Bempp - What's next?

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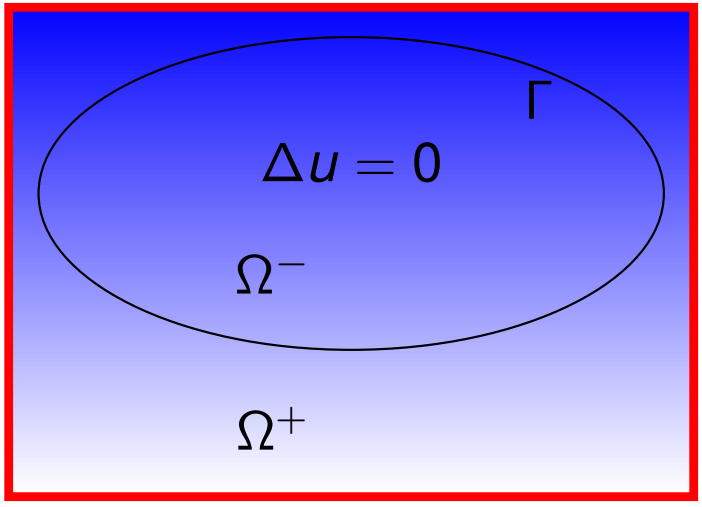
A primer on boundary integral equations



Green's fct. for Laplace equation

$$g(x,y) = \frac{1}{4\pi|x-y|}$$

For Helmholtz equation:

$$g(x,y) = \frac{e^{ik|x-y|}}{4\pi|x-y|}$$

Representation formula

$$u(x) = \int_\Gamma g(x,y)\, \gamma_1 u(y)\, ds(y) - \int_\Gamma \frac{\partial g(x,y)}{\partial n(y)}\, \gamma_0 u(y)\, ds(y), \quad x \in \Omega^-$$

Neumann trace

Dirichlet trace

Trace + Representation Formula ⇝ Calderón identities

Calderón identities

Take the Dirichlet and Neumann trace to obtain

$$V = \begin{bmatrix} \gamma_0 u & \gamma_1 u \end{bmatrix}^T$$

$$A = \begin{bmatrix} -K & V \\ W & K' \end{bmatrix}$$

Interior Problem

$$V = \left[\frac{1}{2} I + A \right] V$$

Exterior Problem

$$V = \left[\frac{1}{2} I - A \right] V$$

Calderón identities...

- Projection Property

$$\left[\frac{1}{2}I \pm A\right]^2 V = \left[\frac{1}{2}I \pm A\right] V$$

  for any possible pair of boundary data V.
- Regularisation Property

$$(2A)^2 = I$$

How to discretise a boundary integral operator?

Consider single-layer operator $V : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$

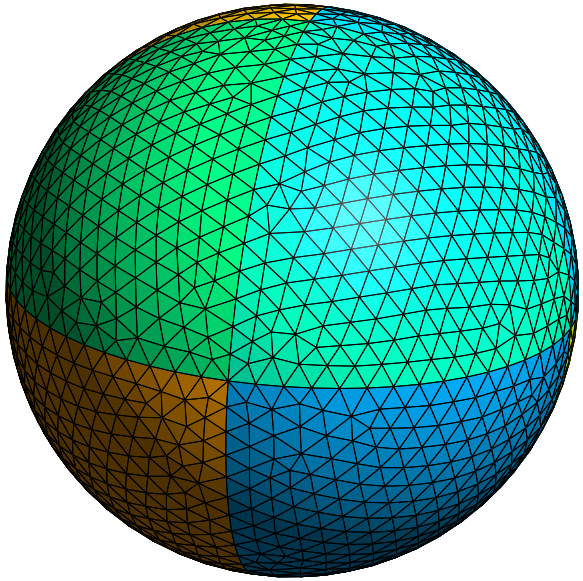
$$[V\phi](x) = \int_\Gamma g(x,y)\phi(y)ds(y).$$

