Computational challenges in state-of-the-art beam dynamics

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SciDAC2: COMPASS Collaboration

Community Petascale Project for Accelerator Science and Simulation

A Proposal Submitted to the DOE Office of Science

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8 laboratories
5 universities
1 company

Topics

- Accelerators at the leading edge of HEP
  - Fermilab complex, LHC, ILC
    - acronyms spelled out later...
  - Gross features of models
- Rudiments of accelerator physics
  - single-particle effects
  - collective effects
- Overview of Synergia2
- Issues in current development

Accelerators at the leading edge of HEP

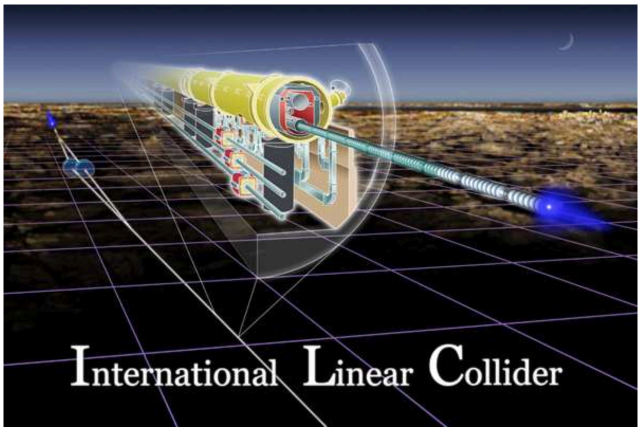
- The Fermilab Tevatron is currently the highest energy machine in the world: 1TeV protons on 1TeV antiprotons

Accelerators at the leading edge of HEP, cont.

- When the CERN Large Hadron Collider (LHC) enters high-energy mode (expected in 2008), it will be the world's new highest energy machine: 7TeV protons on 7TeV protons

Accelerators at the leading edge of HEP, cont.

- The International Linear Collider (ILC) is currently in the planning stages. It will collide 250GeV electrons with 250GeV positrons.



Gross features

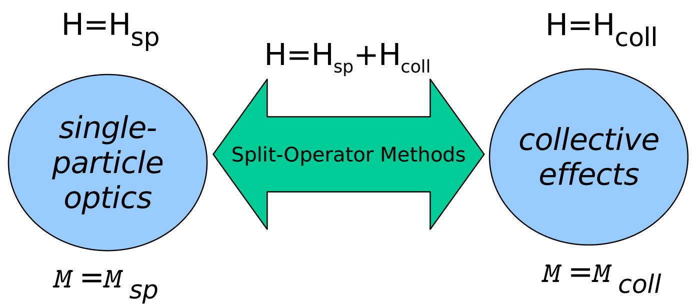
- Accelerators are complex devices
  - e.g., The Tevatron is made up of roughly 4000 individual elements
- Accelerator operations are complex processes
  - Component parameters may ramp according to programs/feedback loops
  - Beams are injected/manipulated to join, separate, etc.
  - etc., etc., etc.

Rudimentary Accelerator Physics

- Take the Fermilab Booster:
  - O(10^11) particles in a bunch
  - O(10^2) bunches in the machine
- Good news:
  - particle-machine interactions are dominant
  - “single-particle optics”
- Bad news:
  - particle-particle interactions are not negligible
  - “collective effects”

Separating single-particle and collective effects

- Combination of particle-in-cell (PIC) and split-operator techniques allow us to separate single-particle optics from collective effects



$$M(t) = M_{sp}(t/2)\, M_{coll}(t)\, M_{sp}(t/2) + O(t^3)$$

A look ahead at the bottom line

- We need to take O(100) steps per revolution in a circular accelerator
  - Machine cycle may be O(10^4 – 10^7) revolutions
  - interesting physics can be found in O(1000) revolutions
- Beam being modeled is a relatively smooth, oscillating blob in a pipe that is O(few) times larger than the blob
- Precision accuracy (in collectives) not usually necessary

