# *Large Scale Beam Dynamics Simulations on High Performance Computers*

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# A) Project Overview

**Project Title: Community Petascale Project for Accelerator Science and Simulation (ComPASS)**

**Principal Investigator:** Panagiotis Spentzouris

**Affiliation:** Fermi National Accelerator Laboratory

**Project webpage:** http://compass.fnal.gov

## Participating Institutions and Co-Investigators:

Argonne National Laboratory - Michael Borland, Lois Curfman McInnes
Brookhaven National Laboratory - Alexei Fedotov, Wolfram Fischer
Fermi National Accelerator Laboratory - James Amundson, Panagiotis Spentzouris
Lawrence Berkeley National Laboratory - William Fawley, Esmond Ng, Ji Qiang, Robert Ryne
Stanford Linear Accelerator Center - Lie-Quan Lee, Cho Ng
Tech-X Corporation - David L. Bruhwiler, John R. Cary
Thomas Jefferson National Accelerator Facility - Rui Li, Haipeng Wang
University of California, Los Angeles - Viktor Decyk, Warren Mori, Sven Reiche
University of Maryland - Tom Antonsen
University of Southern California - Tom Katsouleas

**Funding Partners:** Office of Science — High Energy Physics, Advanced Scientific Computing Research, Nuclear Physics, and Basic Energy Sciences

## Science goals:

This project will develop a comprehensive computational infrastructure for accelerator modeling and optimization. This project will advance accelerator computational capabilities from the terascale to the petascale to support DOE priorities for the next decade and beyond.

