Large-Scale Computing for MAP

Robert D. Ryne

RDRyne@lbl.gov

Center for Beam Physics

Accelerator and Fusion Research Division, LBNL

MAP Winter Meeting

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Goals of this talk

- Start a discussion about how large-scale, parallel accelerator modeling can impact MAP
- Describe some important topics in accelerator theory and simulation that can impact MAP
- Provide background on SciDAC/ComPASS project, and on codes & capabilities in LBNL Center for Beam Physics, that are related to the above

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 on present supercomputers
  - 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

Given the power of present and future high performance computing platforms, there is opportunity for significant impact to MAP activities

- More realistic simulations (multi-physics, high-resolution)
- tools for design optimization
- faster turn-around
- ability to perform simulations that are otherwise impossible

Important methodologies (old and new) in accelerator theory can also have a major impact

- eigen-emittance analysis and beam manipulation schemes
- Hamiltonian/symplectic methods
- methods for nonlinear map computation
- …

Some examples

- Parallel beam-beam optimization applied to LHC
- Parallel study of space-charge effects in proposed CERN PS2
- Parallel beam-beam modeling in support of Tevatron
- Parallel, self-consistent e-cloud modeling of CERN SPS
- Parallel LHC beam-beam modeling w/ wire compensation
- Eigen-emittance analysis to understand dynamics of systems w/ coupling among the phase planes

Parallel parameter scans and parallel optimization

- Have developed capabilities to use, e.g., 1000 processors for a point-design, and to *simultaneously* scan a multi-dimensional parameter space, or to optimize parameters
  - uses 2-level parallelism based on MPI Groups
  - present: single objective function differential evolutionary algorithm
  - future: multi-objective 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**	

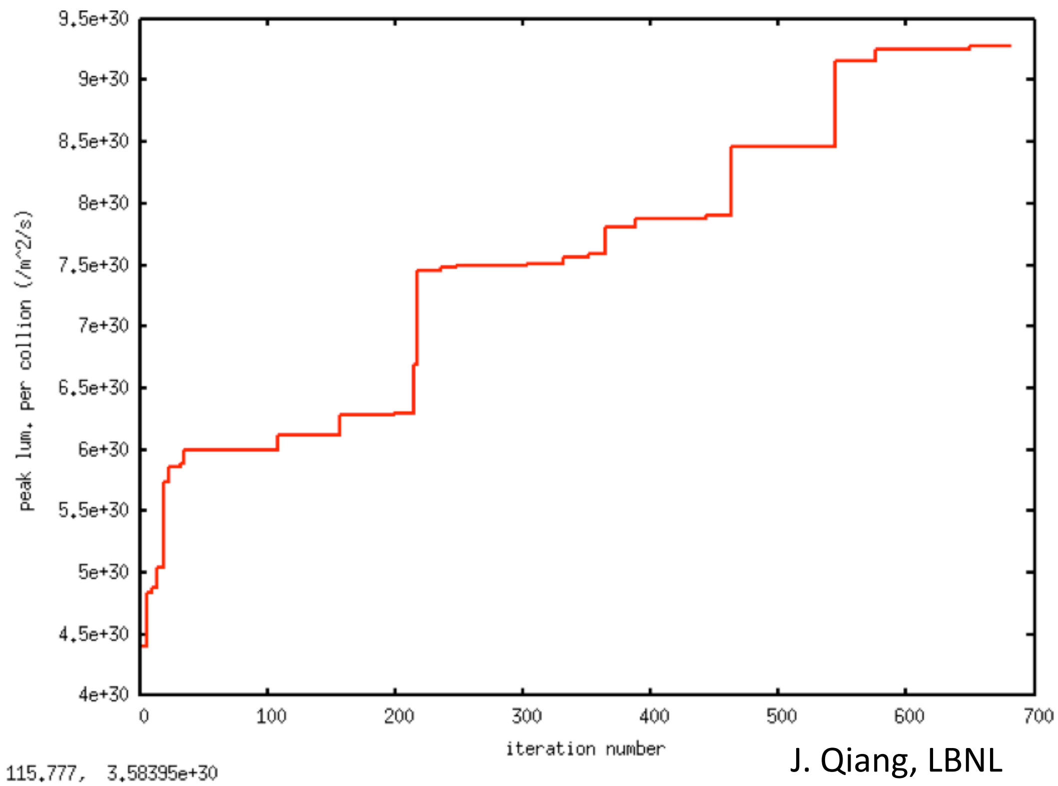
Testing on Cray XT-5 at NCCS shows good scalability up to 100K processors

