MACH-B: Fast Multipole Method Approaches in Particle Accelerator Simulations for the Computational and Intensity Frontiers

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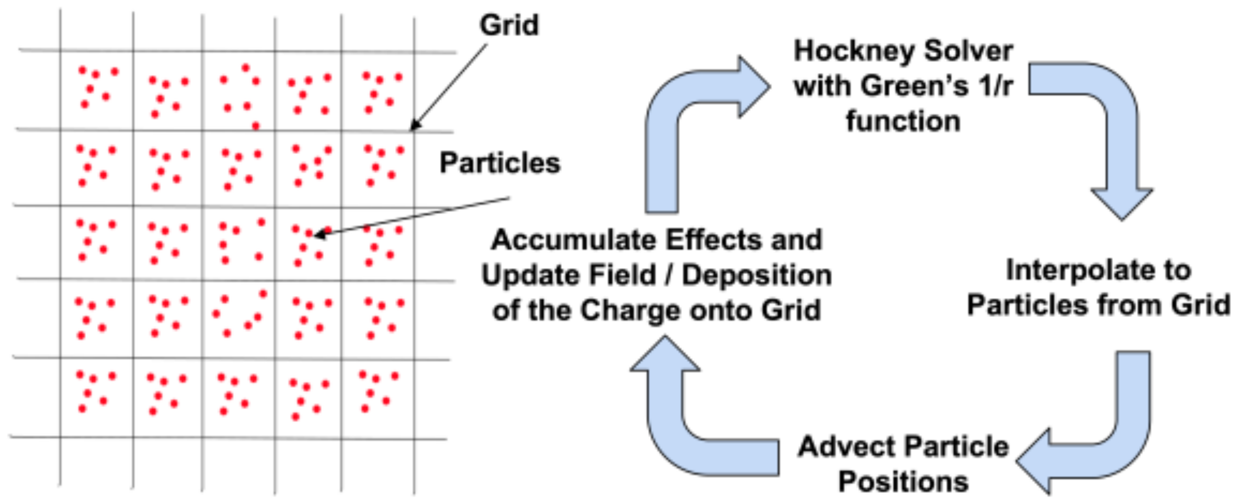
Contribution

The **MACH-B** (**Multipole Accelerator Codes for Hadron Beams**) project is developing a highly-scalable Fast Multipole Method [1, 2, 6] (FMM)-based tool for higher fidelity modeling of particle accelerators for high energy physics within the next generation of FermiLab's Synergia [3] software system on heterogeneous architectures. By incorporating advanced, highly-scalable, high-performance and generally-applicable FMM-based algorithms [6] for accurately modeling space-charge effects in high intensity hadron beams as well as handling singular effects near the beam pipe using advanced quadratures with boundary integral approaches [7], MACH-B enables researchers to more accurately predict beam loss. Further, by introducing an abstraction layer to hide the complexities associated with the implementation and parallelization of FMM algorithms, adding MACH-B implementations into Synergia removes one of the key impediments to the adoption of FMMs for the accelerator community.

Classic Particle Simulations

The majority of numerical approaches for accelerator multiparticle tracking solve the macro-scale problem by employing Particle-In-Cell (PIC) (or Particle-Mesh) methods [3, 4, 5].



PIC methods are seen in simulations of particles that are advected through some domain: it is a sensible initial choice for the accelerator community. Other common examples for these approaches include vortex methods for simulating fluids and simulating electrostatic fields for the summation of potentials from charge distributions. These methods incorporate an Eulerian method for solving the necessary equations and Lagrangian techniques to advect particles through the domain. The specific differences in PIC methods are in how mesh values and particle values are mapped back and forth.

Needs of Advanced Tools

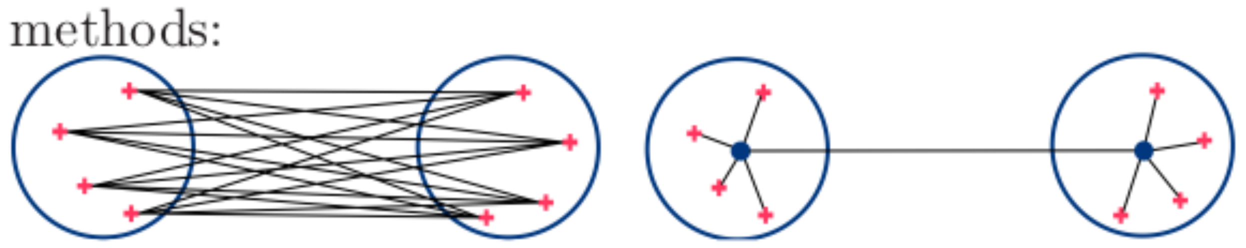
Space-charge modeling in high intensity hadron beams for the accelerator community requires scalable and high-fidelity algorithmic approaches, possessing the following qualities:

- **Inherently multiscale**, handling a variety of particle, field, and material distributions.
- **Exploit locality** to provide scientists with greater control over near-field interactions.
- **Reduce the expense of non-locality** by decreasing the computational expense of far-field interactions while increasing efficiency and maintaining accuracy.
- **Guarantee high accuracy where needed** when smoothing, macroparticles, or self-interactions are introduced.
- **Handle a variety of complex geometries** such that methods are extensible to complex geometries for solving boundary-dependent problems.

