A fast multipole formulation for elastic wave propagation in semi-infinite media

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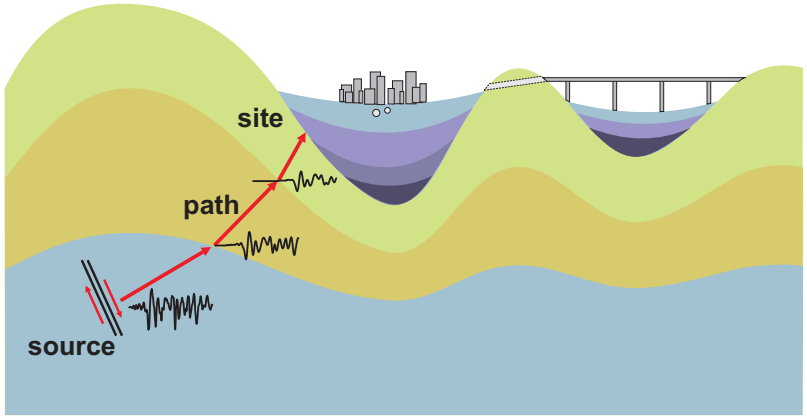
Bon anniversaire Martin !

Outline

1. Motivations and background
2. Formulation of the Elastic Half-space Fundamental solutions
3. New Fast Multipole Formulation for the Elastic Half-space
4. Accuracy and complexity
5. Example: incident plane P wave on a spherical cavity in a half-space
6. Conclusions and future work

Motivation

Modelling of elastic wave propagation in large/unbounded domains



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

Pros and cons of Boundary Element Methods for seismic waves

Domain methods (FEM, SEM, ...)
→ Domain mesh
→ Approx. radiation conditions
→ Sparse matrix

BEM
→ Surface mesh (i.e. reduced dim.)
→ Exact radiation conditions
→ Fully-populated matrix

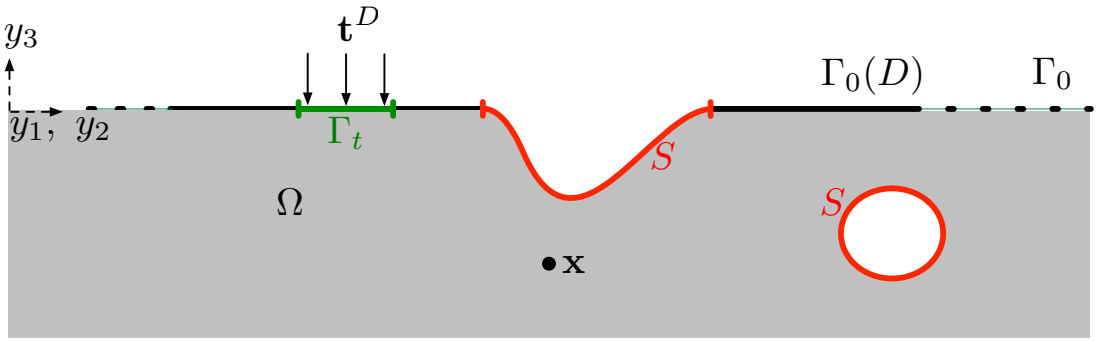
→ BEM adequate for large (unbounded) media, simple (linear) prop
→ Fully-populated BEM influence matrix: severe limiting factor

BIE for semi-infinite media

Formulation with the **full-space** fundamental solutions (FS)

$$\boldsymbol{c}(\boldsymbol{x})\cdot\boldsymbol{u}(\boldsymbol{x}) + (\text{P.V.}) \int_{S\cup\Gamma_t\cup\Gamma_0} \boldsymbol{u}(\boldsymbol{y})\cdot\boldsymbol{T}_\infty(\boldsymbol{x},\boldsymbol{y};\omega)\,\mathrm{d}S_{\boldsymbol{y}} - \int_S \boldsymbol{t}(\boldsymbol{y})\cdot\boldsymbol{U}_\infty(\boldsymbol{x},\boldsymbol{y};\omega)\,\mathrm{d}S_{\boldsymbol{y}}$$

$$= \int_{\Gamma_t} \boldsymbol{t}^{\mathrm{D}}(\boldsymbol{y})\cdot\boldsymbol{U}_\infty(\boldsymbol{x},\boldsymbol{y};\omega)\,\mathrm{d}S_{\boldsymbol{y}} \quad (\boldsymbol{x}\in S\cup\Gamma_t\cup\Gamma_0)$$



BIE for semi-infinite media

Formulation with the **half-space** fundamental solutions (FS)

$$\boldsymbol{c}(\boldsymbol{x})\cdot\boldsymbol{u}(\boldsymbol{x}) + (\text{P.V.})\int_S \boldsymbol{u}(\boldsymbol{y})\cdot\boldsymbol{T}^{\text{HS}}(\boldsymbol{x},\boldsymbol{y};\omega)\,\mathrm{d}S_{\boldsymbol{y}} - \int_S \boldsymbol{t}(\boldsymbol{y})\cdot\boldsymbol{U}^{\text{HS}}(\boldsymbol{x},\boldsymbol{y};\omega)\,\mathrm{d}S_{\boldsymbol{y}}$$
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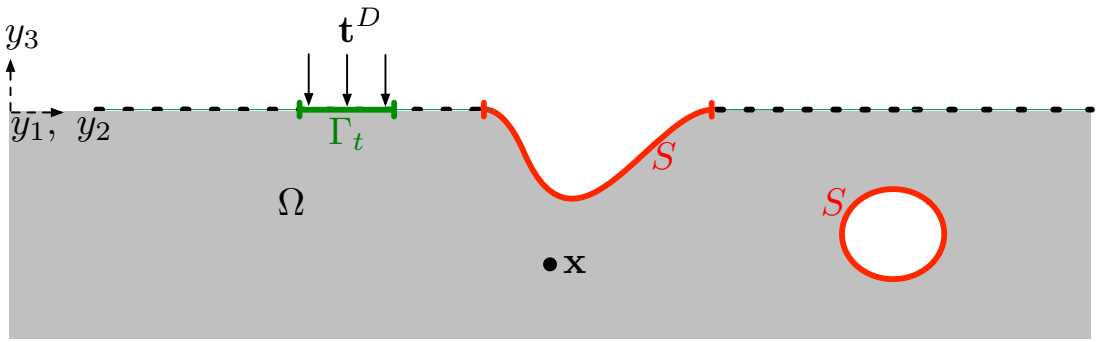

U^{HS} and T^{HS} satisfy traction-free condition on free surface $y_3 = 0$

Numerical advantages and issues

+ No truncation issue (S is a bounded surface)
+ # DOFs drastically reduced compared to full-space FS

– Closed-form of U^{HS} and T^{HS} not available
– Substantial CPU time (integrals of oscillating functions over infinite intervals)

Fast Multipole accelerated BEM

Fast Multipole Method (FMM):

- Accelerates standard BEM and reduces memory requirements
- Fast, approximate method for evaluating the linear integral operator (matrix-vector product, called by iterative solver)

[1] [Chaillat *et al.*, CMAME, 2008]

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FMM using **full-space** elastodynamics FS

- Full-space elastodynamic FS uses (derivatives of) Helmholtz FS:

$$\boldsymbol{U}(\boldsymbol{x},\boldsymbol{y};\omega) = (k_S^2\mu)^{-1}\left[(\nabla\nabla - \boldsymbol{I}\Delta)G_S(\boldsymbol{x}-\boldsymbol{y}) - \nabla\nabla G_P(\boldsymbol{x}-\boldsymbol{y})\right]$$

$$\boldsymbol{T}(\boldsymbol{x},\boldsymbol{y};\omega) = \boldsymbol{n}(\boldsymbol{y})\cdot\boldsymbol{\mathcal{C}}:\nabla_y\boldsymbol{U}(\boldsymbol{x},\boldsymbol{y};\omega)$$

$$\text{with}\quad G_\alpha(\boldsymbol{r}) = \frac{\exp(ik_\alpha|\boldsymbol{r}|)}{4\pi|\boldsymbol{r}|} \qquad \text{(Helmholtz FS, } \alpha = P, S\text{)}$$

- Extension of FMM for Helmholtz to elastodynamics[1]

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FMM using **half-space** elastodynamics FS:

- No multipole expansion of the FS currently available
- Need to derive half-space FS in form enabling fast computation
- Need to formulate a new FMM for the elastic half-space FS

[1] [Chaillat *et al.*, CMAME, 2008]

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2 Formulation of the Elastic Half-space Fundamental solutions

