Title
High Performance Computing in Accelerator Science: Past Successes. Future Challenges

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Publication Date
2011-10-24

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B. Carlsten, D. Higdon, N. Yampolsky,
Los Alamos National Laboratory

Acknowledgements: This work was supported by the Director, Office of Science, High Energy Physics as well as Advanced Scientific Computing Research, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

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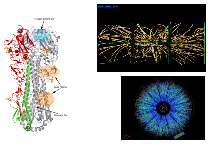
Importance of Accelerators and Accelerator Modeling

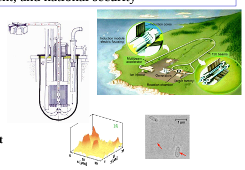
Particle accelerators are among the most versatile instruments of scientific discovery

- materials science
- chemistry
- biosciences
- high energy physics
- nuclear physics



Particle accelerators have important applications in energy, environment, and national security

- interrogation systems to detect nuclear material, explosives in cargo
- accelerator-driven energy production
- studying materials and organisms relevent to energy and the environment

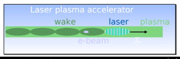


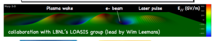
Particle accelerators have a huge impact on the quality of people's lives

- medical irradiation therapies
- pharmaceutical drug design
- medical radio-isotope production

Advanced computing is essential to advancing the frontiers of accelerator science and technology

- cost & risk reduction for upgrades and new projects
- design optimization
- testing new ideas, exploring & gaining incite where measurement/expt is expensive or impossible
- developing advanced accelerator concepts
  - Laser-Plasma Accelerators (LPA's) will revolutionize accelerator technology
    - compact LPA-based accelerators: huge impact to US science, industry, medicine
    - staged LPA's to reach energy frontier





Recognizing the importance of accelerators to the nation, DOE/SC has strongly supported advanced computing for accelerator modeling

- HEP-led DOE SciDAC projects in collab w/ ASCR, NP, BES
- BES accelerator R&D project on future light source modeling
- Strong collaboration between ASCR-supported researchers and accelerator physicists across DOE/SC

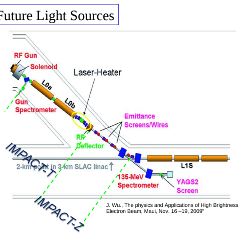
Future Challenges & Opportunities

- Accelerators:
  - Future light sources: advanced injectors; beam manipulation; novel seeding schemes; energy recovery linacs, emittance control, beam loss, halos
  - LPA's: enhanced beam quality control; 10 GeV stages; toward an LPA collider
  - Novel accelerators: e-ion colliders, FRIB, muon accelerators
- Modeling:
  - multicore, hybrid systems – programmability, performance
  - scalability to ~1M cores – algorithms; extreme scale I/O, data analysis, visualization
  - statistical methods for fast emulators
  - HPC in control rooms for near-real-time feedback to experiments

Selected Applications to Accelerator Projects

Modeling Present and Future Light Sources

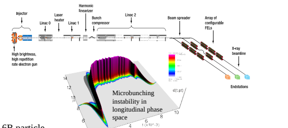
- Parallel, multi-physics, multi-scale modeling:
  - space charge, synch. radiation, nonlinear optics
  - interaction of lasers, plasma, and beams
  - wide spatial and temporal range
- Needed for:
  - predicting microbunching instability, predicting emittance dilution
    - optimization mitigation schemes
  - predicting & optimization injector performance
  - exploring & optimizing novel seeding schemes
  - exploring novel beam manipulation systems



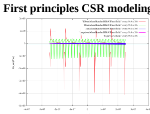
J. Wu., The physics and Applications of High Brightness Electron Beam, Maui, Nov. 16 –19, 2009"

Applications:

