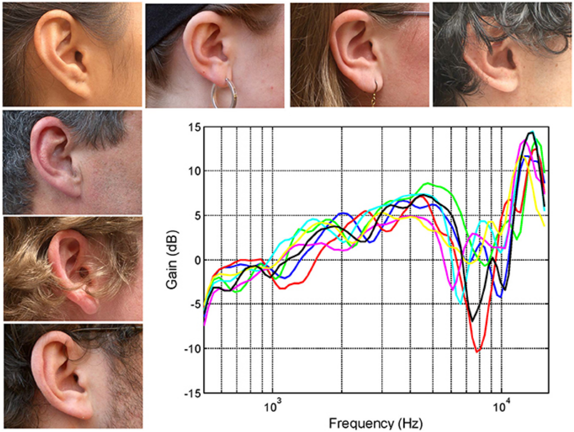
Fast Boundary Elements Methods and Applications

François Alouges Matthieu Aussal

Centre de Mathématiques Appliquées de l'École Polytechnique
Route de Saclay - 91128 Palaiseau CEDEX France

New Trends in Integral Equations
February 4th-5th 2016

Industrials needs for 3D audio

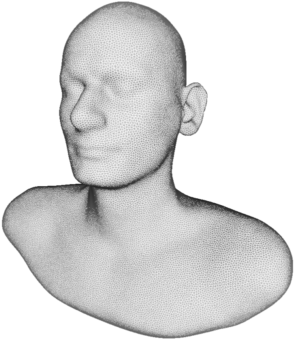


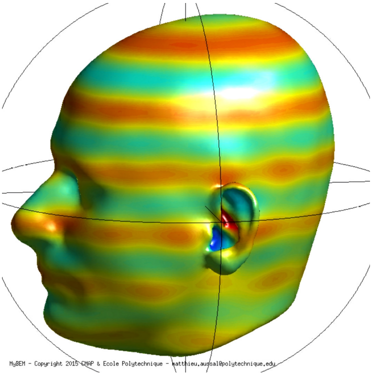
Individual frequency filters functions of space and morphology :

$$
\begin{array}{ccc}
\mathbb{R}^3 \times \mathbb{R}^+ \times \mathbb{M} & \rightarrow & \mathbb{C} \\
(\mathbf{x}, \quad f, \quad \mathbf{m}) & \rightarrow & HRTF(\mathbf{x}, f, \mathbf{m})
\end{array}
$$

Numerical simulation of HRTF

Microsoft Kinect and SYMARE mesh





Solve Helmholtz equation

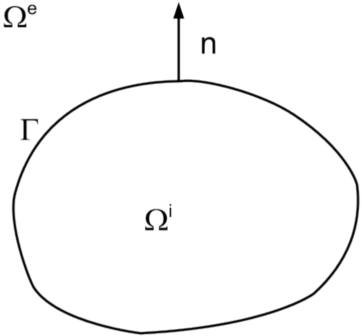
for scattering problem

Acoustic scattering problem

Notations :

Let a solution u defined in the full space $\mathbb{R}^3 \setminus \Gamma$ with :

- Γ smooth and oriented,
- $u^i = u|_{\Omega_i}$ and $u^e = u|_{\Omega_e}$,
- $\mu = [u] = u^e - u^i$ and $\lambda = [\partial_n u] = \partial_n u^e - \partial_n u^i$.



Theorem of integral representation

If u satisfies Helmholtz equation and Sommerfeld radiation condition :

$$\left\{\begin{array}{rcl} -(\Delta u^i + k^2 u^i) & = & 0 \in \Omega^i, \\ -(\Delta u^e + k^2 u^e) & = & 0 \in \Omega^e, \\ \lim\limits_{r \to +\infty} r\,(\partial_r u^e + iku^e) & = & 0, \end{array}\right.$$

then u satisfies :

$$\begin{array}{rcll} u(\mathbf{x}) & = & \mathcal{D}\mu(\mathbf{x}) - \mathcal{S}\lambda(\mathbf{x}) & \forall \mathbf{x} \in \Omega^i \cup \Omega^e, \\ \frac{1}{2}(u^i(\mathbf{x}) + u^e(\mathbf{x})) & = & D\mu(\mathbf{x}) - S\lambda(\mathbf{x}) & \forall \mathbf{x} \in \Gamma, \\ \frac{1}{2}(\partial_n u^i(\mathbf{x}) + \partial_n u^e(\mathbf{x})) & = & H\mu(\mathbf{x}) - D^t\lambda(\mathbf{x}) & \forall \mathbf{x} \in \Gamma. \end{array}$$

Boundary Element Method

- Single layer potential (idem for Double layer) :

$$\mathcal{S}\lambda(\mathbf{x}) = \int_\Gamma G(\mathbf{x},\mathbf{y})\lambda(\mathbf{y})d\Gamma_y, \quad G(\mathbf{x},\mathbf{y}) = \frac{e^{-ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}.$$

- Boundary finite elements $(\phi_n(\mathbf{x}))_{1\leq n\leq N_{dof}}$:

$$\lambda(\mathbf{x}) \sim \lambda_\phi(\mathbf{x}) = \sum_{n=1}^{N_{dof}} \lambda_n\phi_n(\mathbf{x}).$$

- Discretization of Γ with a quadrature $(\mathbf{y}_q,\gamma_q)_{1\leq q\leq N_q}$:

$$\mathcal{S}\lambda(\mathbf{x}) \sim G\star\lambda_\phi(\mathbf{x}) = \sum_{q=1}^{N_q} \gamma_q G(\mathbf{x},\mathbf{y}_q)\lambda_\phi(\mathbf{y}_q).$$

