# Hierarchical Matrices for 3D Helmholtz problems in multi-patch IGA-BEM setting

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SIGMA 2023

Luminy, France - October 28 – November 1, 2024

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# Outline

- Boundary element methods and integral formulation (BIE)
- Isogeometric setting (IGA-BEM) and multi-patch geometries
- Hierarchical matrix formulation
- Low rank approximation of admissible blocks
- Some numerical results
- Current developments.

# Boundary Element Methods

- Boundary Element Methods are numerical methods to solve PDEs and can be seen in some cases as a valid alternative to classical domain methods as Finite Element or Finite Difference methods.
- The differential problem is reformulated into Boundary Integral Equations which require suitable and efficient *quadrature formulae* for their solution

- Advantages:
  - Reduced dimension of the computational domain: easier computation on complex geometries (no domain mesh generation!)
  - Simplicity to solve external problems: easier treatment of unbounded domains

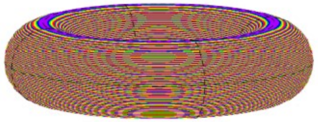
- Disadvantages:
  - Fundamental solution of the PDE problem is needed beforehand
  - Singular kernels (singular integrals)
  - Fully populated matrices

# 3D Acoustic model problem

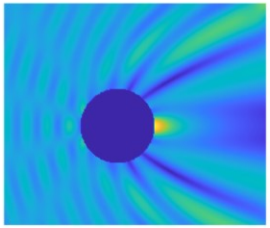
- We consider 3D acoustic problems described by the Helmholtz equation, with Neumann boundary conditions:

$$\begin{cases} \Delta u(\boldsymbol{x}) + \kappa^2 u(\boldsymbol{x}) = f(\boldsymbol{x}) & \text{in } \Omega \subset \mathbb{R}^3 \\ \dfrac{\partial u(\boldsymbol{x})}{\partial \boldsymbol{n}_x} = u_N(\boldsymbol{x}) & \text{on } \Gamma \end{cases}$$

Sound vibration



Sound scattering



Acoustic parameters: $\omega$ angular frequency, $c$ speed of the wave
Frequency–domain: $\kappa = \omega/c$ , wave number, $\lambda = 2\pi/\kappa$, wave length

- For exterior problems, the acoustic domain Ω is infinite. ⇨ the unknown function u at infinity must satisfy the Sommerfeld radiation condition:

$$\lim_{|\boldsymbol{x}|\to\infty} |\boldsymbol{x}| \left( \nabla u(\boldsymbol{x}) \cdot \frac{\boldsymbol{x}}{|\boldsymbol{x}|} - \boldsymbol{i}\kappa u(\boldsymbol{x}) \right) = 0$$

- any radiated or scattered acoustic wave has to converge towards zero when the radius tends to infinity.

# Boundary integral equation

- Setting null the external body forces (f=0), we consider a direct integral representation formula for u.

$$u(\boldsymbol{x}) = \int_{\Gamma} \frac{\partial}{\partial \boldsymbol{n}_y} \mathcal{G}_\kappa(\boldsymbol{x},\boldsymbol{y})\, u(\boldsymbol{y})\, d\gamma_y - \int_{\Gamma} \mathcal{G}_\kappa(\boldsymbol{x},\boldsymbol{y}) \frac{\partial u}{\partial \boldsymbol{n}}(\boldsymbol{y})\, d\gamma_y \qquad \boldsymbol{x} \in \Omega \setminus \Gamma$$

double layer potential single layer potential

- The integral representation formula is strictly connected to the definition of the fundamental solution $\mathcal{G}$ and its normal derivative. Setting $r = \|\boldsymbol{x} - \boldsymbol{y}\|$

$$\mathcal{G}_\kappa(\boldsymbol{x},\boldsymbol{y}) := \frac{e^{i\kappa r}}{4\pi r}, \qquad \frac{\partial}{\partial \boldsymbol{n}_y} \mathcal{G}_\kappa(\boldsymbol{x},\boldsymbol{y}) = \frac{e^{i\kappa r}}{4\pi r}\left(-\frac{1}{r} + i\kappa\right)\frac{\partial r}{\partial \boldsymbol{n}_y}, \qquad \frac{\partial r}{\partial \boldsymbol{n}_y} = -\frac{\boldsymbol{r}\cdot\boldsymbol{n}_y}{r}$$

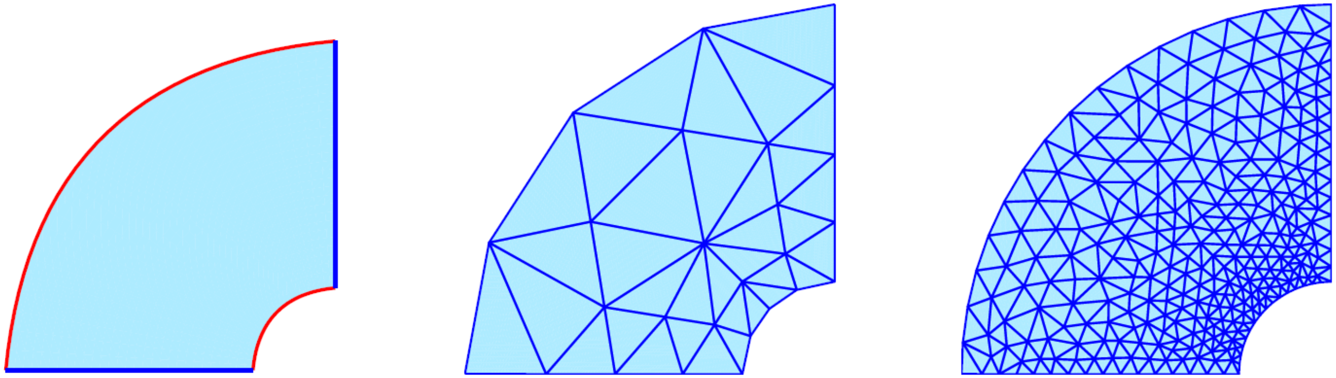
- applying the trace operator we get the Conventional Boundary Integral Equation CBIE:

$$\int_{\Gamma} \mathcal{G}_\kappa(\boldsymbol{x},\boldsymbol{y})\, u_N(\boldsymbol{y})\, d\gamma_y = \frac{1}{2}\varphi(\boldsymbol{x}) + \int_{\Gamma} \frac{\partial}{\partial \boldsymbol{n}_y} \mathcal{G}_\kappa(\boldsymbol{x},\boldsymbol{y})\, \varphi(\boldsymbol{y})\, d\gamma_y \qquad \boldsymbol{x} \in \Gamma, \varphi := u_{|\Gamma}$$

- The radiation condition is included in the integral formulation

# Isogeometric analysis

- Standard approach: CAD geometry is replaced by FEM geometry (mesh)
- The mesh is an approximate geometry: many problems (thin shell structures, boundary layer in fluids) are very sensitive to geometric imperfections



- Isoparametric approach:

  *the solution space for dependent variables is represented in terms of the same functions which represent the geometry"* **[Cottrell, Hughes, Bazilevs; CMAME 2005]**

- The goal was to develop an analysis framework based on functions capable of exactly representing geometry
- IDEA: exploit CAD techniques and representations

# IgA-BEM

- Isogeometric Analysis has led a new interest also in possible applications in the BEM context (previously only considered in FEM)
- The possibility of describing accurately both the geometry and the solution has been studied also in the BEM approach (IGA-BEM)

**[Politis, Ginnis, Kaklis et al, 2009], [ Simpson, Scott, et al., 2012, 2014]**

- The use of IgA in the BEM context can radically improve the corresponding numerical schemes because of the additional smoothness of NURBS and B-splines in comparison to $C^0$-continuous piecewise polynomials
- Representation of 3D objects only needs to be encompassed by their *boundary surfaces* based on Boundary representation (B-rep).
- To approximate accurately the integrals coming from the IGA-BEM formulation we have constructed new appropriate quadrature schemes, tailored on B-splines.

**[Aimi, Calabrò, Falini, S., Sestini,** CMAME **2020]**

**[Falini, Giannelli, Kanduc, S., Sestini,** Int.J. Num.Met. Eng. **2019]**

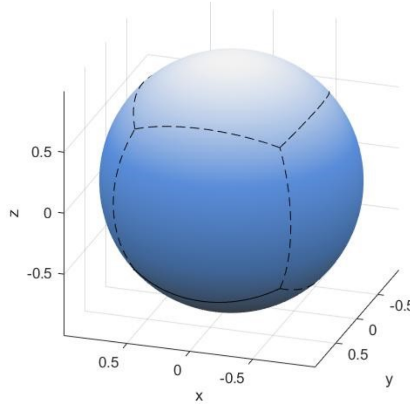
# IgA multi-patch boundary representation

- The boundary $\Gamma$ is a union of $M$ patches $\Gamma = \bigcup_{\ell=1}^{M} \Gamma^{(\ell)}, \; \ell \neq k \;\; \Rightarrow \begin{cases} \Gamma^{(\ell)} \cap \Gamma^{(k)} = \emptyset \\ \partial\Gamma^{(\ell)} \cap \partial\Gamma^{(k)} = \text{common edge, corner point or empty set} \end{cases}$

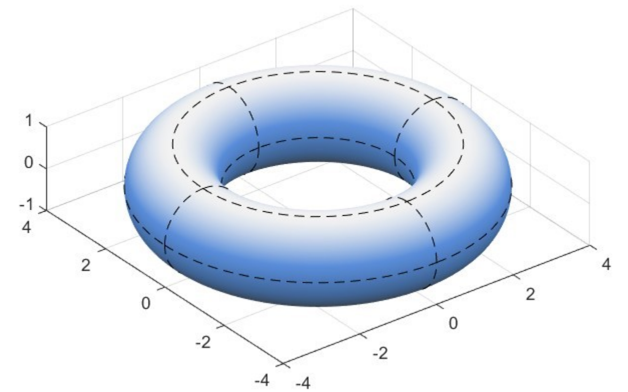
$\bar{\Gamma}^{(\ell)} = Image(\mathbf{F}^{(\ell)}), \quad \mathbf{F}^{(\ell)} : [0,1]^2 \to \bar{\Gamma}^{(\ell)}$ geometric mapping

$$\mathbf{F}^{(\ell)}(\mathbf{t}) = \frac{\sum_{\mathbf{i}\in\mathcal{I}_g^{(\ell)}} w_{\mathbf{i}}^{(\ell)} \mathbf{Q}_{\mathbf{i}}^{(\ell)} \hat{B}_{\mathbf{i},\mathbf{d}_g}^{(\ell)}(\mathbf{t})}{\sum_{\mathbf{i}\in\mathcal{I}_g^{(\ell)}} w_{\mathbf{i}}^{(\ell)} \hat{B}_{\mathbf{i},\mathbf{d}_g}^{(\ell)}(\mathbf{t})}, \quad \mathbf{t} \in [0,1]^2, \quad \text{NURBS representation}$$

