SciDAC Advances and Applications in Computational Beam Dynamics

D. Abell[7], A. Adelmann[6], J. Amundson[2], C. Bohn[5], J. Cary[7], P. Colella[4], D. Dechow[7], V. Decyk[9], A. Dragt[10], R. Gerber[4], S. Habib[3], D. Higdon[3], T. Katsouleas[11] K.-L. Ma[8], P. McCorquodale[4], D. Mihalcea[5], C. Mitchell[10], W. Mori[9], C. T. Mottershead, F. Neri[3], I. Pogorelov[4], J. Qiang[4], R. Ryne[4], R. Samulyak[1], D. Serafini[4], J. Shalf[4], C. Siegerist[4], P. Spentzouris[2], P. Stoltz[7], B. Terzic[5], M. Venturini[4], P. Walstrom[3]

[1]BNL, [2]FNAL, [3]LANL, [4]LBNL, [5]NIU, [6]PSI, [7]Tech-X, [8]UCD, [9]UCLA, [10]U. Md., [11]USC

Abstract

SciDAC has had a major impact on computational beam dynamics and the design of particle accelerators. Particle accelerators -- which account for half of the facilities in the DOE Office of Science *Facilities for the Future of Science* 20 Year Outlook -- are crucial for US scientific, industrial, and economic competitiveness. Thanks to SciDAC, accelerator design calculations that were once thought impossible are now carried routinely, and new challenging and important calculations are within reach. SciDAC accelerator modeling codes are being used to get the most science out of existing facilities, to produce optimal designs for future facilities, and to explore advanced accelerator concepts that may hold the key to qualitatively new ways of accelerating charged particle beams. In this poster we present highlights from the SciDAC Accelerator Science and Technology (AST) project Beam Dynamics focus area in regard to algorithm development, software development, and applications.

CODE DEVELOPMENT

Beam Dynamics codes developed under the SciDAC AST project include:

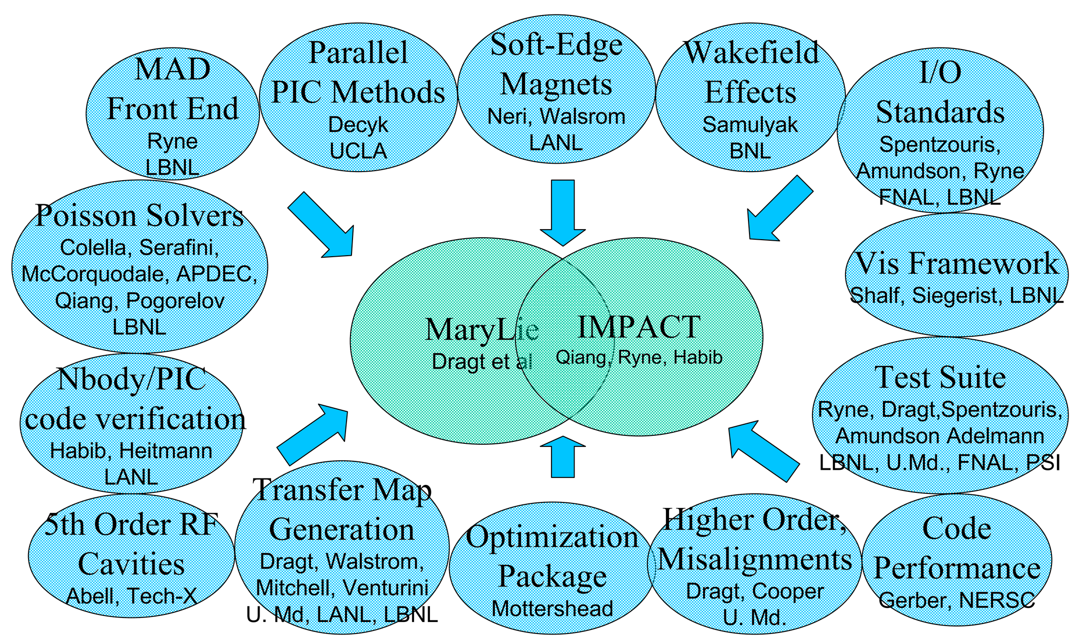
• IMPACT: An integrated suite of codes consisting of 2 PIC codes, a linac design code, and an envelope code. This package was originally developed to model high intensity ion linacs. Its functionality has been greatly enhanced so that it is now able to model high brightness electron beam dynamics (e.g. photocathodes), ion beam dynamics, and multi-species transport through a wide variety of transport systems.