- Galerkin formulation (**dense**) :

$$[S]_{i,j} = \int_\Gamma\int_\Gamma \phi_i(\mathbf{x})G(\mathbf{x},\mathbf{y})\phi_j(\mathbf{y})d\Gamma_x d\Gamma_y.$$

Vectorized formalism for Matlab computation

Final galerkin formalism used :

$$\mathcal{S}\lambda(\mathbf{x}) \sim \Phi_l \cdot G_{xy} \cdot \Phi_r$$

with :

- Φ_l : **sparse** integration matrix, from dof to $\mathbf{x}$ quadrature,
- G_{xy} : **full** interaction matrix between $\mathbf{x}$ and $\mathbf{y}$ quadrature,
- $\Phi_r = \Phi_l^t$: **sparse** from $\mathbf{y}$ quadrature to dof.

Singular interactions for $|\mathbf{x} - \mathbf{y}| < \epsilon$ are done with semi-analytical corrective patch :

$$\mathcal{S}\lambda(\mathbf{x}) \sim \Phi_l \cdot (G_{xy} \cdot \Phi_r + G_{xddl}),$$

where G_{xddl} is also **sparse** matrix.

Galerkin finite elements $\Rightarrow$ Points to points interactions

Points to points interactions

With N_0 depending on computer used :

- **Direct method** : Computing and storing dense matrix ...
  ... $O(N^2)$ **operations, impossible for** $N \geq N_0$.
- **Iterative method** : Only computing dense matrix ...
  ... $O(N^2)$ **operations, slow for** $N \geq N_0$.
- **Fast iterative method** : Split the variables $\mathbf{x}$ and $\mathbf{y}$ in $G(\mathbf{x}, \mathbf{y})$...
  ... $O(N)$ **operations, fast for** $N \geq N_0$.

Example with a regular kernel

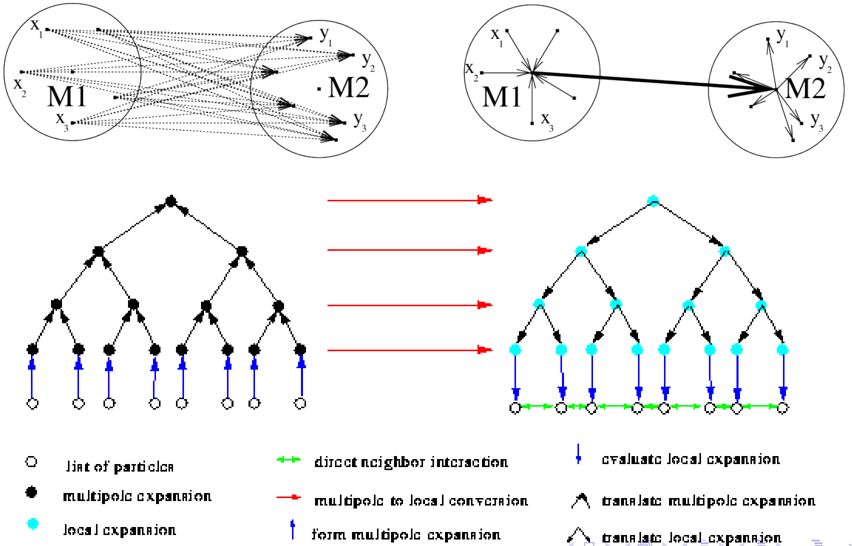
If $G(\mathbf{x},\mathbf{y}) = |\mathbf{x}-\mathbf{y}|^2 = |\mathbf{x}|^2 - 2\mathbf{x}\cdot\mathbf{y} + |\mathbf{y}|^2$, then

$$\forall i,\ \ v_i = \sum_j G(\mathbf{x}_i,\mathbf{x}_j)u_j = |\mathbf{x}_i|^2 \sum_j u_j - 2\mathbf{x}_i \cdot \sum_j \mathbf{x}_j u_j + \sum_j |\mathbf{x}_j|^2 u_j$$

- Separation of the variables $\mathbf{x}$ et $\mathbf{y}$ $\rightarrow$ **Compression !**
- **(A lot of) numerical and technical difficulties** ...
  ... **Complexity** $\rightarrow O(N \log N)$.

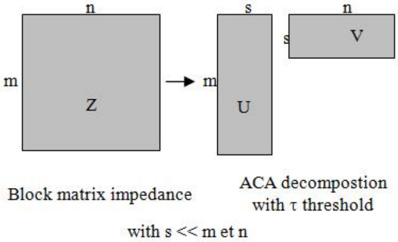
The Fast Multipole Method (FMM)

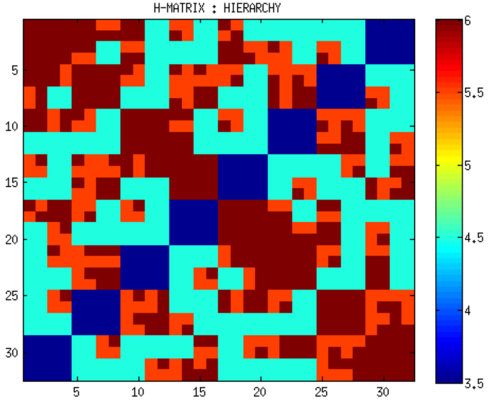
Firstly introduced by L. Greengard in 1987 for Laplace kernel.



