Fast Multipole Method Approaches in Particle Accelerator Simulations for the Computational and Intensity Frontiers: SnowMass 2021 Letter of Interest

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In high intensity hadron beam accelerators, the space-charge effect from the interactions between charged particles can have significant impact on beam dynamics, including particle loss along the accelerator. At the beam pipe, these effects and losses can be especially pronounced. As the facilities for high energy physics grow in size and cost (in building, maintenance, and simulation energy usage), and as the constraints on beam loss increase, *it is becoming more important for the Computational and Intensity Frontiers to be able to accurately predict the space-charge effect on beam loss with higher-fidelity computational approaches.*

Reservoir Labs is working on a project titled MACH-B (Multipole Accelerator Codes for Hadron Beams)[1], in which we are developing a highly-scalable Fast Multipole Method (FMM)-based tool for higher fidelity modeling of particle accelerators for high energy physics within the next generation of the Synergia software [1, 24] system on heterogeneous architectures, which will rely further on the Kokkos [4] abstraction layer to provide source level portability of our code base between CPUs and GPUs. We will deploy new particle simulation capabilities and accurately model space charge through HPC software with the following components:

- *Fast Multipole Methods (FMMs)*: Originally designed for Coulomb interactions, FMM schemes achieve linear scaling [9, 12]. In the class of tree codes, FMMs separate near- and far-field interactions on a hierarchy of spatial scales using octree (3D) data structures. Because they achieve arbitrary precision at modest cost with straightforward error estimates, FMMs are best suited for large problems requiring high degrees of accuracy at scale such as those necessary in particle accelerator simulations. We are designing our FMM techniques to be kernel-independent [14, 15, 16, 17, 29, 30] to allow for maximum flexibility for multiple PDEs and has been shown to scale well to hundreds of thousands of processors.
- *Boundary Integral Solvers (BIS) and Boundary Conditions*: For smooth/piecewise-smooth boundaries, such as those often seen near particle accelerator pipe walls, boundary integral equation approaches (1) require no need for complex mesh generation for calculating potentials, (2) allow far-field boundary conditions to be satisfied, and (3) result in higher degrees of accuracy [13]. At the beam pipe, a BIS can be specifically designed to couple with our domain-based FMM solver for an embedded boundary solver (EBS) [3, 18, 19, 26, 30]. In cases where periodic or mixed boundary conditions may be required, FMMs can be tailored to handle these [27, 28]. These boundary solvers are designed to work with unstructured geometries, can perform on-the-fly quadratures for singular and hypersingular kernels, and can be hierarchically parallelized.

In order to achieve the demands of the Computational and Intensity Frontiers in the next 10-20 years, it will be imperative to introduce more flexible and higher-fidelity schemes such as Fast Multipole Methods for simulation purposes.

1 Overview of the Needs for FMMs and Current Approach

Despite the importance of simulating N-body interactions at the micro-scale, macro-scale level problems such as those involving modeling the space-charge effect in accelerators involve a number of degrees of freedom (N), too

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large to simulate even with the exascale resources that are driving DOE applications [2, 5]. For such macro-scale problems, multiscale approaches involving different solvers integrated at various spatial hierarchies must be employed to reduce the computational complexity to a tractable level. The majority of numerical approaches for accelerator multi-particle tracking solve the macro-scale problem by employing Particle-In-Cell (PIC) (or Particle-Mesh (PM)) methods [6, 10, 23, 25]. PIC methods are often seen in simulations of particles that are advected through some domain, so it is a sensible initial choice for the accelerator community.

While PIC methods are good for calculating long-range interactions, they interpolate all particles in a cell to the grid and back. One possible solution for improving near-field accuracy in PIC is the Particle-Particle, Particle-Mesh Method (P^3M), which splits the potential for each particle into two parts: a normal particle-mesh (PM) interaction for distant particle interactions and a particle-particle (PP) summation for near-field interactions [8]. Even though the P^3M method or some variant is necessary for high-accuracy, choosing the near-field radius for the PP calculations takes some finesse [10], made even more complicated in high energy beam dynamics simulations [7, 20]. Despite being *problematic in terms of numerical accuracy and resolution*, PIC codes lend themselves to good strong and weak scalings and have been adopted for large-scale DOE SciDAC-funded, parallel beam dynamics software packages [1]. But, numerical accuracy is difficult to manage and diminishes further at scale.

It is clear that better numerical simulation approaches and tools are necessary for the DOE HEP initiatives in terms of being able to improve the state of the art for particle accelerators in the following ways:

1. More accurately model and simulate higher fidelity models for accelerators;
2. Better predict beam loss and model space-charge effects in high intensity hadron beam environments;
3. Maintain inherent scalability for large degrees of freedom;
4. Ensure that any novel approaches and tools are able to address conditions at the boundary of the beam pipe and be able to perform efficient multiparticle tracking.

In the field of HEP, novel approaches beyond PIC that have shown promise include symplectic multiparticle space-charge simulations [21, 22] as well as Fast Multipole Method (FMM)-based approaches [31].

As described above, space charge modeling in high intensity hadron beams for the accelerator community requires multiscale algorithmic approaches. We believe the most powerful modern multiscale algorithm for such problems is the FMM, which exploits locality to reduce computations for a naive N-body solver from $O(N^2)$ to $O(N)$, and which reduces communication in parallel solvers, critical for exascale computing and macro-scale simulations. Due to the perceived implementation and usage complexity, however, FMM approaches are not employed as often as they should be. In our current effort, we are working to remove these barriers to entry by providing good codes inside of Synergia [1] that scale well and provide clear interfaces and simple parameter tuning for ease-of-use.

Our current efforts include implementing a high-performance generally-applicable FMM-based algorithm for accurately modeling space-charge effects in high intensity hadron beams as well as handling singular effects near the beam pipe. These advances in incorporating multiscale FMMs and advanced quadratures into boundary integral solvers and simulations for beam dynamics software will enable researchers to more accurately predict beam loss, especially as accelerators push to higher average power and the limit of $1W/m$ losses becomes a tighter constraint. 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 with Kokkos [4] will remove one of the key impediments to the adoption of FMMs for the accelerator community.

The core technical objectives of our current effort are as follows:

- **Objective 1: FMM Library**. Research and development of a kernel-independent FMM library [14, 16, 17, 29, 30], built with Kokkos [4] to interface as a module within Synergia [1].
- **Objective 2: BIS and Boundary Conditions**. Research and development of periodic and mixed boundary conditions [13, 27, 28], including incorporation of a boundary solver library built from QBX [11, 26] principles. We will also build an Embedded Boundary Solver library with black-box API and tunable parameter access.
- **Objective 3: FMM, BIS, and EBS Parallelization, Enhancements and Metrics**. Based on our success in highly-scalable FMMs [16, 17, 30], we will complete our FMM and BIS solvers while focusing on maximumizing parallelization and minimumizing communication for scaling to many cores.
- **Objective 4: Library Testing and Evaluation**. We will consult with Fermilab's Accelerator Simulation (AS) Group and Scientific Computing scientists to focus on data for analyzing the codes from Objectives 1-3 against standard Synergia codes for accuracy and parallel scaling results. As part of this objective, we plan to publish results, reporting ongoing and intermediate metrics.

Our current work is showing the potential for new techniques to accelerate the state of the art for accelerator simulations, and we feel that in order to remain competitive in terms of achieving accurate and scalable results in the next decade (and beyond), focusing on Fast Multipole Method approaches for particle simulations in accelerators will be necessary.

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