Introduce (weak) variational form

$$\langle V\phi, \psi\rangle_\Gamma = \int_\Gamma \psi(x) \int_\Gamma g(x,y)\phi(y)ds(y)ds(x), \ \psi \in H^{-1/2}(\Gamma).$$

Compute matrix elements

$$\mathbf{V}_{ij} = \int_{\tau_i}\int_{\tau_j} g(x,y)ds(y)ds(x)$$



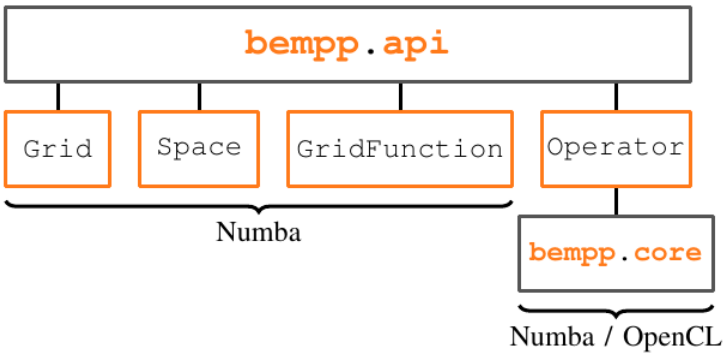
The Bempp software package

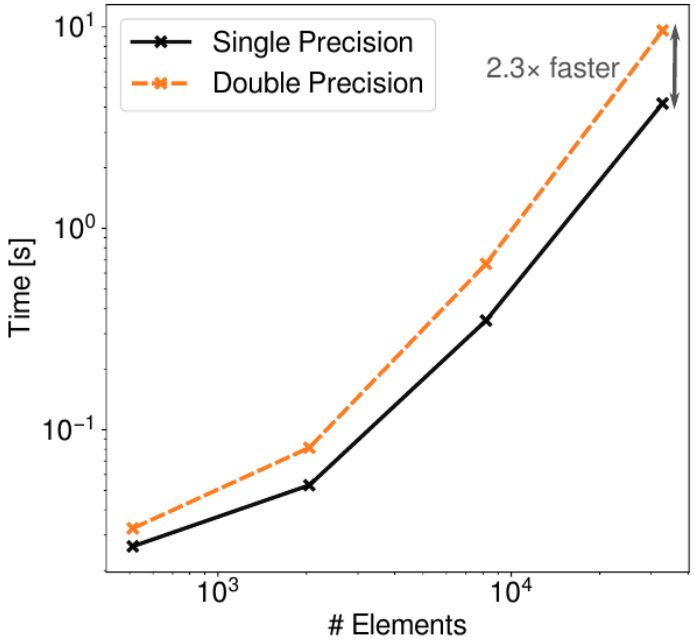
- Originally developed as C++ library, later moved to Python (Bempp-cl)
- Support for Laplace, Helmholtz, Maxwell operators
- FEM/BEM coupling with FEnics
- Old C++ Bempp has support for Hierarchical-Matrix acceleration
- New Bempp supports Fast Multipole Method

Bempp-cl

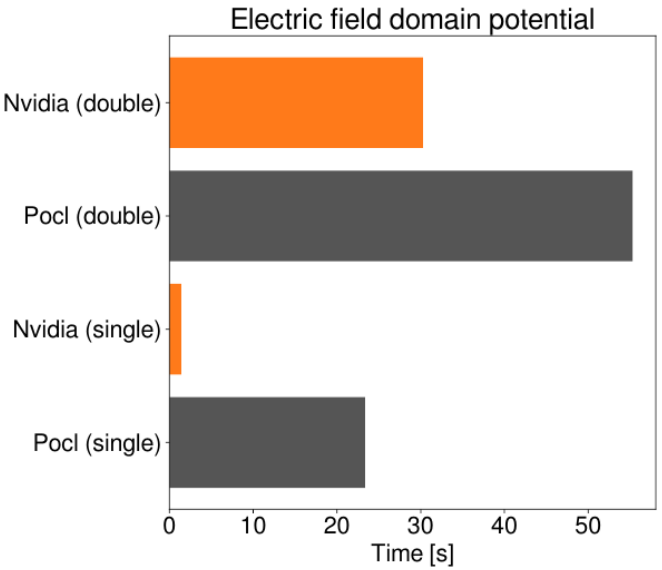
- Successor of the Bempp boundary element library.
- Fully developed using Python with fast OpenCL kernels for computational routines.
- Galerkin discretisation of operators for Laplace, Helmholtz, and Maxwell problems.
- Compute kernels can be run on CPU or offloaded to GPU.
- Core routines optimised for fast dense assembly of opertors.
- Library provides coupling interfaces to Exafmm, can be easily adapted to other fast particle summation libraries.