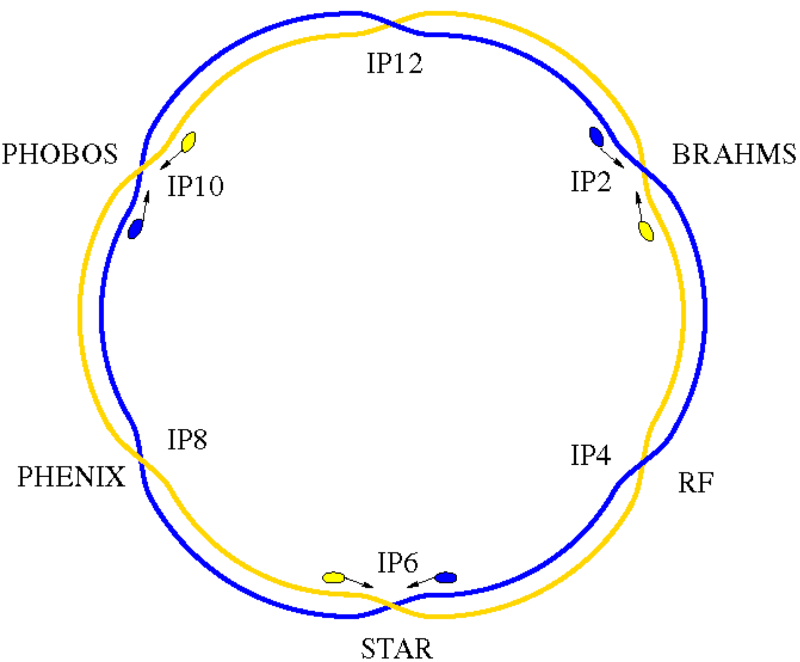
# B) Science Lesson

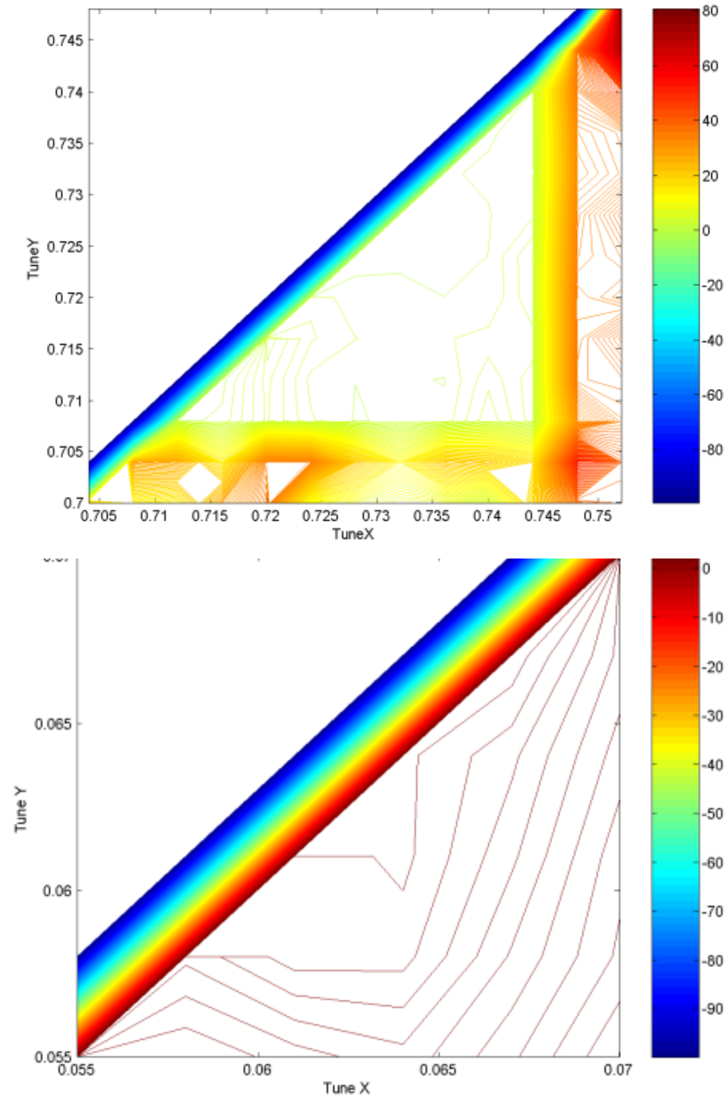
- What does the application do, and how?

- This simulation suite will contain a comprehensive set of interoperable components for beam dynamics, electromagnetics, electron cooling, and advanced accelerator modeling. Beam dynamics studies will include developing an understanding of the lifetime limits from beam collisions in colliders. Electromagnetics modeling will be used to optimize cavity shapes for increased accelerating gradient and beam current. Electron cooling computations will determine the configuration of cooling systems needed for mitigating beam-beam effects. Advanced accelerator modeling is needed to develop concepts for HEP accelerators beyond the ILC and to develop tabletop electron accelerators for BES and NP projects.

- In the beam dynamics simulation area, we use a parallel particle-in-cell approach to for multi-physics self-consistent simulations