Single-particle optics

- (This is a very simplified discussion)
- Analytic and numerical theory of single-particle optics is a mature subject
- We can consider transverse and longitudinal dynamics separately
- Transversely, the main accelerator components are (de-)focusing quadrupole magnets and drifts (empty space)
- Individual particles oscillate back in forth in x- and y-coordinates as a harmonic oscillator with varying strength
  - The number of complete oscillations per turn in a circular accelerator is the *tune*
    - *Booster x,y tunes ~7*
    - *Tevatron x,y tunes ~20*
      - *never an integer or even a simple ratio!*
- The overall shape of the beam "breathes" as it goes through the lattice

Transverse breathing

- A properly *matched* beam breathes according to the lattice (magnet) parameters.
  - The animation shows the transverse (x,y) beam density as a function of time
    - z is always along the beam pipe
- A *mismatched* beam would superimpose a second frequency (determined by the tune.)

Single-particle optics, cont.

- The quadrupole/drift combinations are repeated in n identical/similar periods around a ring
  - n=24 for Booster
- Longitudinally, the dynamics are dominated by RF cavities
- Beams may be bunched, debunched, bunching or debunching

Modeling single-particle optics

- We usually model a section of a beam
  - single bunch
  - multiple bunches
  - slice of uniform beam
- Our modeled section is usually a relatively simple blob
- Transversely
  - shape oscillates
  - particles move within envelope
- Longitudinally
  - shape might expand, contract, or stay the same
  - particles may or may not oscillate

Collective effects

- Space charge (Fermilab Booster, ILC damping ring)
  - interaction of beam particles with themselves
  - requires Poisson solve
- Electron cloud (Fermilab Main Injector, ILC Damping ring, LHC)
  - interaction of beam with electrons knocked off accelerator walls
  - requires Poisson solve
- Beam-beam (Fermilab Tevatron, LHC, ILC interaction point)
  - interaction of colliding beams with each other
  - requires Poisson solve
- Wake fields (Fermilab Booster, ILC damping ring)
  - interaction of beam with currents generated by beam in pipe

Why bother?

- All effects are proportional to intensity
  - single-particle optics are independent of intensity
- More intensity -> more physics
- Collective effects are often the limiting factor in increasing beam intensity

Synergia2

- Synergia2 combines a state-of-the-art implementation of single-particle optics (CHEF, from FNAL) with the current state-of-the-art implementation of space charge effects (IMPACT, from LBNL and other solvers developed at FNAL)
- Really a Python framework
  - Components can be mixed and matched
  - Simulations are simple Python programs, allowing for arbitrarily complex simulations