Characteristics of Bempp-cl



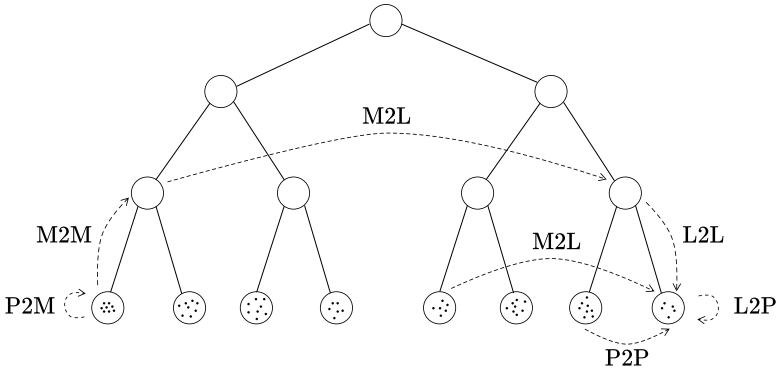


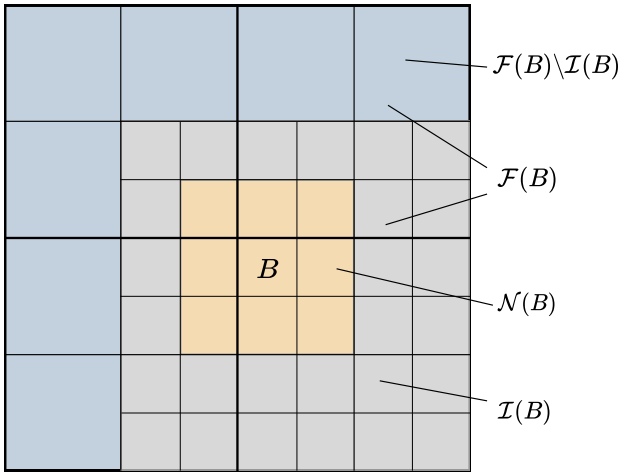
- Top: Structure of Bempp-cl
- Top-Right: AVX acceleration in Bempp-cl
- Bottom-Right: Offloading of a domain potential operator

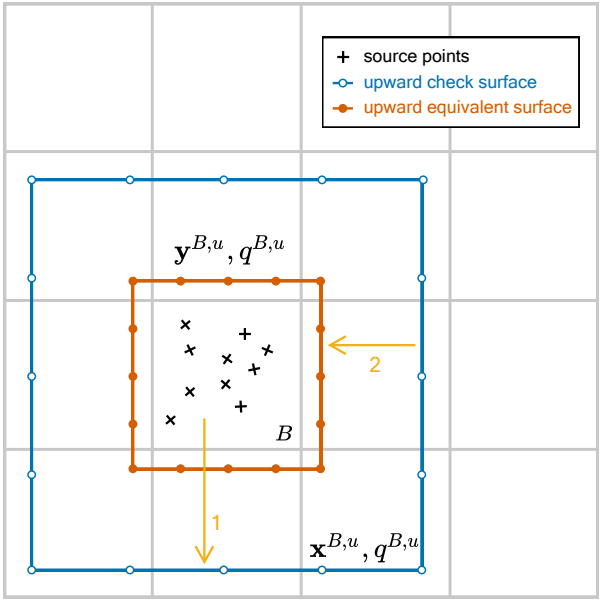


FMM Acceleration with Exafmm-t

- Kernel-Independent FMM library.
- Developed by T. Wang & L. Barba
- Written in C++, Provides Python Interface.
- Highly efficient at higher accuracies.