- LCLS
  - R. Akre et al., Commissioning the Linac Coherent Light Source injector, PRST-AB, 11, 030703
  - K. Bane et al., Measurements and modeling of CSR and its impact on the LCLS electron beam, PRST-AB, 12, 030704
  - J. Qiang et al., 3D quasistatic model for high brightness beam dynamics simulation, PRST-AB, 9, 044204
- Future XFEL's
  - Next generation light source
  - MaRIE XFEL
- Photoinjectors, streak camera design
- First principles CSR modeling



Microbunching instability in longitudinal phase space



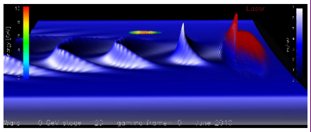
High resolution, 6B particle simulations of CSR enhancement in a microbunched beam (B. Carlsten, R. Ryne, N. Yampolsky)

Parallel multi-billion particle simulation of a FEL linac concept using the IMPACT code suite. Ji Qiang et al., "High resolution simulation of beam dynamics in electron linas for x-ray free electron lasers," PRST-AB, 12, 100702

Modeling Laser-Plasma Accelerators (LPA's)

Lorentz-boosed frame algorithm has enabled up to 1 million times peformance gain for LPA modeling

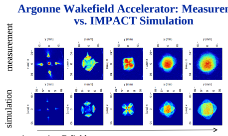
- Lorentz boost technique is applicable to LPAs, free electron lasers (FEL's), electron-cloud effects
- Introduced in 2007, now widely adopted
  - Original paper: J.-L. Vay, Phys. Rev. Lett. 98, 130405 (2007)
  - First direct simulations of LPA stages up to 1 TeV: J.-L. Vay, C. G. R. Geddes, E. Cormier-Michel, D. P. Grote, accepted by Physics of Plasmas Letters
- Large-scale modeling used to guide present LOASIS expts, support design of BELLA facility including future 10 GeV stages



VayPRL07, AAC10, PoP & JCP submitted,.
related: Bruhwiler (Tech X), Martins (UCLA/IST)

Comparison of Large-Scale Simulations with Experiment

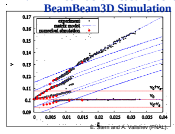
Argonne Wakefield Accelerator: Measurement vs. IMPACT Simulation



increasing B field

M. Rihaoui (ANL), PRST-AB 12, 124201 (2009).

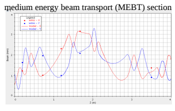
VLEPP collider: Measurement vs. BeamBeam3D Simulation



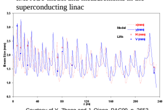
E. Stern and A. Valishev (FNAL).

Spallation Neutron Source linac: Measurement vs. IMPACT Simulation.

IMPACT model and measurements in the medium energy beam transport (MEBT) section



IMPACT model and measurements in the superconducting linac



Courtesy of Y. Zhang and J. Qiang, PAC09, p. 2653.

Collaboration w/ applied math, comp sci, data & vis experts is essential

- ExaHDF5 team: parallel I/O, analysis, vis.
  - Chou, Wu, Rubel, Howison, Qiang, Prabhat, Austin, Bethel, Ryne, Shoshani, *Parallel Index and Query for Large Scale Data Analysis*, to appear in SuperComputing 2011.
- E. Wes Bethel et al (VACET): beam path analysis for LPA
  - O. Rubel, C. G. R. Geddes, E. Cormier-Michel, K. Wu, Prabhat , G. H. Weber, D. M. Ushizima, P. Messmer, H. Hagen, B. Hamann, E. W. Bethel, *Automatic beam path analysis of laser wakefield particle acceleration data*, Computational Science & Discovery, vol. 2, 015005 (2009)
- X. Li: multi-core performance optimization
- H. Shan et al: code performance optimization
  - H. Shan, E. Strohmaier, J. Qiang, D. Bailey, K. Yelik, *Performance Modeling and Optimization of a high energy colliding beam simulation code*, Proc. Supercomputing'06
- D. Higdon et al: statistical methods for inference, forecasting
  - D. Higdon et. al, *Combining Field Data and Computer Simulations for Calibration and Prediction*, SIAM J. Sci. Comput. Vol. 26, No. 2, pp. 448-466 (2004).
- J. Meza: parallel optimization methods