The Hierarchical Matrices ($\mathcal{H}$-Matrix)

Firstly introduced by
W. Hackbusch in 1999





6 level hierarchy for 6 000 particles

The Sparse Cardinal Sine Decomposition (SCSD)

- Introduced by F. Alouges & M. Aussal in 2014.
- Convolution in space $\Leftrightarrow$ Product in Fourier domain.
- Fourier transform of the cardinal sine (S^2 = unit sphere) :

$$\mathcal{F}\left(\frac{\sin(|\mathbf{z}|)}{|\mathbf{z}|}\right) = 2\pi^2\delta_{S^2} \qquad \forall \mathbf{z} \in R^3.$$

- Integral representation :

$$\frac{\sin(|\mathbf{z}|)}{|\mathbf{z}|} = \frac{1}{4\pi}\int_{S^2} e^{i\mathbf{s}\cdot\mathbf{z}} ds \qquad \forall \mathbf{z} \in \mathbb{R}^3.$$

- Imaginary part of G_{xy}, setting $\mathbf{z} = k(\mathbf{x}-\mathbf{y})$ for all $(\mathbf{x},\mathbf{y}) \in \mathbb{R}^3$:

$$\mathfrak{Im}\left(G(\mathbf{x},\mathbf{y})\right) = \frac{\sin(k|\mathbf{x}-\mathbf{y}|)}{4\pi|\mathbf{x}-\mathbf{y}|} = \frac{k}{(4\pi)^2}\int_{S^2} e^{ik\mathbf{s}\cdot\mathbf{x}} e^{-ik\mathbf{s}\cdot\mathbf{y}} d\mathbf{s}.$$

- Simple separation of the variables $\mathbf{x}$ and $\mathbf{y}$.

First step towards a fast convolution

- Convolution for the imaginary part :

$$\mathfrak{Im}\,(G) \star \lambda_\phi(\mathbf{x}_r) = \sum_{q=1}^{N_q} \gamma_q \left[\frac{k}{(4\pi)^2} \int_{S^2} e^{ik\mathbf{s}\cdot\mathbf{x}_r} e^{-ik\mathbf{s}\cdot\mathbf{y}_q} d\mathbf{s} \right] \lambda_\phi(\mathbf{y}_q).$$

- After discretization of S^2 with a quadrature $(\mathbf{s}_p; \sigma_p)_{1\leq p\leq N_p}$:

$$\mathfrak{Im}\,(G)\star\lambda_\phi(\mathbf{x}_r) \sim \frac{k}{(4\pi)^2} \sum_{p=1}^{N_p} e^{ik\mathbf{s}_p\cdot\mathbf{x}_r} \sigma_p \left[\sum_{q=1}^{N_q} e^{-ik\mathbf{s}_p\cdot\mathbf{y}_q} \gamma_q \lambda_\phi(\mathbf{y}_q) \right]_p .$$

- **Fast** evaluation thanks to a Non Uniform 3D Fourier Transform (**NUFFT 3D type-III**), in space $\mathbf{x}_n$ and frequencies ξ_p :

$$NUFFT(f)_p = \sum_{n=1}^{N} e^{\pm i\xi_p\cdot\mathbf{x}_n}\, f_n$$

- **Complexity $O(N \log N)$!**

Trick for the real part of the Green kernel

- **Principle :** $\mathfrak{Re}(G)$ is expressed using $\mathfrak{Im}(G)$
- Fourier transform of the cardinal cosine :

$$\mathcal{F}\left(\frac{\cos(|\mathbf{z}|)}{|\mathbf{z}|}\right) = \frac{4\pi}{|\xi|^2 - 1} \qquad \forall(\mathbf{z}, \xi) \in \mathbb{R}^3 \times \mathbb{R}^3.$$

- Integral representation of the Green kernel :

$$\frac{\cos(|\mathbf{z}|)}{|\mathbf{z}|} = \frac{1}{2\pi^2} \int_{\mathbb{R}^3} \frac{1}{|\xi|^2 - 1} \; e^{i\xi\cdot\mathbf{z}} d\xi.$$

- Change variables from Cartesian to Spherical :

$$\frac{\cos(|\mathbf{z}|)}{|\mathbf{z}|} = \frac{1}{2\pi^2} \int_{\mathbb{R}^+} \frac{\rho^2}{\rho^2 - 1} \left(\int_{S^2} \; e^{i\rho\mathbf{s}\cdot\mathbf{z}} d\mathbf{s} \right) d\rho.$$

- Expression 1D of cosc as a function of sinc :

$$\frac{\cos(|\mathbf{z}|)}{|\mathbf{z}|} = \frac{2}{\pi} \int_{\mathbb{R}^+} \frac{\rho}{\rho^2 - 1} \frac{\sin(\rho|\mathbf{z}|)}{|\mathbf{z}|} d\rho.$$

Quadrature

$$\frac{\cos(|\mathbf{z}|)}{|\mathbf{z}|} = \frac{2}{\pi}\int_{\mathbb{R}^+} \frac{\rho}{\rho^2-1}\frac{\sin(\rho|\mathbf{z}|)}{|\mathbf{z}|}d\rho.$$

- We look for points and weights $(\rho_m;\alpha_m)_{1\leq m\leq M}$

$$\frac{\cos(|\mathbf{z}|)}{|\mathbf{z}|} \sim \sum_{m=1}^{M}\alpha_m\frac{\sin(\rho_m|\mathbf{z}|)}{|\mathbf{z}|}.$$