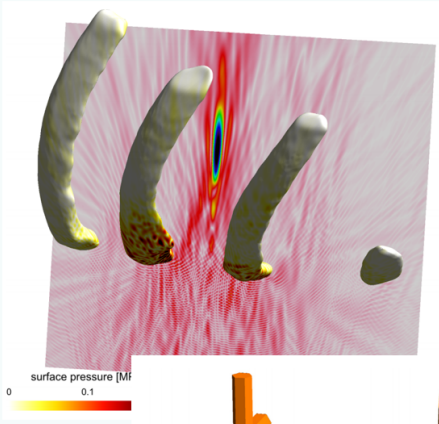
Interfacing Bempp-cl and Exafmm

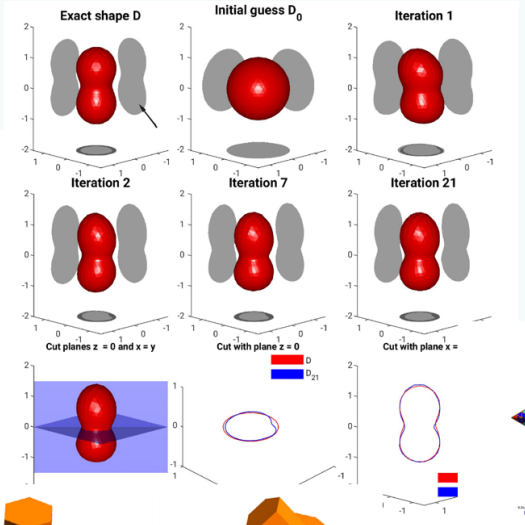
Let A be the matrix representation of a Galerkin discretised boundary integral operator. Let x be any vector. Reformulate Ax as

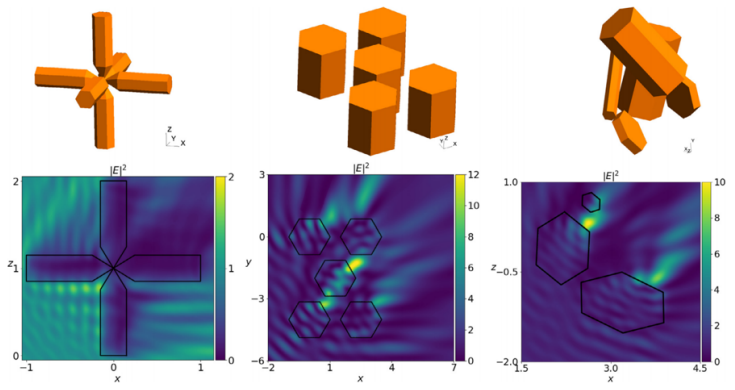
$$Ax = P_{test}^T (G - C) P_{dom} x + Sx$$

- P_{test} and P_{dom} highly sparse matrices that map function space coefficients to particle weights at quadrature points.
- G is black-box operator evaluating particle sums over weights across all quadrature points across all elements.
- C is sparse matrix that contains the particle interactions between neighboring triangles.
- S is sparse matrix containing all singular Galerkin integrals in adjacent elements.

Applications







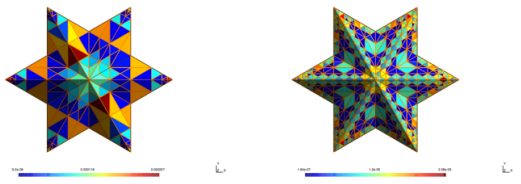


FIGURE 17. Example 3.3: Mesh $\mathcal{T}_\ell$ and distribution of the error estimator η_ℓ^2 for $\ell = 10$ (left) with 360 elements and $\ell = 15$ (right) with 1524 elements.

