Present and Future Computing Requirements for NERSC repository m327: “Parallel Simulation of Electron Cooling Physics and Beam Transport”

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Workshop: Large Scale Computing and Storage Requirements for Nuclear Physics

May 26, 2011

Work supported by the US DOE Office of Science, Office of Nuclear Physics, including grant No.’s DE-FC02-07ER41499 and DE-SC0000835. Resources of NERSC were used.
1. m327 Project Overview

- PI: David Bruhwiler (Tech-X Corporation)
- Summarize scientific objectives through 2014
  - Provide computational support to BNL and Jlab
  - Reduce technical risk for future Electron-Ion Collider
    - eRHIC (BNL concept) and ELIC (JLAB concept)
- Present focus is in three areas
  - electron cooling of relativistic hadron beams (increase luminosity)
  - beam-beam collisions (effect on beam dynamics, luminosity)
  - spin-tracking (how to keep polarized beam fraction high)
- In the next 3 years we expect to …
  - support CeC proof-of-principle experiment underway at BNL
  - larger-scale to support near-term RHIC efforts & also EIC
  - beam-beam to support RHIC, LHC, ELIC design
Coherent e- Cooling (CeC) is a priority for RHIC & the future Electron-Ion Collider

• 2007 Nuclear Science Advisory Committee (NSAC) Long Range Plan:
  – recommends “…the allocation of resources to develop accelerator and detector technology necessary to lay the foundation for a polarized Electron-Ion Collider.”

• 2009 Electron-Ion-Collider Advisory Committee (EICAC):
  – selected CeC as one of the highest accelerator R&D priorities
  – EIC Collaboration website: http://web.mit.edu/eicc

• Alternative cooling approaches
  – stochastic cooling has shown great success with 100 GeV/n Au$^{+79}$ in RHIC
    • Blaskiewicz, Brennan and Mernick, “3D stochastic cooling in RHIC,” PRL 105, 094801 (2010).
    • however, it will not work with 250 GeV protons in RHIC
  – high-energy unmagnetized electron cooling could be used for 100 GeV/n Au$^{+79}$
    • S. Nagaitsev et al., PRL 96, 044801 (2006). Fermilab, relativistic antiprotons, with $\gamma \sim 9$
    • Cooling rate decreases as $1/\gamma^2$; too slow for 250 GeV protons
  – CeC could yield six-fold luminosity increase for polarized proton collisions in RHIC
    • This would help in resolving the proton spin puzzle.
    • Breaks the $1/\gamma^2$ scaling of conventional e- cooling, because it does not depend on dynamical friction
Staging of all-in-tunnel e-RHIC
e− energy increases from 5 to 30 GeV by building-up SRF linacs

RHIC: 325 GeV p or 130 GeV/u Au

The most cost effective design

Computing for DOE/NP– May 11, 2011
Coherent Electron Cooling (CeC) system:

- Uses FEL to combine electron & stochastic cooling concepts
- A CEC system has three major subsystems
  - **Modulator**: the ions imprint a “density bump” on e- distribution
  - **Amplifier**: FEL interaction amplifies density bump by orders of magnitude
  - **Kicker**: the amplified & phase-shifted e- charge distribution is used to correct the velocity offset of the ions

1.b. Limited Scope of this Presentation

• m327 is not the only repo supporting accelerator technology
  • Other relevant NP activities in accelerator modeling and design:
    • SLAC
      • FEM modeling of SRF cavities at JLab, MSU/FRIB
    • LBL
      • parallel particle tracking & beamline design
      • additional beam-beam simulations for JLab, RHIC, LHC, EIC
    • ANL
      • FEM modeling of SRF cavities for FRIB
      • parallel particle tracking & beamline design for FRIB
      • Vlasov/Poisson algorithm development
    • Tech-X
      • FDTD modeling of SRF cavities for JLab
      • inverse cyclotron for light-ion stopping at FRIB
      • electron gun modeling for BNL (diamond amplifier project)
2.a. Current HPC Methods

• Algorithms used
  • coherent electron cooling (CeC)
    • ES PIC; δf PIC; Vlasov (all use FDTD, Poisson, unif. mesh)
  • beam-beam and spin-tracking
    • pushing particles through complicated external fields
    • Poisson solves used in some cases for “space charge kicks”

• Codes
  • The parallel VORPAL framework (Tech-X and collab’s)
    • particle-in-cell; fluids; geometry; multi-physics; vlasov
    • electromagnetics, electrostatics
  • Trilinos, PETSc, parallel HDF5, new algorithm development
    • electron cooling, SRF cavities, laser-plasma, fusion, beams
  • DOE/NP, HEP, BES, OFES applications; also DOD
  • BeamBeam3D and IMPACT-T (LBL and collab’s)
  • SimTrack (BNL and collab’s)
  • Teapot-SpinTrack (part of UAL framework) (BNL and Tech-X)
2.b. Current HPC Methods

• Quantities that affect problem size, scale of simulations (electron cooling only)

• δf PIC uses macro-particles to represent deviation from assumed equilibrium distribution
  – much quieter for simulation of beam or plasma perturbations
  – implemented in VORPAL for Maxwellian & Lorentzian velocities