3 New Fast Multipole Formulation for the Elastic Half-space

4 Accuracy and complexity

5 Example: incident plane P wave on a spherical cavity in a half-space

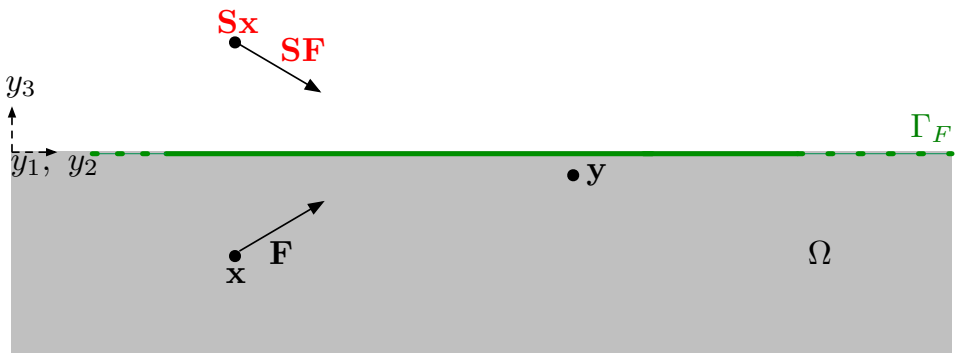
6 Conclusions and future work

Introduction of a complementary FS

Additive decomposition of half-space FS into three parts:

$$\boldsymbol{U}^{HS}(\boldsymbol{x},\boldsymbol{y}) = \boldsymbol{U}_{\infty}(\boldsymbol{x},\boldsymbol{y}) + \bar{\boldsymbol{U}}_{\infty}(\boldsymbol{x},\boldsymbol{y}) + \boldsymbol{U}_{C}(\boldsymbol{x},\boldsymbol{y})$$
$$\boldsymbol{T}^{HS}(\boldsymbol{x},\boldsymbol{y}) = \boldsymbol{T}_{\infty}(\boldsymbol{x},\boldsymbol{y}) + \bar{\boldsymbol{T}}_{\infty}(\boldsymbol{x},\boldsymbol{y}) + \boldsymbol{T}_{C}(\boldsymbol{x},\boldsymbol{y})$$

- $\boldsymbol{U}_{\infty}, \boldsymbol{T}_{\infty}$: elastic full-space FS
- $\bar{\boldsymbol{U}}_{\infty}, \bar{\boldsymbol{T}}_{\infty}$: image elastic full-space FS
  (image point force applied at the mirror image source point)



- $\boldsymbol{U}_{C}, \boldsymbol{T}_{C}$: complementary FS

Contrary to the scalar case, the method of images allows to only partially satisfy the traction-free condition on the free-surface

Decomposition of the operators

Induced decomposition of integral operators

$$\mathcal{S}[\boldsymbol{t}](\boldsymbol{x}) := \int_S \boldsymbol{t}(\boldsymbol{y}) \cdot \boldsymbol{U}^{\mathrm{HS}}(\boldsymbol{x}, \boldsymbol{y}; \omega)\, \mathrm{d}S_{\boldsymbol{y}}, \qquad \mathcal{S}[\boldsymbol{t}](\boldsymbol{x}) = \mathcal{S}_\infty[\boldsymbol{t}](\boldsymbol{x}) + \bar{\mathcal{S}}_\infty[\boldsymbol{t}](\boldsymbol{x}) + \mathcal{S}_{\mathrm{C}}[\boldsymbol{t}](\boldsymbol{x})$$

$$\mathcal{D}[\boldsymbol{u}](\boldsymbol{x}) := \int_S \boldsymbol{u}(\boldsymbol{y}) \cdot \boldsymbol{T}^{\mathrm{HS}}(\boldsymbol{x}, \boldsymbol{y}; \omega)\, \mathrm{d}S_{\boldsymbol{y}}, \qquad \mathcal{D}[\boldsymbol{u}](\boldsymbol{x}) = \mathcal{D}_\infty[\boldsymbol{u}](\boldsymbol{x}) + \bar{\mathcal{D}}_\infty[\boldsymbol{u}](\boldsymbol{x}) + \mathcal{D}_{\mathrm{C}}[\boldsymbol{u}](\boldsymbol{x})$$

Fast computation of the three contributions to $\mathcal{S}[\boldsymbol{t}](\boldsymbol{x})$ and $\mathcal{D}[\boldsymbol{t}](\boldsymbol{x})$

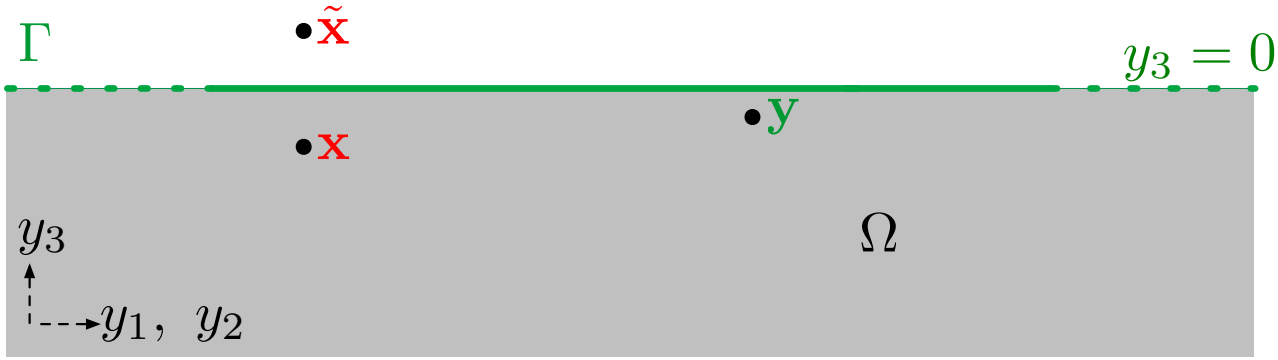
- Evaluation of $\mathcal{S}_\infty$, $\bar{\mathcal{S}}_\infty$, $\mathcal{D}_\infty$ and $\bar{\mathcal{D}}_\infty$: "standard" FMM (diagonal form-based decomposition of full-space FS[2])
- Remaining difficulty: compute contributions $\mathcal{S}_{\mathrm{C}}$, $\mathcal{D}_{\mathrm{C}}$ involving the complementary FS $\boldsymbol{U}_{\mathrm{C}}$ and $\boldsymbol{T}_{\mathrm{C}}$.

Goals

- Formulate $\boldsymbol{U}_{\mathrm{C}}$ and $\boldsymbol{T}_{\mathrm{C}}$ in a form which enables fast computations
- Define a fast algorithm to compute $\mathcal{S}_{\mathrm{C}}[\boldsymbol{t}](\boldsymbol{x})$ and $\mathcal{D}_{\mathrm{C}}[\boldsymbol{u}](\boldsymbol{x})$

[2] [Chaillat *et al.*, CMAME, 2008]

Formulation of half-space FS in Fourier space



- Partial Fourier transform:

$$\hat{\boldsymbol{u}}(\xi_1, \xi_2, y_3) = \frac{1}{4\pi^2} \int_{\mathbb{R}^2} e^{-\mathrm{i}(\xi_1 y_1 + \xi_2 y_2)} \boldsymbol{u}(y_1, y_2, y_3)\, \mathrm{d}y_1 \mathrm{d}y_2$$

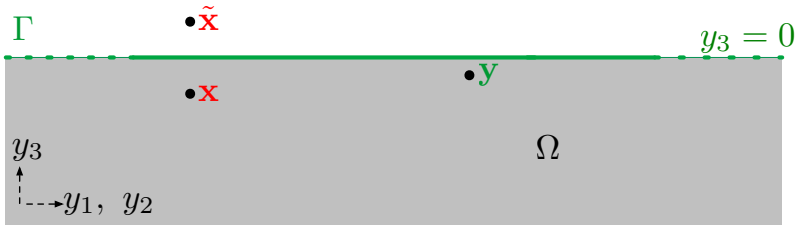
For gradients: $\widehat{\nabla \boldsymbol{u}}(\boldsymbol{\xi}, y_3) = \mathrm{i}\boldsymbol{\xi} \otimes \hat{\boldsymbol{u}}(\boldsymbol{\xi}, y_3) + \boldsymbol{e}_3 \otimes \hat{\boldsymbol{u}}'(\boldsymbol{\xi}, y_3)$

- Classical result for Helmholtz FS (for $r_3 < 0$)

$$\frac{exp(ik|\boldsymbol{r}|)}{4\pi|\boldsymbol{r}|} = \frac{1}{2\pi} \int_0^{\infty} \int_0^{2\pi} e^{-r_3\sqrt{\xi^2 - k^2}}\, e^{\mathrm{i}\xi\left(r_1 \cos\alpha + r_2 \sin\alpha\right)} \frac{\xi}{\sqrt{\xi^2 - k^2}} d\xi d\alpha$$

[Greengard *et al.*, IEEE Comp. Science. Engrg, 1998]