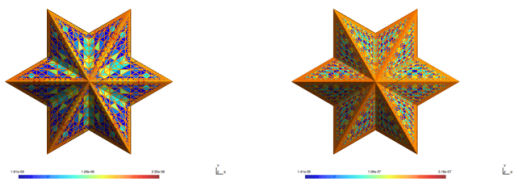


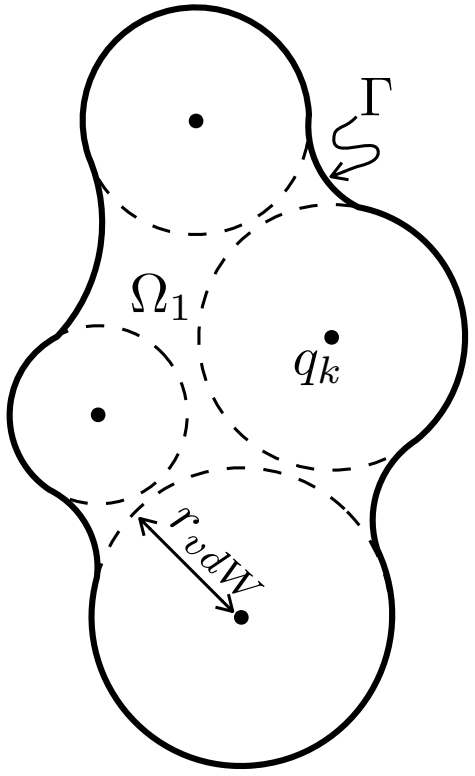
FIGURE 18. Example 3.3: Mesh $\mathcal{T}_\ell$ and distribution of the error estimator η_ℓ^2 for $\ell = 20$ (left) with 5754 elements and $\ell = 25$ (right) with 20304 elements.

Poisson-Boltzmann for virus simulations

Solve Poisson-Boltzmann equation

$$\Delta\phi_1 = \frac{1}{\epsilon_1}\sum_k q_k \delta(\mathbf{r}, \mathbf{r}_k) \text{ in } \Omega_1$$

$$(\Delta - \kappa^2)\phi_2 = 0 \text{ in } \Omega_2$$



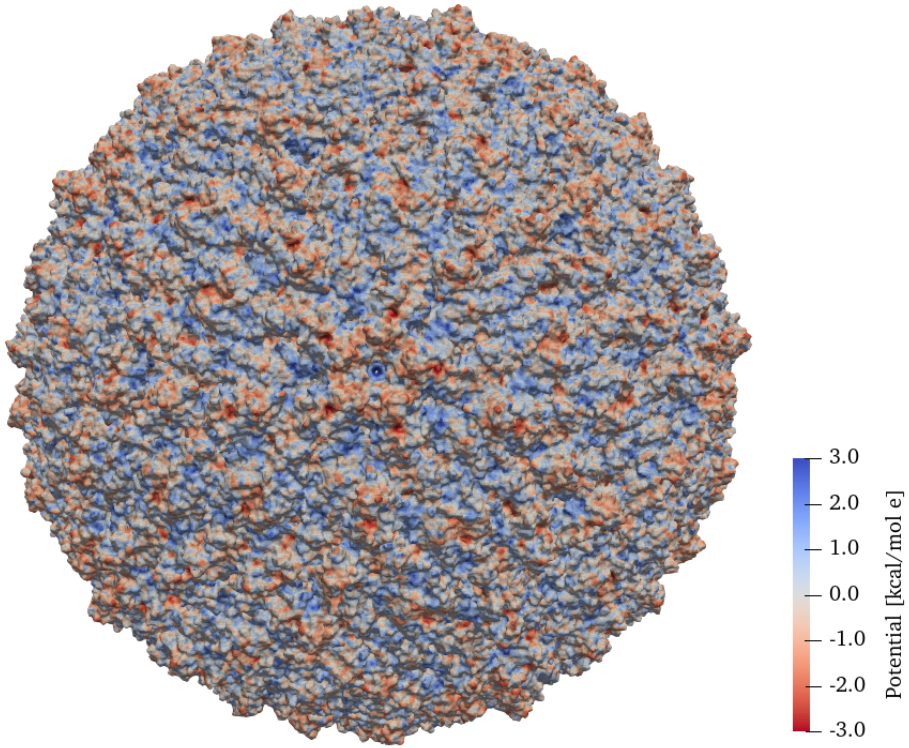
Interface conditions on Γ:

$$\phi_1 = \phi_2,$$
$$\epsilon_1 \frac{\partial\phi_1}{\partial\mathbf{n}} = \epsilon_2 \frac{\partial\phi_2}{\partial\mathbf{n}}$$