•BeamBeam3D: A code for modeling beam-beam effects in colliders. This code contains multiple models (weak-strong, strong-strong) and multiple collision geometries (head-on, long-range, crossing angle). It has been used to model the Tevatron, PEP-II, RHIC, and LHC.

•MaryLie/IMPACT: A code that combines the high-order optics modeling capabilities of the MaryLie Lie algebraic beam transport code with the parallel PIC capabilities of IMPACT. It is able to model space-charge effects in large circular accelerators such as the ILC damping rings.

•Synergia: A parallel beam dynamics simulation framework based on modern programming design. Synergia combines multiple functionality, such as the space-charge capabilities of IMPACT and the high-order optics capabilities of MXYZPLT, along with a "humane" user interface and standard problem description. (For additional information see the poster "Simulation of the Fermilab Booster using Synergia," by P. Spentzouris.)

Codes developed under SciDAC typically involve large multidisciplinary teams. An example is illustrated below for the MaryLie/IMPACT code.



Code modules and developers for the MaryLie/IMPACT parallel beam dynamics code.

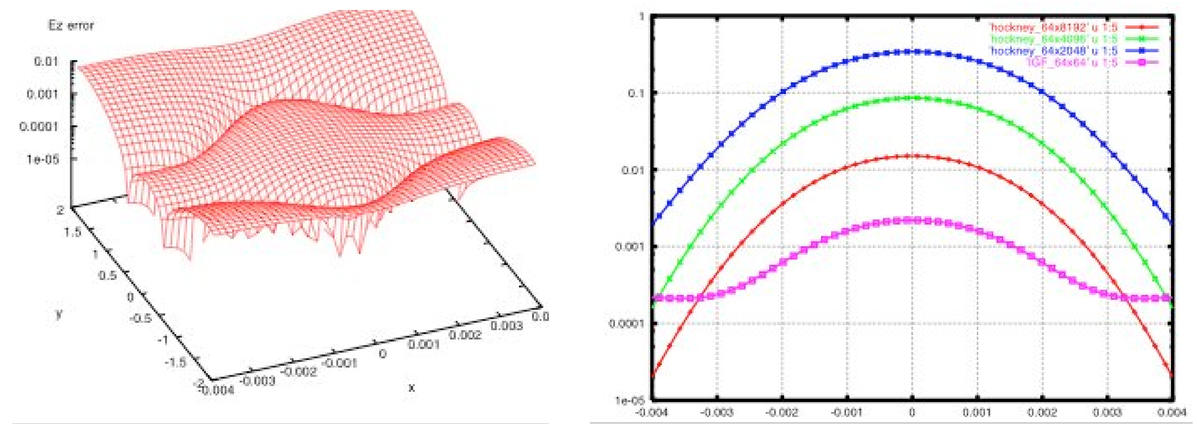
ALGORITHMS DEVELOPMENT; ISIC AND SAPP COLLABORATIONS

RECENT HIGHLIGHTS

- APDEC solvers incorporated into ML/I code; progress on AMR/PIC (P. Colella, D. Serafini, P. McCorquodale)
- Developed shifted Green function for long-range beam-beam, cathode images (J. Qiang, LBNL)
- Developed integrated Green function for high aspect ratio situations (J. Qiang, R. Ryne, LBNL)
- Wavelet solver developed and incorporated into IMPACT (I. Pogorelov, LBNL, B. Terzic, NIU)
- Multigrid solver developed and used to model RIA beam formation & transport (J. Qiang, LBNL)
- Wakefield module developed and incorporated into ML/I (R. Samulyak, BNL)
- Statistical methods for phase space reconstruction from data (D. Higdon, LANL)
- Hybrid high performance visualization of particle data w/ large range of density scale (K.-L. Ma, UC Davis)
- PARTVIEW/H5PART tools for large-scale data management and visualization in parallel PIC codes (J. Shalf, C. Siegerist, LBNL; A. Adelmann, PSI)