$\left\{ \hat{B}_{\mathbf{i},\mathbf{d}_g}^{(\ell)}, \mathbf{i} \in \mathcal{I}_g^{(\ell)} \right\} =$ tensor product B-spline basis of bi-degree $\mathbf{d}_g$ (clamped knot vectors)



6–patch quartic NURBS



16–patch quadratic NURBS

# Discretization

$S_{\mathbf{d},h} := \text{span}\left\{B^{(\ell)}_{\mathbf{j},\mathbf{d}} : j \in \mathcal{J}^{(\ell)}, 1 \le \ell \le M\right\}$ IgA spline discretization space

$B^{(\ell)}_{\mathbf{j},\mathbf{d}}(\mathbf{x}) = \hat{B}^{(\ell)}_{\mathbf{j},\mathbf{d}} \circ \mathbf{F}^{(\ell)^{-1}}(\mathbf{x}) \qquad \mathbf{x} \in \Gamma^{(\ell)}$ lifted bases

- Free knot vector selection on each patch ⇨ inter-patch adaptivity

$$N_{DOF} = \sum_{\ell=1}^{M} \left|\mathcal{J}^{(\ell)}\right| \qquad \varphi := u_{|_\Gamma}$$

$$\varphi_h \approx \varphi, \qquad \varphi_h(\boldsymbol{x}) := \sum_{\ell=1}^{M} \sum_{\boldsymbol{j} \in \mathcal{J}^{(\ell)}} \alpha_{\boldsymbol{j}}^{(\ell)} B^{(\ell)}_{\boldsymbol{j},\boldsymbol{d}}(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma$$

# The linear system

- Domain is parametrized with M patches:

$$\boldsymbol{F}^{(\ell)} = [0,1]^2 \rightarrow \mathbb{R}^3$$ *geometry mapping*

$$\boldsymbol{x}^{(\ell)} = \boldsymbol{F}^{(\ell)}(\boldsymbol{s}), \quad \boldsymbol{s} = (s_1, s_2)$$ *collocation point*

$$\boldsymbol{y}^{(\ell)} = \boldsymbol{F}^{(\ell)}(\boldsymbol{t}), \quad \boldsymbol{t} = (t_1, t_2)$$ *integration point*

$$J^{(\ell)}(\boldsymbol{t}) := \left\| \frac{\partial \boldsymbol{F}^{(\ell)}}{\partial t_1} \times \frac{\partial \boldsymbol{F}^{(\ell)}}{\partial t_2} \right\|$$ *surface area element*

$$\varphi_h(\boldsymbol{x}) := \sum_{\ell=1}^{M} \sum_{\boldsymbol{j} \in \mathcal{J}} \alpha_{\boldsymbol{j}}^{(\ell)} (\hat{B}_j \circ \boldsymbol{F}^{(\ell)-1})(\boldsymbol{x}) \Rightarrow \boxed{\mathbb{A}\,\boldsymbol{\alpha} = \boldsymbol{\beta}}$$

A: M x M block matrix

- The matrix entries are of type

$$\mathbb{A}_{ij}^{(\ell,k)} = \int_{[0,1]^2} \frac{\partial}{\partial \boldsymbol{n}_y} \mathcal{G}_\kappa(\boldsymbol{s}_i^{(\ell)}, \boldsymbol{F}^{(k)}(\boldsymbol{t}))\, \hat{B}_{j,\boldsymbol{d}}^{(k)}(\boldsymbol{t})\, J^{(k)}(\boldsymbol{t})dt + \frac{1}{2} \hat{B}_{j,\boldsymbol{d}}^{(k)}(\boldsymbol{s}_i^{(\ell)})$$

- The right hand side entries:

$$\boldsymbol{\beta}_{ij}^{(\ell)} = \sum_{k=1}^{M} \int_{[0,1]^2} \mathcal{G}_\kappa(\boldsymbol{s}_i^{(\ell)}, \boldsymbol{F}^{(k)}(\boldsymbol{t}))\, u_N\left(F^{(k)}(\boldsymbol{t})\right) J^{(k)}(\boldsymbol{t})dt$$

# IGA-BEM pipeline

- Discretization of the surface $\Gamma$
  - Multi-patch parametric representation by tensor product splines (B-splines or NURBS)
  - patch topology conforming meshes ($C^{-1}$ or $C^{0}$)
- Discretization of the BIE (N= #DoF)
  - Collocation method

**[Degli Esposti, Falini, Kanduc, S, Sestini,** CAMWA, **2024]**

- Construction and solution of the linear system
  - regular, singular and near-singular quadrature based on the spline product formula and quasi-interpolation. Quadrature always developed on B-spline supports
  - non-symmetric and fully-populated matrix
- Representation formula to evaluate quantities in the exterior domain
  - cost reduced to a matrix/vector multiplication

**Limitations of standard IGA-BEM**

- to improve accuracy we have to use finer meshes ⟹ high costs in terms of memory and CPU time
- limited geometric complexity and frequency range (due to the size of the final linear system)