Synergia2

We do not believe in re-inventing the wheel

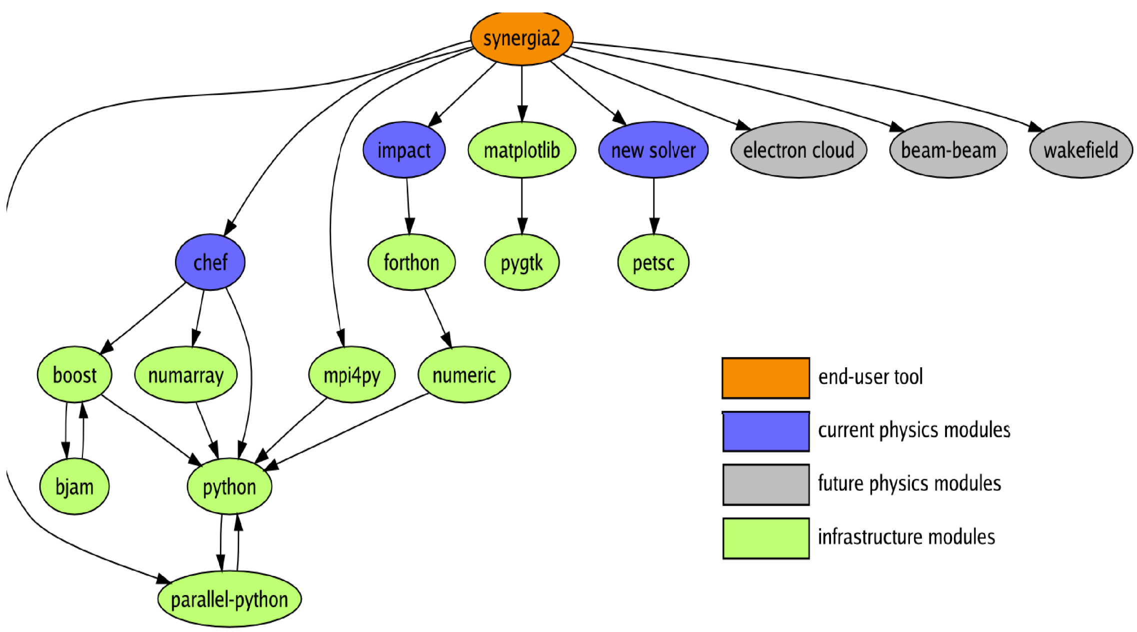
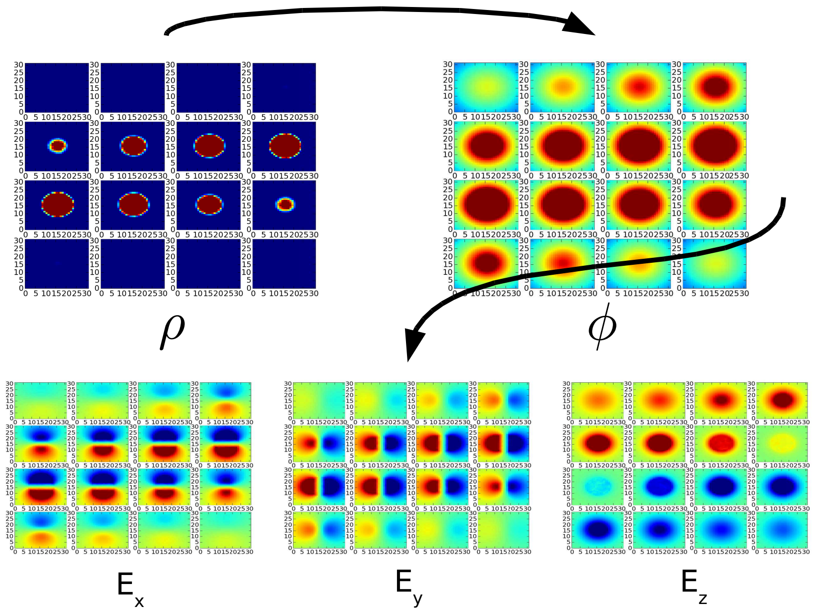


Diagram (mostly) generated by meta-build tool Contractor

Poisson solvers

Prototypical element of collective effect simulation:
Poisson solver

Use space charge as an example application



Parallel FFT-based Poisson solvers

- IMPACT
  - F90
  - State-of-the-art for a long time
    - established, benchmarked
- New FFTW-based solver
  - C++
  - Uses FFTW3.2 (currently in alpha release)
    - First FFTW3 with MPI parallelism
    - “Fastest Fourier Transform in the West”
    - Actively maintained
      - widely used, tested
  - Can also use FFTW2
    - previous stable *parallel* FFTW