- We solve in $(\rho_m;\alpha_m)_{1\leq m\leq M}$ with a least square approximation, and $\rho_m = \frac{\pi}{b}(2m-1)$

$$\forall|\mathbf{z}_i| \in [a,b]: \quad \sum_{m=1}^{M}\alpha_m \sin(\rho_m|\mathbf{z}_i|) = \cos(|\mathbf{z}_i|) \Rightarrow A(\rho)\alpha = B.$$

- **Fundamental result :**

$$M \propto \frac{a+b}{a}|\log(\epsilon)|$$

Final SCSD-formalism

- For $k|\mathbf{x}-\mathbf{y}| \in [a,b]$:

$$\frac{\cos(k|\mathbf{x}-\mathbf{y})|)}{4\pi|\mathbf{x}-\mathbf{y}|} \sim \sum_{m=1}^{M} \alpha_m \frac{\sin(\rho_m k|\mathbf{x}-\mathbf{y})|)}{4\pi|\mathbf{x}-\mathbf{y}|}.$$

- We append $(\rho_m; \alpha_m)$ with $\alpha_{M+1} = -i$ and $\rho_{M+1} = 1$:

$$\frac{e^{-ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \sim \sum_{m=1}^{M+1} \frac{\alpha_m}{4\pi} \frac{\sin(\rho_m k|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|} = \sum_{m=1}^{M+1} \frac{\alpha_m}{(4\pi)^2} \int_{S^2_{k\rho_m}} e^{i\mathbf{s}\cdot\mathbf{x}} e^{-i\mathbf{s}\cdot\mathbf{y}} d\mathbf{s}.$$

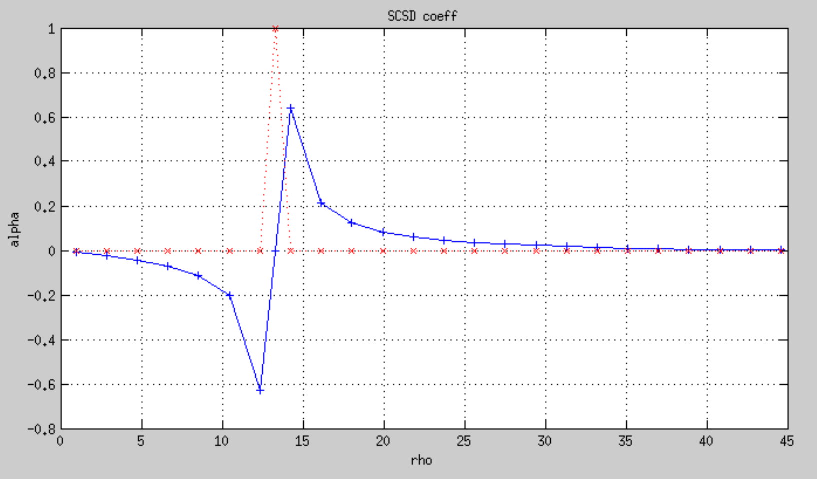
- Quadrature of $\mathbb{R}^3$ with $(\xi_p \in \cup S^2_{k\rho_m}; \omega_p)_{1\leq p\leq N_p}$:

$$G \star \lambda_\phi(\mathbf{x}) \sim \frac{1}{(4\pi)^2} \sum_{p=1}^{N_p} e^{i\xi_p\cdot\mathbf{x}} \omega_p \left[\sum_{q=1}^{N_q} e^{-i\xi_p\cdot\mathbf{y}_q} \gamma_q \lambda_\phi(\mathbf{y}_q) \right]_p .$$

- **Fundamental result :** $N_p \propto \left(\frac{b}{a}|\log(\epsilon)|\right)^3$

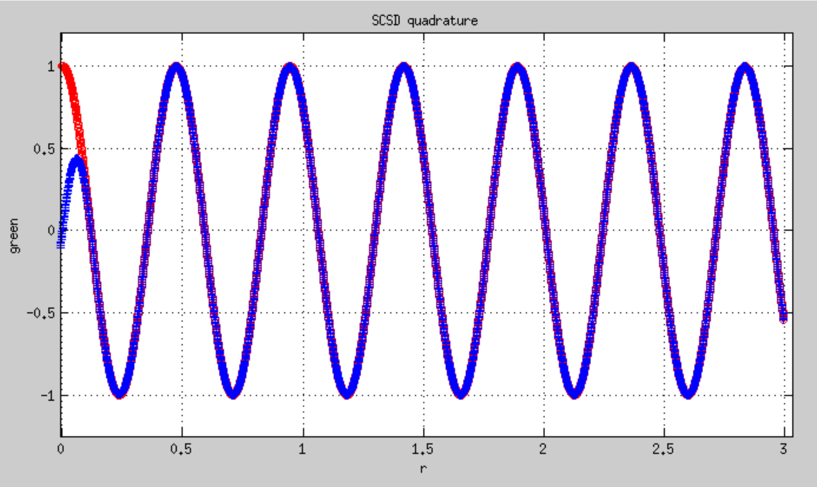
Exemple of SCSD cosine quadrature (1)

Quadrature $(\rho_m; \alpha_m)_{1\leq m\leq M}$ for unit sphere with $k = 13$.



Exemple of SCSD cosine quadrature (2)

Cosine approximation by a sum of sine function => Regular in 0.