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

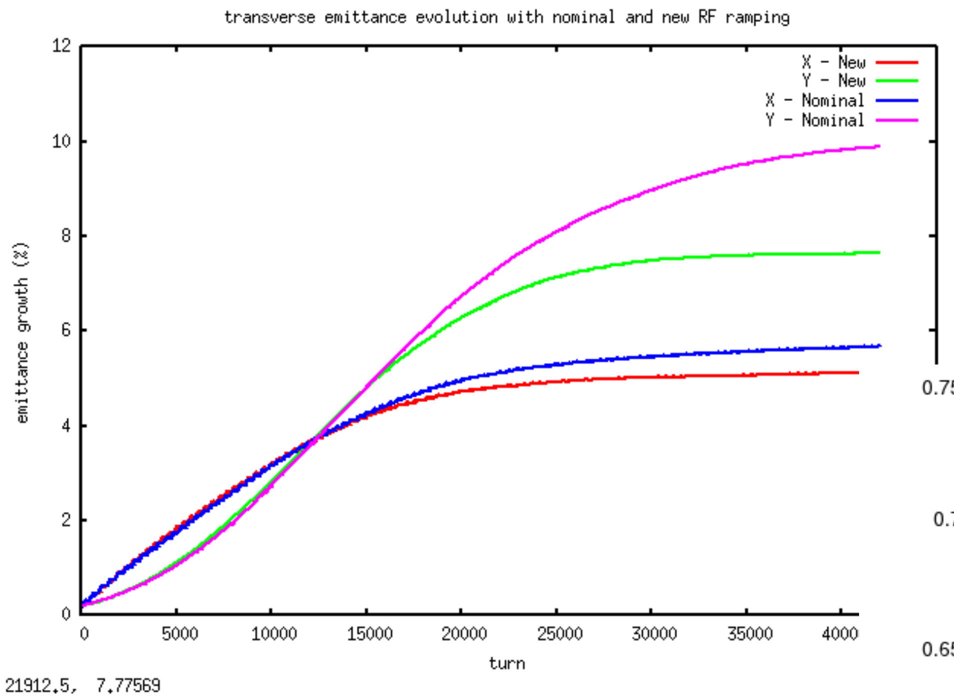
• 3 hr simulation would have taken 12 days w/ serial optimizer, 2 yrs w/ serial code



