and **low-rank approximation** through **truncated** multipole expansion

$$\frac{1}{\|\xi - \mathbf{x}\|} = \sum_{n=0}^{\textcolor{red}{p}} \sum_{m=-n}^n R_{n,m}(\mathbf{x} - \mathbf{x}_0) \sum_{n'=0}^{\textcolor{red}{p}} \sum_{m'=-n'}^{n'} (-1)^n \overline{S_{n+n', m+m'}(\xi_0 - \mathbf{x}_0)} R_{n', m'}(\xi - \xi_0)$$

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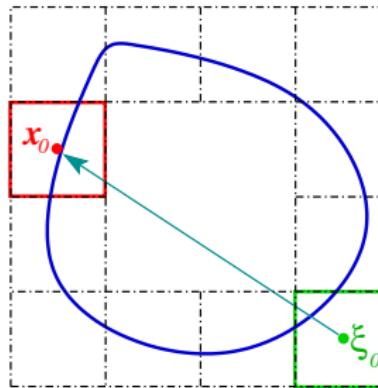
Adaptive cross approximation

Kernel-independent acceleration via kernel interpolation

In many cases:

- ▶ Fundamental solution available (not necessarily in closed form);
Availability of high-order derivatives problematic at best
→ Taylor-based expansion impractical
- ▶ Analytic expansion (e.g. multipole, exponential) not available
→ FMM treatment impossible

Idea: **polynomial interpolation** of $G(\mathbf{x}, \xi)$ in product of two non-adjacent cells
 $(\mathbf{x} \in \mathcal{C}_x, \xi \in \mathcal{C}_\xi)$



Kernel-independent acceleration via kernel interpolation

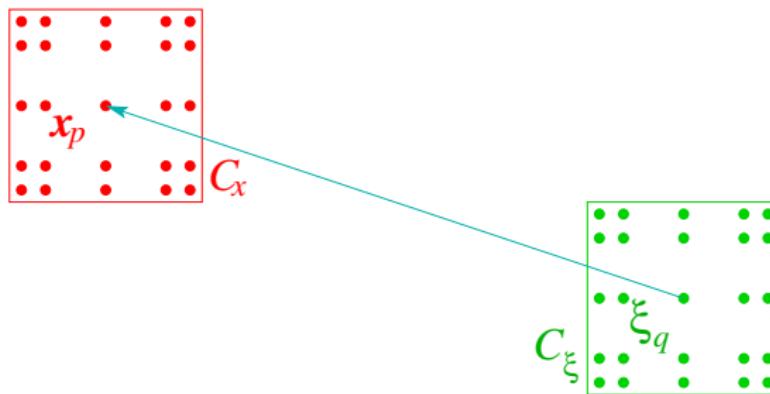
$$G(\mathbf{x}, \boldsymbol{\xi}) \approx \sum_{p=1}^P \sum_{q=1}^Q P_p(\mathbf{x}) G(\mathbf{x}_p, \boldsymbol{\xi}_q) Q_q(\boldsymbol{\xi})$$

\mathbf{x}_p : interpolation nodes in C_x (Cartesian product of 1-D set of nodes);

$P_p(\mathbf{x})$: interpolation polynomials (e.g. Cartesian product of 1-D Lagrange polyn.);

$\boldsymbol{\xi}_q$: interpolation nodes in C_ξ (Cartesian product of 1-D set of nodes);

$Q_q(\boldsymbol{\xi})$: interpolation polynomials (e.g. Cartesian product of 1-D Lagrange polyn.);



Kernel-independent acceleration via kernel interpolation

Evaluation of

$$\mathcal{S}[\varphi, \partial\Omega]^{\text{far}}(\mathbf{x}) = \sum_{\mathcal{C}_\xi \in \mathcal{A}(\mathcal{C}_x)} \int_{\partial\Omega \cap \mathcal{C}_\xi} G(\mathbf{x}, \boldsymbol{\xi}) \varphi(\boldsymbol{\xi}) dS_\xi$$

- ▶ Multipole moments:

$$M_q(\boldsymbol{\xi}_0) = \int_{\partial\Omega \cap \mathcal{C}_\xi} Q_q(\boldsymbol{\xi}) \phi(\boldsymbol{\xi}) dS_\xi$$

- ▶ M2L translation:

$$L_p(\mathbf{x}_0) = \sum_{q=1}^Q G(\mathbf{x}_p, \boldsymbol{\xi}_q) M_q(\boldsymbol{\xi}_0)$$

- ▶ M2M (upward) translations by expressing the $Q_q^{(\ell-1)}(\boldsymbol{\xi}; \boldsymbol{\xi}_0^{(\ell-1)})$ in terms of the $Q_q^{(\ell)}(\boldsymbol{\xi}; \boldsymbol{\xi}_0^{(\ell)})$ (e.g. Taylor expansion for polynomials)
- ▶ L2L (downward) translations similarly

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 - Adaptive cross approximation

Adaptive cross approximation

Aim: find recursively a low-rank approximation of a $m \times n$ block \mathbf{A} of the form:

$$\mathbf{A} = \mathbf{R} + \mathbf{S}, \quad \mathbf{S} = \sum_{k=1}^r \mathbf{u}_k \mathbf{v}_k^\top, \quad \|\mathbf{R}\|_F \leq \epsilon$$

To be used in conjunction with a \mathcal{H} -matrix block clustering.

- ▶ BEBENDORF, M., Rjasanov, S.. Adaptive low-rank approximation of collocation matrices. *Computing*, **70**:1–24 (2003).