• Typical 3D simulation size
  – 3D domain, 40 $\lambda_D$ on a side; 10 cells per $\lambda_D \rightarrow \sim 10^8$ cells
  – 300 ptcls/cell to accurately model temp. effects $\rightarrow \sim 2 \times 10^{10}$ ptcls
  – $dt \sim (dx/v_{th,x}) / 5$; $\omega_{pe} \sim v_{th} / \lambda_D \rightarrow \tau_{pe} \sim 300$ time steps
  – 1 µs/ptcl/step $\rightarrow \sim 1,000$ processor-hours for $\frac{1}{2}$ plasma period
2.c. Current HPC Requirements (electron cooling only)

- Architectures currently used
  - Franklin, Hopper, small clusters
- Compute/memory load
  - 1,000 proc-hours per run; ~1,000 runs per year (param. scans)
  - 5 GB aggregate memory
- Data read/written
  - reading: input file (negligible size)
  - \(20 \times 5 = 100\) GB (i.e. 20 restart dumps for movie generation)
- Necessary software, services or infrastructure
  - parallel i/o via HDF5; Trilinos; python; VisIt; IDL
- Known limitations/obstacles/bottlenecks
  - none at present or in next year; major problems are looming
- Hours requested/allocated/used in 2011
  - 2.2 million hours requested for FY 2011
  - 0.5 million allocated on Franklin; 0.7 million for Hopper
  - 0.35 million hours used so far (many free hours on Hopper)
3.a. HPC Usage & methods for next 3-5 years

• Upcoming changes to codes/methods/approaches to satisfy science goals (electron cooling only)
  • Large-scale Vlasov/Poisson sim’s for e- cooling to benchmark PIC
  • Move beyond $10^5$ cores for PIC, Vlasov and spin-tracking
    • in part via move towards effective use of GPUs
    • beginning exploration of OpenMP for hybrid parallelism

• Changes to Compute/memory load
  • more resolution & PPC needed in future to model realistic e- beams
    • 50,000 proc-hours per run; ~1,000 runs per year
    • 30 GB aggregate memory
  • full 3D3V Vlasov/Poisson (6D mesh) to benchmark/verify $\delta f$ PIC
    • 300,000 proc-hours per run; ~100 runs per year
    • 150 GB aggregate memory

• Changes to Data read/written
  • $\delta f$ PIC: $20*30 = 600$ GB (i.e. 20 restart dumps for movie generation)
  • Vlasov: $20*150 = 3$ TB
3.b. HPC Usage & methods for next 3-5 years

• Changes to necessary software, services or infrastructure
  • we may need assistance with visualizing 4D and 6D fields
  • assistance with the obstacles listed below may be necessary

• Anticipated limitations/obstacles/bottlenecks on 10K-1M PE system
  • I/O is not now a bottle neck, but it does not appear to scale, so…
  • dynamic load balancing may be required for good efficiency
  • must move to smaller surface-to-volume ratios for MPI domains
    • communication-related overhead will become a bottle neck
    • fault tolerance will become a major concern
VORPAL shows good efficiency at 4k Franklin cores for electrostatic PIC (strong scaling; production simulations of electron cooling)
Strategy for New Architectures

• How are you dealing with, or planning to deal with, many-core systems that have dozens or hundreds of computational cores per node?
  - beginning to explore benefits of OpenMP for hybrid parallelism
  - hoping that MPI-3 will alleviate the problem (perhaps temporarily)

• How are you dealing with, or planning to deal with, systems that have a traditional processor augmented by some sort of accelerator such as a GPU or FPGA or similar?
  - VORPAL electromagnetics (w/ boundaries) is ported to multiple GPUs
  - electrostatic PIC has been prototyped on NVIDIA Fermi architecture
  - BNL codes TEAPOT and Spink were rewritten to use cuda
    - 100x speedup with 10,000 particles has enabled new physics
4.a. Summary I

- What new science results might be afforded by improvements in NERSC computing hardware, software and services?
  - Faster beam-beam and spin-tracking simulations, with greater physical fidelity, could provide physical insight that points to beam dynamics changes that significantly increase the luminosity of RHIC, with greater polarization
    - This would reduce the time/cost required for obtaining important nuclear physics results, and perhaps enable new results
  - Providing computational support to the CeC proof-of-principle experiment at BNL could help that effort succeed, resulting in a fundamentally new and important technique to increase the luminosity of RHIC or of any future EIC facility by orders of magnitude
4.b. Summary II

- Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science
  - present architecture and configuration should work well in the near future
  - Major changes in architecture (e.g. GPU or hybrid CPU/GPU) will require a great deal of additional software development
    - however, we are working to prepare for this transition
- NERSC generally acquires systems with roughly 10X performance every three years. What significant scientific progress could you achieve over the next 3 years with access to 50X NERSC resources?
  - would allow us to use full 3D3V (i.e. 6D mesh) Vlasov/Poisson to benchmark/verify our 3D δf PIC simulations for realistic e- distrib.’s
    - important; otherwise we have less confidence in our δf PIC results
- What "expanded HPC resources" are important for your project?
  - convenient 4D and 6D visualization of fields
  - GPU hardware, supporting libraries, consulting