Methodology to derive FS in Fourier space



1. Full-space FS: Derive stress vector $\hat{\boldsymbol{T}}_\infty(y_3 = 0)$ from $\boldsymbol{U}_\infty(\boldsymbol{x}, \boldsymbol{y}; \omega)$;
2. Image full-space FS: Derive stress vector $\hat{\tilde{\boldsymbol{T}}}_\infty(y_3 = 0)$
3. Complementary term:
   - Solve (partial-Fourier form of) elastodynamic Navier equation
   - Apply boundary condition

$$\hat{\boldsymbol{T}}_\infty + \hat{\tilde{\boldsymbol{T}}}_\infty + \hat{\boldsymbol{T}}_C = \boldsymbol{0} \qquad (y_3 = 0)$$

4. Obtain FS $\hat{\boldsymbol{U}}_C$ in Fourier space
5. Deduce FS $\hat{\boldsymbol{T}}_C$ in Fourier space (using constitutive equation)

$$\hat{\boldsymbol{T}}_C = \boldsymbol{e}_3 \cdot \boldsymbol{\mathcal{C}} : \widehat{\nabla_y \boldsymbol{U}_C}$$

Expression in Fourier space: $\boldsymbol{U}_{\mathrm{C}}$

$$\hat{\boldsymbol{U}}_{\mathrm{C}}(\xi, y_3, \boldsymbol{x}) = \frac{s_{\mathrm{P}}(\xi)}{4\pi^2\delta(\xi)\mu k_{\mathrm{S}}^2}\left[2\boldsymbol{V}_{\mathrm{S}}^{+}(\xi)e^{s_{\mathrm{S}}y_3} + \beta\boldsymbol{V}_{\mathrm{P}}^{+}(\xi)e^{s_{\mathrm{P}}y_3}\right]$$
$$\otimes \left[2\boldsymbol{V}_{\mathrm{S}}^{-}(\xi)\, e^{\boldsymbol{q}_{\mathrm{S}}^{-}\cdot\boldsymbol{x}} + \beta\boldsymbol{V}_{\mathrm{P}}^{-}(\xi)\, e^{\boldsymbol{q}_{\mathrm{P}}^{-}\cdot\boldsymbol{x}}\right] \quad (\xi^2 := \xi_1^2 + \xi_2^2)$$

Remarks on $\hat{\boldsymbol{U}}_{\mathrm{C}}$:

- Expressed as product of a function of $\boldsymbol{x}$ and a function of $\boldsymbol{y}$;
- Exponential decay ($y_3, x_3 \leq 0$)

$$s_a(\xi) := \sqrt{\xi^2 - k_a^2}, \quad \boldsymbol{q}_a^{\pm}(\xi) := \pm \mathrm{i}\boldsymbol{\xi} + s_a(\xi)\boldsymbol{e}_3 \quad (a = \mathrm{P,S});$$

- Matrix $\hat{\boldsymbol{U}}_{\mathrm{C}}(\xi, y_3, x)$ has rank one: tensor product of two vectors, where

$$\boldsymbol{V}_{\mathrm{S}}^{\pm}(\boldsymbol{\xi}) := \pm\left[\, s_{\mathrm{S}}(\xi)\, \boldsymbol{q}_{\mathrm{S}}^{\pm}(\boldsymbol{\xi}) + k_{\mathrm{S}}^2\boldsymbol{e}_3 \,\right], \quad \boldsymbol{V}_{\mathrm{P}}^{\pm}(\boldsymbol{\xi}) := \pm s_{\mathrm{P}}^{-1}(\xi)\boldsymbol{q}_{\mathrm{P}}^{\pm}(\boldsymbol{\xi});$$

- k_{R} such that $\delta(k_{\mathrm{R}}) = 0$: Rayleigh wavenumber ($k_{\mathrm{P}} < k_{\mathrm{S}} < k_{\mathrm{R}}$)

$$\beta(\xi) := k_{\mathrm{S}}^2 - 2\xi^2, \qquad \delta(\xi) := \beta^2(\xi) - 4\xi^2 s_{\mathrm{P}}(\xi)s_{\mathrm{S}}(\xi)$$

Expression in Fourier space: $\boldsymbol{T}_{\mathrm{C}}$

$$\hat{\boldsymbol{T}}_{\mathrm{C}}(\boldsymbol{\xi}, y_3, \boldsymbol{x}) = \frac{1}{4\pi^2 \delta(\xi) k_{\mathrm{S}}^2} \left[2\boldsymbol{W}_{\mathrm{S}}(\boldsymbol{\xi}) e^{s_{\mathrm{S}} y_3} + \beta \boldsymbol{W}_{\mathrm{P}}(\boldsymbol{\xi}) e^{s_{\mathrm{P}} y_3} \right]$$
$$\otimes \left[2\boldsymbol{V}_{\mathrm{S}}^{-}(\boldsymbol{\xi})\, e^{\boldsymbol{q}_{\mathrm{S}}^{-} \cdot \boldsymbol{x}} + \beta \boldsymbol{V}_{\mathrm{P}}^{-}(\boldsymbol{\xi})\, e^{\boldsymbol{q}_{\mathrm{P}}^{-} \cdot \boldsymbol{x}} \right] \quad (\xi^2 := \xi_1^2 + \xi_2^2)$$

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$$\beta(\xi) := k_{\mathrm{S}}^2 - 2\xi^2, \quad \delta(\xi) := \beta^2(\xi) - 4\xi^2 s_{\mathrm{P}}(\xi) s_{\mathrm{S}}(\xi)$$

Expressions in physical coordinates

$$\boldsymbol{U}_C(\boldsymbol{x},\boldsymbol{y}) = \int_{\mathbb{R}^2} e^{i(\xi_1 y_1+\xi_2 y_2)}\,\hat{\boldsymbol{U}}_C(\boldsymbol{\xi}, y_3, \boldsymbol{x})\,d\xi_1 d\xi_2$$

$$\boldsymbol{T}_C(\boldsymbol{x},\boldsymbol{y}) = \int_{\mathbb{R}^2} e^{i(\xi_1 y_1+\xi_2 y_2)}\,\hat{\boldsymbol{T}}_C(\boldsymbol{\xi}, y_3, \boldsymbol{x})\,d\xi_1 d\xi_2$$

FMM-suitable formulation: integrand involves product of a function of $\boldsymbol{x}$ and a function of $\boldsymbol{y}$ $\rightarrow$ essential feature for fast evaluation

Numerical evaluation:

Introduce polar coordinates $\boldsymbol{\xi} = (\xi_1, \xi_2) = \xi(\cos\alpha, \sin\alpha)$

$$\boldsymbol{U}_C(\boldsymbol{x},\boldsymbol{y}) = \int_0^{+\infty}\int_0^{2\pi} e^{i\xi(\cos\alpha y_1+\sin\alpha y_2)}\,\hat{\boldsymbol{U}}_C(\xi\cos\alpha, \xi\sin\alpha, y_3, \boldsymbol{x})\,\xi\,d\alpha d\xi$$

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Numerical evaluation

$$\boldsymbol{U}_C(\boldsymbol{x},\boldsymbol{y}) = \int_0^{+\infty} \underbrace{\int_0^{2\pi} e^{\mathrm{i}\xi(\cos\alpha y_1 + \sin\alpha y_2)}\, \hat{\boldsymbol{U}}_C(\xi\cos\alpha, \xi\sin\alpha, y_3, \boldsymbol{x})\xi \,\mathrm{d}\alpha}_{\mathbf{I}_C(\xi,\boldsymbol{x},\boldsymbol{y})} \mathrm{d}\xi$$

Evaluation for standard BEM (not suitable for FMM)

- Integration over α analytical (yields $J_i(\xi|\boldsymbol{y}-\boldsymbol{x}|)$, $0 \leq i \leq 2$)
- Destroys separation of variables $\boldsymbol{x}$ and $\boldsymbol{y}$

Numerical integration for FM-BEM: double integral in (α, ξ) space

- Quadrature rule over α (angular integral)
  Smooth, periodic functions $\Rightarrow$ simple trapezoidal rule
- Quadrature rule over ξ (integrand: $\mathbf{I}_C(\xi, \boldsymbol{x}, \boldsymbol{y})$)
  - Oscillatory functions: difficult to integrate numerically
  - Singularity due to Rayleigh pole
  - Quadrature for $\boldsymbol{x}$ and $\boldsymbol{y}$ lying in a prescribed parameter space

  $\Rightarrow$ Non-classical quadrature rule necessary:
  generalized Gaussian quadrature (GGQ)

Generalized Gaussian quadrature rules

$\Rightarrow$ Well suited to FMMs, already implemented for Helmholtz:

- Definition of a FMM at low frequencies [Greengard *et al.*, 1998]
- Definition of a wideband FMM [Cheng et al. , 2006]

$\Rightarrow$ Construction of quadrature rule is involved and integrand-specific

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Principle for constructing GGQ rule [Bremer *et al.*, 2010]

$$I_\ell(p) := \int_0^{\xi_{max}} \phi_\ell(\xi, p)\, d\xi \quad (1 \leq \ell \leq m, p \in \mathcal{P})$$