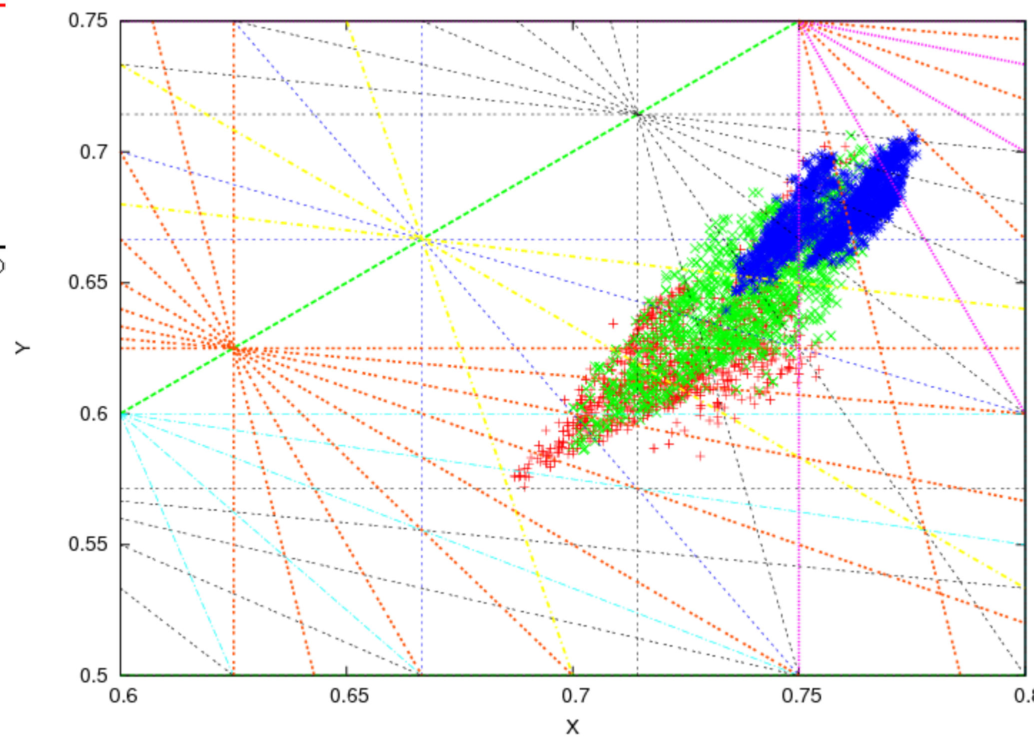
J. Qiang, LBNL

Parallel simulation of proposed CERN PS2 using IMPACT

Transverse emittance growth with different RF ramping schemes



Tune footprints at different acceleration energy



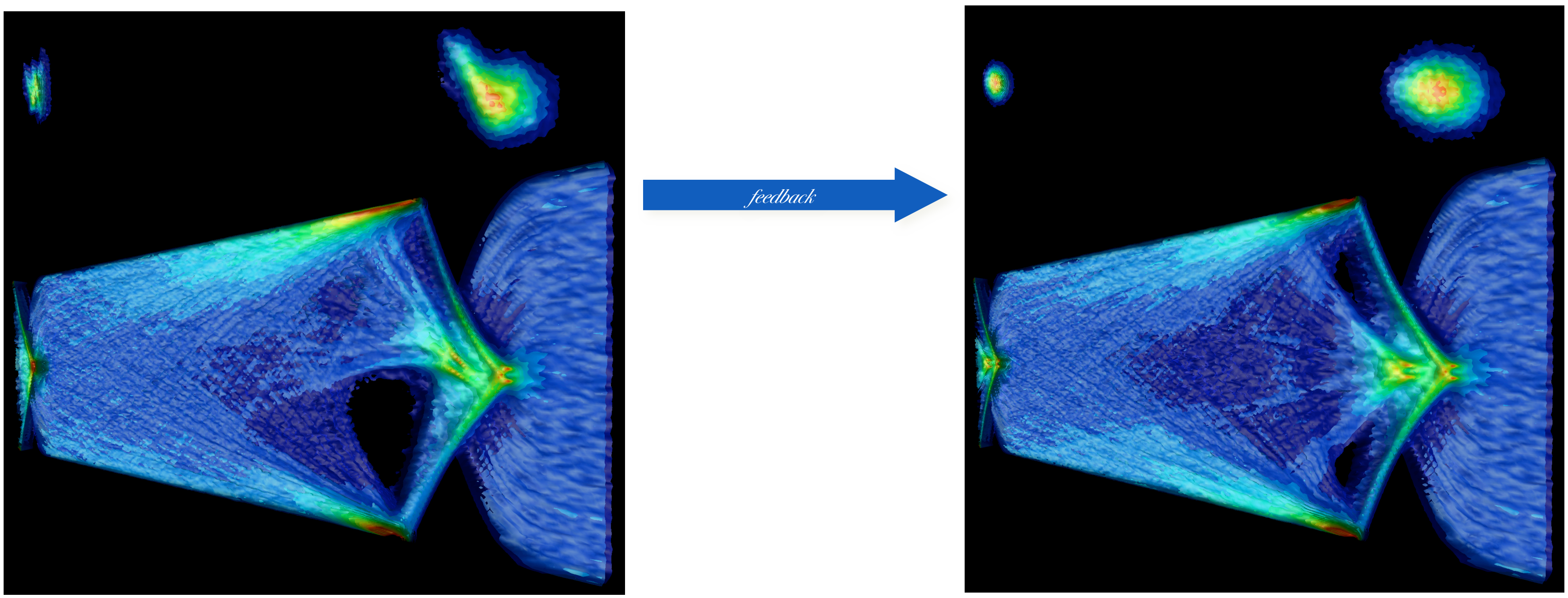
IMPACT simulation, Ji Qiang, LBNL, and Uli Wienands, SLAC

Parallel beam-beam simulation in support of Tevatron

- BeamBeam3D code installed at FNAL
- Code enhancements and benchmarking performed by FNAL staff (E. Stern)
- Code used to help understand beam-beam effects in Tevatron
- Results of simulations successfully used in Tevatron ops to support change of chromaticity during the transition to collider mode optics, leading to a factor of 2 decrease in proton losses, improved reliability of collider operations
  - E. G. Stern, J. F. Amundson, P. G. Spentzouris, and A. A. Valishev , "Fully 3D multiple beam dynamics processes simulation for the Fermilab Tevatron," Phys. Rev. ST Accel. Beams 13, 024401 (2010)

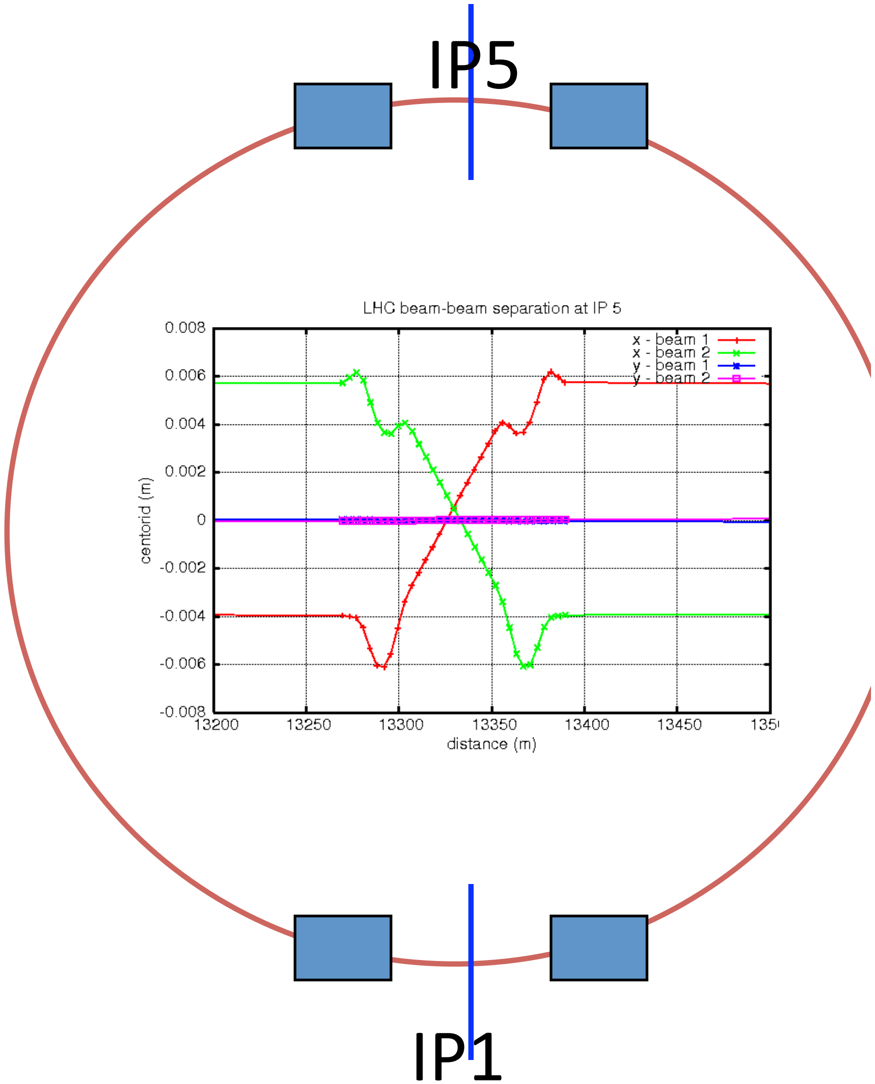
Parallel 3D e-cloud modeling to assess feedback system to mitigate beam instability

