Advanced Computing for MAP

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Goals of this talk

- Continue discussion about how large-scale parallel accelerator modeling, and other advanced computational methods, can impact MAP

Trends in HPC

- Multi-core systems
  - already have >100K cores in supercomputers
  - expect >1M cores in the near future
  - need hybrid prog. for best performance (not just MPI)
- Heterogeneous systems
  - GPUs provide potential for ~50-100x performance gains
- Sustained multi-petaflop coming soon
- What all this means for you:
  - "easy" to get access to ~~1000's cores~~ 10K – few 10's K cores now
  - expect many more in the future
    - » some day "small" will mean "< 100K cores"

Computational resources

- DOE/SC HEP provides substantial computational resources at NERSC (5M hours this year) for accelerator modeling; also, resources available at Argonne LCF and Oak Ridge LCF

If you need parallel computing time for large-scale simulations for MAP-related activities, contact the ComPASS project; we will request an account for you at NERSC and provide access to the ComPASS repository

Several issues relevant to MAP could benefit from advanced computing

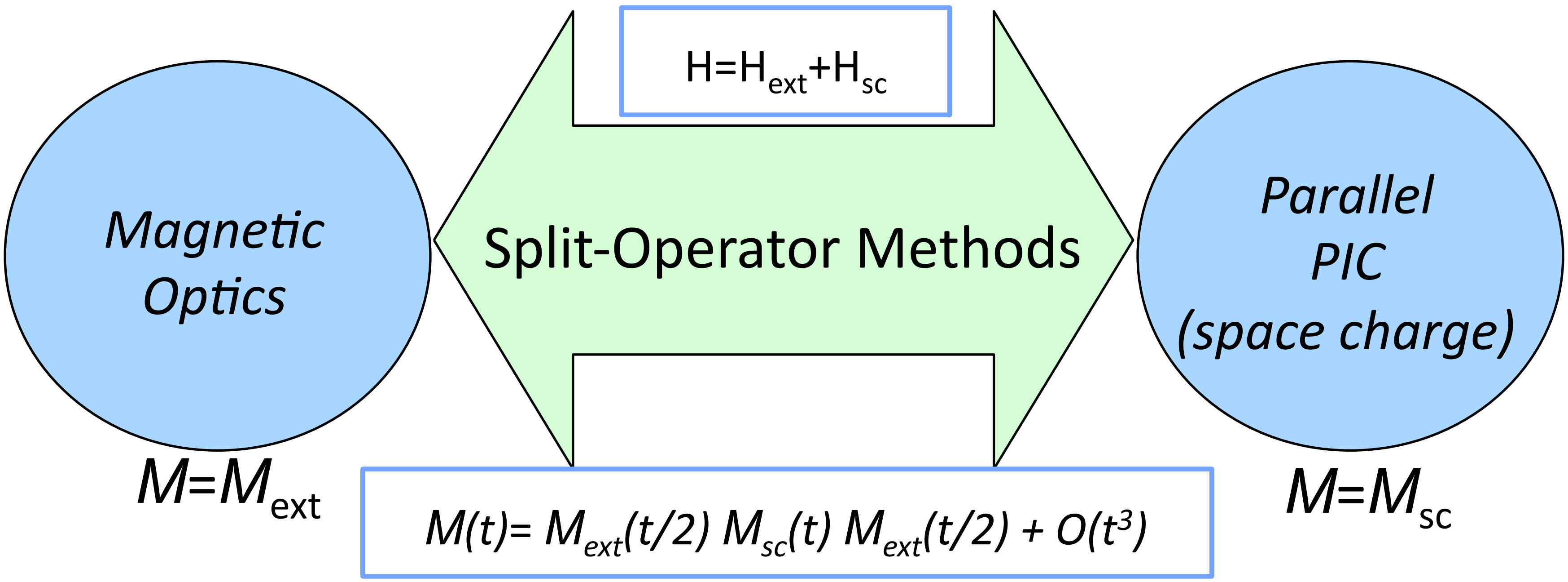
- Space-charge effects
- Beam-beam effects
- Wakefield effects
- CSR effects
- Large-scale EM design
- Tools for design optimization
- Parallelization of cooling
- Nonlinear dynamics in systems with unconventional geometries (helical) and unconventional parameter regimes (large energy spread)