Adaptive cross approximation: partially-pivoted ACA

1. Initialization: $\mathbf{S} = \mathbf{0}$, $\mathcal{K} = \emptyset$, $r = 0$

2. Recursion:

(a) $k = \text{Min}\{j, j \notin \mathcal{K}\}$, $\mathcal{K} = \mathcal{K} \cup \{k\}$; STOP if $|\mathcal{K}| = n$,

(b) Row generation: $\mathbf{a} = \mathbf{A}_{k\bullet}$,

(c) Row of residual, pivot column: $\mathbf{R}_{k\bullet} = \mathbf{a} - \sum_{i=1}^r \mathbf{v}_i (\mathbf{u}_i)_k$, $\ell = \text{Argmax} |R_{k\ell}|$,

(d) Test: if $\text{Max} |R_{k\ell}| = 0$, go to 2(a),

(e) Column generation: $\mathbf{a} = \mathbf{A}_{\bullet\ell}$,

(f) Column of residual, pivot row: $\mathbf{R}_{\bullet\ell} = \mathbf{a} - \sum_{i=1}^r \mathbf{u}_i (\mathbf{v}_i)_\ell$, $k = \text{Argmax} |R_{k\ell}|$,

(g) New vectors: $\mathbf{u}_{m+1} = (R_{k\ell})^{-1} \mathbf{R}_{\bullet\ell}$, $\mathbf{v}_{m+1} = \mathbf{R}_{k\bullet}$,

(h) Stopping criterion: $\|\mathbf{u}_{r+1}\|_F \|\mathbf{v}_{r+1}\|_F \leq \epsilon \|\mathbf{S}\|_F$,

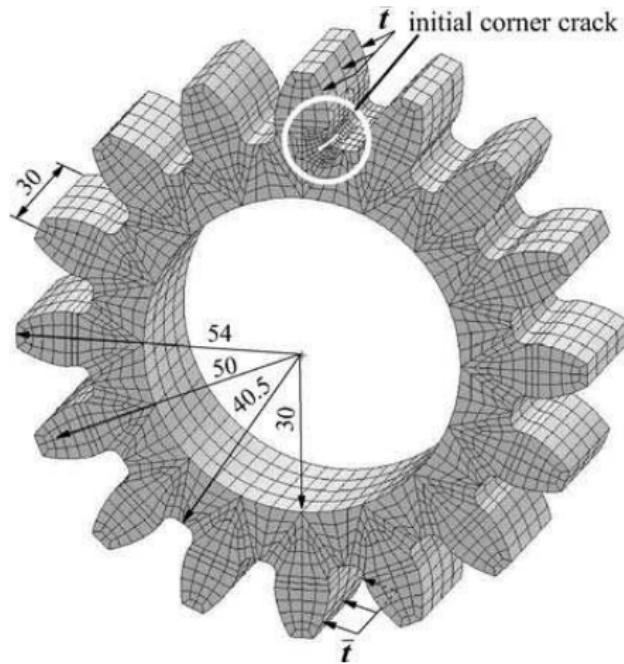
(i) New approximation of block: $\mathbf{S} = \mathbf{S} + \mathbf{u}_{r+1} \mathbf{v}_{r+1}^\top$,

(j) Recursion: $r = r + 1$, go to 2(b)

- ▶ Algorithm requires $O(r^2(m+n))$ operations,
- ▶ Complete ACA requires $O(N^{1+\delta} \epsilon^{-\delta})$ operations for any $\delta > 0$ if kernel asymptotically smooth

[Kurz, Rain, Rjasanov, 2006]

Example: crack propagation analysis



- ▶ $N \approx 45000$,
- ▶ CPU ≈ 4500 s
- ▶ RAM = 1.5GB

- ▶ KOLK, K., WEBER, W., KUHN, G. Investigation of 3D crack propagation problems via fast BEM formulations. *Comp. Mech.*, **37**:32–40 (2005).

1. Review of boundary integral equation formulations

Electrostatics

Laplace

Elastostatics

Frequency-domain wave equations

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The multi-level fast multipole method

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8. Preconditioning

- Diagonal preconditioner $M_{ij} = A_{ij}\delta_{ij}$;
- Sparse matrix of near contributions in FMM;
- Incomplete LU factorization of \mathbf{A} ;
- Sparse approximate inverses;
- Multigrid approaches;
- Fast BEM solution method (e.g. FMM, ACA) with **low** truncation;
- Preconditioners exploiting specific features of the problems, e.g. single-inclusion case for many-inclusion problems.

Sparse approximate inverse (SPAI)

- ▶ Definition:

$$[A^\#] = \arg \min_{[E]} \| [I] - [E][A] \|_F^2 \quad [E] \in \mathbb{R}^{N \times N} \text{ sparse}$$

where $[A^\#]$ has a **sparsity pattern** (either predefined or found iteratively).

- ▶ Hence each column of $[A^\#]$ solves an uncoupled, small minimization problem:

$$\{A_k^\#\} = \arg \min_{\{E\}} \| \{e_k\} - \{E\}[A] \| \quad \{E\} \in \mathbb{R}^{1 \times N} \text{ sparse}$$

- ▶ **Simplification:** choose number m of nonzero entries in each row of $[A^\#]$ and find SPAI of $\tilde{[A]}$:

$$\{\hat{A}_i^\#\} = \arg \min_{\{\hat{E}\} \in \mathbb{R}^{1,m}} \left\{ \| \{E\}[\tilde{A}_i] \|^2 - 2 \operatorname{trace}(\{E\}[\tilde{A}_i]) + 1 \right\} \quad (1 \leq i \leq N)$$

where $\tilde{[A]}$ is the sparse matrix made of the m largest entries of $[A]$.

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