# Fast solvers for IGA-BEM

- Need of an efficient approximate method to evaluate the matrix entries, that allows to define a fast solver
- Hierarchical matrices, or $\mathcal{H}$-matrices, have been introduced in the BEM setting by Hackbusch as a technique to produce sparse-data representation of dense matrices, which carries improvements in terms of storage and computational cost with respect to the usual matrix operations

**[Hackbusch,** *Computing*, **1993]**

⟹ $\mathcal{H}$-matrices:

- representation of the BEM matrix with an $\mathcal{H}$-matrix structure
- reduction of the memory cost: low-rank approximation of large blocks
- optimization of the CPU times by using the $\mathcal{H}$-matrix/vector product

- Pure algebraic approach
- Alternative approach to Fast Multipole Method **[Greengard & Rokhlin,** *J. Comp. Phys*, **1987]**
  - For the Helmholtz problem a diagonal FFM has been developed **[Rokhlin,** *Appl. Comp. Harm*, **1993]**
  - Different formulations for low and high frequencies

# Hierarchical clustering of DoF

- $\mathcal{H}$-matrix representation of the system matrix

- Preliminary clustering of row and columns based on the geometry (physical distance):
- definition of two Binary Trees, $\mathcal{T}_1^{(\ell)}$ and $\mathcal{T}_2^{(\ell)}$ whose depth is determined by a parameter $n\_leaf$
  - rows ↔ collocation points =reference points
  - columns ↔ basis support ↔ basis referred points=reference points

  $\mathcal{T}_i^{(\ell)}$ i=1,2

    - initial box : bounding box of the patch reference points
    - dyadic subdivision into balanced small boxes
    - stop subdivision when a minimum number of points per box is reached

  - Remark: negligible cost

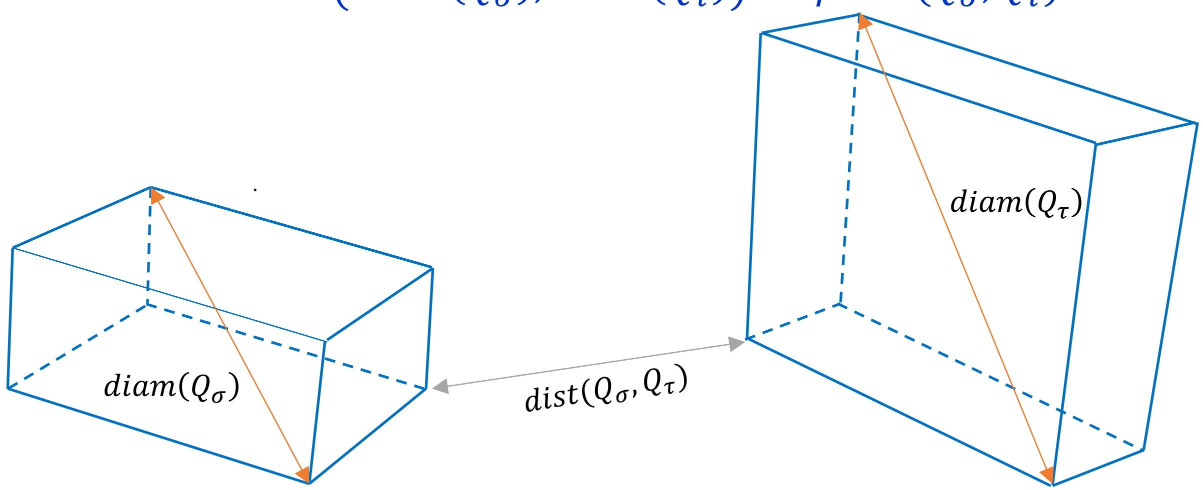
- In total we have to construct 2M cluster trees
- The interaction of any two of these cluster trees form a block cluster tree

# Cluster tree algorithm

- Subdivision of the IgA-BEM matrix (Block Cluster Tree): definition of sub-matrices, again Euclidean distance based
- We have to define a criterion the determine whether a block has a suitable *low-rank approximation:*
  - The block should be as large as possible
  - Computing explicitly the rank of the blocks is too expensive

- A block associated to the cluster indices $(\sigma, \tau)$, with $\sigma \in \mathcal{T}_1^{(\ell)}$ and $\tau \in \mathcal{T}_2^{(\ell)}$ is admissible if