# BeamBeam3D applied to RHIC



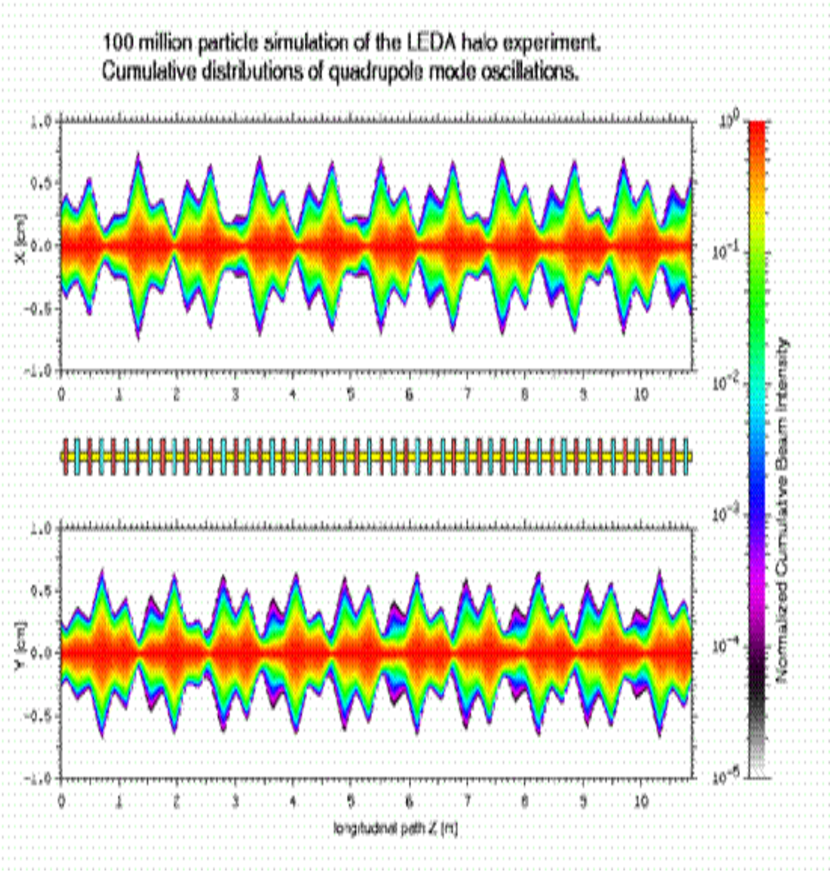




Emittance growth scan in tune space for a nominal working point (top right) and for a new working point (bottom right) at RHIC from BeamBeam3D simulation

J. Qiang, LBNL, W. Fischer, BNL

# IMPACT-Z

- Parallel PIC code using coordinate "z" as the independent variable
- Key Features
  - Detailed RF accelerating and focusing model
  - Multiple 3D Poisson solvers
    - Variety of boundary conditions
    - 3D Integrated Green Function
  - Multi-charge state
  - Machine error studies and steering
  - Wakes
  - CSR (1D)
  - Run on both serial and multiple processor computers