Parallel 3D space charge

- IMPACT, Synergia
  - high order optics + parallel 3D space charge + wakes + …
  - 3D space charge is challenging
    - currently able to treat a variety of boundary conditions
- Build upon these codes, add:
  - particle decay
  - interfaces to parallel cooling codes
  - algorithms for large energy spread, helical geometry

Combining parallel space-charge modeling w/ other effects in a Hamiltonian framework

- Use split operator method to combine high order optics w/ parallel particle-in-cell



High order, if desired, using Yoshida method

Including parallel space charge in serial optics code

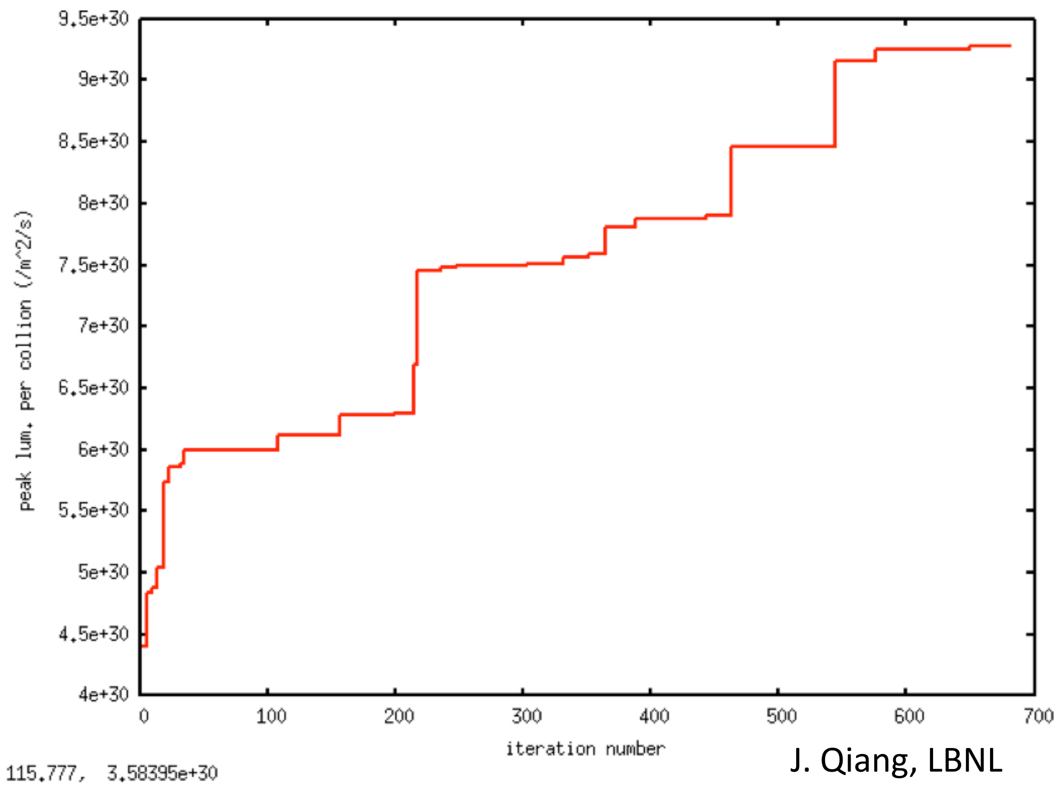
- Easy to parallelize the single particle dynamics
- Inclusion of parallel space charge is complicated
  - significant effort required for performance optimization
  - various parallelization approaches
    - domain decomposition, particle decomp, hybrid decomp
- But it is easy to include space charge if you replicate the grid and solve Poisson serially
  - good first step to produce code quickly that works
  - but it will not scale

BeamBeam3D: Parallel Strong-Strong / Strong-Weak Simulation

- Multiple-slice model for finite bunch length effects
- Novel algorithm -- shifted Green function -- efficiently models long-range parasitic collisions
- Parallel particle-based decomposition to achieve perfect load balance
- Lorentz boost to handle crossing angle collisions
- Arbitrary closed-orbit separation (static or time-dep)
- Independent beam parameters for the 2 beams
- Multiple bunches, multiple collision points
- Conducting wire, crab cavity compensation model
- Parallel parameter scans and parallel optimization
- …

