Berkeley Lab Accelerator Simulation Toolkit

Detailed modeling of:
• beams, plasmas, laser-plasma inter., linacs, rings, injectors, plasma accelerators, traps, ...

Using state-of-the-art codes:
• BEAMBEAM3D, IMPACT, INF&RNO, POSINST, WARP.

With original advanced algorithms:
• boosted frame, IGF, laser envelope, SEY, AMR, relativ. particle pusher, EM spectral Circ, ...

http://blast.lbl.gov
IMPACT: Integrated Map and Particle Tracking Code

• The IMPACT(-Z depend.) started around middle of 90s (R. Ryne) including:
  - Drift, Quadrupole, RF linear transfer map
  - one 3D space-charge solver with open BCs
  - a few thousand lines of High Performance Fortran (HPF) code

• Redesign of the IMPACT code around the end of 90s (J. Qiang):
  - object-oriented design and implementation using F90
  - domain decomposition parallelization using MPI
  - multiple 3D space-charge solvers with open BCs, periodic BCs, conducting pipes
IMPACT: Recent Advances

• Current Features (with >100,000 lines of code) include:
  – Z dependent and T dependent tracking
  – Detailed 3D RF accelerating and focusing model, dipole, solenoid, multipole, ...
  – Multiple charge states, multiple bunches
  – 3D shifted-integrated Green’s function space-solver
  – 3D spectral finite difference multigrid space-solver
  – Structure + resistive wall wakefields
  – CSR/ISR
  – Gas ionization
  – Photo-electron emission
  – Machine errors and steering

• Can be used to model beam dynamics in:
  – Photoinjectors
  – Ion beam formation and extraction
  – RF linacs
  – Rings
Governing Equations in the IMPACT Code

\[
\frac{\partial f (\vec{r}, \vec{p}, t)}{\partial t} + \vec{r} \frac{\partial f (\vec{r}, \vec{p}, t)}{\partial \vec{r}} + \vec{p} \frac{\partial f (\vec{r}, \vec{p}, t)}{\partial \vec{p}} = 0
\]

\[
\dot{\vec{r}} = \frac{\partial H}{\partial \vec{p}}
\]

\[
\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{r}}
\]

\[
H \doteq H_{\text{ext}} + H_{\text{sc}}
\]

\[
\nabla^2 \phi = -\rho / \varepsilon \quad \rho = \iiint f(r, p, t) \, d^3 p
\]
Split-Operator Method for Particle Advance

\[ H = H_{\text{ext}} + H_{\text{sc}} \]

\[ M(t) = M_{\text{ext}}(t/2)M_{\text{sc}}(t)M_{\text{ext}}(t/2) + O(t^3) \]

• Rapidly varying s-dependence of external fields is decoupled from slowly varying space charge fields
• Leads to very efficient particle advance:
  - Do not take tiny steps to push millions - billions of particles
  - Do take tiny steps to compute maps; then push particles w/ maps

Magnetic Optics

Multi-Particle Simulation

(high order possible via Yoshida)
Different Boundary/Beam Conditions Need Different Efficient Numerical Algorithms $O(N\log(N))$ or $O(N)$

FFT based Green function method:
- Standard Green function: low aspect ratio beam
- Shifted Green function: separated particle and field domain
- Integrated Green function: large aspect ratio beam
- Non-uniform grid Green function: 2D radial non-uniform beam

Fully open boundary conditions

Spectral-finite difference method:
2D open boundary
Transverse regular pipe with longitudinal open

Multigrid spectral-finite difference method:

Transverse irregular pipe

Green Function Solution of Poisson’s Equation (I) (open boundary conditions)

\[ \phi(r) = \int G(r, r') \rho(r') dr' ; \quad r = (x, y, z) \]

\[ (r_i) = h \sum_{i'=1}^{N} G(r_i, r_{i'}) (r_{i'}) \]

\[ G(x, y, z) = \frac{1}{\sqrt{(x^2 + y^2 + z^2)}} \]

Direct summation of the convolution scales as \( N^2 \) !!!!

\( N \) – total number of grid points

**FFT based Hockney’s Algorithm / zero padding:- scales as \( (2N)\log(2N) \)**


\[ c(r_i) = h \sum_{i'=1}^{2N} G_c(r_i, r_{i'}) c(r_{i'}) \]

\[ (r_i) = c(r_i) \quad \text{for } i = 1, N \]
Integrated Green Function Method (II)
(large aspect ratio beam with open boundary conditions)

\[ c(r_i) = \sum_{i'=1}^{2N} G_i(r_i, r_{i'}) c(r_{i'}) \]

\[ G_i(r, r') = \int G_s(r, r') dr' \]

Integrated Green function

Standard Green function

Comparison between the IG and SG for a beam with aspect ratio of 30

Integrated Green’s function is needed for modeling large aspect ratio beams!