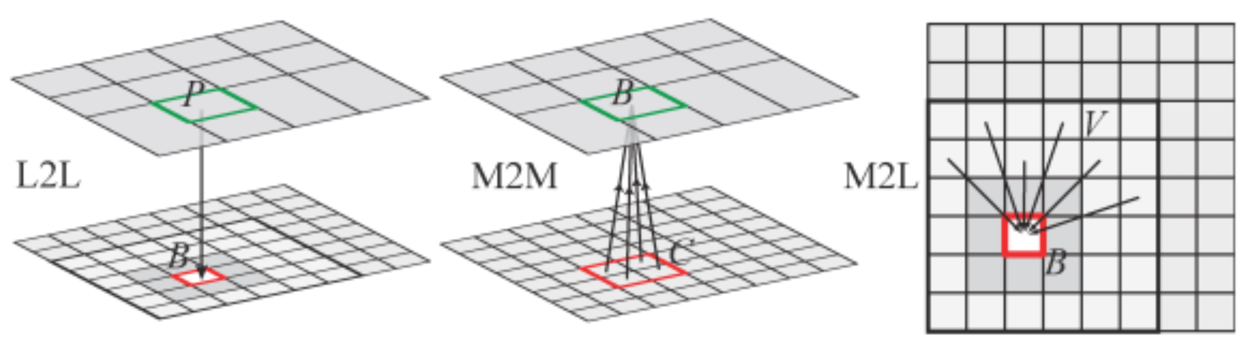
FMMs possess all of these qualities and are well-suited for computational particle accelerator simulations.

Fast Multipole Method (FMM)

FMM computes the total field at target domain B as the sum of (a) the field due to the sources contained in its near field $\mathcal{N}^B$ and (b) its far field $\mathcal{F}^B$. The contributions from $\mathcal{N}^B$ are computed directly using a dense summation, while the contributions from $\mathcal{F}^B$ are obtained by evaluating approximating expansion coefficients. These coefficients are constructed to achieve far-field low-rank approximations at pre-specified levels of accuracy for computationally-efficient and provably-accurate methods:



FMM uses *upward* and *downward passes* on a hierarchical tree structure, employing multiple operators for converting various expansion (multipole and local) coefficients to **achieve optimal linear complexity**. Example from [2] for 2D data flow:



FMM Results in Synergia

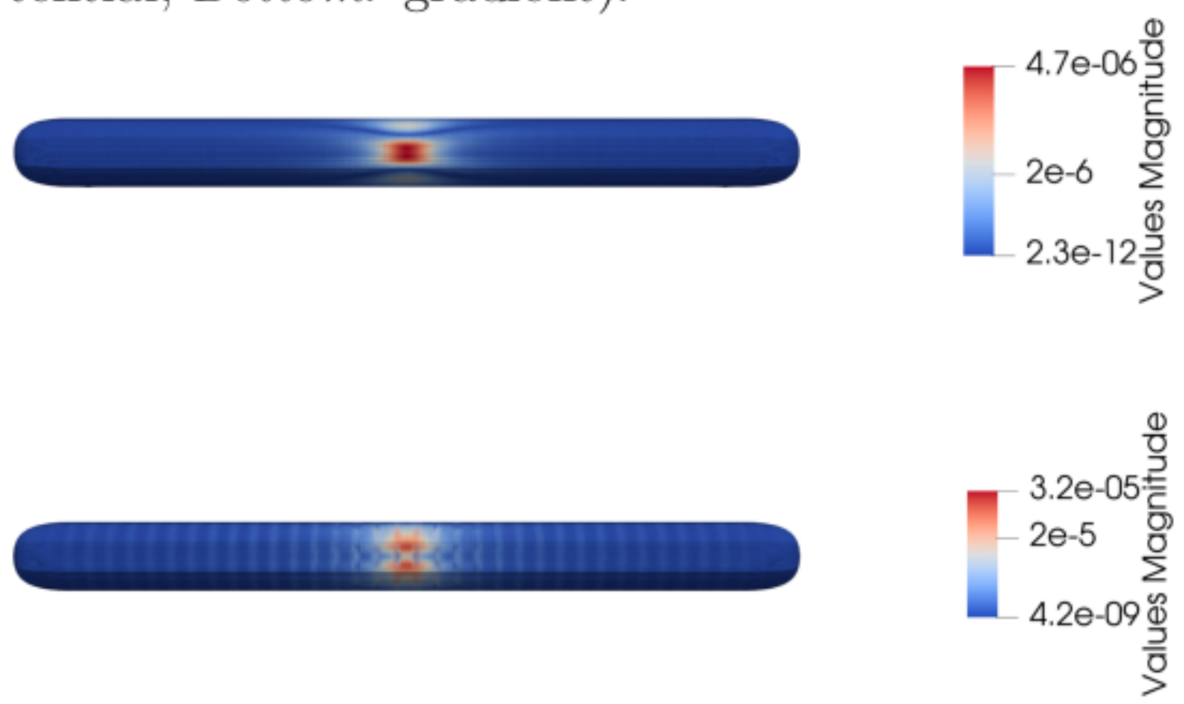
Using 32768 particles per grid cell (M) with $p = 8$ digits of requested accuracy in the FMM expansions, we compare Synergia's Hockney-based PIC solver as interpolated from the grid to particle locations versus MACH-B's FMM tools incorporated into Synergia.