Let $\phi_1 = \phi_{reac} + \phi_{coul}$ (ϕ_{coul} is potential generated from the point charges only). Then want to compute the solvation energy.

$$\Delta G^{polar}_{solv} = \frac{1}{2}\sum_{k=1}^{N_q} q_k \phi_{reac}(\mathbf{r}_k)$$

Results for Zika Virus



10m surface elements. 40 Core Compute node. Total time: 139.5 minutes, GMRES time: 80 minutes, 18 GMRES iterations, Max RAM use: 43GB, $\Delta G_{solv} = -116254.9 kcal/mol$. Diagonal preconditioner through inverse of mass matrix with mass lumping.

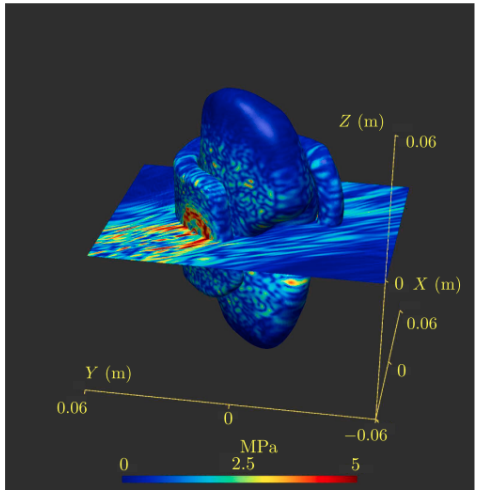
Joint work with T. Wang, C. Cooper, L. Barba

High-Intensity Focused Ultrasound Treatment Planning

Single-trace transmission formulation

$$\left(A^j_{k_0} + \widetilde{A^j_{k_j}}\right)\gamma^{j,+}p_{tot} + \sum_{i\neq j} A^{ji}_{k0}\gamma^{i,+}p_{tot} = \gamma^{j,+}p_{inc}$$

- Standard single-trace formulation ill-conditioned
- Not suitable for large iterative solvers



Precondition with

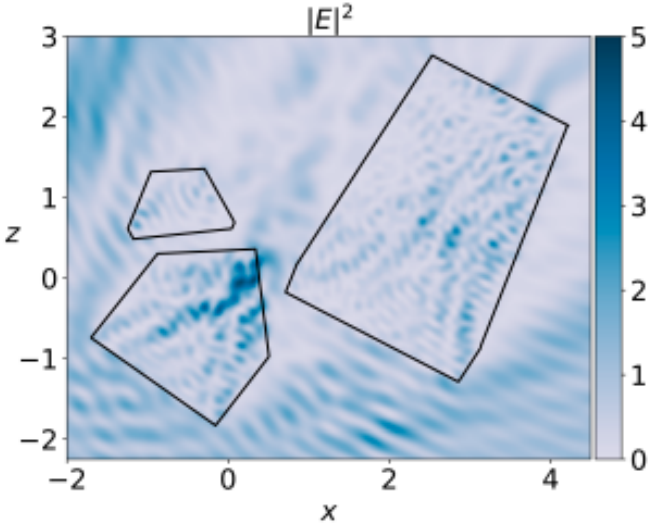
$$C_j := \begin{bmatrix} \widetilde{DtN}^{j,+} & \\ & \widetilde{NtD}^{j,+} \end{bmatrix}$$