Modeling High Intensity Beams with High Aspect Ratios

Issue: Modeling beam stability, halo formation, and ultra-low beam loss in high intensity accelerators.
Challenge: Need high statistics simulations, high performance codes, and ability to model systems that may have very high aspect ratios
Solution: Development of Integrated Green Function (IGF) approach exhibits > 100x performance improvement in high aspect ratio systems

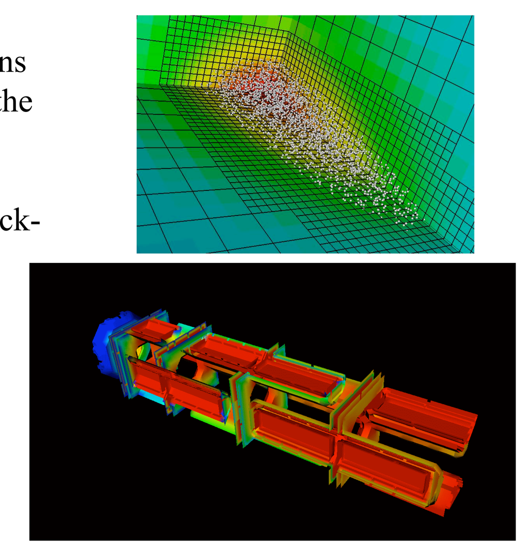


Simulation of a high-aspect ratio bunch using an integrated Green Function (IGF) algorithm and a conventional algorithm (Hockney). Left: Electric field error using IGF is below 1% using a 64x64 grid. Right: IGF on a 64x64 grid (purple) is more accurate than a standard calculation using 64x2048 (blue), 64x4096 (green), and 64x8192 (red). (R. Ryne, LBNL)

Collaboration with the APDEC ISIC

• Members of the Applied Partial Differential Equations Center (APDEC) are developing new capabilities for the AST project's beam dynamics codes
•Goal: Develop a flexible suite of fast solvers for PIC codes based on APDEC's Chombo framework for block-structured AMR
•Key technologies include
  •Method of local corrections (MLC)
  •Solvers for infinite boundary conditions
  •AMR/PIC methods
•Benefits
  •Fast, efficient solvers
  •Accurate representation of complex geometries

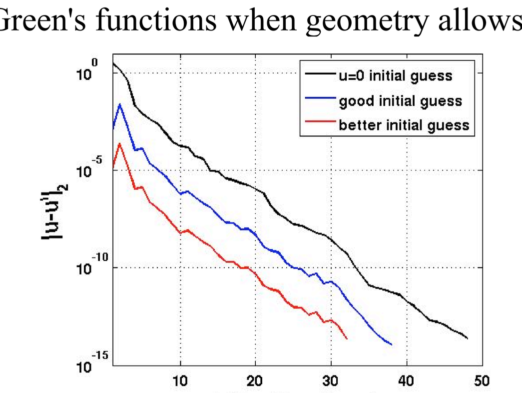
•Additional information can by found in the poster "Advanced 3D Poisson solvers and Particle-in-Cell Methods for Accelerator Modeling" by David Serafini.