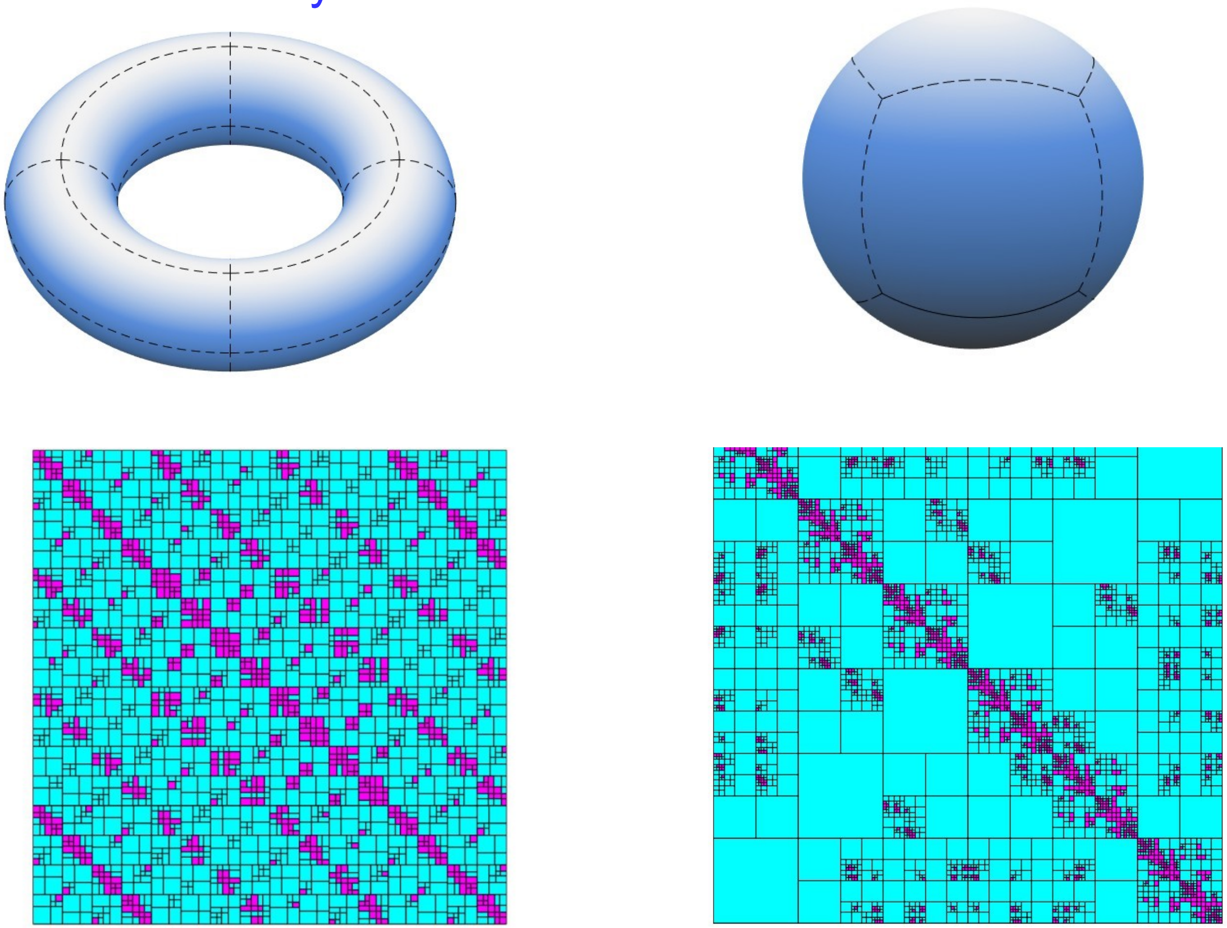
$$min\big(diam(Q_\sigma), diam(Q_\tau)\big) \leq \eta\ dist(Q_\sigma, Q_\tau)$$




- 3 kinds of blocks: leaves (full- or low-rank matrices) and non-leaves (H-matrices)

# Structure of the H-matrix representation

- The structure of the H-matrix representation of the BEM matrix depends only on the geometry and the admissibility condition



# Low-rank representation

- The reduction of the memory storage of the IgA-BEM is related to the possibility of writing a *low-rank representation* or degenerate expansion of the fundamental solution $\mathcal{G}_\kappa$ , i.e.

$$\mathcal{G}_\kappa(\boldsymbol{x},\boldsymbol{y}) = \sum_{k=0}^{r} \varphi_k(\boldsymbol{x})\,\psi_k(\boldsymbol{y}) \quad + R_r(\boldsymbol{x},\boldsymbol{y}),$$

where $R_r(\boldsymbol{x},\boldsymbol{y})$ is the residuum and tends to zero for $r \to \infty$ **[Bebendorf, 2008]**

- For the Helmholtz kernel it can be proved that if the admissibility condition is satisfied, the residuum can be bounded from above.

$$|R_r(\boldsymbol{x},\boldsymbol{y})| \le \frac{c_1}{c_2\,\|\boldsymbol{x}-\boldsymbol{y}\|^m}\,\frac{(\sqrt{3}\,\gamma\,\eta)^r}{1-\sqrt{3}\,\gamma\,\eta} \qquad \gamma = \frac{1+\kappa\|\boldsymbol{x}-\boldsymbol{y}\|}{c_2}$$

- When $\kappa\, diam(\Gamma)$ is small $\longrightarrow \gamma \cong \frac{1}{c_2}$. Existence of a a pre-asymptotic regime for which the low-rank representation is efficient

**[Chaillat, Desiderio, Ciarlet,** J. Comp. Phys, **2017]**

# Computation of low-rank representation

- Given an admissible block $\mathbb{A}_{\sigma,\tau}^{(\ell,\bar{\ell})} \in C^{m\times n}$ we approximate it as the product of matrices of small rank

$$\mathbb{A}_{\sigma,\tau}^{(\ell,\bar{\ell})} = \mathbb{S}_r + \mathbb{R}_r$$

with $\mathbb{S}_r = \mathbb{U}\,\mathbb{V}^H$ where $\mathbb{U}$ and $\mathbb{V}$ are both $N \times r$ matrices and the residuum $\mathbb{R}_r$ is such that

