Convolution-Based Solvers for Modeling Space Charge and Radiation: OpenSC, CSR3D, LW3D

Robert D. Ryne

May 7-9, 2018

Berkeley, CA

USA

1 st



workshop







ENERGY Office of Science

Lawrence Berkeley National Laboratory

Outline

- Introduction
- OpenSC
- CSR3D/LW3D







Overview

- Software for calculating
 - 3D space-charge fields (OpenSC)
 - 3D space-charge and radiation (CSR3D/LW3D)
- OpenSC is a library of 3D Poisson solvers for use in accelerator codes
 - Originally developed for use in Warp
 - Adopted and modified for use in Bmad
- CSR3D was originally written to compute CSR fields
 - Uses a Lienard-Wiechert approach
- LW3D is a prototype code that extends CSR3D to self-consistent modeling





Review of Convolution-Based Space-Charge Method

- Beam dynamics codes with Poisson solvers are widely used in the accelerator community for rf accelerator design with space charge
- Many problems involving space-charge can be treated by a model that assumes
 - simple boundary conditions
 - electrostatic in the beam frame
- Convolution-based approach solves for the potential (or fields) by calculating

$$\int \rho(\vec{x}\,')\vec{G}(\vec{x}-\vec{x}\,')\,d\vec{x}\,'$$









Discretization of the Green Function

• Simplest discretization simply uses G at values of grid-point separation,

$$\int \rho(\vec{x}') \vec{G}(\vec{x} - \vec{x}') d\vec{x}' \Longrightarrow \sum \rho_j G_{i-j}$$

- Use FFTs to perform the discrete convolution
 - turns O(N²) problem into O(N log N)
 - This is a mathematical trick (not a spectral algorithm)
- Having found the potential, compute the E field
 Or could perform 3 convolutions to compute E directly
- ES PIC codes normally compute B assuming the beam is mainly unidirectional (only ${\rm A_z})$





Better: Use an Integrated Green Function (IGF)

- Simplest discretization can produce erroneous results when grid aspect ratio is large
 - Issue is not really aspect ratio; the root cause involves the variation of G within a grid cell
 - Results can be wrong but not garbage; not obvious that the code is wrong
- Use of an Integrated Green function (IGF) solves the problem
 - Robust solver, little sensitivity to grid aspect ratio
 - Accuracy depends on choosing a fine enough grid to resolve ρ



Many people want to put 3D space-charge in their code. To avoid people "reinventing the wheel" we developed OpenBC

- Parallel, reusable, convolution-based, 3D space-charge library
- Currently supports
 - Free-space boundary conditions
 - Rectangular waveguide boundary conditions
- Parallel 3D FFT uses the package by S. Plimpton, SNL
- Build system, OpenMP support, other enhancements by C. Mayes (SLAC)
- Current version of OpenBC is on github; will be incorporated into Picsar



















OpenBC uses the Parallel 3D FFT package by S. Plimpton. Tested on up to 131K cores of Edison at NERSC







9

CSR3D: A massively parallel code for studying 3D CSR effects

- Originally developed by R. Ryne in collab. with B. Carlsten, C. Mitchell, and J. Qiang
- Two versions: (1) Point-to-grid, and (2) Convolution-based
- Convolution-based version uses a Lienard-Wiechert Particle-Mesh (LWPM) method
- Has been to study aspects of CSR, especially 3D effects and stochastic effects, that would be difficult or impossible to simulate with other codes
- References:
 - R. Ryne et al., "Large Scale Simulation of Synchrotron Radiation using a Lienard-Wiechert Approach," Proc IPAC 2012
 - R. Ryne et al., "Using a Lienard-Wiechert Solver to Study Coherent Synchrotron Radiation Effects," Proc FEL2013
- In 2017 used by B. Garcia (SLAC) for comparison with an analytical model of CSR
 - B. Garcia, T. Raubenheimer, and R. Ryne, "Stochastic Effects from Classical 3D Synchrotron Radiation," Proc FEL2017
- Marinelli et al plan to use to study a new method for eSASE
- Interest in 3D CSR modeling is picking up discussion at IPAC18; Slack channel...





A sample of CSR3D results

mm

BERKELEY LAB





CSR3D Status

- CSR3D can be run at NERSC
- It only computes fields, it's not a self-consistent code

- This was my first attempt to model 3D CSR
- The coding is not pretty
- Some have looked at the source code, with unfortunate results...









ENERGY Office of Science





The LW3D code

- CSR3D is being modified to be easier to maintain and to enhance its functionality for modeling realistic problems
- The new code is called LW3D in recognition of the fact that it is a Lienard-Wiechert code, not just a code for CSR
- LW3D will be capable of self-consistent modeling
- A prototype exists and is being debugged
- In the meantime CSR3D is available at NERSC







Acknowledgements

- C. Mitchell, J. Qiang (LBNL), C. Mayes (SLAC), B. Carlsten (LANL)
- US DOE Office of Science, Office of HEP
- US DOE Office of Science, Office of BES
- LANL LDRD (2012)
- NERSC resources have been essential to this effort