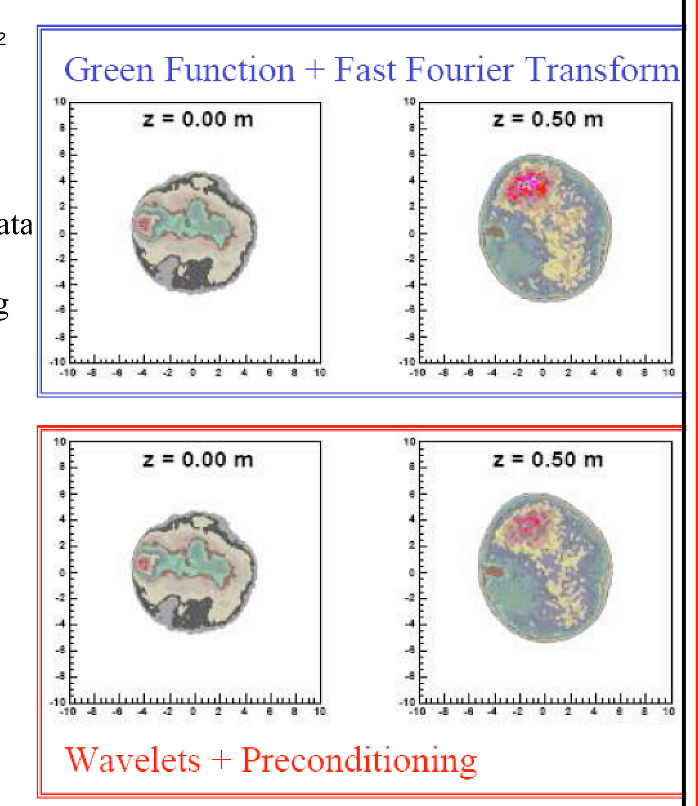


Top: Image showing the Chombo-based adaptive mesh along with a subset of particles from a particle simulation. The 2 level grid has a refinement ratio of 4. Bottom: AMR mesh for a simulation of a Heavy Ion Fusion Injector

WAVELET-BASED POISSON SOLVER

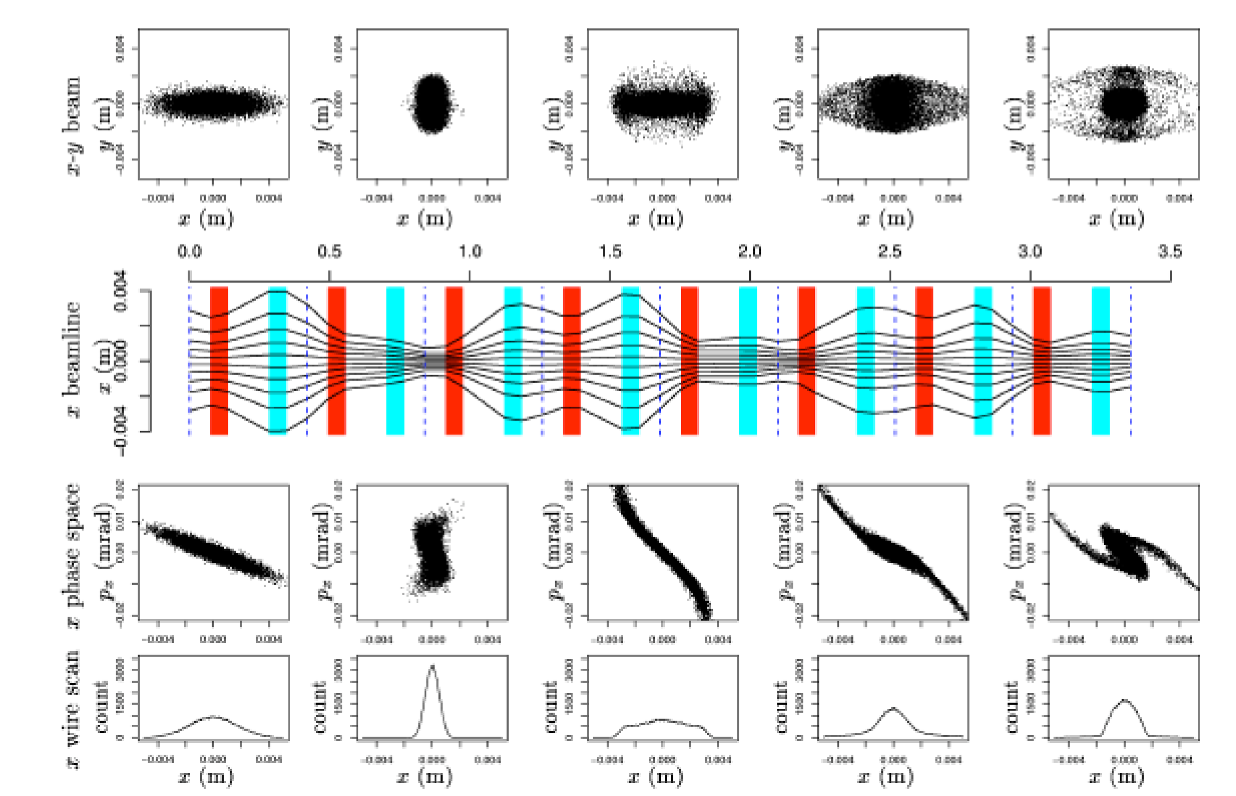
• iterative solver with convergence $\|U-U^i\|_2 \le \left(\frac{\sqrt{k}-1}{\sqrt{k}+1}\right)^i \|U\|_2$
k - condition number of the operator L
• initial approximation: U at previous time step
• diagonal (efficient) preconditioner in wavelet space
• strengths:
  •compact/sparse representation of operators and data
  •removing numerical noise *while* compressing
  •convergence greatly improved by preconditioning
• weakness:
  •need potential on the surface of the grid
  (use Green's functions when geometry allows)