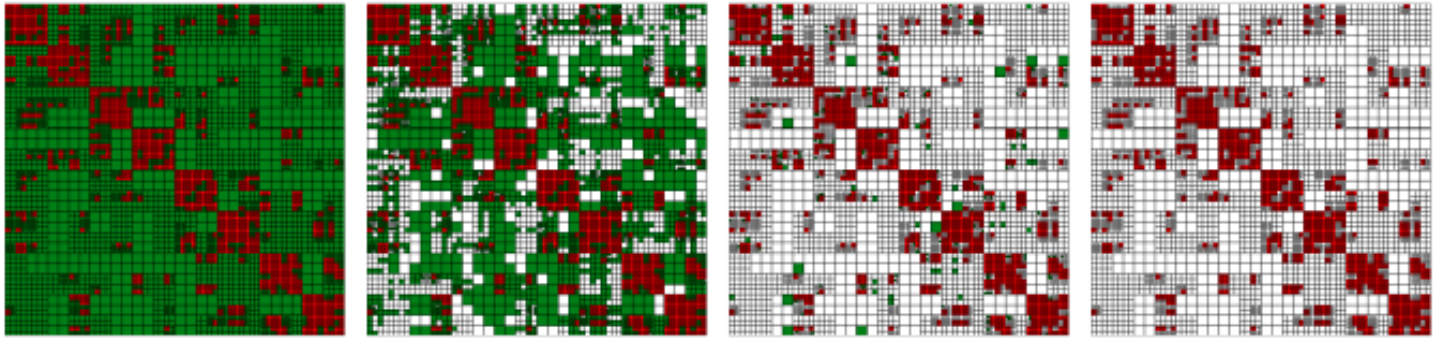
$$\widetilde{DtN} = ik\sqrt{1 + \frac{\Delta_\Gamma}{k_\epsilon^2}}$$

S. R. Haqshenas, et. al. Ultrasonics 110 (2021)

Electromagnetic scattering through ice crystals

- Right: Electromagnetic scattering through ice crystals
- Bottom: Preconditioning by removing far-field contributions





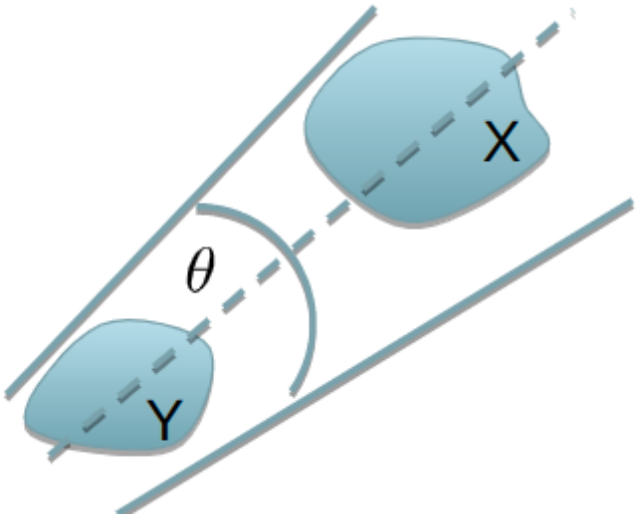
A. Kleanthous, et. al., J. Comp. Phys. 458 (2022)

Why is high-frequency complicated?

Fast boundary element methods rely on far-field compression.
Let $x \in X$ (targets), and $y \in Y$ (sources) For $g(x,y) = \frac{e^{ik|x-y|}}{4\pi|x-4|}$ have

$$\|g(x,y) - \sum_{j=1}^{t_\epsilon} g_j(x)h_j(y)\| < \epsilon, \; t_\epsilon \sim k^2$$

Number of terms in expansion grows quadratically with k



- Require $\theta \sim k^{-1}$ to guarantee compressibility
- Fast algorithms based on this compression proposed by Michielssen, Ying, Engquist, Bebendorf, Boerm, ...

Designing scalable BEM for next gen HPC

UCL

Goal: Create a fast solver framework for fast parallel forward evaluation and approximate inversion of integral operators (`https://github.com/rusty-fast-solvers/roadmap`)

All component libraries developed in Rust with Rayon (multithreading) and MPI (across nodes) for parallelization.