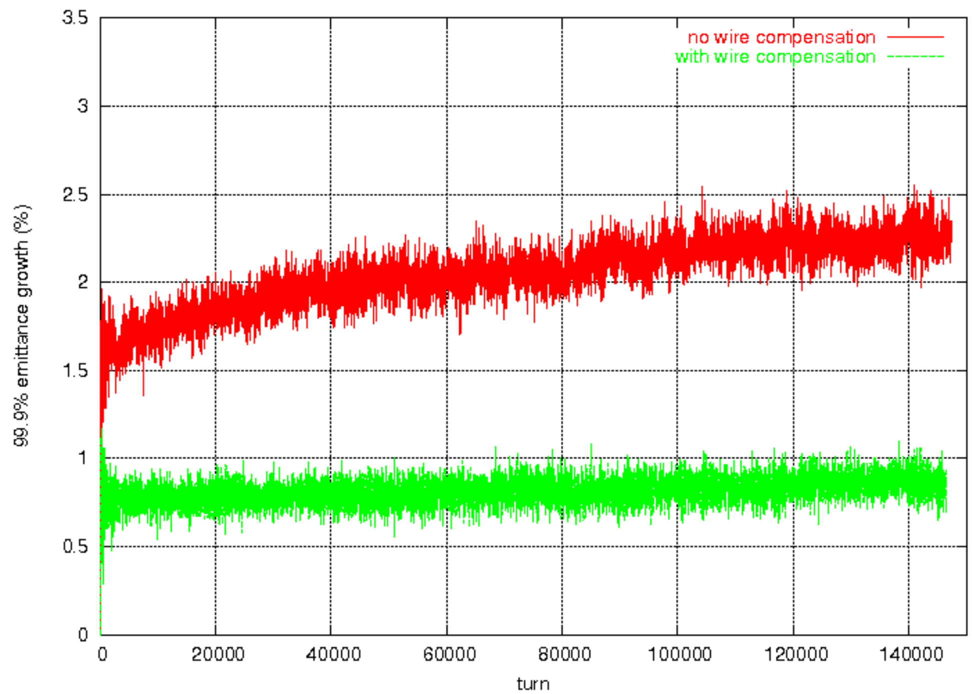
The CERN SPS is currently the bottleneck to providing higher intensity beams for the LHC. Parallel self-consistent e-cloud simulations are being used to study the effectiveness of a feedback system in the CERN SPS.



Warp-POSINST simulation, J.-L. Vay, LBNL

Strong-Strong Beam-Beam Simulation LHC Wire Compensation (2 Head-On + 64 Long Range)





J. Qiang, LBNL

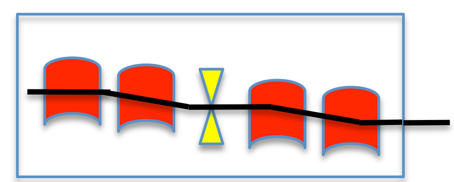
Advanced techniques for phase space analysis and beam manipulation

- Eigen-emittances, λ_j , are the generalization of the usual rms emittances, ε_j , to systems where there may be correlations between the phase space planes.
- Eigen-emittances are derived from beam 2nd moment matrix, Σ. Namely, the eigenvalues of $J\Sigma$ are $\pm i\,\lambda_j$

$$J = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}$$

- If there are no correlations (or if they are removed at some location in a beamline), the eigen-emittances *are* the rms emittances
- Eigen-emittances are invariant under linear symplectic transformations, but they can be *exchanged* among the phase planes, i.e., they are not tied to a specific plane
  - Emittance exchangers exemplify this

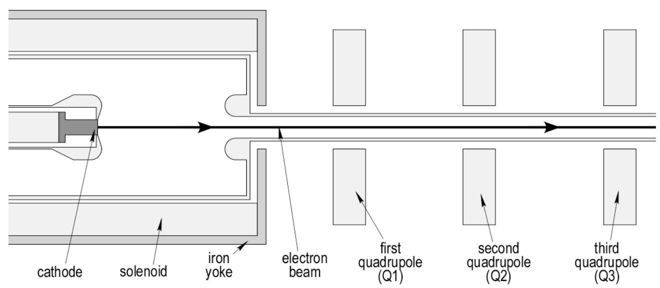
$$M_{eex} = \begin{bmatrix} 0 & 0 & a & b \\ 0 & 0 & c & d \\ e & f & 0 & 0 \\ g & h & 0 & 0 \end{bmatrix}$$



Given strong interest in longitudinal/transverse coupling and beam cooling, MAP beam dynamics codes should print eigen-emittances