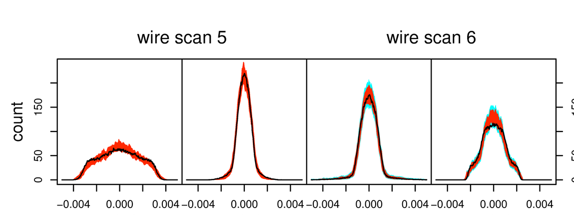


Left: Convergence of wavelet-based preconditioned conjugate gradient (PCG) solver as a function of initial approximation. Right: Comparison between IMPACT-T (upper plots) and IMPACT-T with PCG (lower plots) shows preserved level of detail in wavelet-based solver. (B. Terzic, NIU, and I. Pogorelov, LBNL).

STATISTICAL METHODS FOR CALIBRATION AND FORECASTING



Above: Simulation of a high intensity proton beam through a series of quadrupole magnets. Statistical techniques were used to combine 1D profile monitor data with simulations to infer the 4D beam distribution. Right: The figure shows the 90% intervals for the predicted profile at scanner #6 (shaded regions), and, for comparison, the observed data (black line). Only data from the odd numbered scanners were used to make the prediction. (D. Higdon, LANL).



PARTVIEW/H5PART: TOOLS FOR MANAGING & VISUALIZATING DATA SETS FROM PARALLEL PARTICLE CODES

• PARTVIEW capabilities/features:
  •Allows the user to project 6D time-series data into 3D space by selecting which dimensions will be represented spatially and which will be particle attributes
  •Allows construction of complex transfer functions for representing attributes
  •Contains hooks to connect with a parallel back-end that is able to provide remote file access, progressive streaming, and parallel rendering
•H5PART capabilities/features:
  •HDF5-based parallel I/O library with C++, C, and Fortran bindings
  •Allows management of time-series data

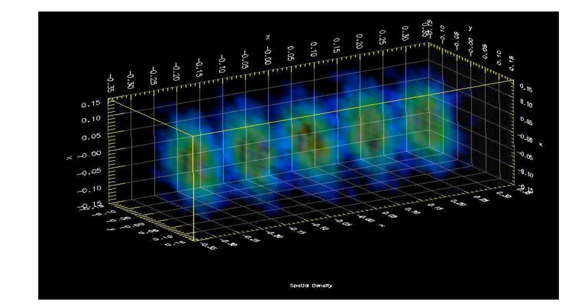
Preliminary performance results, looking at global data (GD) and local data (LD) rates for a test problem on 64 IBM SP3 nodes writing 51 million particles. The performance of PARTVIEW is very good even with respect to raw MPI. (J. Shalf and C. Siegerist, LBNL; A. Adelmann, PSI).