Summary

- Quadrature of $\mathbb{R}^3$ with $(\xi_p \in \cup S^2_{k\rho_m}; \omega_p)_{1\leq p\leq N_p}$:

$$G \star \lambda_\phi(\mathbf{x}) \sim \frac{1}{(4\pi)^2} \sum_{p=1}^{N_p} e^{i\xi_p\cdot\mathbf{x}} \omega_p \left[\sum_{q=1}^{N_q} e^{-i\xi_p\cdot\mathbf{y}_q} \gamma_q \lambda_\phi(\mathbf{y}_q) \right]_p .$$

- Mimicks

$$\begin{aligned} G \star \lambda_\phi(\mathbf{x}) &= \mathcal{F}^{-1}\left(\hat{G}(\xi)\mathcal{F}(\lambda_\phi\delta_\Gamma)\right) \\ &= \int_{\mathbb{R}^3} e^{i\xi\cdot\mathbf{x}} \hat{G}(\xi) \left[\int_\Gamma e^{-i\xi\cdot\mathbf{y}} \lambda_\phi(\mathbf{y})\, d\mathbf{y} \right] d\xi \end{aligned}$$

- **Theoretical complexity :**
  Ball : $O(N \log N)$
  Sphere : $O(N^{6/5} \log N)$

Algorithm

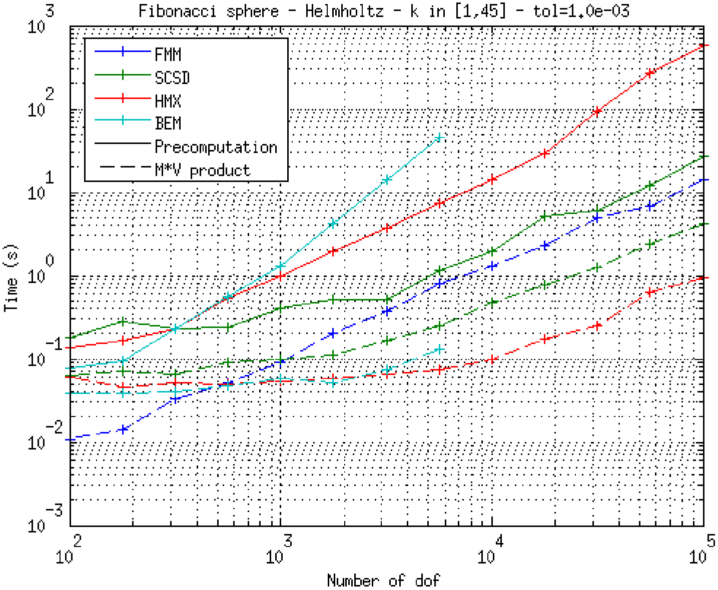
1. SCSD quadrature for **far** interactions (in $[a, b]$) : $(\xi_p \in \mathbb{R}^3; \omega_p)_{1 \leq p \leq N_p}$.
2. Type-III NUFFT $(\mathbf{y}_q)_{1 \leq q \leq N_q}$ to $(\xi_p)_{1 \leq p \leq N_p}$ on $(\gamma_q \lambda_\phi(\mathbf{y}_q))_{1 \leq q \leq N_q}$.
3. Weighting of the result ② with $(\omega_p)_{1 \leq p \leq N_p}$.
4. Type-III NUFFT $(\xi_p)_{1 \leq p \leq N_p}$ to $(\mathbf{x}_i)_{1 \leq i \leq N_i}$ on the result ③ : $G_{far} \star \lambda_\phi(\mathbf{x}_i)_{1 \leq i \leq N_i}$.
5. **Close** interactions correction (in $[0, a]$) : $G_{corr} \star \lambda_\phi(\mathbf{x}_i)_{1 \leq i \leq N_i}$.
6. $G \star \lambda_\phi(\mathbf{x}_i)_{1 \leq i \leq N_i} \sim (G_{far} + G_{corr}) \star \lambda_\phi(\mathbf{x}_i)_{1 \leq i \leq N_i}$.

Context

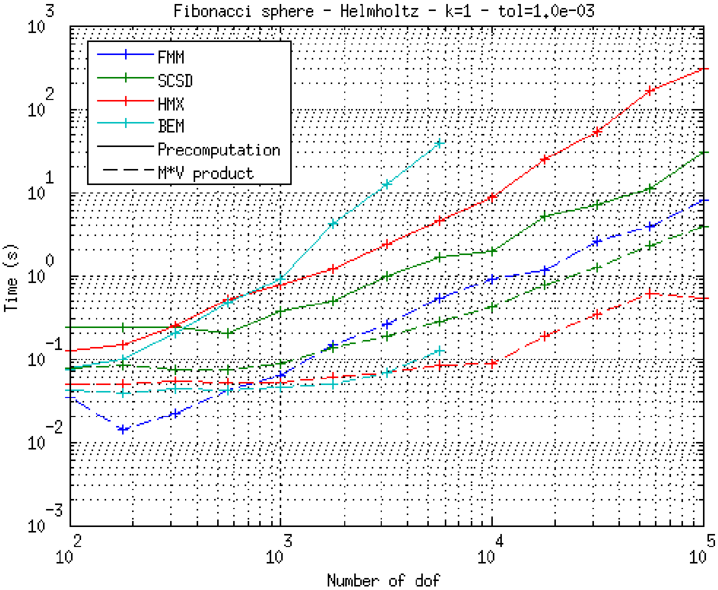
- 4 cores at 2.7 GHz with 32 Go ram,
- Galerkin single layer operator $\mathcal{S}\lambda$,
- BEM, SCSD and $\mathcal{H}$-Matrix in native Matlab,
- FMM and NuFFT in native fortran [1],
- Full parallelism except for NuFFT,
- Up to 10^5 dof, equivalent to 6.10^5 particles