Flat Beam Transformers

- Eigen-emittance techniques are ideally suited to analyzing flat beam transformers (FBTs) and other systems w/ coupling between the phase planes
- FBTs convert beam w/ equal intrinsic $\varepsilon_{x,rms}$, $\varepsilon_{y,rms}$ born at a photo-cathode immersed in a B field into a beam w/ asymmetric $\varepsilon_{x,rms}$, $\varepsilon_{y,rms}$



- Carlsten et al have shown how to
  - generalize FBTs to beams w/ asymmetric intrinsic emittances
  - generalize the concept of x-y FBT's to x-z FBT's

Choice of variables and units

(followup to yesterday's discussion about canonical variables)

- Eigen-emittance analysis requires results in canonical variables (except for approximate treatment)
- "t-code" : $(x,\gamma\beta_x mc-qA_x,y,\gamma\beta_y mc-qA_y,z,\gamma\beta_z mc-qA_z)$ (t)
- "z-code" : $(x,\gamma\beta_x mc-qA_x,y,\gamma\beta_y mc-qA_y,t,-\gamma mc^2-q\varphi)$ (z)
- Most codes use dimensionless variables; also some use dimensionless deviations; for the variables to remain canonical, they cannot be scaled arbitrarily. Use:

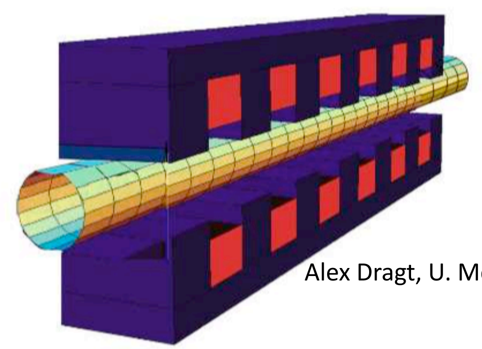
$$x \leftarrow (x - x_0)/l, \qquad p_x \leftarrow (p_x - p_{x0})/\delta,$$
$$y \leftarrow (y - y_0)/l, \qquad p_y \leftarrow (p_y - p_{y0})/\delta,$$
$$t \leftarrow \omega(t - t_0), \qquad p_t \leftarrow (p_t - p_{t0})/(\omega l \delta).$$

- Problems w/out acceleration typically set $\delta=\gamma_0\beta_0$mc (where $\gamma_0\beta_0$ = design momentum = constant)
- Problems with acceleration: set δ=mc
- When δ=mc, quantities such as emittances computed from simulated particle distributions are automatically normalized

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, …

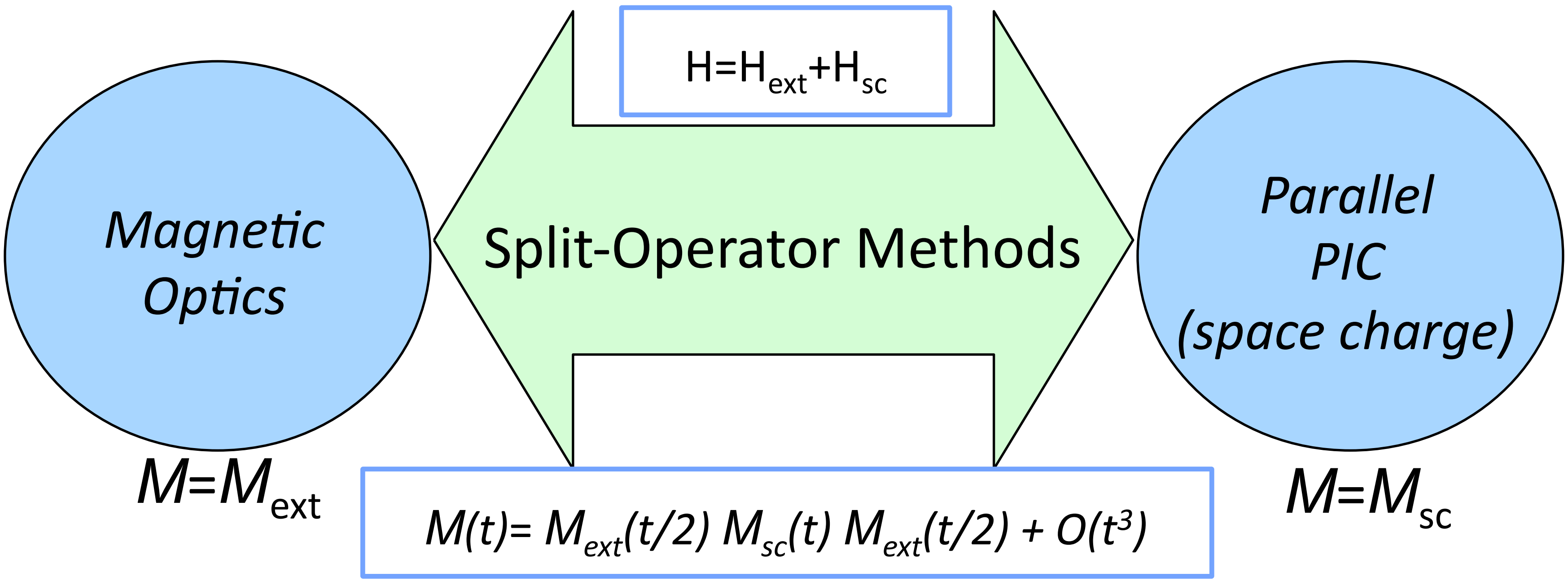
Given the large emittances in muon systems, and the importance of correct inclusion of nonlinear effects, the use of surface methods would be highly beneficial to MAP



Alex Dragt, U. Md.