Quadrature integrating collection of input functions $\phi_1, \ldots, \phi_m$

- m square integrable functions (m large for a good accuracy)
- Reproduce the singular and oscillatory behaviors of integrand
- Integrand is a linear combination of the input functions

Large number of sampled values p_k in the parameter domain $\mathcal{P}$

- Source and observation points ($\boldsymbol{x}$, $\boldsymbol{y}$) for which FS are computed
- Frequencies of interest

Overview of the methodology

1. Adaptive construction of an oversized quadrature
   - Integrates all products of input functions $\phi_1, \ldots, \phi_m$
   - Piecewise-Legendre quadrature rules of (very large) size p
2. Compression of $\{\phi_i\}_{1 \leq i \leq m}$ (sampled at Legendre pts.) to rank r
   - Redundant information in the $\phi_i(\hat{\xi}_k)$
   - Rank-revealing QR decomposition of matrix B (to evaluate $r \ll p$), where
     $$B \in \mathbb{R}^{r \times p}, \quad B_{ik} := u_i(\hat{\xi}_k)\sqrt{\hat{w}_k} \quad \Rightarrow I = BB^*$$
   - Orthonormal basis $u_1, \ldots, u_r$ is built
3. Extraction of r-point quadrature rule from p-point quadrature
4. Point-by-point further reduction of rule size using optimization
   - Quadrature points and weights satisfy nonlinear system
   - Sort the nodes according to their expected significance
   - Try (iteratively) to remove one node (Gauss-Newton iterations)

Output: n_ξ-point GGQ quadrature rule ($n_\xi \approx 15 - 50$ usually)

Developed a version of GGQ custom-tailored to the numerical evaluation of the FS $\boldsymbol{U}_C$ or $\boldsymbol{T}_C$ (2 different quadratures)

Removing the singularities

$$\boldsymbol{U}_{\mathrm{C}}(\boldsymbol{x},\boldsymbol{y}) = \int_0^{+\infty}\int_0^{2\pi} \frac{e^{\mathrm{i}\xi(\cos\alpha y_1+\sin\alpha y_2)}\boldsymbol{s}_{\mathrm{P}}(\xi)}{4\pi^2\delta(\xi)\mu k_{\mathrm{S}}^2}\left[2\boldsymbol{V}_{\mathrm{S}}^{+}(\boldsymbol{\xi})e^{s_{\mathrm{S}}y_3}+\beta\boldsymbol{V}_{\mathrm{P}}^{+}(\boldsymbol{\xi})e^{s_{\mathrm{P}}y_3}\right] \otimes \left[2\boldsymbol{V}_{\mathrm{S}}^{-}(\boldsymbol{\xi})\,e^{\boldsymbol{q}_{\mathrm{S}}^{-}\cdot\boldsymbol{x}}+\beta\boldsymbol{V}_{\mathrm{P}}^{-}(\boldsymbol{\xi})\,e^{\boldsymbol{q}_{\mathrm{P}}^{-}\cdot\boldsymbol{x}}\right]\xi\,\mathrm{d}\alpha\mathrm{d}\xi$$

Two kinds of singularities

- Rayleigh pole: $\xi = k_{\mathrm{R}} \Rightarrow \delta(\xi) = 0$
- Singularity of half-order: term $(\xi^2 - k_{\mathrm{P}}^2)^{-1/2}$ in $\boldsymbol{V}_{\mathrm{P}}^{+}(\boldsymbol{\xi}) \otimes \boldsymbol{V}_{\mathrm{P}}^{-}(\boldsymbol{\xi})$

Standard approaches to remove the singularities

- Deform the integration path to avoid the singularities
- Consider elasticity as the limiting case of viscoelasticity
- Extract the singular contributions

Removing the singularity due to Rayleigh pole

$$\boldsymbol{U}_{\mathrm{C}}(\boldsymbol{x},\boldsymbol{y}) = \int_0^{+\infty}\int_0^{2\pi} Z_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}},\boldsymbol{y},\boldsymbol{x})\,\mathrm{d}\alpha\mathrm{d}\xi, \quad \hat{\boldsymbol{\xi}} := \boldsymbol{\xi}/\xi = (\cos\alpha,\sin\alpha)$$

Removing the singularity due to Rayleigh pole:

$$Z_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}},\boldsymbol{y},\boldsymbol{x}) = \left(Z_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}},\boldsymbol{y},\boldsymbol{x}) - \boldsymbol{A}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})\frac{\varphi_R(\xi)}{\xi - k_{\mathrm{R}}}\right) + \boldsymbol{A}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})\frac{\varphi_R(\xi)}{\xi - k_{\mathrm{R}}}$$

$$\text{where } \boldsymbol{A}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x}) := \lim_{\xi\to k_{\mathrm{R}}}(\xi - k_{\mathrm{R}})Z_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})$$

Requirements on φ_R

(i) Regular function
(ii) Satisfy $\varphi_R(k_{\mathrm{R}}) = 1$ (for correct singularity removal)
(iii) Make $(\xi - k_{\mathrm{R}})^{-1}\varphi_R(\xi)$ integrable at infinity

Removing the singularity due to Rayleigh pole

$$\boldsymbol{U}_{\mathrm{C}}(\boldsymbol{x},\boldsymbol{y}) = \int_0^{+\infty}\int_0^{2\pi} Z_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}},\boldsymbol{y},\boldsymbol{x})\,\mathrm{d}\alpha\mathrm{d}\xi, \quad \hat{\boldsymbol{\xi}} := \boldsymbol{\xi}/\xi = (\cos\alpha,\sin\alpha)$$

Removing the singularity due to Rayleigh pole:

$$Z_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}},\boldsymbol{y},\boldsymbol{x}) = \left(Z_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}},\boldsymbol{y},\boldsymbol{x}) - \boldsymbol{A}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})\frac{\varphi_R(\xi)}{\xi - k_{\mathrm{R}}}\right) + \boldsymbol{A}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})\frac{\varphi_R(\xi)}{\xi - k_{\mathrm{R}}}$$

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Requirements on φ_R in the present FMM context:

(i) Regular function
(ii) Satisfy $\varphi_R(k_{\mathrm{R}}) = 1$ (for correct singularity removal)
(iii) Make $(\xi - k_{\mathrm{R}})^{-1}\varphi_R(\xi)$ integrable at infinity
(iv) Keep the variables $\boldsymbol{y}$ and $\boldsymbol{x}$ separated: $\varphi_R(\xi)$
(v) Keep the exponential decay (to truncate the infinite integral)

$$\varphi_R(\xi) = \exp\left(2(-\xi + k_{\mathrm{R}}) \times \max|x_3|\right)$$

Removing the singularities

$$\boldsymbol{U}_{\mathrm{C}}(\boldsymbol{x},\boldsymbol{y}) = \int_0^{+\infty}\int_0^{2\pi} \boldsymbol{Z}_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}},\boldsymbol{y},\boldsymbol{x})\,\mathrm{d}\alpha\mathrm{d}\xi, \quad \hat{\boldsymbol{\xi}} := \boldsymbol{\xi}/\xi = (\cos\alpha,\sin\alpha)$$

Removing the singularity due to half-order pole: similar approach

$$\boldsymbol{B}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x}) := \lim_{\xi\to k_{\mathrm{P}}} (\xi^2-k_{\mathrm{P}}^2)^{1/2}\boldsymbol{Z}_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})$$

$$\text{and } \varphi_P(\xi) = \xi\exp\Big(-2(\xi^2-k_{\mathrm{P}}^2)^{1/2}\max|x_3|\Big)k_{\mathrm{P}}^{-1}$$

Final expression of $\boldsymbol{U}_{\mathrm{C}}$ free of singularities (cost: similar to adding 2 points to the radial GGQ rule):

$$\boldsymbol{U}_{\mathrm{C}}(\boldsymbol{y},\boldsymbol{x}) = \int_0^{\xi_{max}}\int_0^{2\pi}\Big(\boldsymbol{Z}_{\mathrm{C}}(\xi,\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x}) - \boldsymbol{A}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})\frac{\varphi_R(\xi)}{\xi-k_{\mathrm{R}}} - \boldsymbol{B}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})\frac{\varphi_P(\xi)}{(\xi^2-k_{\mathrm{P}}^2)^{1/2}}\Big)d\alpha d\xi$$

$$+\,\mathrm{Ei}\big(-2k_{\mathrm{R}}\max|x_3|\big)\int_0^{2\pi}\boldsymbol{A}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})d\alpha$$

$$+\,\frac{\exp(-i2k_{\mathrm{P}}\max|x_3|)}{2k_{\mathrm{P}}\max|x_3|}\int_0^{2\pi}\boldsymbol{B}(\hat{\boldsymbol{\xi}};\boldsymbol{y},\boldsymbol{x})d\alpha$$

