SUPERCALCOLO, DATA SCIENCE E AI: DALL'INNOVAZIONE AL TRASFERIMENTO TECNOLOGICO FIRENZE
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OS Osservatorio sulle tendenze e le applicazioni del Supercalcolo

ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

UNIVERSITÀ DEGLI STUDI FIRENZE

Advances in the efficiency of high-order schemes for integral equations in 2D and 3D

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Multi-patch collocation IgA-BEM for Helmholtz problems in 3D

Solutions to the **3D Helmholtz equation** $\Delta u + \kappa^2 u = 0$ in the interior/exterior of a sufficiently regular domain can be found by solving the boundary integral equation

$$\int_\Gamma \mathcal{G}(\mathbf{x},\mathbf{y})\frac{\partial u}{\partial \mathbf{n}}(\mathbf{y})\,d\Gamma_\mathbf{y} = \frac{1}{2}u(\mathbf{x}) + \int_\Gamma \frac{\partial \mathcal{G}}{\partial \mathbf{n_y}}(\mathbf{x},\mathbf{y})u(\mathbf{y})\,d\Gamma_\mathbf{y}, \quad \mathcal{G}(\mathbf{x},\mathbf{y}) = \frac{e^{i\kappa\|\mathbf{x}-\mathbf{y}\|}}{4\pi\,\|\mathbf{x}-\mathbf{y}\|}.$$

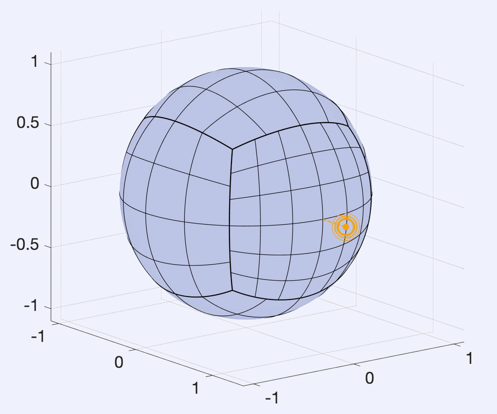
Collocation Boundary Element Method (BEM): the solution is approximated as a linear combination of N basis functions B_j, and the integral equation is imposed at N boundary points $\boldsymbol{x}_i$. This leads to a dense non-symmetric linear system.

Isogeometric Analysis (IgA) paradigm: the multi-patch boundary Γ and the basis functions B_i are both represented using bivariate B-splines (or NURBS) of degree d.

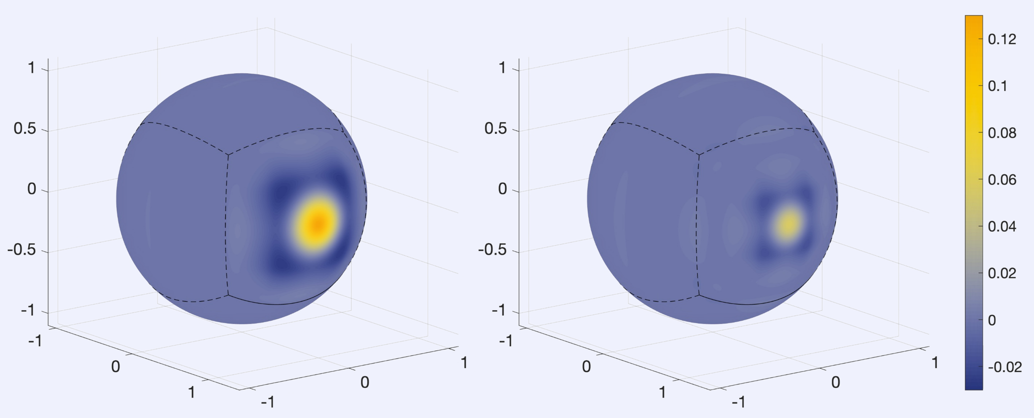
Function-by-function assembly and non-conforming C^0 spline spaces

Assembly of the linear system requires evaluation of the surface integrals for all collocation nodes $\boldsymbol{x}_i$ and basis functions B_j. Some integrals are singular or nearly-singular. In [1], a novel **singularity subtraction technique** based on series expansion around $\boldsymbol{x}_i$ is used. The subtracted part can be integrated in closed form. The residual is approximated by splines using **quasi-interpolation** in the parameter space of each patch. This new approach leads to efficient function-by-function assembly instead of element-by-element approach with e.g. Gaussian formulas.

Linear constraints based on spline knot removal conditions introduced in [1] allow the resolution of B-splines on each patch to be chosen almost independently, without losing global continuity of the solution. **Non-uniform refinement** is an efficient strategy for allocating degrees of freedom when u has localized features.