Parameter (M/p)	Relative error (PIC/FMM)
32/8	$0.14089 / 2.65552 \cdot 10^{-7}$
64/8	$0.12279 / 2.65552 \cdot 10^{-7}$
128/8	$0.0991695 / 2.65552 \cdot 10^{-7}$
256/8	$0.0656299 / 2.65552 \cdot 10^{-7}$

Comparing 3D STKFMM, 3D Hockney (Synergia) and naive force computations on arbitrary point clouds, the FMM preserves its accuracy regardless of the particle distribution, whereas the PIC-based methods, when macroparticles are absent, suffer from significant numerical errors associated with interpolation and finite differences.

Boundary Integral Solver

MACH-B incorporates FMM-based boundary integral solvers based on the `hedgehog` software package [7], studying relative accuracy when evaluating potential and gradient solutions to Laplace's equation with Dirichlet boundary conditions (*Top*: potential; *Bottom*: gradient):

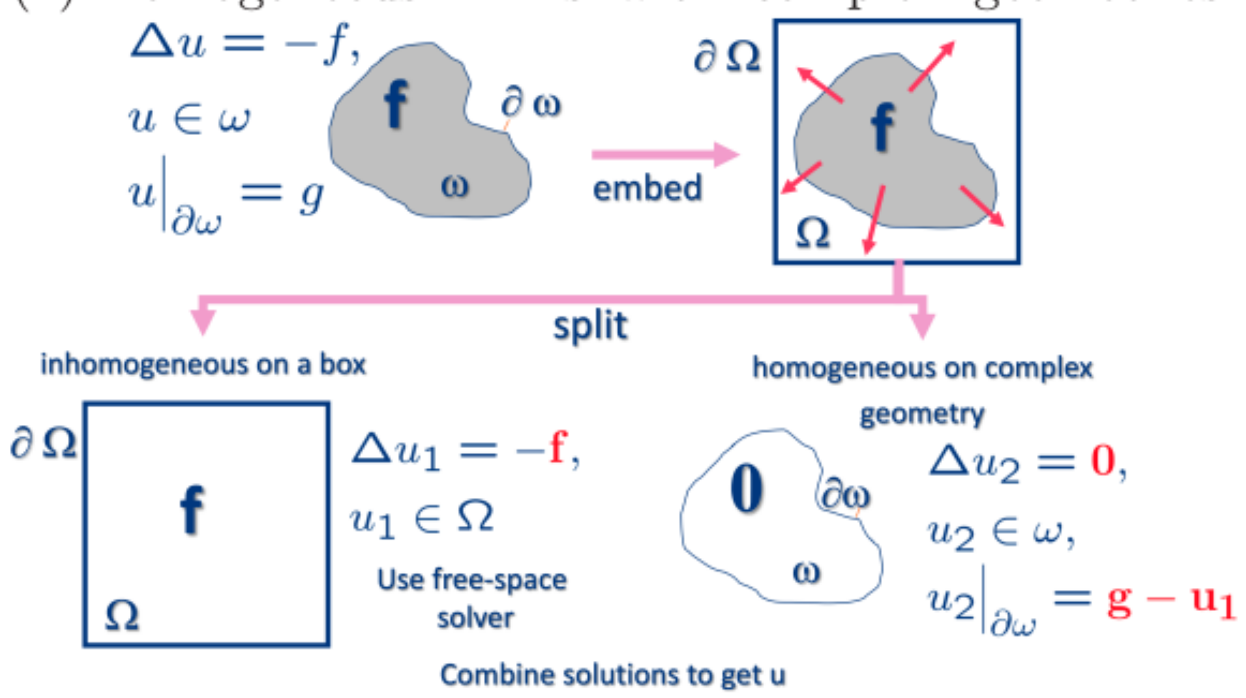


We studied the behavior of the boundary solver for a cylinder with radius 0.5 and length 10. For a fixed distance δ and a point $\mathbf{y}$ on the discretized boundary, we have the interior point $s(\mathbf{y})$, $s(\mathbf{y}) = \mathbf{y} - \delta n(\mathbf{y})$. We considered an FMM accuracy of $1e-8$ and increasing levels of surface discretization (*Number of patches*).

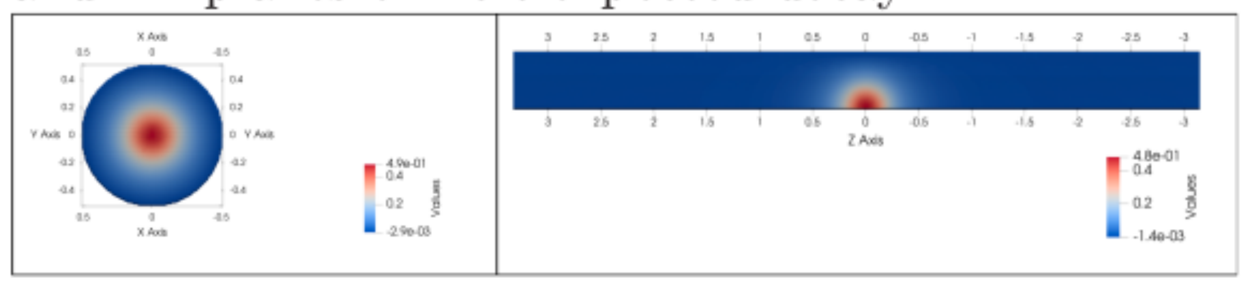
		Number of patches		
Kernel	δ	168	672	2688
Potential	0.05	6.27×10^{-5}	4.68×10^{-6}	8.87×10^{-7}
	0.1	1.70×10^{-5}	3.56×10^{-6}	6.54×10^{-7}
	0.2	9.07×10^{-6}	1.79×10^{-6}	3.20×10^{-7}
Gradient	0.05	8.43×10^{-3}	3.17×10^{-5}	5.84×10^{-6}
	0.1	8.49×10^{-5}	1.96×10^{-5}	3.86×10^{-6}
	0.2	5.53×10^{-5}	1.20×10^{-5}	2.25×10^{-6}