- Singularities integrated analytically
- Separation of variables $\boldsymbol{y}$, $\boldsymbol{x}$ preserved
- Exponential decay of the term into brackets preserved

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Diagonal form-based decomposition

New Multipole Expansion: displacement complementary FS

$$\boldsymbol{U}_{\mathrm{C}}(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{4\pi^2 k_{\mathrm{S}}^2 \mu} \sum_{a,b=\mathrm{P,S}} \int_0^{\xi_{max}} \xi A_{ab}(\xi) \Bigg\{ \int_0^{2\pi} \left[\exp(\boldsymbol{q}_a^+(\xi,\alpha)\cdot\boldsymbol{y})\, \boldsymbol{V}_a^+(\xi,\alpha) \right] \otimes \left[\exp(\boldsymbol{q}_b^-(\xi,\alpha)\cdot\boldsymbol{x})\, \boldsymbol{V}_b^-(\xi,\alpha) \right] \mathrm{d}\alpha \Bigg\} \mathrm{d}\xi$$

with $A_{\mathrm{PP}}(\xi) := \dfrac{\beta^2(\xi) s_{\mathrm{P}}(\xi)}{\delta(\xi)}$, $A_{\mathrm{PS}}(\xi) = A_{\mathrm{SP}}(\xi) := \dfrac{2\beta(\xi) s_{\mathrm{P}}(\xi)}{\delta(\xi)}$, $A_{\mathrm{SS}}(\xi) := \dfrac{4 s_{\mathrm{P}}(\xi)}{\delta(\xi)}$

New Multipole Expansion: traction complementary FS

$$\boldsymbol{T}_{\mathrm{C}}(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{4\pi^2 k_{\mathrm{S}}^2} \sum_{a,b=\mathrm{P,S}} \int_0^{\xi_{max}} \xi A_{ab}(\xi) \Bigg\{ \int_0^{2\pi} \left[\exp(\boldsymbol{q}_a^+(\xi,\alpha)\cdot\boldsymbol{y})\, \boldsymbol{W}_a(\xi,\alpha) \right] \otimes \left[\exp(\boldsymbol{q}_b^-(\xi,\alpha)\cdot\boldsymbol{x})\, \boldsymbol{V}_b^-(\xi,\alpha) \right] \mathrm{d}\alpha \Bigg\} \mathrm{d}\xi$$

Advantages of the Multipole Expansions

- FMM-suitable formulation: separation of $\boldsymbol{x}$ and $\boldsymbol{y}$
- Tensor product of 2 vectors: rank one formulation

New Algorithm for Complementary term

$$\mathcal{S}_C[\boldsymbol{t}](\boldsymbol{x}) := \int_S \boldsymbol{t}(\boldsymbol{y}) \cdot \boldsymbol{U}^{HS}(\boldsymbol{x}, \boldsymbol{y}; \omega)\, dS_{\boldsymbol{y}}, \quad \mathcal{D}_C[\boldsymbol{u}](\boldsymbol{x}) := \int_S \boldsymbol{u}(\boldsymbol{y}) \cdot \boldsymbol{T}^{HS}(\boldsymbol{x}, \boldsymbol{y}; \omega)\, dS_{\boldsymbol{y}}$$

Fast Multipole Algorithm for Complementary term

1. Computation of multipole moments $(a, b = \mathrm{P}, \mathrm{S})$

$$\mathcal{R}^t_a(\xi_i, \alpha_j) := \frac{1}{4\pi^2 k_S^2 \mu} \left\{ \int_S \exp(\boldsymbol{q}^+_a(\xi_i, \alpha_j) \cdot \boldsymbol{y})\, \boldsymbol{t}(\boldsymbol{y})\, dS_{\boldsymbol{y}} \right\} \cdot \boldsymbol{V}^+_a(\xi_i, \alpha_j$$

$$\mathcal{R}^u_a(\xi_i, \alpha_j) := \frac{1}{4\pi^2 k_S^2} \left\{ \int_S \exp(\boldsymbol{q}^+_a(\xi_i, \alpha_j) \cdot \boldsymbol{y})\, \boldsymbol{u}(\boldsymbol{y})\, dS_{\boldsymbol{y}} \right\} \cdot \boldsymbol{W}_a(\xi_i, \alpha_j)$$

2. Evaluation at observation points (quadrature in Fourier space)

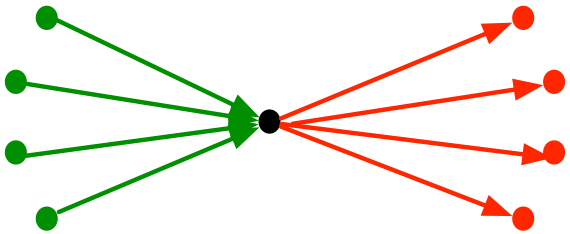
$$\mathcal{S}_C[\boldsymbol{t}](\boldsymbol{x}) = \sum_{a,b=\mathrm{P,S}} \sum_{i=1}^{n_\xi} w^\xi_i \xi_i A_{ab}(\xi_i) \left\{ \sum_{j=1}^{n_\alpha} w^\alpha_j \mathcal{R}^t_a(\xi_i, \alpha_j) \left[\exp(\boldsymbol{q}^-_b(\xi_i, \alpha_j) \cdot \boldsymbol{x})\, \boldsymbol{V}^-_b(\xi_i, \alpha_j) \right] \right\}$$

$$\mathcal{D}_C[\boldsymbol{u}](\boldsymbol{x}) = \sum_{a,b=\mathrm{P,S}} \sum_{i=1}^{n_\xi} w^\xi_i \xi_i A_{ab}(\xi_i) \left\{ \sum_{j=1}^{n_\alpha} w^\alpha_j \mathcal{R}^u_a(\xi_i, \alpha_j) \left[\exp(\boldsymbol{q}^-_b(\xi_i, \alpha_j) \cdot \boldsymbol{x})\, \boldsymbol{V}^-_b(\xi_i, \alpha_j) \right] \right\}$$

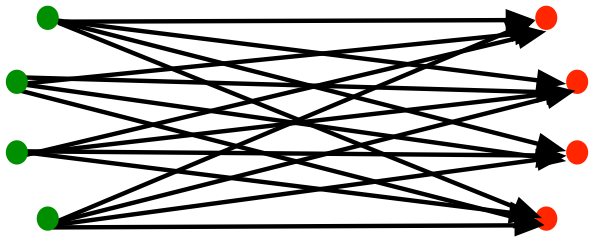
Complexity

Fast Evaluation of the complementary term

FM-BEM



BEM



Complexity for evaluation of $\mathcal{S}_C[\boldsymbol{t}](\boldsymbol{x})$ and $\mathcal{D}_C[\boldsymbol{u}](\boldsymbol{x})$:

- N: number of BE DOFs
- n_α, n_ξ: number of quadrature points angular and radial integrals

- For each quadrature point and each DOF
- Evaluating $\mathcal{S}_C[\boldsymbol{t}](\boldsymbol{x})$ and $\mathcal{D}_C[\boldsymbol{u}](\boldsymbol{x})$ costs $O(n_\xi n_\alpha N)$

Complexity estimated via numerical (empirical) tests:
$n_\xi n_\alpha = O(N^{0.55})$

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Accuracy of the multipole expansions

Comparisons with the code provided by B.B. Guzina[3](FS of the layered elastic half-space)

$$\varepsilon_{ij} = \frac{||\boldsymbol{U}_{ij}^{HS} - (\boldsymbol{U}_{ij}^{HS})_{guz.}||_2}{||(\boldsymbol{U}_{ij}^{HS})_{guz.}||_2} \qquad \text{(if angular integral very accurate)}$$