High Performance I/O

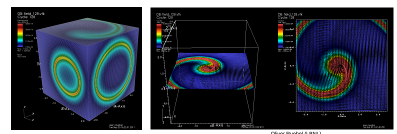
- Using H5Part as data model for ease of use and high performance parallel writes on hopper
- IMPACT-Z generated 56TB dataset on 10,000 franklin cores at NERSC
  - 5GB/s write performance
- Collaboration with ASCR funded *ExaHDF5* project Prabhat (LBL), Koziol (HDF5) and Schuchardt (PNNL)

Data Analysis

- Using FastBit to accelerate queries of interesting particles
  - Halo particles, center slice particles
- Using Parallel FastQuery infrastructure to execute queries on 56 TB dataset
  - Resolved queries in ~10 seconds
  - Queries run on 5,760 hopper cores
- *"Parallel Index and Query for Large Scale Data Analysis"*, by Chou, Wu, Rubel, Howison, Qiang, Prabhat, Austin, Bethel, Ryne, Shoshani. To appear in SuperComputing 2011.

Large Data Visualization

- Exploring massive data sets
  - Billions of particles in 6D phase space, EM fields, 1000's of time steps
  - study mechanisms of halo formation and emittance dilution
  - study complex processes in LPA's
- Collaboration with SciDAC VACET (Wes Bethel, PI)



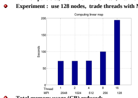
Oliver Ruebel (LBNL)

Parallel visualizations of coherent synchrotron radiation (CSR) using VisIt on Hopper

MPI + OpenMP analysis of computational kernels

MPI + OpenMP : time to compute H_ext

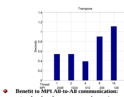
- Hopper @ NERSC, 24 cores per node
- 1 billion particles, 129 x 129 x 2048 mesh, 2 turns
- Experiment : use 128 nodes, trade threads with MPI tasks



- Total memory usage (GB) reduced:
  - 410 → 313 → 241 → 214→201

MPI + OpenMP : transpose time in 3D FFT

- hopper @ NERSC, 24 cores per node
- 1 billion particles, 129 x 129 x 2048 mesh
- Experiment : use 128 nodes, trade threads with MPI tasks



- Benefit to MPI All-to-All communication:
  - Involves fewer messages, larger size per message
  - Reduced from 70% to 40% of the transpose time

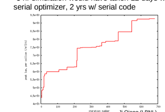
Xiaoye Li (LBNL)

Multi-level parallel implementation for multi-objective design optimization

# processors	time (sec)	problem size	efficiency
6400	2522	100	1
12800	2611	200	0.97
25600	2700	400	0.93
51200	2890	800	0.87
102400	2710	1600	0.93

Testing on Cray XT-5 at NCCS shows good scalability up to 100K procs

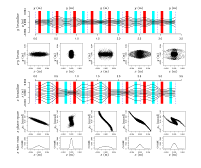
- Parallel, differential evolutionary algorithm to select best working point in tune space
- 3 hr simulation would have taken 12 days w/ serial optimizer, 2 yrs w/ serial code

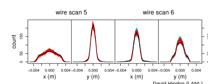


Ji Qiang (LBNL)

Parallel design optimization to maximize LHC luminosity

Model Calibration & Forecasting





David Higdon (LANL)

Simulation of a high intensity proton beam through a series of quadrupole magnets (left). Bayesian techniques were used to combine 1D profile monitor data with simulations to infer the 4D beam distribution. The above figure shows the 90% intervals for the predicted profile at scanner #6 (shaded regions), and, for comparison, the observed data (black line). For this analysis, data from wire scan 6 were not used to make this prediction. (D. Higdon et al.)