(O(N log N))

Evolutionary Algorithm for Global Optimization

Differential Evolution Algorithm

- A population of control parameter vectors are randomly generated from the control parameter space.
- A new perturbed vector $\vec{v}_i$ is generated for each parent $\vec{x}_i$ using one of several mutation strategies.
- A trial control parameter vector is generated by:
  
  $\vec{U}_i = (u_{i1}, u_{i2}, \ldots, u_{iD})$
  
  $u_{ij} = \begin{cases} v_{ij}, & \text{if } \text{rand}_j \leq CR \text{ or } j = \text{mbr}_i \\ x_{ij}, & \text{otherwise} \end{cases}$
  
  rand$_j \in [0, 1]$  
  mbr$_i \in \{1, 2, \ldots, D\}$

- If the trial vector produces a better objective function value than $\vec{x}_i$, it will be put into the next generation. Otherwise, the original parent vector is kept in the next generation.

An Adaptive Unified Differential Evolution Algorithm

Some standard DE mutation strategies:

- **DE/rand/1:** $\bar{v}_i = \bar{x}_{r1} + F_{xc} (\bar{x}_{r2} - \bar{x}_{r3})$
- **DE/rand/2:** $\bar{v}_i = \bar{x}_{r1} + F_{xc} (\bar{x}_{r2} - \bar{x}_{r3}) + F_{xc} (\bar{x}_{r4} - \bar{x}_{r5})$
- **DE/current-to-best/1:** $\bar{v}_i = \bar{x}_i + F_{cr} (\bar{x}_{b} - \bar{x}_i) + F_{xc} (\bar{x}_{r1} - \bar{x}_{r2})$
- **DE/current-to-rand/1:** $\bar{v}_i = \bar{x}_i + F_{cr} (\bar{x}_{r1} - \bar{x}_i) + F_{xc} (\bar{x}_{r2} - \bar{x}_{r3})$
- **DE/rand-to-best/1:** $\bar{v}_i = \bar{x}_i + F_{cr} (\bar{x}_{b} - \bar{x}_i) + F_{xc} (\bar{x}_{r2} - \bar{x}_{r3})$

Unified DE mutation strategy (uDE):

$$\bar{v}_i = \bar{x}_i + F_1 (\bar{x}_{b} - \bar{x}_i) + F_2 (\bar{x}_{r1} - \bar{x}_i) + F_3 (\bar{x}_{r2} - \bar{x}_{r3}) + F_4 (\bar{x}_{r4} - \bar{x}_{r5})$$

Encompasses standard DE mutation strategies as special cases. Four control parameters + CR.


1. Define the minimum size, $N_{min}$ and the maximum size, $N_{max}$ of the parent population. Define the maximum size of external storage, $N_{ext}$.
2. Generate an initial population of $N_{init}$ parameter vectors randomly to uniformly cover the entire solution space.
3. Generate an offspring population using the differential evolutionary algorithm.
4. Check the new population against boundary conditions and constraints.
5. Combine the new population with the existing parent population from external storage and determine the non-dominated solutions ($N_{dom}$).
   - Move min($N_{dom}$, $N_{ext}$) solutions back into external storage. Pruning is used if $N_{dom} > N_{ext}$.
   - Select $NP$ parent solutions from this group of solutions for next generation production.
6. If $N_{init} = N_{dom} = N_{max}$, $NP = N_{dom}$. Otherwise, $NP = N_{init}$ if $N_{dom} < N_{init}$ and $NP = N_{max}$ if $N_{dom} > N_{max}$.
7. If the stopping condition is met, stop. Otherwise, return to Step 3.

A comparison of the optimal test solutions from VPES-PMDE and the popular code NSGA-II

A Fully Symplectic Multi-Particle Tracking Model with Space-Charge Effects

multi-particle Hamiltonian

\[ H = \sum_i \frac{p_i^2}{2} + \frac{1}{2} \sum_i \sum_j q \phi(r_i, r_j) + \sum_i q \psi(r_i) \]

\[ \frac{d\mathbf{r}_i}{ds} = \frac{\partial H}{\partial p_i} \]
\[ \frac{d\mathbf{p}_i}{ds} = -\frac{\partial H}{\partial \mathbf{r}_i} \]

Coulomb potential

\[ \frac{d\zeta}{ds} = -[H, \zeta] \]

A formal single step solution

\[ \zeta(\tau) = \exp(-\tau(:H:))\zeta(0) \]

\[ \zeta(\tau) = \exp(-\tau(:H_1:+:H_2:))\zeta(0) \]
\[ = \exp(-\frac{1}{2}\tau:H_1:) \exp(-\tau:H_2:) \exp(-\frac{1}{2}\tau:H_1:)\zeta(0) + O(\tau^3) \]

\[ \zeta(\tau) = \mathcal{M}(\tau)\zeta(0) \]
\[ = \mathcal{M}_1(\tau/2)\mathcal{M}_2(\tau)\mathcal{M}_1(\tau/2)\zeta(0) \]

space-charge  external focusing/acceleration
Single Step Symplectic Map for $H_2$