Mode	GD [MB/s]	LD [MB/s]
MPI-IO (one file)	241	3.7
One file per proc	1288	20
H5Part (one file)	773	12

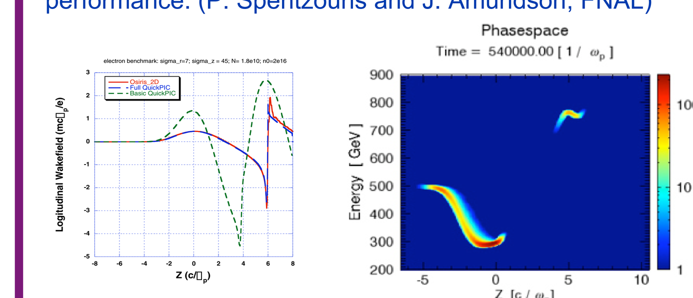
APPLICATIONS

SciDAC AST beam dynamics codes have been applied to several important projects within the DOE Office of Science. Examples include existing colliders (Tevatron, RHIC, PEP-II), future colliders (LHC, under construction), proposed linear colliders (ILC, and previously NLC), high intensity machines (the Fermilab booster, and the SNS ring under construction), linacs for radioactive ion beams (RIA, proposed), and electron linacs for 4th generation light sources (LCLS, under construction).

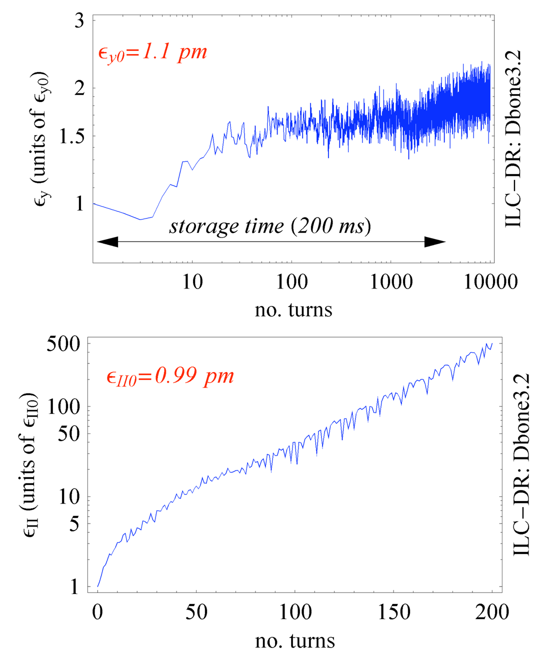
SAMPLE APPLICATIONS OF SCIDAC CODES TO THE HEP PROGRAM



FNAL booster simulation results using Synergia showing the merging of 5 microbunches. SciDAC team members are working closely with experimentalists at the booster to help understand and improve machine performance. (P. Spentzouris and J. Amundson, FNAL)

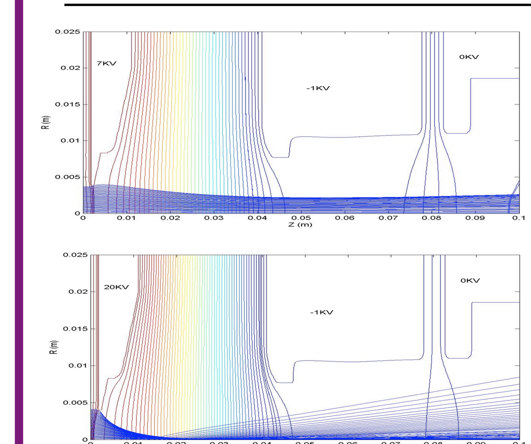


Progress in the Advanced Accelerator portion of the SciDAC AST project is having an impact on beam dynamics modeling. The code QuickPIC uses innovative algorithms to achieve up to 100x performance increase over 3D EM PIC codes with comparable accuracy for some problems (left). QuickPIC has been used to model electron-cloud formation in the LHC. It has also been used to study plasma afterburner concepts (right). (W. Mori and T. Katsouleas, UCLA and USC). EM PIC codes (OSIRIS and VORPAL) have been used to model ongoing LWFA experiments. Further information about the Advanced Accelerator effort can be found in the poster, "Massively Parallel Particle-in-Cell Simulation of Advanced Particle Accelerator Concepts," by D. Bruhwiler.