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

R. D. Ryne, LBNL

Including parallel space charge in a code that has no other collective effects

- 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
- Ultimately need to decide whether to
  - put parallel space charge in existing MAP codes, or
  - put MAP capabilities (cooling, helices,…) in existing parallel codes

Conclusion

- Advances in large-scale computing and in accelerator theory can have a major impact on MAP
- SciDAC3 will likely be announced this summer
  – now is the time to open discussions between MAP and SciDAC/ComPASS to ensure that future ComPASS activities address needs of MAP
- Researchers in LBNL Center for Beam Physics have developed state-of-the-art parallel beam dynamics codes and are involved in developing new, powerful techniques in accelerator theory and modeling
  – we are redirecting our activities to play a stronger role in MAP

Extra Material

- Overview of SciDAC/ComPASS project
- Material on LBNL Center for Beam Physics parallel beam dynamics codes
- Additional material on eigen-emittances

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

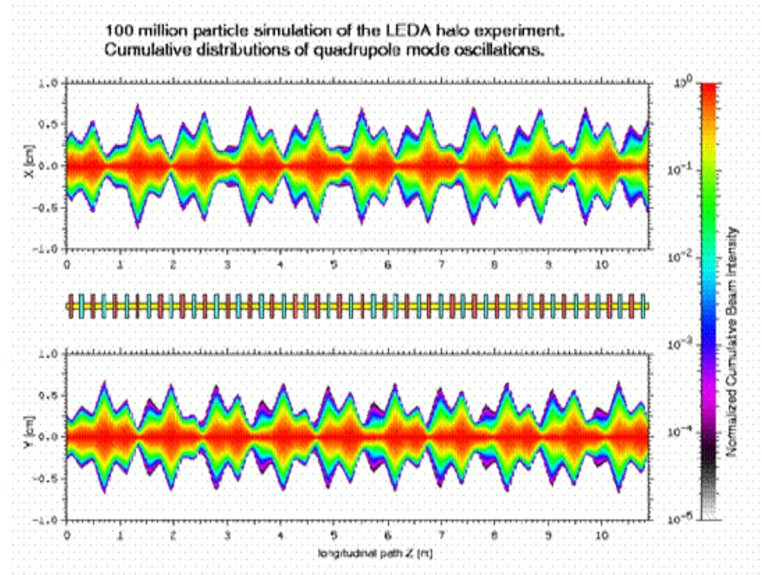
LBNL Center for Beam Physics parallel beam dynamics codes

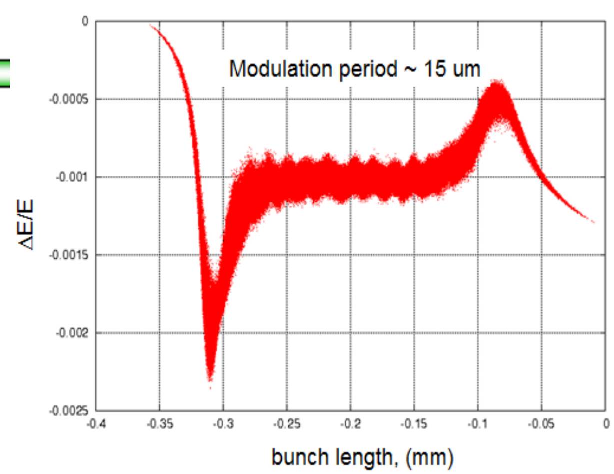
- IMPACT
- BeamBeam3D
- MaryLie/IMPACT
- WARP*, WARP-POSINST

*Developed and maintained by LBNL staff in HIF-VNL in collaboration w/ CBP

IMPACT code suite

- IMPACT-Z: parallel PIC code (z-code)
- IMPACT-T: parallel PIC code (t-code)
- Envelope code, pre- and post-processors,…
- Optimized for parallel processing
- Applied to many projects: SNS, JPARC, RIA, FRIB, PS2, future light sources, advanced streak cameras,…
- Has been used to study photoinjectors for BNL e-cooling project, Cornell ERL, FNAL/A0, LBNL/APEX, ANL, JLAB, SLAC/LCLS





One Billion Macroparticle Simulation of an FEL Linac (~2 hrs on 512 processors)

BeamBeam3D: Parallel Strong-Strong / Strong-Weak Simulation

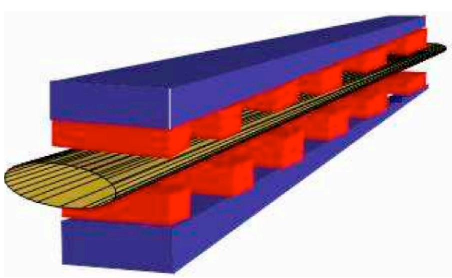
- Beam-Beam forces – integrated, shifted Green function method with FFT – O(N log(N)) computational cost
- Multiple-slice model for finite bunch length effects
- Parallel particle-based decomposition to achieve perfect load balance
- Lorentz boost to handle crossing angle collisions
- Arbitrary closed-orbit separation (static or time-dep)
- Multiple bunches, multiple collision points
- Linear transfer matrix + one turn chromaticity+thin lens sextupole kicks
- Conducting wire, crab cavity, and electron lens compensation
- Parallel tune scan and optimization