Embedded Boundary Solvers

FMM tools allow us to solve advanced problems in complex domains and shapes by combining two problems they can handle well: (1) free-space PDEs with inhomogeneous force distributions and (2) homogeneous PDEs with complex geometries:



In MACH-B, we model the potential of a single-bunch, Gaussian distribution of charges within a cylindrical conducting pipe. Approximated open boundary conditions at the ends (when a source distribution is concentrated locally) are achieved by extending the length of the pipe. Results for the x-y and x-z planes exhibit expected decay.



References

[1] L. Greengard and V. Rokhlin: *A Fast Algorithm for Particle Simulations*, J. Comp. Phys., 73:2, 325–348, 1987.

[2] M.H. Langston, L. Greengard, D. Zorin: *A Free-Space Adaptive FMM-Based PDE Solver in Three Dimensions*, Comm. in Appl. Math. and Comp. Sci., 6:1, 79–122, 2011.

[3] J. Amundson, P. Spentzouris, J. Qiang and R. Ryne: *Synergia: An Accelerator Modeling Tool with 3-D Space Charge*, J. Comp. Phys., 211:1, 229–248, 2006.

[4] A. Friedman, D.P. Grote, and H. Irving: *Three-Dimensional Particle Simulation of Heavy-Ion Fusion Beams*, Phys. Fluids B, 4, 2203–2210, 1992.

[5] R. Hockney and J. Eastwood: *Computer Simulation Using Particles*, CRC Press, 1988.

[6] D. Malhotra and G. Biros: *PVFMM: A Parallel Kernel Independent FMM for Particle and Volume Potentials*, Comm. in Comp. Phys., 18:3, 808–830, 2015.

[7] M.J. Morse, A. Rahimian and D. Zorin: *A Robust Solver for Elliptic PDEs in 3D Complex Geometries*, arXiv:2002.04143, 2020.

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