Development Status:

- rusty-green-kernel AVX accelerated direct evaluation of Laplace, Helmholtz Green's functions. Usuable.
- rusty-tree Serial and parallel Octree implementations. Serial tree implemented. Parallel tree early stages. Partially implemented.
- rusty-compression Fast randomized compression routines for approximate low-rank matrices. Mostly finished.
- rusty-translation Implementation of M2M, M2L, L2L, P2M, L2P operators based on numerical field compressions (KIFMM, etc.) In planning
- rusty-fmm Serial and parallel FMM loops In planning
- rusty-inverse Evaluation of approximate inverses Not yet started

Fast Green's function evaluation

Efficiently evaluate sums of the form

$$f(x_i) = \sum_j c_j g(x_i, y_j), \quad g(x, y) = \frac{e^{ik|x-y|}}{4\pi|x-y|}, k \in \mathbb{C}$$

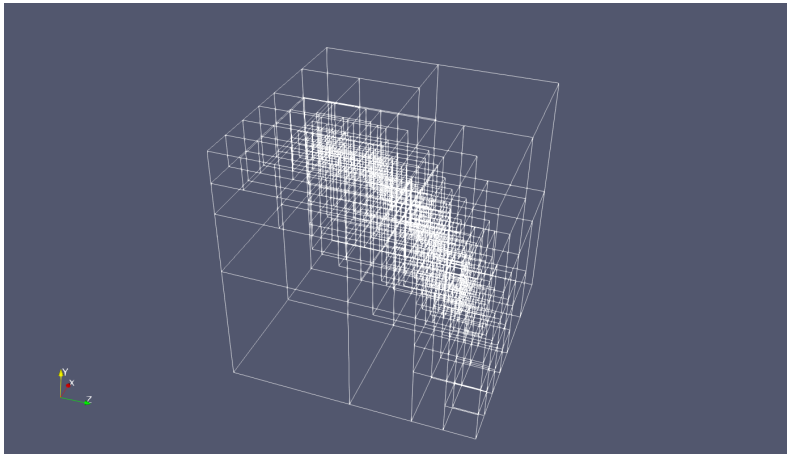
rusty-green-kernel offers

- SIMD accelerated evaluation in single precision and double precision
- Optional multithreaded evaluation
- Needed for
  - Fast evaluation of nearfield interactions
  - Generation of translation operators

Distributed octrees with rusty-tree

- Require adaptive hierarchical domain partitioning for organising nearfield and farfield data.
- Adaptive load-balanced setup of Octrees on distributed platforms (Sundar/Sampar/Biros 2008)
- Have developed working MPI parallelized library

- Initial experimental runs with 1 billion points on ARCHER2
- Right: Small occtree for quarter sphere



Joint work with Sri Kailasa, publication in preparation

Field translation operators

Let $y_0 \in Y$ be in the set of sources, $x_0 \in X$ in the set of targets. B_{y_0} Octree box around source. B_{x_0} octree box around target.

Field in the exterior of B_{y_0}

$$f(x) \approx \sum_{j=1}^{N} c_j^{(s)} g(x, y_j), \; x \in \mathbb{R}^3 \backslash \overline{B_{y_0}}$$

Field in the interior of B_{x_0}

$$f(x) \approx \sum_{j=1}^{N} c_j^{(t)} g(x, y_j), x \in B_{x_0}$$

Field translation operator A

$$c^{(t)} = A c^{(s)}$$

Implementation of translation operators

- Analytical multipole expansions, etc. (Greengard, Rohklin, ...)
- Algebraic techniques
  - Chebychev series representations: Black-Box FMM (Darve, ...)
  - Fundanetal solution approximations: KIFMM (Ying, ...)

rusty-compression: Low-rank approximate translation operators

$$A \approx UV^T,\ U, V^H \in \mathbb{C}^{N \times k}$$

rusty-field: Evaluate various types of translation operators

Final words

- Large-scale acoustic/electromagnetic integral equation solvers significant undertaking
- Good results with Bempp for single node problems, but natural limits for larger applications
- We are building a new scalable and highly parallel code base from scratch that addresses the needs of very large scattering problems
- Further problems: FEM/BEM Coupling, Domain decomposition methods, High-order surface representations,...