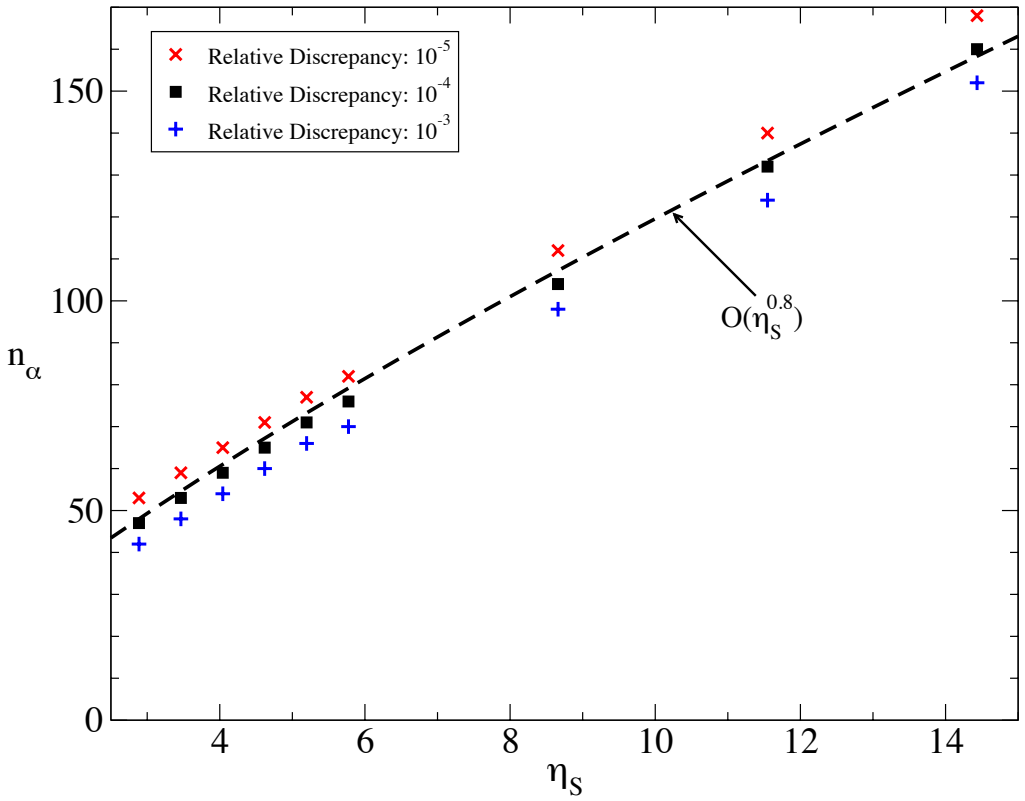
Accuracy w.r.t N_ξ (fixed $\eta_S = 1/\sqrt{3}$)

N_ξ	ε_{11}	ε_{12}	ε_{13}	ε_{31}	ε_{33}
12	$4.1\ 10^{-2}$	$1.9\ 10^{-2}$	$1.5\ 10^{-1}$	$2.1\ 10^{-1}$	$2.7\ 10^{-2}$
15	$4.4\ 10^{-3}$	$3.1\ 10^{-3}$	$2.3\ 10^{-2}$	$4.8\ 10^{-2}$	$1.8\ 10^{-2}$
16	$1.9\ 10^{-3}$	$6.3\ 10^{-4}$	$4.8\ 10^{-3}$	$6.3\ 10^{-3}$	$1.5\ 10^{-3}$
17	$1.2\ 10^{-3}$	$4.2\ 10^{-4}$	$3.2\ 10^{-3}$	$4.5\ 10^{-3}$	$1.4\ 10^{-3}$
23	$5.5\ 10^{-5}$	$1.9\ 10^{-4}$	$1.7\ 10^{-4}$	$1.6\ 10^{-4}$	$1.8\ 10^{-4}$

$\Rightarrow$ Better accuracy if # points in the radial integral increases

[3][B.B. Guzina and Pak, QJMAM, 2001])

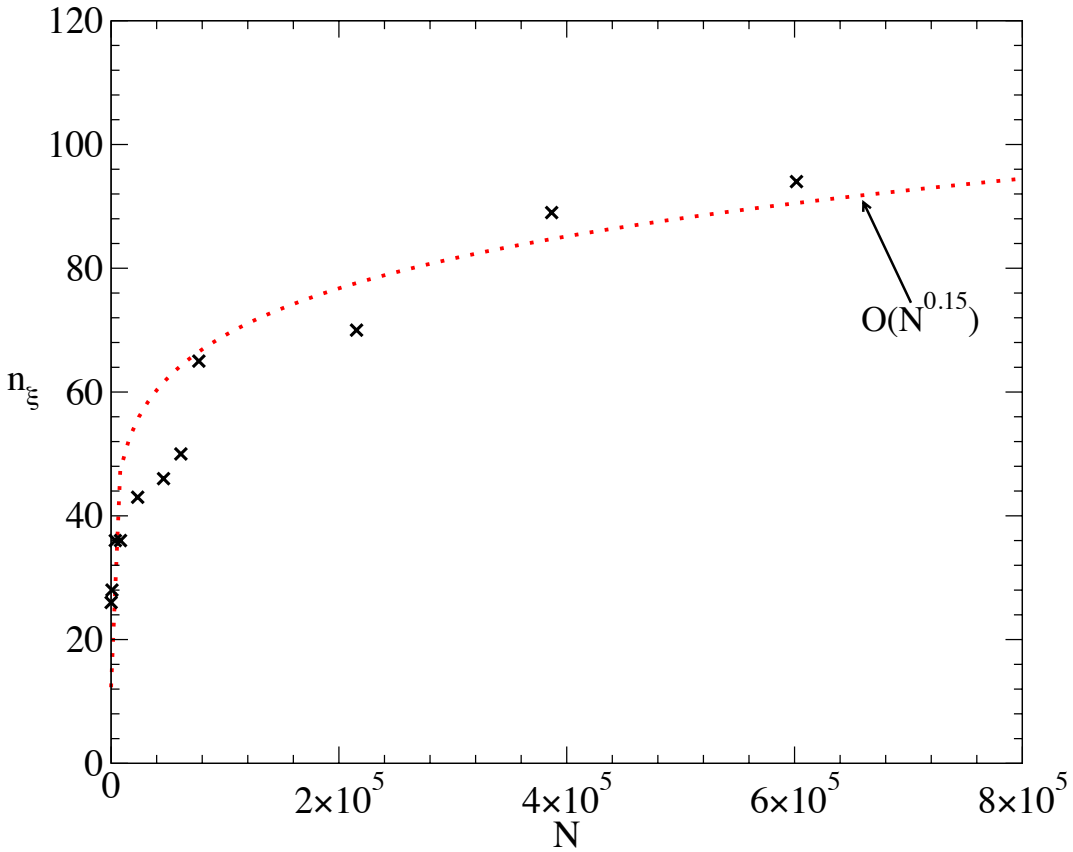
Trapezoidal rule for angular integration



$$n_\alpha = O(\eta_S^{0.8}) = O(N^{0.4})$$

Relative Discrepancy on $\sum_j \boldsymbol{U}_C(\boldsymbol{x}_i, \boldsymbol{y}_j)\mathbf{t}(\boldsymbol{y}_j)$ with a ref. solution ($N_\alpha = 250$)

Generalized Gaussian Quadrature



n_ξ observed to be of order $n_\xi = O(\eta_S^{0.3}) = O(N^{0.15})$

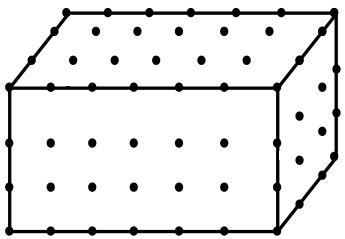
Verification of the complexity estimate

Complexity of the matrix-vector product

$$\sum_{j}^{N} \boldsymbol{U}^{HS}(\boldsymbol{x}_i, \boldsymbol{y}_j)\mathbf{t}(\boldsymbol{y}_j) \quad \text{(for given sets of points } x_i, y_j \quad 1 \leq i, j \leq N)$$

Discretization: Fixed density of points per S-wavelength $\Rightarrow$ N set by choice of ω

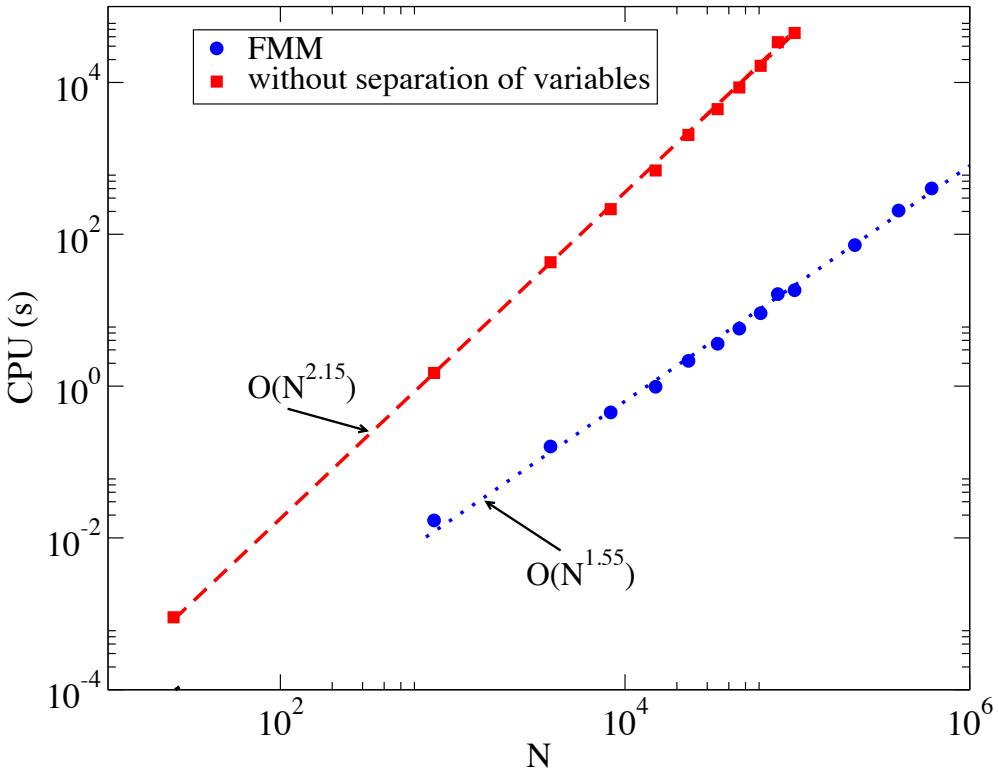
Rectangular box: (non-dimensional spatial coordinates)