1. Mex-file from L. Greengard : www.cims.nyu.edu/cmcl

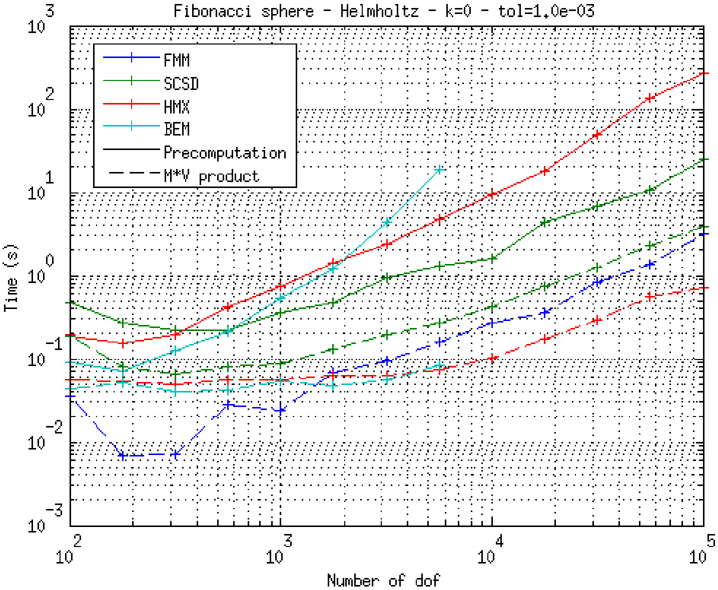
Helmholtz problem with adaptive wave number



Helmholtz problem at low frequency (k=1)



Laplace problem (k=0)



Validation on the unit sphere : Radar Cross Section

- **Boundary conditions :** Homogeneous Dirichlet or Neumann,
- **Excitation :** Plane wave

$$u_{pw}(\mathbf{x}) = e^{-i\mathbf{k}\cdot\mathbf{x}},$$

- **Integral equation :** Brackage-Werner formulation with $\beta \in \mathbb{C}$

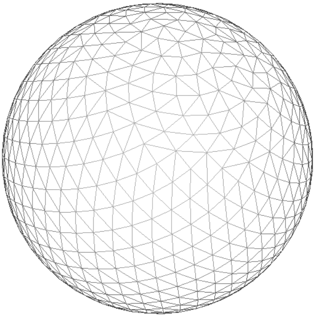
$$\begin{cases} [ik\beta S - (\frac{Id}{2} + D)]\mu(\mathbf{x}) &= -u_{pw}(\mathbf{x}) \qquad \forall \mathbf{x} \in \Gamma, \\ \lambda(\mathbf{x}) &= ik\beta\mu(\mathbf{x}), \end{cases}$$

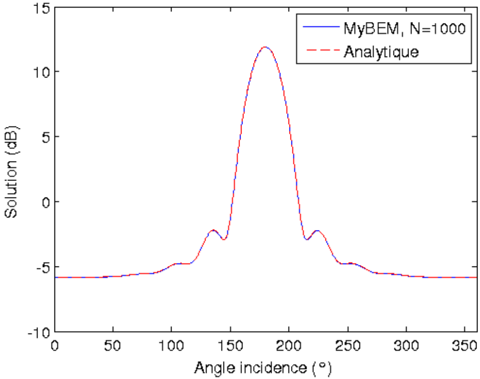
$$\begin{cases} [-H - ik\beta(\frac{Id}{2} - D^t)]\mu(\mathbf{x}) &= -\partial_n u_{pw}(\mathbf{x}) \qquad \forall \mathbf{x} \in \Gamma, \\ \lambda(\mathbf{x}) &= ik\beta\mu(\mathbf{x}). \end{cases}$$

- **Radiation at infinity**

RCS of the unit sphere at 1 000 dof (SCSD)

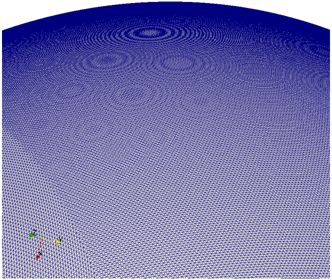
Helmholtz problem - Dirichlet Brackage Werner
Mesh generated with Matlab - 1 000 degrees of freedom
0.3 kHz - 5 iterations - 2 seconds