Non-conforming refinement near acoustic source in orange.

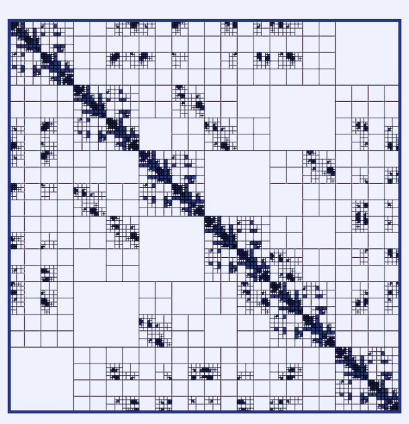


On-surface error before and after refinement for rigid scattering problem with spherical acoustic source, $d = 2$ and $\kappa = 2$.

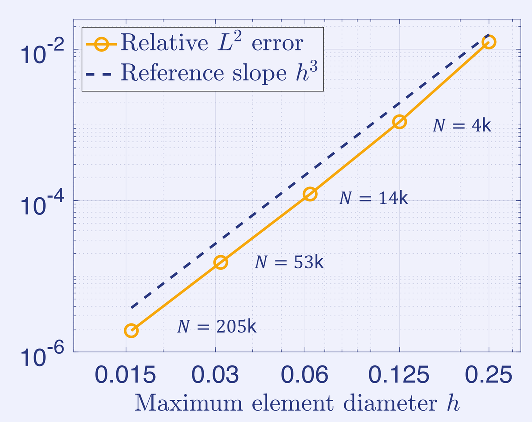
Hierarchical matrices compression

BEM tradeoff: dimension reduction from 3D to 2D, but the system matrix A is full. However, any sub-block of A that satisfies a suitable distance condition between its own collocation nodes and spline supports admits accurate low-rank approximation. An **H-matrix** is built by recursively subdividing A until the distance condition is satisfied, or a minimum size is reached. **Adaptive cross approximation** (ACA) allows low-rank approximations to be found without precomputing the whole sub-blocks.

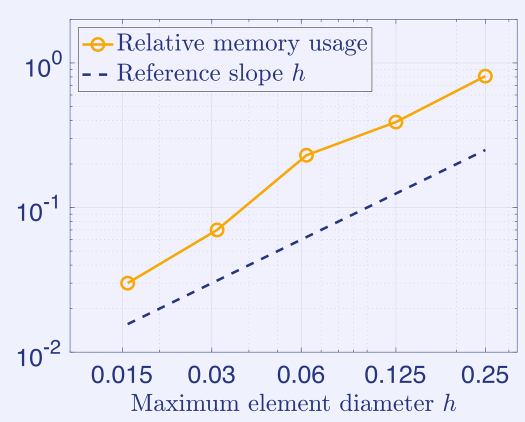
In [2], the synergy between H-matrices and function-by-function IgA-BEM assembly is shown, leading to **large improvements in memory usage and computation times**.



H-matrix structure on a sphere. Only dark blocks have full rank.



Errors for rigid scattering of a plane wave on a torus, $d = 2$.



Compression ratio of H-matrix for rigid scattering on a torus.

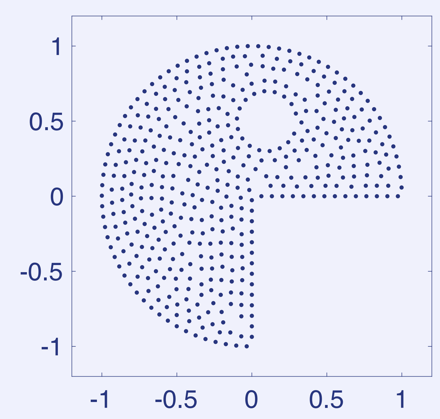
Decoupled Nyström method for Fredholm integral equations in 2D

Replacing the integral in a **Fredholm equation of the second kind** with a quadrature formula (w, Y) over a domain or manifold Ω leads to the semidiscretization

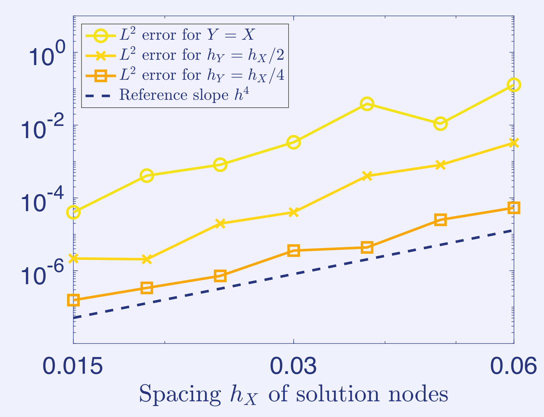
$$\lambda u(\mathbf{x}) - \int_\Omega k(\mathbf{x},\mathbf{y})\,u(\mathbf{y})\,d\mathbf{y} = f(\mathbf{x}) \quad\longrightarrow\quad \lambda u(\mathbf{x}) - \sum_{i=1}^{|Y|} w_i\,k(\mathbf{x},\mathbf{y}_i)\,u(\mathbf{y}_i) = f(\mathbf{x}). \qquad (1)$$