Parallel optimization example: finding machine settings to optimize LHC luminosity

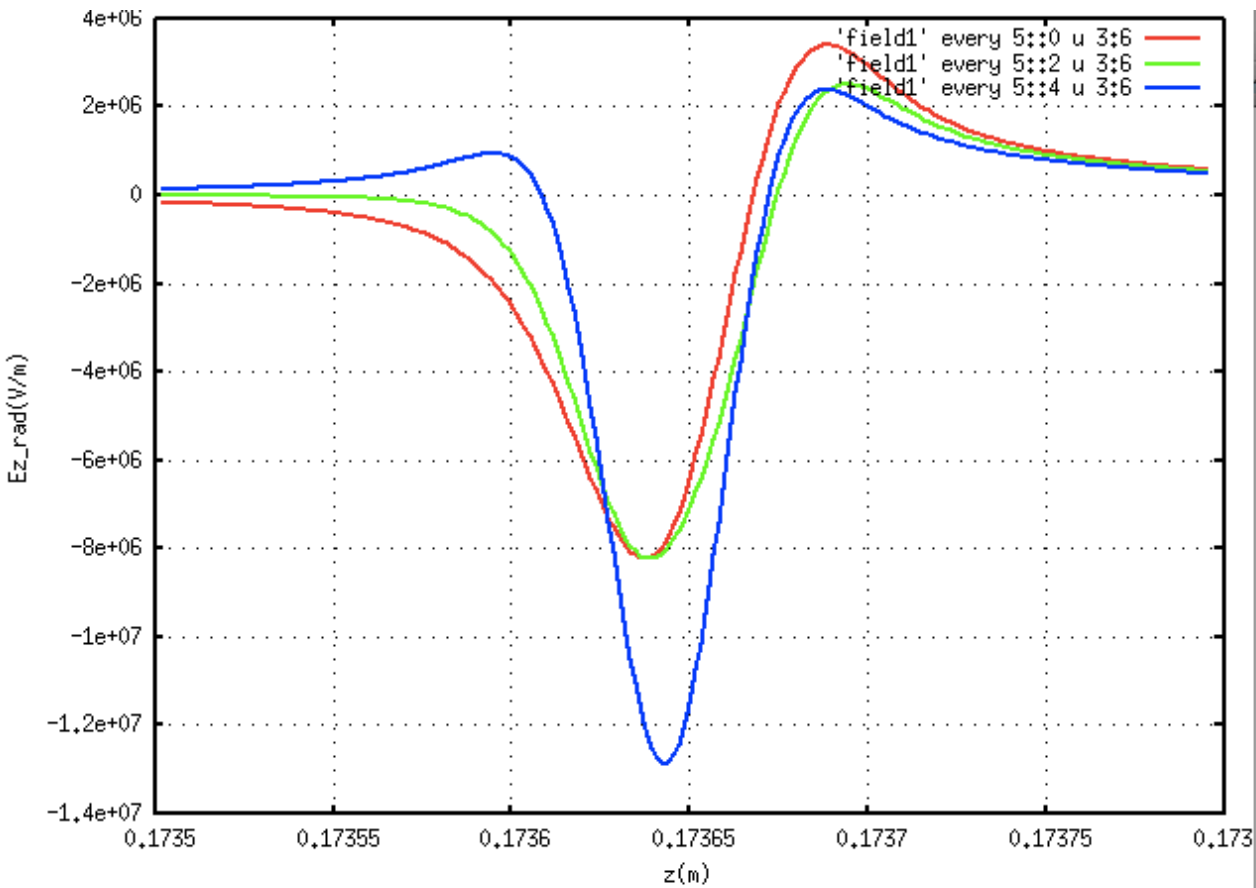
- Parallel, differential evolutionary algorithm to select best working point in tune space
- 12800 procs on Franklin at NERSC; pop. size = 100, procs/pop_member = 128
- 3 hr simulation would have taken 12 days w/ serial optimizer, 2 yrs w/ serial code



J. Qiang, LBNL

Radiation from accelerating charges

- 3D effects of CSR explored on parallel computers via (not self-consistent) Lienard-Wiechert
  - important in future light sources