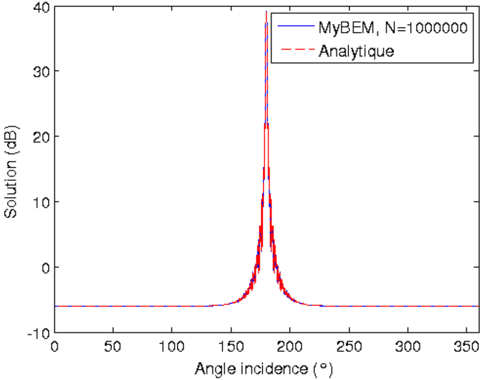




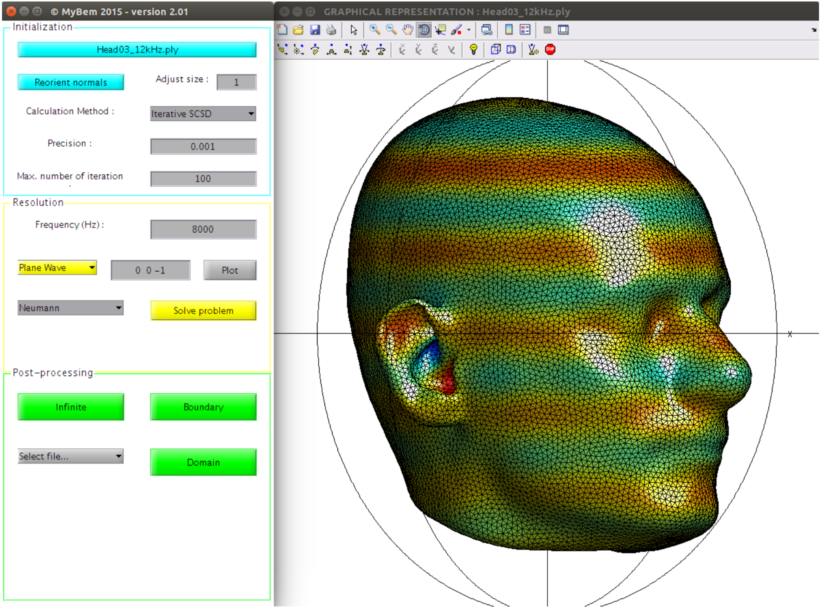
RCS of the unit sphere at 1 000 000 dof (SCSD)

Helmholtz problem - Dirichlet Brackage Werner
Mesh generated with Matlab - 1 000 000 degrees of freedom
10 kHz ($kr_{max} = 369$) - 12 iterations - 20 minutes





MyBEM - A Matlab fast BEM library



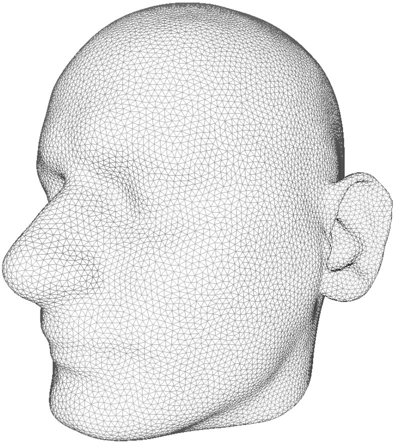
Main features

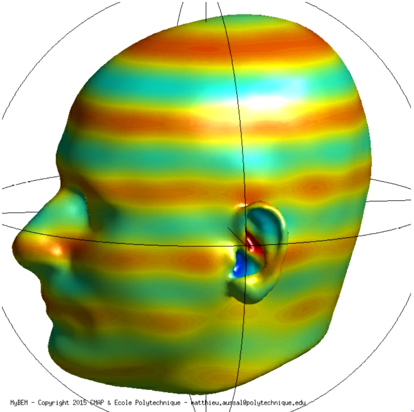
- Galerkin approximation with Finite Elements type P^1 and RT on triangles
- Semi-analytical for singular integrations in close interaction
- New fast method SCSD with NUFFT mexfile [1]
- Fast Multipole Method [1] and $\mathcal{H}$-Matrix for comparisons
- Infinite, volumic and surfacic radiation
- LU preconditioning and Brackage-Werner regularization
- Indirect jump formulations
- Object-Oriented Programming
- High-level script call or standalone GUI
- Parallel loops (*parfor*)
- Non regression tests

1. Mex-file from L. Greengard : www.cims.nyu.edu/cmcl

Ears modes of human head

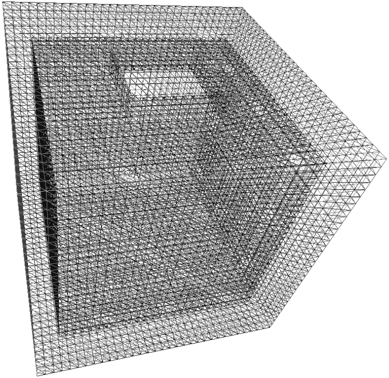
Helmholtz Problem - Neumann Brackage Werner
Mesh from SYMARE project - 20 000 degrees of freedom
8 kHz - 17 iterations - 54 seconds

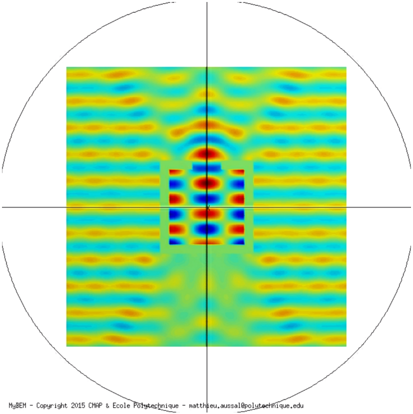




Resonance in a 3D cubic cavity

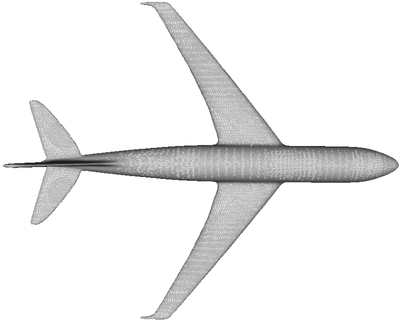
Helmholtz problem - Neumann Brackage Werner
Mesh generated with Matlab - 10 000 degrees of freedom
600 Hz - 56 iterations - 1 minute

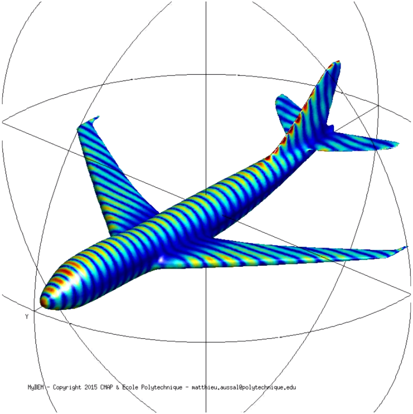




Surface current on Boeing 747

Maxwell problem - PEC CFIE
Mesh from Gamma project - 150 000 degrees of freedom
5 GHz - Vertical polarisation - 164 iterations - 16 minutes