MaryLie/IMPACT (ML/I)

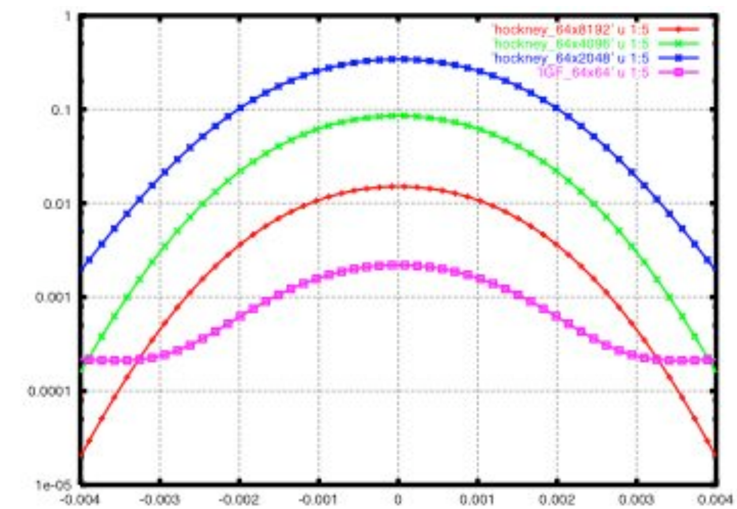
- Combines capabilities of MaryLie code (A. Dragt, U Md) with IMPACT code (J. Qiang, R. Ryne, LBNL) + new features
- Multiple capabilities in a single unified environment:
  - Map generation
  - Map analysis
  - Particle tracking w/ 3D space charge
  - Envelope tracking
  - Fitting and optimization
- Recent applications: ERL for e-cooling @ RHIC; CERN PS2

- Parallel
- 5th order optics
- 3D space charge
- 5th order rf cavity model
- 3D integrated Green func
- Photoinjector modeling
- “Automatic” commands
- MAD-style input
- Test suite
- Contributions from LBNL, UMd, Tech-X, LANL,…

Map computation from surface data

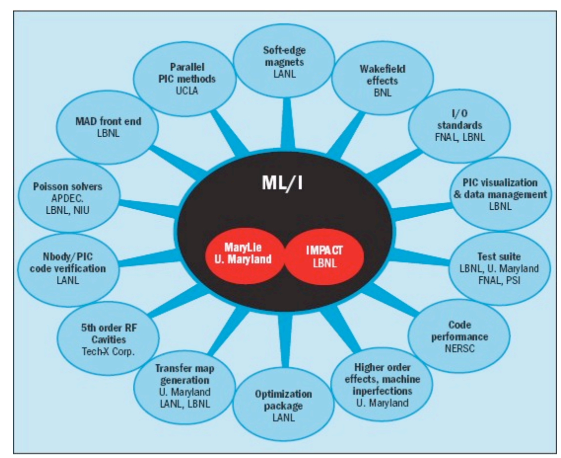


Alex Dragt, U. Md.



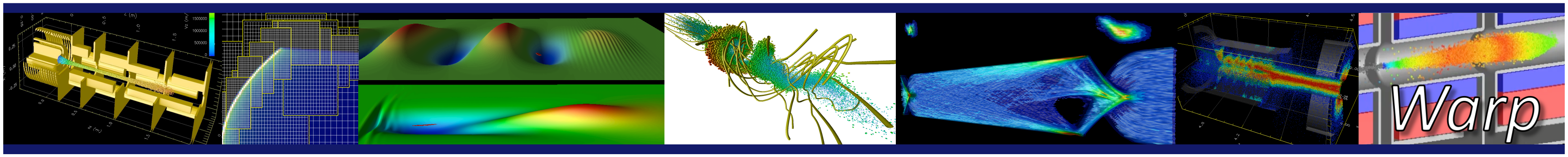
Error in E-field computed w/ different algorithms applied to a 2D Gaussian elliptical distribution w/ 500:1 aspect ratio

Integrated Green Function on 64x64 grid is more accurate than Hockney on 64x2048, 64x4096, 64x8192.



Warp: a parallel framework combining features of plasma (Particle-In-Warp) and accelerator codes

- **Geometry:** 3D (x,y,z), 2D-1/2 (x,y), (x,z) or axisym. (r,z)
- **Python and Fortran:** "steerable," input decks are programs
- **Field solvers:** Electrostatic/Magnetostatic - FFT, multigrid; AMR; implicit
  Electromagnetic - Yee, Cole-Kark.; PML; AMR
- **Parallel:** MPI (1, 2 and 3D domain decomposition)
- **Boundaries:** "cut-cell" --- no restriction to "Legos"
- **Lattice:** general; non-paraxial; can read MAD files
  - solenoids, dipoles, quads, sextupoles, linear maps, arbitrary fields, acceleration
- **Bends:** "warped" coordinates; no "reference orbit"
- **Particle movers:** Boris, large time step "drift-Lorentz", novel relativistic Leapfrog
- **Reference frame:** lab, moving-window, Lorentz boosted
- **Surface/volume physics:** secondary e^-/photo-e^- emission, gas emission/tracking/ionization
- **Diagnostics:** extensive snapshots and histories
- **Misc.:** **trajectory** tracing; quasistatic & steady-flow modes; space charge emitted emission; "equilibrium-like" beam loads in linear focusing channels; maintained using CVS repository.