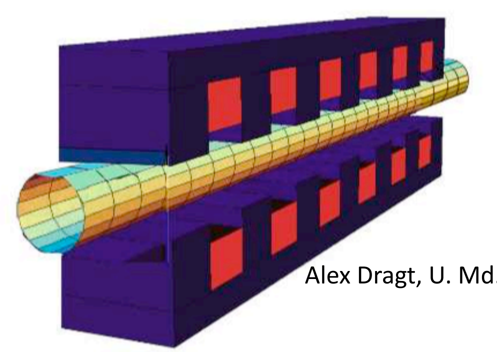
6.24 billion macroparticle simulation (real-world nC)

Simulations up to 96K procs

Using surface data to compute nonlinear transfer maps

- The computation of nonlinear transfer maps involves high order derivatives of axial field data Ez, Bz
- Numerical differentiation of axial grid data to high order is hopeless
- The best approach is to use surface data to compute on-axis generalized gradients
  - surfaces corresponding to cylinders, ellipsoids, bent boxes,…
  - applicable to magnets and rf cavities
  - see papers of A. Dragt, M. Venturini, C. Mitchell, P. Walstrom, D. Abell, …

Given the large emittances in muon systems, and the importance of correct inclusion of nonlinear effects, the use of surface methods would be highly beneficial to MAP



Conclusion

- Advanced computing can have a major impact on MAP
- SciDAC3 will likely be announced this summer
  - continue discussions between MAP and SciDAC/ ComPASS to ensure that future ComPASS activities address needs of MAP

Extra Material

- Overview of SciDAC/ComPASS project

SciDAC overview

- SciDAC=Scientific Discovery through Advanced Computing
- DOE/SC ASCR-led initiative w/ HEP, NP, BES, BER, FES
- Strongly multi-disciplinary
- SciDAC1, SciDAC2, SciDAC3
  - 5 yr programs starting in 2001, 2006, 2011
- http://www.scidac.gov

"… SciDAC research projects are collaborative efforts involving teams of physical scientists, mathematicians, computer scientists, and computational scientists working on major software and algorithm development for and application to problems in the SC core programs, namely, BES, HEP, NP, ASCR, FES, and BER. Research funded under the SciDAC program must address the interdisciplinary problems inherent in ultrascale computing, problems that cannot be addressed by a single investigator or small group of investigators."

ComPASS overview

- ComPASS=Community Petatscale Project for Accelerator Science and Simulation
  - HEP-led SciDAC project; mainly HEP+ASCR, also smaller contributions from NP and BES
  - develop advanced computational capabilities driven by needs of high priority HEP projects
  - http://compass.fnal.gov
  - Contacts/Project mgmt Team:
    - P. Spentzouris (PI), J. Cary (Tech-X), L. McInnes (ANL), W. Mori (UCLA), C. Ng (SLAC), E. Ng (LBNL), R. Ryne (LBNL)

ComPASS codes

- Beam Dynamics including ES-PIC:
  – IMPACT suite
  – Synergia
  – BeamBeam3D
  – MaryLie/IMPACT
  – WARP-POSINST
- Electromagnetics including EM-PIC:
  – ACE3P
  – VORPAL
- Laser/Plasma Accel:
  – OSIRIS, QuickPIC
  – VORPAL
  – WARP

Info on EM codes

- For info on ACE3P, see talk by Zenghai Li at this meeting; www.slac.stanford.edu/grp/acd/ace3p.html

- For info on VORPAL, see www.txcorp.com

Info on Beam Dynamics codes

- Parallel, large-scale, multi-physics
  - 3D space-charge, high-order optics (MaryLie, CHEF), beam-beam, wakes, e-cloud effects, e-cooling, 1D CSR,…

- An example of what is being done now:
  - Using IMPACT, start-to-end simulation of beam delivery system for a future light source, w/ real-world # of particles (~5 billion) requires ~10 hrs on few thousand procs

- Contacts:
  - IMPACT, BeamBeam3D: J. Qiang, JQiang@lbl.gov
  - Synergia: P. Spentzouris, spentz@fnal.gov
  - MaryLie/IMPACT: R. D. Ryne, RDRyne@lbl.gov
  - WARP-POSINST: J.-L. Vay, JLVay@lbl.gov

END OF EXTRA MATERIAL