Abstract
PSI-COFUND Proposal: Efficient and Precise Simulation of Particle Accelerators using Adaptive Meshes

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1 Problem domain

In this project we will address research in the area of particle accelerator science, in particular regarding the High Intensity Proton Facility (HIPA) and the Swiss Free Electron Laser (SwissFEL), and in the domain of parallel numerical methods. We will investigate two fundamental problems in particle accelerator science:

1. the quantitative and efficient evaluation of the effects of *halo particles* (caused by space charge) in high intensity hadron accelerators, and
2. the quantitative and efficient evaluation of the effects of *space charge* in the *low energy part* of FEL's.

For both problems, in state of the art models, the particles (by means of their densities) and fields are defined on *regular grids* and the further development of both applications is hindered by the large memory requirements of regular grids and the prohibitive time to solution.

The challenge in the domain of parallel numerical methods is based on the fact, that proper grid refinement based on both particles *and* fields is non-trivial and conflicting in nature. Existing approaches based on *adaptive mesh refinement* (AMR) have successfully tackled particles or fields separately; but not much work has been done to combine the two.

Today, both applications are based on a Particle-In-Cell (PIC) approach implemented on block structured grids in the efficient three-dimensional particle tracking framework Object Oriented Parallel Accelerator Library [1](OPAL) [1].

2 A new AMR approach

We propose to extend our existing approach of mesh and particle handling in OPAL with memory efficient and scalable AMR capabilities where the adaptation takes into account both field strength and particle density. The emerging new technique will allow us to increase the level of detail of our simulations without compromising memory consumptions and time to solution. In consequence, this will allow us to perform start-to-end simulations with a sufficient level of detail in an acceptable amount of time, which would not be feasible otherwise.

The aim of this research project is to extend this approach by a *massively parallel* and *memory efficient* block structured elliptic AMR solver taking into account

1. refinement based on halo particles (density fluctuations),
2. refinement based on field gradients, and
3. optimal load balancing of particles and fields.

The challenge of *finding an optimal load balance among particles* ***and*** *fields* within an AMR framework, which is targeted toward massive parallel scaling and memory efficiency was never met. It will be addressed in this research project. A prior research among available core frameworks, leads us to `p4est` [2], a massive parallel octree framework, which we plan to use as the kernel for our new AMR solver.

[1] OPAL is used at PSI for precise particle accelerator modeling and worldwide by an growing user community, counting at the moment in the order of 30 users and close to 10 developers, in 5 different laboratories and universities.

3 Primary application domains

In Fig. 1 dark current (green) and the electron bunch (red) are shown in the electron source for the SwissFEL. From the picture it can be seen that (1) a high quality approximation of bunch and dark current requires a very fine grid and that (2) the area where the grid actually has to be fine (i.e. the area with the colored particles) is very small. Therefore, a uniform grid is direfully inefficient. In fact, it consumes so much memory that due limited grid resolution the accuracy is insufficient at places it is desired the most.

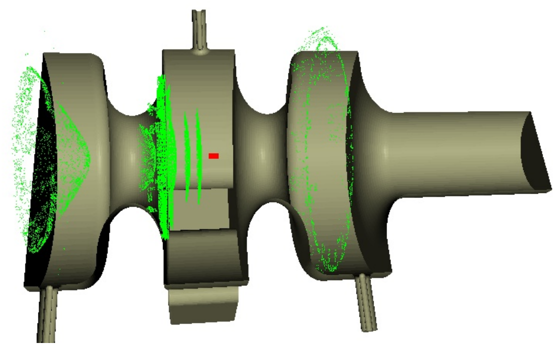

Figure 1: The SwissFEL electron gun under design, showing the primary beam in red and the dark current electrons in green.

With the current uniform discretization we are forced to utilize all the available memory which subsequently results in prohibitive execution times. By consequence, at the moment a full 3D model of dark current including the electron bunch is not possible.

In [3] we showed for the first time that neighboring bunches have an influence on the beam dynamics of high power cyclotrons. In Fig. 2, 2D charge density projections for different numbers of neighboring bunches are shown. It is clearly visible that there are particles (halo) in the space between neighboring bunches.

Given the fact that all high power cyclotrons are limited by their losses, it is of utmost importance to properly resolve these structures in order to better understand the dynamics at levels 10^{-4} to 10^{-5} of the charge density. Up to now we have to use uniform grids to model the transport, which is very inefficient with respect to memory, numerical resolution, as well as time to solution. This fact limits us to only a small number of neighboring turns, with only modest numbers of particles per bunch. For the next generation of high power cyclotrons, aiming at intensities that are higher by an order of magnitude, the present modeling capabilities are hardly sufficient.

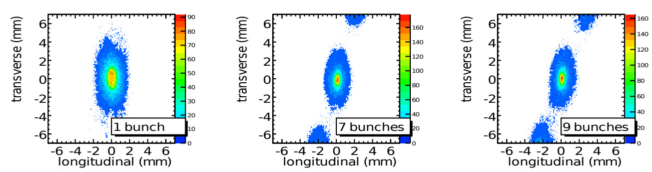

Figure 2: 2D charge density projections of a 1 mA bunch. The results are obtained from simulations with a single bunch (left), 7 bunches (middle), and 9 bunches (right), respectively.

References

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[2] C. Burstedde, L. C. Wilcox, and O. Ghattas. p4est: Scalable Algorithms for Parallel Adaptive Mesh Refinement on Forests of Octrees. *SIAM J. Sci. Comput.*, 33(3):1103, 2011.

[3] J. J. Yang, A. Adelmann, M. Humbel, M. Seidel, and T. J. Zhang. Beam dynamics in high intensity cyclotrons including neighboring bunch effects: Model, implementation, and application. *Phys. Rev. ST Accel. Beams*, 13(6):064201, Jun 2010.