Synergia: a new platform for beam dynamics with multiple bunch interactions

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Synergia

- Synergia is a comprehensive package for beam dynamics
- How comprehensive?
  - Single particle dynamics
  - Single bunch dynamics
  - Multiple-bunch (train) dynamics
  - Dual-train dynamics
    - The newest addition to Synergia

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Logo soup for breakfast

Synergia: A comprehensive accelerator beam dynamics package

http://web.fnal.gov/sites/synergia/SitePages/Synergia%20Home.aspx

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Accelerator Simulation Group

Funded by DOE

Computer time from INCITE and ALCC

The ComPASS Project
High Performance Computing for Accelerator Design and Optimization

https://sharepoint.fnal.gov/sites/compass/SitePages/Home.aspx

Funded by DOE SciDAC

ASCR Leadership Computing Challenge

ALCC

U.S. DEPARTMENT OF ENERGY

INCITE

LEADERSHIP COMPUTING

CAMPAG

Consortium for Advanced Modeling of Particle Accelerators

Funded by DOE
Synergia concept

• The split-operator method combines external fields (magnets) with internal fields (space charge, wakefields)
  – 1/2-step external fields + full step internal kick + 1/2 step external fields
  – External field calculations (single-particle effects)
    • Trivially parallelizable
  – Internal field calculations (collective effects)
    • Particle-in-cell calculation
• Synergia is a framework based on a generalization of the split operator approach
Computational details

- Synergia simulations are (usually) Python applications
  - Synergia functionality is provided in the form of a library of classes
    - Implementation is entirely C++ with Python bindings
  - Pure C++ applications are also possible
- Synergia allows users to implement run-time logic for ramping, feedback, \textit{etc.}
- Synergia provides examples ranging from a trivial FODO cell to real-world accelerators with realistic running conditions
- Synergia simulations are fully checkpointable
  - Including user-provided classes
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CHEF provides single-particle physics for Synergia

• CHEF is a single-particle beam dynamics library by Leo Michelotti (FNAL)
  – magnets, cavities, drifts, etc.
    • direct symplectic tracking
    • (and/or) arbitrary-order polynomial maps
  – utilizes automatic differentiation
    • same code to do tracking and nonlinear map generation
  – many advanced analysis features
    • nonlinear map analysis, including normal forms
    • lattice functions (multiple definitions)
    • tune and chromaticity calculation and adjustment
    • etc.
Normal form analysis

- Linear case (FODO cell) transforms elliptical Poincare phase space plots to circular action-angle representation
Normal form analysis

- Nonlinear case (includes octupole and skew quadrupole)
Aperture model

- Apertures can be associated with elements and/or steps
- 2D model
  - could be extended with slices
- Geometric
  - circular
  - elliptical
  - rectangular
  - polygon
  - wire
- Abstract
  - phase space
  - Lambertson
    - removes particles
- New apertures can be implemented by the end user
Preparing for Exascale (optimizing for Intel Phi)

- libFF is our next-generation single particle implementation
- libFF gives an overall speedup compared to CHEF
- Explicit vectorization gives another overall speedup
  - libFF required for vectorization
- OpenMP allows us to take advantage of all 240 hardware threads
- Overall speedup for quadrupole is 5768x
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Collective effects in Synergia

• Collective effects are Synergia’s *raison d’etre*
• Single bunch collective effects in Synergia include
  – Wakefields
    • Arbitrary wake functions
  – Space charge
    • Variety of boundary conditions and levels of approximation
    • 3D open transverse boundary conditions
    • 3D conducting rectangular transverse boundary
    • 3D conducting circular transverse boundary
    • 2.5D open boundary conditions
      – 2D calculation, scaled by density in longitudinal slices
    • 2D semi-analytic
      – uses Bassetti-Erskine formula, $\sigma_x$ and $\sigma_y$ calculated on-the-fly
• New space charge models can be implemented by the end user
• Resonant extraction in FNAL Debuncher Ring for Mu2e experiment
  – Ramped nonlinear lattice combined with significant space charge effects