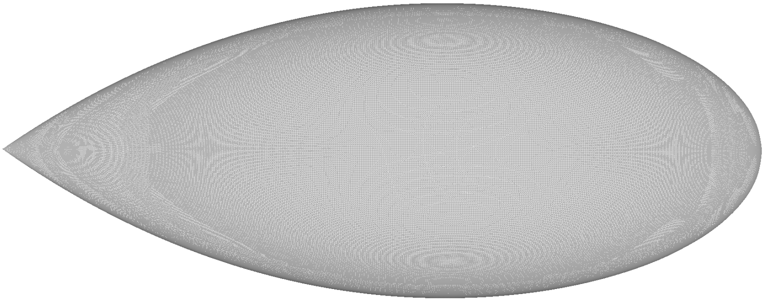


Surface current on NASA Almond

Maxwell problem - PEC CFIE

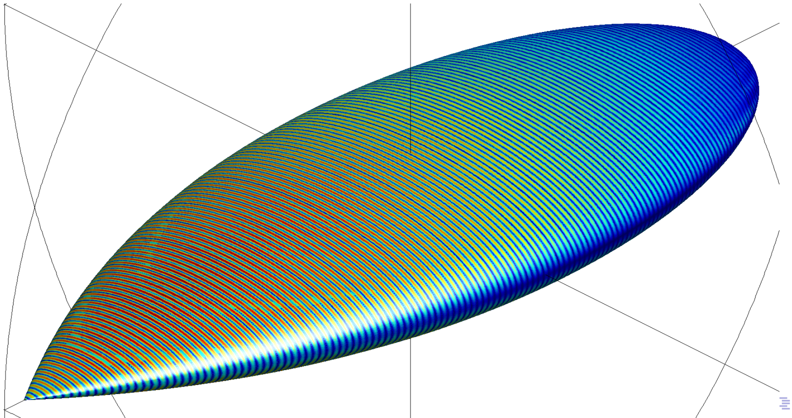
Mesh of an industrial - 1 000 000 degrees of freedom

8.5 GHz ($kr_{max} = 478$) - Vertical polarisation - 112 iterations - 2 hours



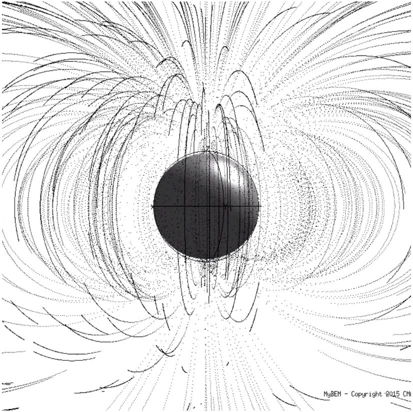
Surface current on NASA Almond

Maxwell problem - PEC CFIE
Mesh of an industrial - 1 000 000 degrees of freedom
8.5 GHz ($kr_{max} = 478$) - Vertical polarisation - 112 iterations - 2 hours



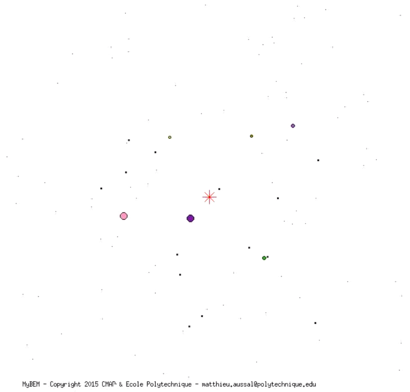
Earth's magnetic field

Laplace problem - Double layer potential
Mesh generated with Matlab - 10 000 degrees of freedom - 3 seconds



Gravitational interactions

Laplace problem - Double layer potential
10 000 degrees of freedom - Runge-Kutta 4 scheme (100 000 time step) - 10 minutes



Conclusion and future works

CONCLUSION :

- New SCSD fast convolution for many equation (Laplace, Helmholtz, Maxwell, Stokes),
- Creation of an object based Matlab library for fast BEM,
- Analytical validation up to 10^6 degrees of freedom.
- Calculation of numerical Head Filters *HRTF* up tu 20 kHz

FUTURE WORKS :

- More kernels...,
- Preconditioning,
- High Performance Computing (parallelization of NuFFT),
- Domain Decomposition Method and coupled FEM/BEM,
- Benchmarks and industrial applications,
- Finish paper(s)...

Thanks for your attention

- Alouges, F., Aussal, M. (2015) *The Sparse Cardinal Sine Decomposotion and its application for fast numerical convolution*. Numerical Algorithms, 1-22.
- Aussal, M. (2014) *Méthodes numériques pour la spatialisation sonore, de la simulation à la synthèse binaurale*. PhD thesis to be published.
- Greengard, L., & Rokhlin, V. (1987). *A fast algorithm for particle simulations*. Journal of computational physics, 73(2), 325-348.
- Greengard, L. (1988). *The rapid evaluation of potential fields in particle systems*. MIT press.
- Greengard, L., & Lee, J. Y. (2004). *Accelerating the nonuniform fast Fourier transform*. SIAM review, 46(3), 443-454.
- Lee, J. Y., & Greengard, L. (2005). T*he type 3 nonuniform FFT and its applications*. Journal of Computational Physics, 206(1), 1-5.