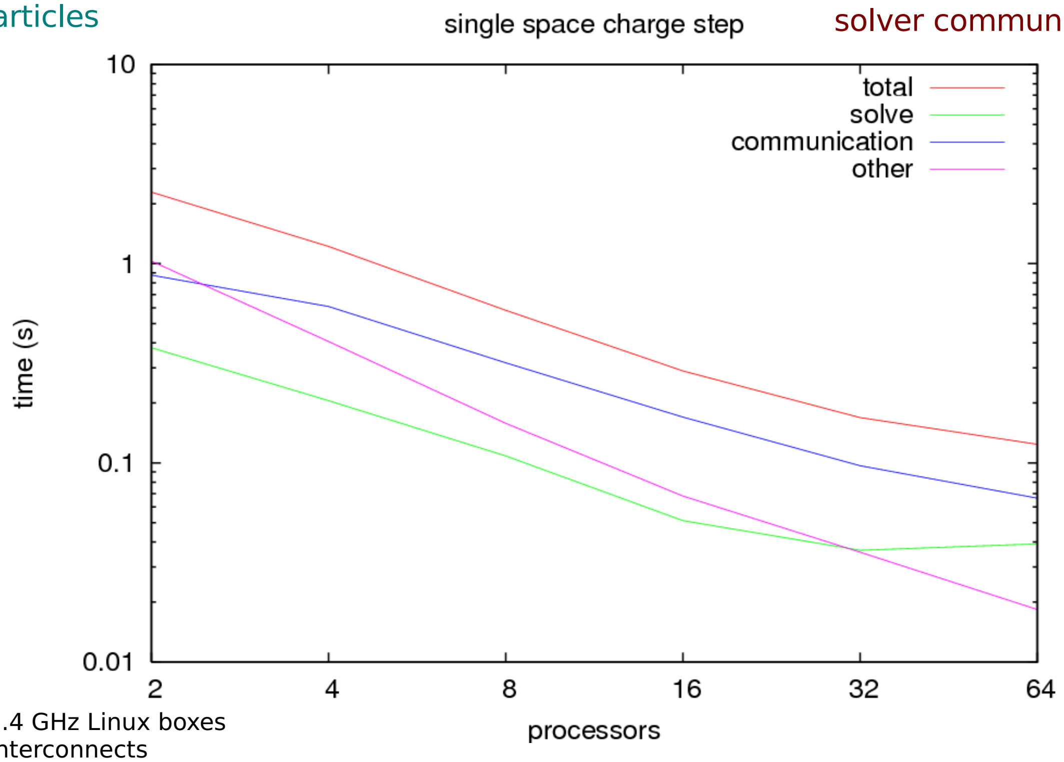
FFT limitations

- Uniform grids
  - ILC beam is highly asymmetric
- Poor parallel scaling
- Limited boundary conditions
  - open
  - square conducting pipe
  - round conducting pipe

Solvers aren't the end of the story

IMPACT solver
32x32x256 grid
1M particles

"communication"
is above and beyond
solver communication



48 dual 2.4 GHz Linux boxes
Myrinet interconnects

Parallel decomposition schemes

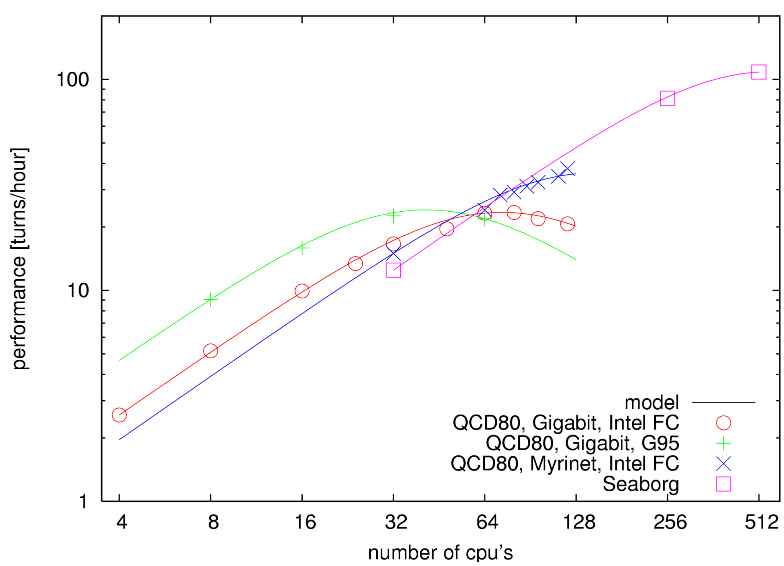
- Particle/field decomposition
  - spatial decomposition of fields
  - spatial decomposition of particles
    - ***performance depends on physics***
  - used in IMPACT
- Field decomposition
  - spatial decomposition of fields
  - particles uniformly, randomly distributed
    - ***performance independent of physics***
  - currently used with new FFTW-based solver