• Study emittance growth over 100,000 revolutions in GSI SIS18 accelerator
  – 7,100,000 steps, 4,194,304 particles
  – 29,779,558,400,000 particle-steps
  – 1,238,158,540,800,000 calls to “drift”

Study of emittance growth and statistical noise
Synergia Single-bunch Space Charge for Theoretical Studies

- Space charge modes provide theoretical framework for space charge studies
- Difficult to extract modes from noise in realistic simulation
- First use of Dynamic Mode Decomposition (DMD) in Beam Dynamics
- Excellent theory/simulation agreement

- Booster simulations also led to discovery of parametric Landau Damping
  - Macridin, Burov, et. al.
  - Fermilab PUB-16-391-APC-CD
Preparing for Exascale

• Communication avoidance
  – Field solves are a fixed size problem
  – More calculation, less communication
  – Allows scaling in number of particles and/or bunches
  – Can use arbitrary unit size, but one node is usually best

• With communication avoidance, we have achieved strong scaling over ~1000x

Single-bunch strong scaling from 16 to 16,384 cores
32x32x1024 grid, 105M particles
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Bunch train dynamics

- Synergia can propagate a *train* of bunches
  - Collective effects can either apply to bunches individually, collectively, or both
  - Space charge is in the first category
  - Wakefields are in the last category
- Bunch train simulations can be very large
  - Synergia shows excellent weak scaling

**ALCF’s Intrepid**
Weak scaling from 64 to 1024 bunches
8192 to 131,072 cores; up to over $10^{10}$ particles
Synergia Bunch Train with Wakefields Example

- Synergia qualitatively reproduces an observed instability in the Fermilab Booster
- The wakefields are large and complicated due to the presence of exposed laminations
- Simulating an entire bunch train was critical
  - Instability only occurs in simulations of at least 14 bunches
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Motivation: Slip Stacking in the Fermilab Recycler and Main Injector

• The Fermilab Recycler and Main Injector are the two largest components of the current Fermilab accelerator complex
• Slip stacking
  – Used to create high-intensity beams
  – Pairs of bunches combined
  – First approximation: periodic boundary conditions to mimic other pairs
  – Realistic simulations will include O(500) pairs
  – Non-trivial structure observed in operation
• Truly a leadership class computing problem.
• Work in progress!
First attempt at slip stacking

- Periodic boundary conditions to simulate infinite, uniform stream of bunches
- Captures some of the physics
- Plots show longitudinal phase space
Dual-train propagation in Synergia

• In order to properly simulate the physics of two slipping trains of particles we have extended the Synergia propagation model to include dual-train propagation
  – Model could also be used for electron cloud-beam dynamics
  – Model could also be used for beam-beam dynamics
    • *Neither yet implemented*

• Simulations include two trains with relative motion
Dual-train Space Charge

First, note that the trains are typically well-separated in phase space, but strongly overlapping in physical space

− Bunches are well-separated longitudinally within a train

Space charge algorithm for dual-train propagation: use superposition

1. Calculate internal space charge for each bunch, saving fields
2. Find overlapping bunches
   − Each primary bunch (batch A) will have 0-2 overlaps with bunches from batch B
     • If bunches are evenly spaced, which they are here, but Synergia also allows uneven spacing
3. For each overlapping pair, exchange fields and kick particles due to other bunch’s field
   − alternate odd/even bunches to avoid contention
First Synergia Results with Dual-train Space Charge

Slip portion of slip stacking for 2x2 bunches in the Fermilab Recycler under realistic conditions

RR Turn 0
Conclusions

• Synergia is a comprehensive framework for beam dynamics simulations.
  – Single-particle physics
  – Single-bunch physics
  – Bunch-train physics
  – Dual-train physics

• We are expanding Synergia to meet the needs of the accelerator community while also preparing for Exascale computing.