$$-4L \leq y_1, y_2 \leq 4L, \quad -4L \leq y_3 \leq -L$$

Complexity estimation

Complexity estimate for evaluation of $\mathcal{S}_C[\boldsymbol{t}]$

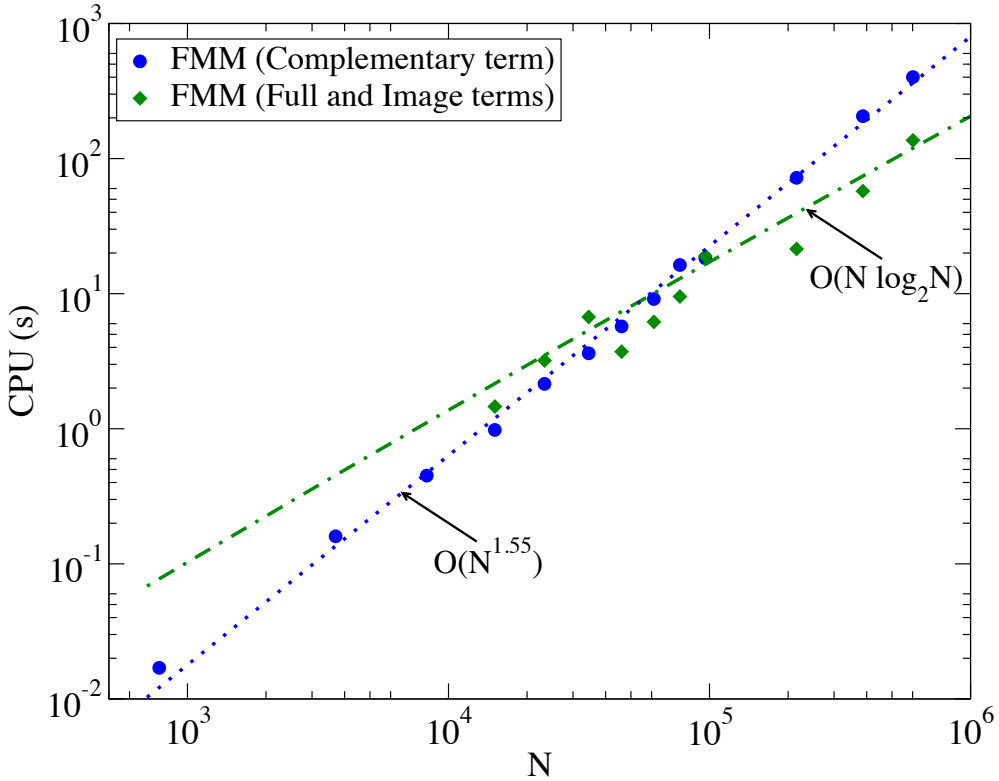


$$n_\xi = O(N^{0.15})$$
$$n_\alpha = O(N^{0.4})$$

- Without separation of variables ***x***, ***y***: $O(N_\xi N^2) \Rightarrow O(N^{2.15})$
- FMM: $O(N_\alpha N_\xi N) \Rightarrow O(N^{1.55})$

Complexity estimation

Complexity estimate for evaluation of $\mathcal{S}[t] = \mathcal{S}_\infty[t] + \bar{\mathcal{S}}_\infty[t] + \mathcal{S}_C[t]$



- "New" FMM to compute $\mathcal{S}_C$: $O(N^{1.55})$
- "Standard" FMM to compute sum of $\mathcal{S}_\infty[t]$ & $\bar{\mathcal{S}}_\infty[t]$: $O(N \log N)$

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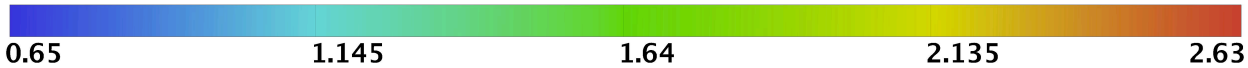
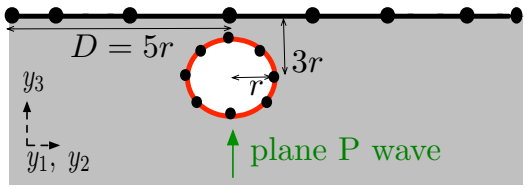
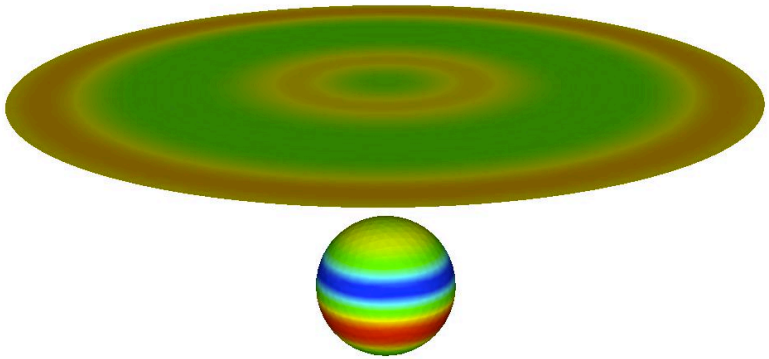
Accuracy of the new half-space FS (BEM)

Comparison between the new formulation based on half-space FS (BEM) with classical formulation based on elastic full-space FS

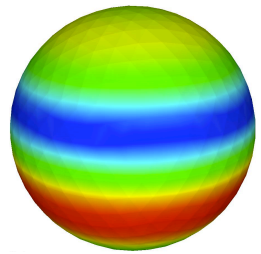
Modulus of vertical component of displacement ($\eta_s = k_s r/\pi = 1$)







Full-space FS (FMM)
N = 20 277



Half-space FS (BEM)
N = 1 926

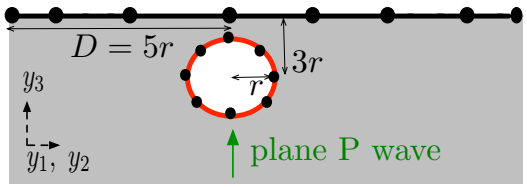
Remarks

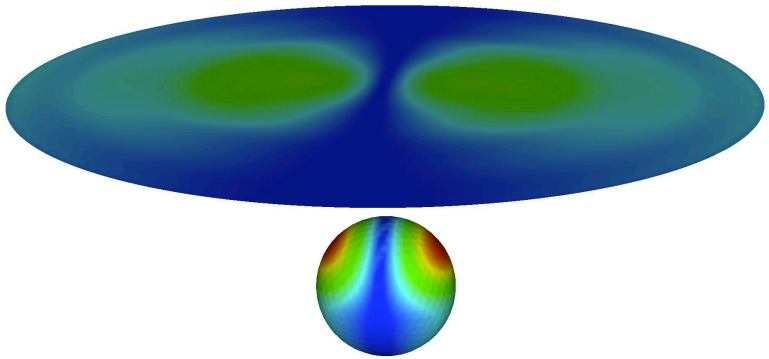
- Full-space solution : approximation due to artificial truncation
- Frequency too small to use FMM for half-space FS
- Need of post-processing to compute displ. on the free surface

Accuracy of the new half-space FS (BEM)

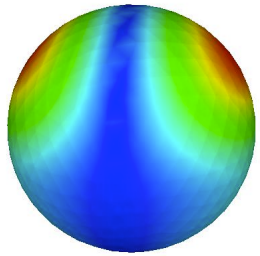
Comparison between the new formulation based on half-space FS (BEM) with classical formulation based on elastic full-space FS

Modulus of horizontal component of displacement ($\eta_s = k_s r/\pi = 1$)