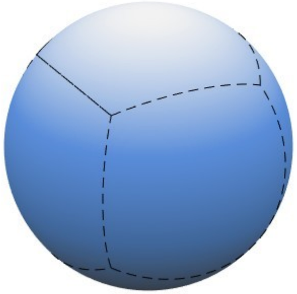
$$\|\mathbb{R}_r\|_F = \left\|\mathbb{A}_{\sigma,\tau}^{(\ell,\bar{\ell})} - \mathbb{S}_r\right\|_F = \left\|\mathbb{A}_{\sigma,\tau}^{(\ell,\bar{\ell})} - \mathbb{U}\,\mathbb{V}^H\right\|_F \le \varepsilon \left\|\mathbb{A}_{\sigma,\tau}^{(\ell,\bar{\ell})}\right\|_F$$

- $r \ll N$ we obtain a drastic reduction of the memory requirement for the storage of $\mathbb{A}_{\sigma,\tau}^{(\ell,\bar{\ell})} \Longrightarrow$ how to compute $\mathbb{U}$ and $\mathbb{V}$ ?
- The best low-rank approximation is given by the truncated SVD. Its computation is too expensive as it requires in input all the entries of the matrix.
- Adaptive Cross Approximation (ACA) produces quasi-optimal low-rank approximations without requiring the assembly of the whole matrix
  - Every matrix of rank r is the sum of r matrices of rank 1
  - Greedy algorithm iteratively adding suitable 1-rank matrices to the current approximation
  - Requires only few entries of the matrix

**[Babendorf,Rjasanow,** Computing, **2003]**

# Example 1: rigid scattering on a sphere

- $\Omega$ =domain exterior to a sphere centered at the origin and with unit radius



- Acoustic pressure produced by a wave vector,

  source at infinity $$p_{inc} = e^{i\kappa(\boldsymbol{v}\cdot\boldsymbol{x})} \qquad \boldsymbol{v} = (1,0,0)$$

- The incident wave hitting the rigid body produces a scattered pressure

$$\begin{cases} \Delta p_s + \kappa^2 p_s = 0 & \text{in } \Omega \\ \partial_n p_s = -\partial_n p_{inc} & \text{on } \Gamma \\ \partial_r p_s - i\kappa p_s = o(1/r) & \text{Sommerfeld r.c.} \end{cases}$$

$$p_{tot} = p_{inc} + p_s$$

$$p_s(\boldsymbol{x}) = \sum_{n=0}^{\infty} \frac{i^n (2n+1) j'(\kappa R)}{h_n'(\kappa R)} P_n(cos(\theta)) h_n(\kappa R) \qquad n = 10$$

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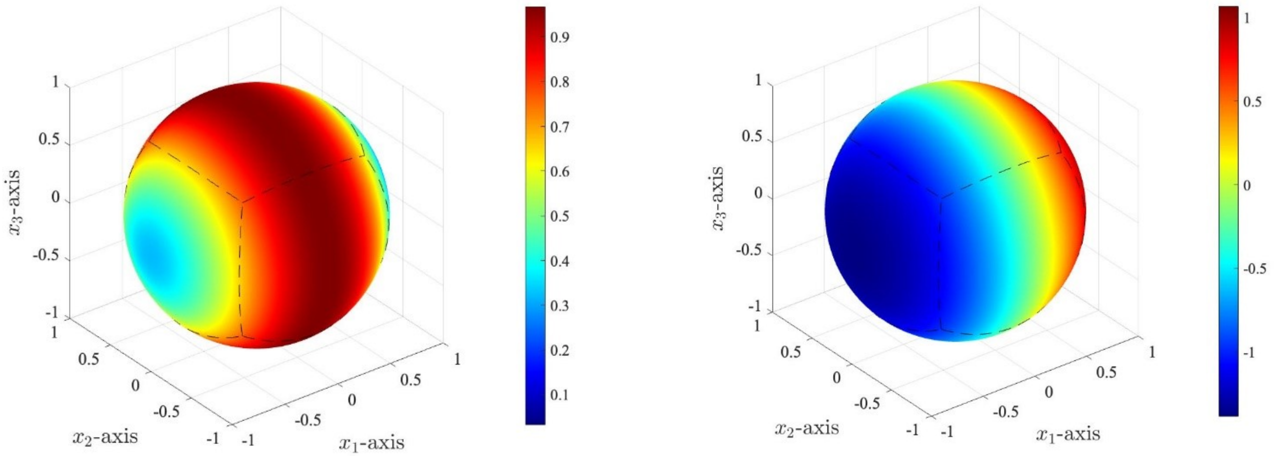
# Rigid scattering on a sphere (low- freq)

$\kappa = 1$
$n_{leaf} = 25$
$\eta = 3$
$\varepsilon_{ACA} = 1.0e-08$
$\varepsilon_{GMRES} = 1.0e-08$