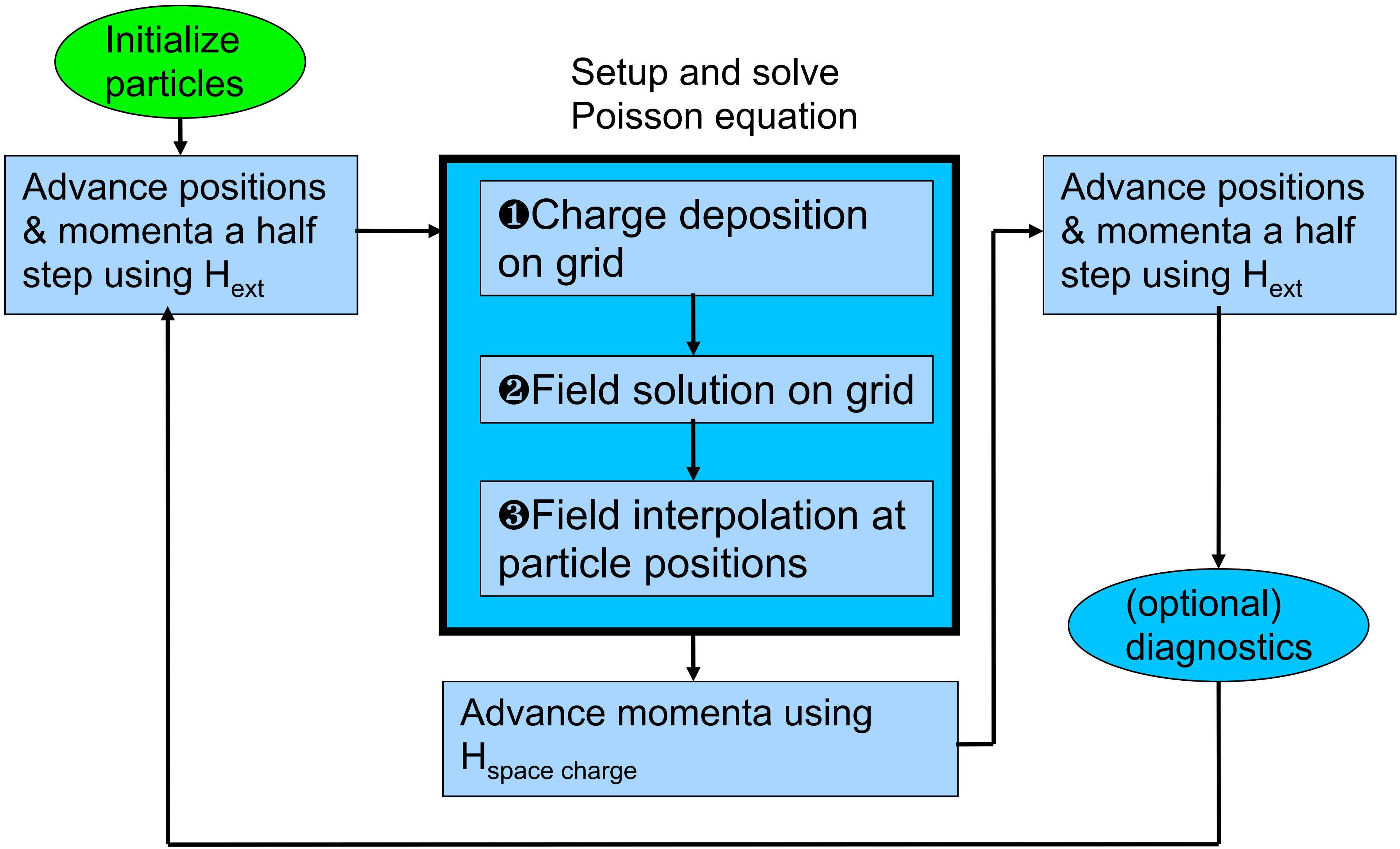
# C) Parallel Programming Model

- MPI
- Fortran 90
- Runtime libraries: hdf5, fftw
- Other infrastructure: python, idl
- What platforms does the application currently run on?
  - Almost all platforms
- Current status & future plans for the programming model
  - MPI+OpenMP+more

# D) Computational Methods

- What algorithms and math libraries do you use?
  - Particle-in-cell, FFT
- Current status and future plans for your computation
  - Currently use uniform grid
  - Plan to develop adaptive mesh solver to calculate Coulomb forces

# Particle-In-Cell Simulation with Split-Operator Method




Courtesy of R. Ryne

# E) I/O Patterns and Strategy

- Input I/O and output I/O patterns
  - One file with information collected from all PEs
  - Each PE output its own file
  - HDF5
- Approximate sizes of inputs and outputs
  - Mbytes to Tbytes
- Checkpoint / Restart capabilities: what does it look like?
  - Macro-particle phase space coordinates
- Current status and future plans for I/O
  - Work on HDF5

# F) Visualization and Analysis

- How do you explore the data generated?
  - Gnuplot, Matlab
- Do you have a visualization workflow?
  - Not yet
- Current status and future plans for your viz and analysis
  - Work with VIS/Analysis team to try VisIT

# G) Performance

- What tools do you use now to explore performance:
  - IPM
- What do you believe is your current bottleneck to better performance?
  - Single PE speed, communication and load balance
- What do you believe is your current bottleneck to better scaling?
  - Communication, load balance

# H) Tools

- How do you debug your code?
  - Manully print-out or use totalview
- Current status and future plans for improved tool integration and support

# I) Status and Scalability

- How does your application scale now?
  - Single simulation on ~k cores
  - Optimization on ~10 k cores
- Where do you want to be in a year?
  - Single simulation on ~ 10 k cores
- What are your top 5 pains? (be specific)
  - Global communication, load imbalance
- What did you change to achieve current scalability?
  - Domain decomposition to Particle-field decomposition,

# J) Roadmap

- Where will your science take you over the next 2 years?
  - New big accelerator design (Project-X, Muon collider, NGLS)
- What do you hope to learn / discover?
  - Improve the code performance
- What improvements will you need to make (algorithms, I/O, etc)?
  - Better Poisson solver, parallel I/O

# Vision for a future light source facility at LBNL

## A HIGH REP-RATE, SEEDED, VUV — SOFT X-RAY FEL ARRAY