Full-space FS (FMM)
N = 20 277



Half-space FS (BEM)
N = 1 926

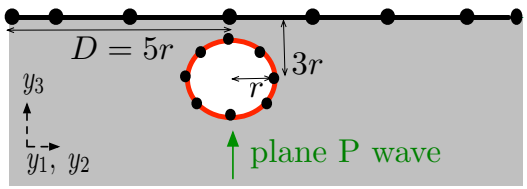
Remarks

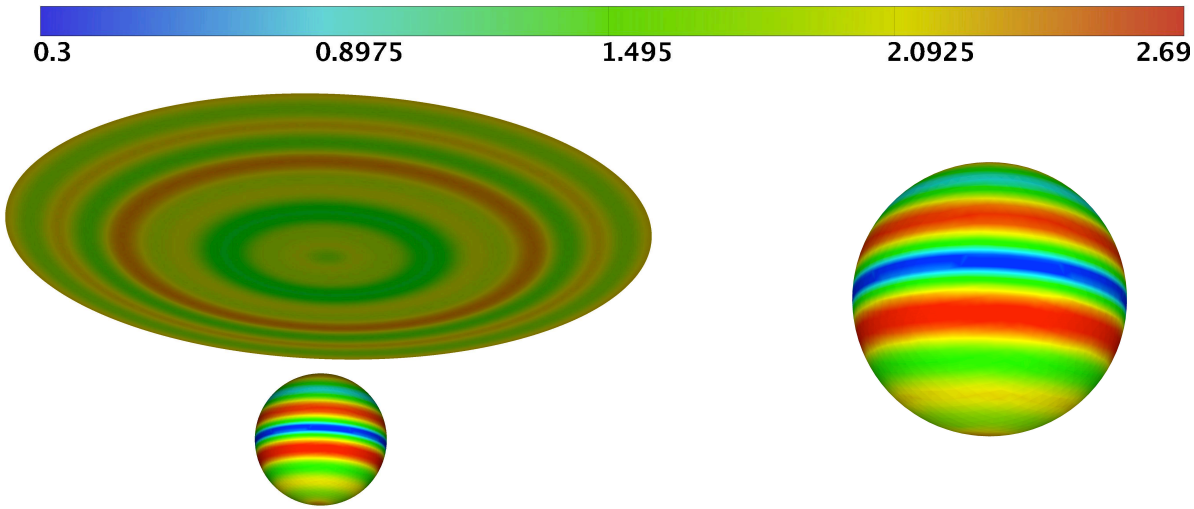
- Full-space solution : approximation due to artificial truncation
- Frequency too small to use FMM for half-space FS
- Need of post-processing to compute displ. on the free surface

Accuracy of the new half-space FS (FM-BEM)

Comparison between the new formulation based on half-space FS (FM-BEM) with classical formulation based on elastic full-space FS

Vertical component of displacement ($\eta_s = k_s r/\pi = 2.5$)





Full-space FS (FMM)
N = 38 934

Half-space FS (FMM)
N = 7 686

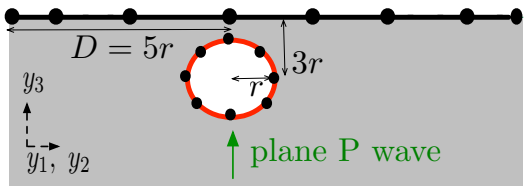
Remarks

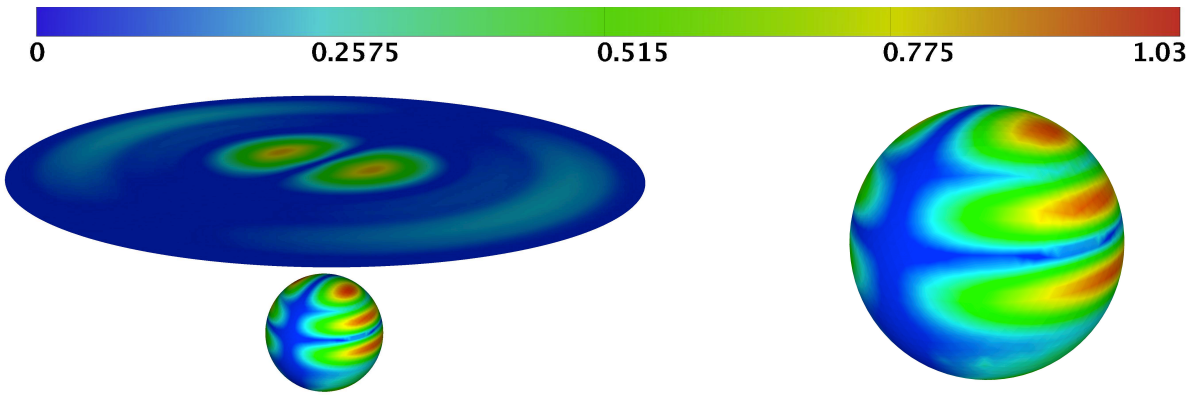
- CPU not compared: implement. of $\mathcal{S}_C[\boldsymbol{t}]$, $\mathcal{D}_C[\boldsymbol{u}]$ not optimized
- Optimal way to compute the image terms $\bar{\mathcal{S}}_\infty[\boldsymbol{t}]$, $\bar{\mathcal{D}}_\infty[\boldsymbol{u}]$?

Accuracy of the new half-space FS (FM-BEM)

Comparison between the new formulation based on half-space FS (FM-BEM) with classical formulation based on elastic full-space FS

Horizontal component of displacement ($\eta_s = k_s r/\pi = 2.5$)





Full-space FS (FMM)
N = 38 934

Half-space FS (FMM)
N = 7 686

Remarks

- CPU not compared: implement. of $\mathcal{S}_C[\boldsymbol{t}]$, $\mathcal{D}_C[\boldsymbol{u}]$ not optimized
- Optimal way to compute the image terms $\bar{\mathcal{S}}_\infty[\boldsymbol{t}]$, $\bar{\mathcal{D}}_\infty[\boldsymbol{u}]$?

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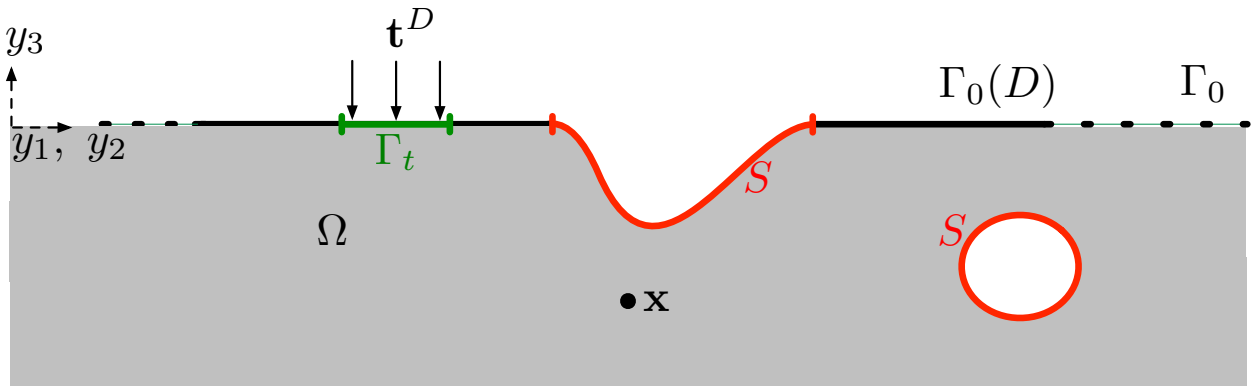
Summary and conclusions

- Formulation of the multipole expansions for the half-space elastodynamic fundamental solutions
- Tailored algorithm to compute Generalized Gaussian Quadrature
- New FMM proposed for elastodynamic problems in semi-infinite media
- Accuracy of new formulation based on half-space FS compared with classical formulation based on elastic full-space FS
- Complexity of a matrix-vector product estimated numerically



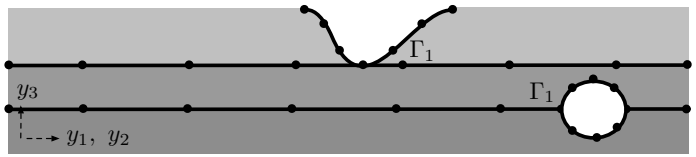
References:

- S. Chaillat, M.B.: A new Fast Multipole formulation for the elastodynamic half-space Green's tensor (submitted to J. Comp. Phys., under revision, 2013)
- S. Chaillat, M.B.: Recent advances on the fast multipole accelerated boundary element method for 3D time-harmonic elastodynamics, Wave Motion, 2013, in press

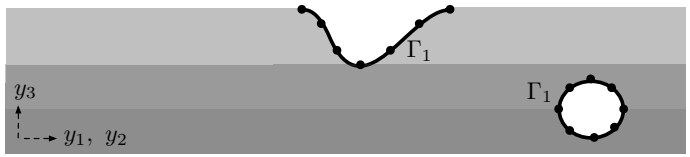
Future work

- Optimize the implementation: computation of the image term?
- Comparisons of numerical efficiency with classical formulation based on elastic full-space FS
- Formulate a FMM for the layered visco-elastic half-space FS

Homogeneous FS



Layered Half-space FS



- Parallelization to run higher frequencies