$\kappa \, diam(\Gamma) < 2\pi$

*Low-freq.*

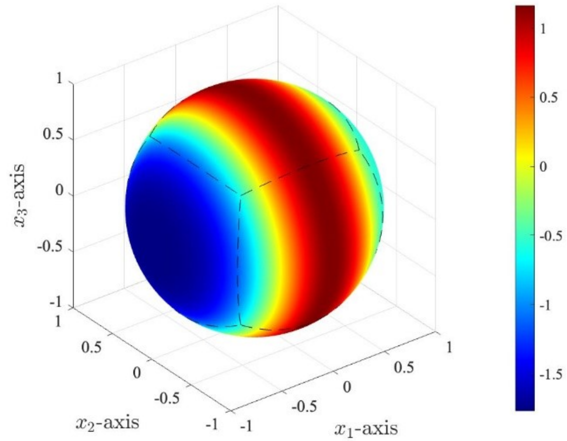


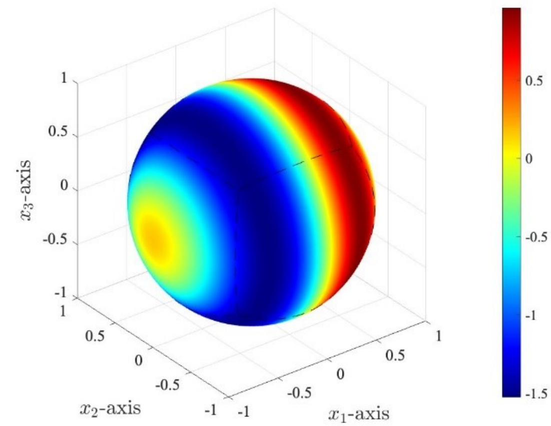

| $N_{DOF}$ | mem (%) | Err |
|---|---|---|
| 864 | 00.73 | 7.43e-05 |
| 2904 | 46.71 | 8.87e-06 |
| 10584 | 78.05 | 1.09e-06 |
| 40344 | 91.99 | 1.45e-07 |
| 157464 | 97.27 | 1.20e-08 |

- An iterative solver (variant of GMRES) for $\mathcal{H}$-matrices is considered.

# Rigid scattering on a sphere (high- freq)

$\kappa = 3$
$n_{leaf} = 25$
$\eta = 3$
$\varepsilon_{ACA} = 1.0e-08$
$\varepsilon_{GMRES} = 1.0e-08$




$\kappa \, diam(\Gamma) > 2\pi$

*High -freq.*

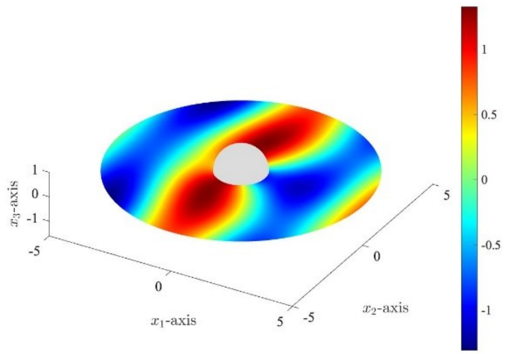
| $N_{DOF}$ | mem (%) | Err |
|---|---|---|
| 864 | -9.29 | 8.03e-04 |
| 2904 | 43.01 | 8.78e-05 |
| 10584 | 77.13 | 1.06e-05 |
| 40344 | 91.69 | 1.11e-06 |
| 157464 | 95.27 | 1.54e-07 |

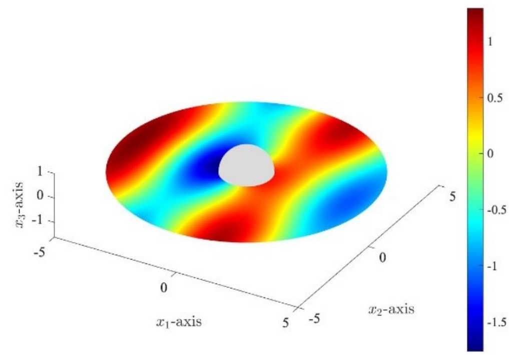
→ Very good accuracy for engineering applications

# Rigid scattering on a sphere

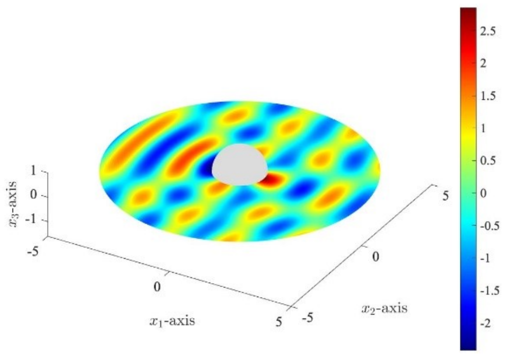
- Reconstructed total field, $N_{dof}$=2904