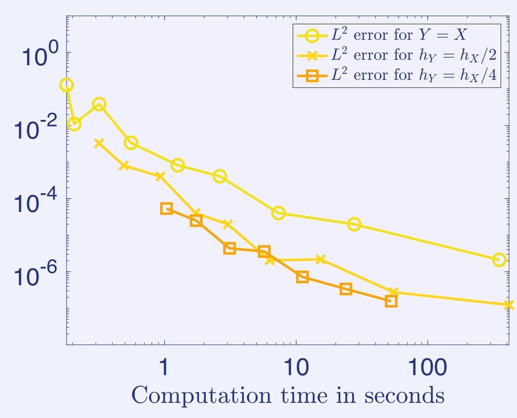
The classical Nyström method collocates (1) at Y. This is inefficient if the kernel k varies more rapidly than u: the $|Y|\times|Y|$ linear system is unnecessarily large. We introduce a **decoupled Nyström method** by collocating (1) at a different set X, potentially smaller than Y. The unknowns become the values of u at X. A linear reconstruction of values at Y from values at X must be introduced in the scheme. Arbitrarily high orders of convergence are still achieved under natural assumptions.

The decoupled scheme is **more efficient**, especially for rapidly-varying k. Numerical experiments so far focus on smooth kernels and 2D domains, and are performed in a **meshless setting**, with X and Y being sets of scattered nodes over Ω with average nodal spacings h_X and h_Y generated by the library NodeGenLib [3]. Reconstructions are done locally using polyharmonic radial basis functions, and quadrature relies on the novel **high-order moment-free approach** described in [4].



Quadrature nodes Y on a disk sector with $h_Y = 0.07$.

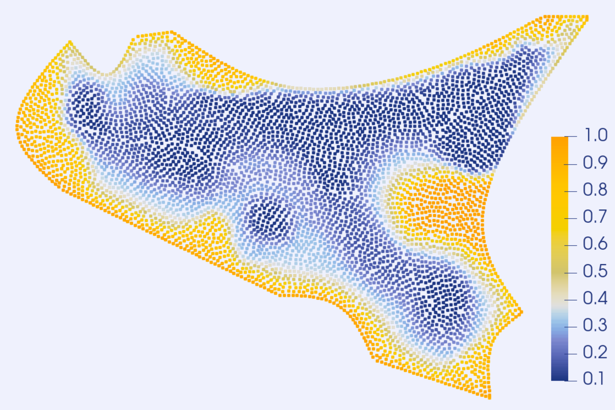




Errors on disk sector with $\lambda = 1$, Gaussian kernel with $\sigma = 0.1$, rhs f equal to Franke's function. Reconstruction and quadrature have order 4.

Integral equations with smooth kernels are used in biology to model **non-local interactions** such as long-range diffusion and excitatory/inhibitory signals. For example, the following equation describes the equilibrium density of a population subject to non-local diffusion and logistic growth with capacity factor $a(\boldsymbol{x})$.

$$\int_\Omega k(\mathbf{x},\mathbf{y})\big(u(\mathbf{y}) - u(\mathbf{x})\big)\,d\mathbf{y} + u(\mathbf{x})\big(a(\mathbf{x}) - u(\mathbf{x})\big) = 0.$$



Equilibrium population over island with $a(\boldsymbol{x})$ chosen as a function of elevation.

Ongoing and future work

The research group is currently focusing on the extension of efficient IgA-BEM techniques to the solution of **wave propagation problems** in 3D unbounded domains, including dissipative effects, using convolution quadrature in time and collocation in space. Matrix blocks can be assembled in parallel, and this enables the use of **High-Performance Computing** (HPC). Decoupled Nyström methods for problems in 3D and with singular kernels are also being investigated.

References

[1] Degli Esposti, B., Falini, A., Kanduč, T., Sampoli, M. L., & Sestini, A. (2023). *IgA-BEM for 3D Helmholtz problems using conforming and non-conforming multi-patch discretizations and B-spline tailored numerical integration*. Computers & Mathematics with Applications.

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[3] Degli Esposti, B. NodeGenLib. https://github.com/BrunoDegliEsposti/NodeGenLib/

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