Particle/Field Decomposition

- Communication pattern consists of many small point-to-point communications
- Benchmarking verifies that the performance is limited by latency

fit to t = aN + b/N

find a ∝ latency

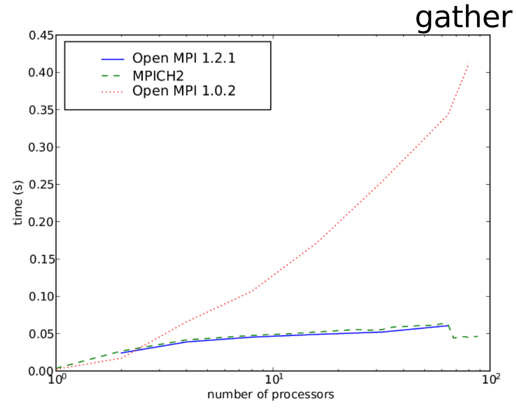


Field decomposition

- No particle movement necessary
  - Charge density requires gather
  - Electric fields must be scattered
- Collective communications on few large messages
  - less sensitive to latency
    - better on commodity networks
  - takes advantage of optimized MPI collectives

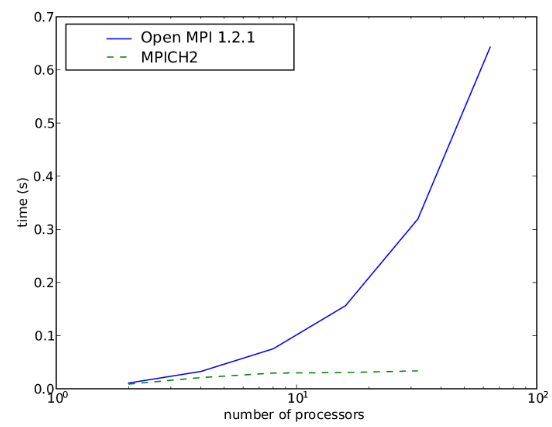
MPI collectives subtleties

gather



- Open MPI 1.0
  - naive collectives
- Open MPI 1.2
  - improved collectives
- MPICH2
  - less convenient, etc.

scatter



- Open MPI 1.2
  - not optimized on all collectives

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Summary

- Collective effect simulations have two pieces
  - The effect
    - the hard part
  - Single-particle optics
    - scaling is trivial
- The problem involves
  - Many solves (O(10^5)) of medium-size
  - Applying results to O(10^6) particles
    - With a varying spatial domain

Extra slides

Synergia single-particle optics

- The simplest way to calculate single particle optics is to extract maps (arbitrary-order Tailor expansions) from CHEF and apply to particles
- Our sparse map application has been demonstrated to scale to at least 15th order
  - a 15th order map has 6^16=2821109907456 possible elements

PIC space charge calculation

- Calculate charge density on a grid in rest frame
  - Typical grid sizes 64^3, 32x32x256
  - Typical number of particles is 10^6
- Solve Poisson Equation for electric potential in rest frame
- Differentiate potential to obtain electric field
- Boost electric field to beam frame
- Apply kicks due to electric field
- Typically perform 4 kicks per cell in FNAL Booster
  - 96 kicks per turn
- Interesting time scales are typically O(1000) turns
  - Booster cycle is 20,000 turns

IMPACT parallel implementation

- Divide processors into 2-d grid according to (y and z coordinates)
- Move particles to appropriate processors
  - Use nearest-neighbor communication
  - charge density, potential and field are all local to processor
  - domains are periodically updated
- Solve Poisson via FFT
  - solution utilizes grid-doubling, so a typical FFT size is 128x128x128