\[ H_2 = \frac{1}{2\varepsilon_0} \frac{8}{abc} w \sum_i \sum_j \sum_l \sum_m \sum_n \frac{1}{\gamma_{lmn}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \sin(\alpha_l x_i) \sin(\beta_m y_i) \sin(\gamma_n z_i) \]

\[
p_{xi}(\tau) = p_{xi}(0) - \tau \frac{1}{\varepsilon_0} \frac{8}{abc} w \sum_j \sum_l \sum_m \sum_n \frac{\alpha_l}{\Gamma_{lmn}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \cos(\alpha_l x_i) \sin(\beta_m y_i) \sin(\gamma_n z_i) \]

\[
p_{yi}(\tau) = p_{yi}(0) - \tau \frac{1}{\varepsilon_0} \frac{8}{abc} w \sum_j \sum_l \sum_m \sum_n \frac{\beta_m}{\Gamma_{lmn}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \sin(\alpha_l x_i) \cos(\beta_m y_i) \sin(\gamma_n z_i) \]

\[
p_{zi}(\tau) = p_{zi}(0) - \tau \frac{1}{\varepsilon_0} \frac{8}{abc} w \sum_j \sum_l \sum_m \sum_n \frac{\gamma_n}{\Gamma_{lmn}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \sin(\alpha_l x_i) \sin(\beta_m y_i) \cos(\gamma_n z_i) \]
Much Less Numerical Emittance Growth Using the Symplectic Spectral Model

- PIC-finite difference model
- Symplectic spectral model
Some Application Examples of the IMPACT Code

• Simulation of a high intensity proton beam halo experiment
• Simulation of space-charge driven coupling resonance in PS
• Simulation of space-charge effects in next generation light sources
Macroparticle Simulation of a Proton Beam Halo Experiment

Evolution of the Normalized Cumulative Beam intensity

J. Qiang et. al, PRST-AB 5, 124201.
Horizontal Beam Profiles at 9 Wire Scanners
(matched case)
Final Emittance Growth with Different Initial Distributions
(same RMS sizes and emittances)

The detail of the initial distribution matters!
“For this purpose increasing levels of complexity have been planned with simulations, first in 2D approximation and up to 2000 turns:
- step (1) in constant focusing approximation;
- step (2) using a linearized version of the AG lattice;
- step (3) using the fully nonlinear lattice of the PS [7];
- step (4) the 21/2 D or 3D bunched beam simulation including all lattice effects;
- step (5) extension up to the full 13,000 turns of the measurements provided that necessary CPU times – presumably of the order of months – are not prohibitive.
At a later point, after suitable code optimization, the even more ambitious dynamical crossing may be addressed, preferably after new measurements are carried out over less than the demanding 44,000 turns of the 2003 experiment.” - I. Hofmann et al., Proceedings of 2005 PAC.

Space-Charge Driven Coupling Resonance at PS

[Graphs and images related to space-charge driven coupling resonance at PS]
Static Montague Resonance Crossing at PS

measurements

emittances (m-rad)

Horizontal tune

IMPACT simulation

emittances (m-rad)

horizontal tune
Dynamics Montague Resonance Crossing at PS

100 ms dynamic Crossing

measurements

IMPACT simulation: fully 3D+nonlinear lattice
IMPACT Application in Electron Linac for Next Generation Light Sources

- Beam manipulation and conditioning
- Beam distribution and individual beamline tuning
- Low-emittance, high rep-rate electron gun
- Laser systems, timing & synchronization
- ~2 GeV CW superconducting linac

FEL Power/undulator length \( \sim f \left( \frac{I_{\text{peak}}}{n} \right) \frac{n}{E} \)

The longitudinal phase space of a beam at the exit of a linac
Longitudinal Space-Charge Effects: Microbunching Instability

- Initial density modulation induces energy modulation through long. impedance $Z(k)$, converted to more density modulation by a chicane $\Rightarrow$ growth of slice energy spread / emittance!

![Diagram showing energy and current modulation](image)

Current modulation

- Gain=10

Courtesy of Z. Huang
Final Longitudinal Phase Space and RMS Slice Energy Spread

J. Qiang et al., PRST-AB 12, 100702, 2012.
Experimental Observation of uBl: Benchmark IMPACT Simulations against LCLS Measurements

D. Ratner et al., PRSTAB 18, 030704 (2015).

J. Qiang et al., In preparation (2016).
First-Time Start-to-End Simulation of FEL X-Ray Radiation Using Real Number of Electrons

- Combined the IMPACT-T code and the IMPACT-Z code into a single code
- Developed a new interface to integrate the Genesis code into the IMPACT code as one computing module for undulator
- The start-to-end multi-physics simulation includes:
  - self-consistent 3D space-charge effects,
  - 1D CSR effects, ISR effects, structure wakefields,
  - self-consistent 3D electron and x-ray radiation interaction
Real Number of Electron Matters: No Need for Shot Noise Model
Evolution of X-Ray FEL Radiation Power

fundamental 1 nm average power evolution (MW)

3rd harmonic 0.333 nm average power evolution (MW)

Thank You!