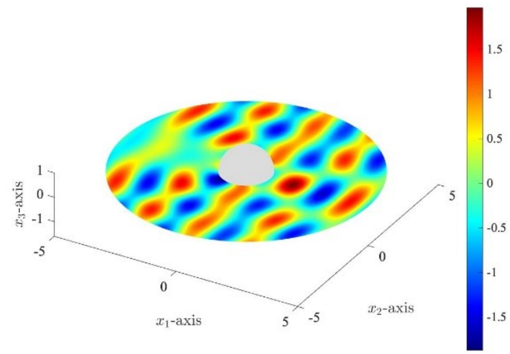
$\kappa = 1$




$\kappa = 3$




real part

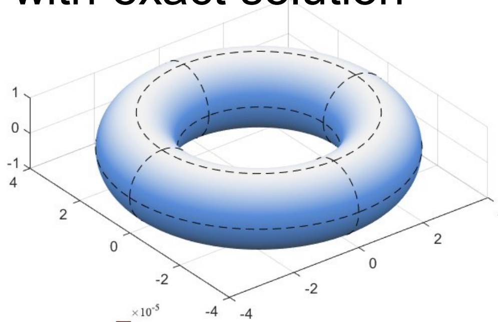
imaginary part

# Example 2: acoustic problem (interior)

- Helmholtz problem interior to a torus, Neumann conditions with exact solution

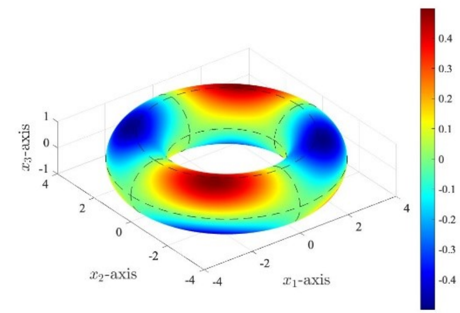
$$\phi(\boldsymbol{x}) = \sin\left(\frac{\kappa x}{\sqrt{3}}\right)\sin\left(\frac{\kappa y}{\sqrt{3}}\right)\sin\left(\frac{\kappa z}{\sqrt{3}}\right), \quad \boldsymbol{x} \in \Gamma$$

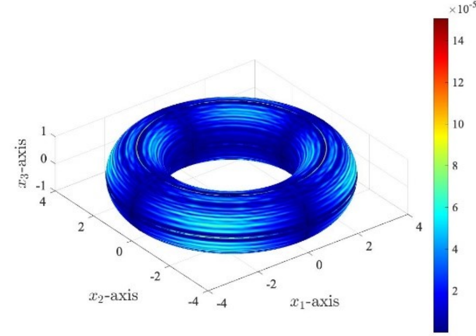
**[Simpson et al. 2014]**



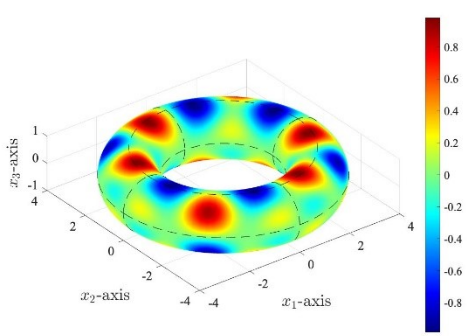
- Multi-patch geometry, $C^{-1}$ joints

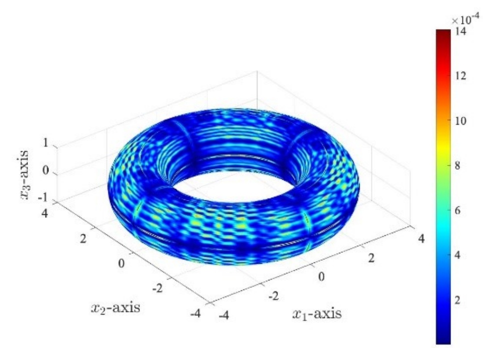
$\kappa = 1$




$\kappa = 3$

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# Example 2: acoustic problem (interior)

$\kappa = 1$
$\varepsilon_{GMRES} = 1.0e-08$

| $N_{DOF}$ | mem ($\mathbb{A}$) | mem ($\beta$) | Err |
|---|---|---|---|
| 864 | −25.84% | −21.01% | 1.16e − 03 |
| 2904 | 30.71% | 32.81% | 1.10e − 04 |
| 10584 | 71.12% | 73.77% | 1.28e − 05 |
| 40344 | 90.02% | 91.19% | 1.57e − 06 |
| 157464 | 96.81% | 97.32% | 1.97e − 07 |

$\kappa = 3$
$\varepsilon_{GMRES} = 1.0e-08$

| $N_{DOF}$ | mem ($\mathbb{A}$) | mem ($\beta$) | Err |
|---|---|---|---|
| 864 | −41.05% | −37.03% | 1.15e − 02 |
| 2904 | 21.63% | 19.52% | 9.91e − 04 |
| 10584 | 67.92% | 69.06% | 1.07e − 04 |
| 40344 | 89.11% | 89.81% | 1.29e − 05 |
| 157464 | 96.57% | 97.11% | 1.65e − 06 |

# Conclusion

- An efficient and accurate numerical strategy to solve 3D Helmholtz problems using isogeometric BEMs on conformal multi-patch smooth geometries and spline discretization spaces by hierarchical matrices.
- It gives good results achieving optimal approximation order with a drastic reduction of the computational cost, in terms of both time and memory requirement.

- Future work:
  - Helmholtz equation for different $\kappa$ (special treatment of highly oscillating singular integrals coming from IgA-BEM)
  - HPC implementation
  - Time-domain problems

**Thank you for your attention**

# SMART 2025

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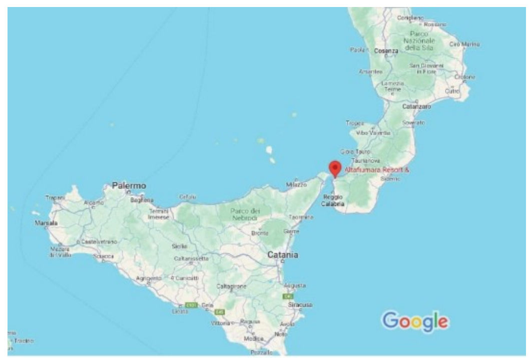


**SAVE THE DATE !!!**

**Confirmed invited speakers**: Keenan Crane, Annie Cuyt, Stefano De Marchi, Carlotta Giannelli, Marjeta Knez, Deepesh Toshniwal, Jungho Yoon

www.smart2025.unirc.it