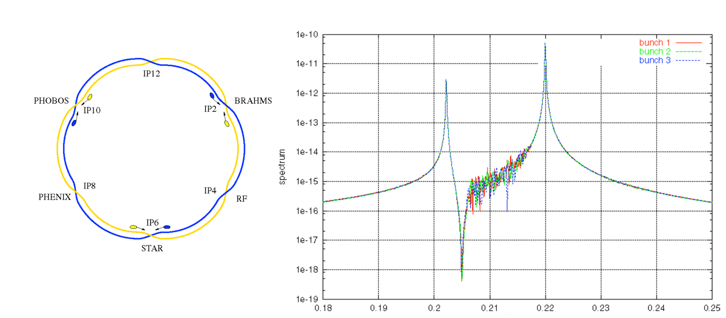


Results of MaryLie/IMPACT simulations of an ILC "dog-bone" damping ring (DR) design showing space-charge induced emittance growth using different space-charge models. Space charge is important for the ILC DR in spite of the high energy because of the combination of small emittance and large (16 km) circumference. Top (nonlinear space charge model): the beam exhibits small emittance growth. Bottom (linear space charge model): the beam exhibits exponential growth due to a synchro-betatron resonance. The instability is a numerical artifact caused by the simplified (linear) space-charge model. (M. Venturini, LBNL)

SAMPLE APPLICATIONS OF SCIDAC CODES TO THE NP PROGRAM

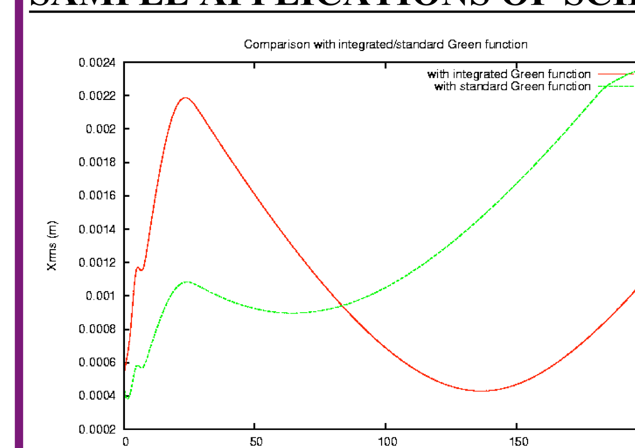


IMPACT-T simulation of the beam emerging from the RIA ECR ion source showing the effect of incorrect electrode voltage (bottom) on the beam quality emerging from the source. (J. Qiang, LBNL)

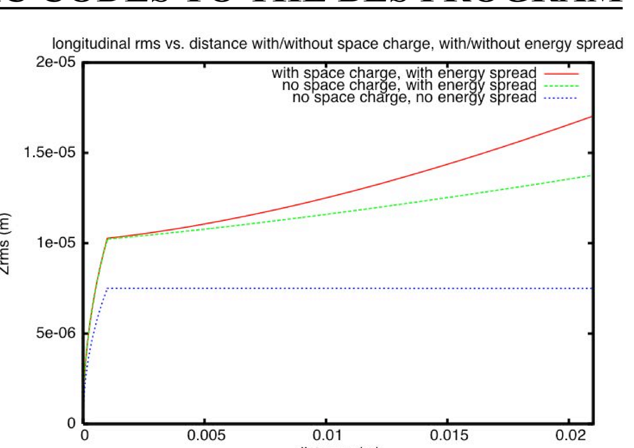


Left: Schematic of the RHIC collider showing the three interaction regions. Right: Power spectrum of horizontal centroid motion of three bunches using a strong-strong (I.e. fully self-consistent model). Prior to SciDAC, it was virtually impossible to perform strong-strong, multi-bunch, multi-IR beam-beam simulations accurately. Under SciDAC, the first-ever million particle, million-turn strong-strong simulation (of LHC) was performed in 2004.

SAMPLE APPLICATIONS OF SCIDAC CODES TO THE BES PROGRAM



LCLS simulation using IMPACT-T: Large effect observed when using Integrated Green function compared with standard Green function (J. Qiang, LBNL and C. Limbourg, SLAC)



Plot of rms bunch length vs distance in the proposed LCLS streak camera showing the effect of space charge on the bunch length (J. Qiang, LBNL)