Extra material on eigen-emittances

What are eigen-emittances*#

- Let z denote a 6-vector of canonical coordinates and moments, $z=(x,p_x,y,p_y,t,p_t)$
- Consider the matrix of 2nd moments, $Z_{ab}=<z_a,z_b>$
- For example, in a 1D system (2D phase space),

$$Z=\begin{pmatrix} <x^2> & <xp_x> \\ <xp_x> & <p_x^2> \end{pmatrix}$$

- Easy to verify that Z is diagonalized via a *symplectic congruency transformation*,

$$AZA^T=\varepsilon_{rms}I_{2x2}$$

where

$$A=\begin{pmatrix} 1/\sqrt{\beta} & 0 \\ \alpha/\sqrt{\beta} & \sqrt{\beta} \end{pmatrix}$$

$$\alpha=-<xp_x>/\varepsilon_{rms}$$

$$\beta=<x^2>/\varepsilon_{rms}$$

$$\gamma=<p_x^2>/\varepsilon_{rms}$$

$$\varepsilon_{rms}^2=<x^2><p_x^2>-<xp_x>^2$$

*Material presented here is from Chapter 8, section 8.37, of the MaryLie manual and in Ch 26 of Alex Dragt's textbook, downloadable from http://www.physics.umd.edu/dsat/

#The earliest reference to "eigen-emittance" that I have found is A. J. Dragt et al., "Lie Algebraic Treatment of Linear and Nonlinear Beam Dynamics," Ann. Rev. Nucl. Part. Sci., Vol. 38, pp 455-496 (1988). The definition in terms of symplectic congruency transformations is found in the MaryLie manual.

See also: A. Dragt, R. Gluckstern, F. Neri, and G. Rangarajan, "Theory of Emittance Invariants", in Lecture Notes in Physics 343: Frontiers of Particle Beams; Observation, Diagnosis, and Correction, M. Month and S. Turner, Eds., Springer Verlag (1989); A. Dragt, F. Neri, and G. Rangarajan, "General moment invariants for linear Hamiltonian systems", Phys. Rev. A, p. 2572 (1992).

Eigen-emittances, cont.

- In the 1D case we found that: $AZA^T = \varepsilon_{rms} I_{2x2}$

- This is a special case of a famous theorem due to Williamson* that states#,
  - *for any real symmetric positive-definite 2nx2n matrix Z, there exists a symplectic matrix A such that*

    $$AZA^T = \Lambda \qquad (\Lambda\text{=diagnonal matrix})$$

  - *Furthermore, the elements of the matrix* Λ *are the modulii of the eigenvalues of JZ*

$$J = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}$$

- In 2D and 3D we will use the notation (note the under-bar) $\underline{\varepsilon}_1 , \underline{\varepsilon}_2 , \underline{\varepsilon}_3$ to denote the elements of Λ, and we will call them "eigen-emittances"
  - $\underline{\varepsilon}_1 , \underline{\varepsilon}_2 , \underline{\varepsilon}_3$ equal the rms emittances if Z is 2x2 block diagonal (i.e. if <xy>, <xp_y>,…, etc., are zero)

*J. Williamson, "On the Algebraic Problem Concerning the Normal Forms of Linear Dynamical Systems," Amer. J. Math. **58** (1) (1936), 141-163.

#See, e.g., the texbook by Maurice de Gosson, "Symplectic Geometry and Quantum Mechanics," 2006.

Eigen-emittances in 3D

- In the 1D case we found that

$$AZA^T = \underline{\varepsilon}_x I_x \qquad I_x = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

- The analgous result in 3D is

$$AZA^T = \underline{\varepsilon}_1 I_1 + \underline{\varepsilon}_2 I_2 + \underline{\varepsilon}_3 I_3$$

$$I_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad I_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad I_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

- Note that the code MaryLie has built-in capabilities to compute eigen-emittances and related quantities.

Invariance of the eigen-emittances under linear symplectic transport*

- Suppose that we have a distribution of particles and compute its 2nd moments to compute the matrix given by $Z_{ab}=\langle z_a, z_b \rangle$
- There exists a symplectic matrix A that diagonizes Z via the congruency relation,

$$AZA^T = \underline{\varepsilon}_1 I_1 + \underline{\varepsilon}_2 I_2 + \underline{\varepsilon}_3 I_3$$

- Suppose we propagate particles to some final location via symplectic matrix M. Then the final 2nd moment matrix (e.g. at the end of the beamline) is

$$Z^f = MZM^T$$

- Now consider the matrix $B=AM^{-1}$:

$$BZ^f B^T = AM^{-1}MZM^T(M^T)^{-1}A^T = AZA^T = \underline{\varepsilon}_1 I_1 + \underline{\varepsilon}_2 I_2 + \underline{\varepsilon}_3 I_3$$

- Hence, the matrix B brings Z^f to normal form. Therefore we can also write:

$$BZ^f B^T = \underline{\varepsilon}_1^f I_1 + \underline{\varepsilon}_2^f I_2 + \underline{\varepsilon}_3^f I_3$$

- We conclude that

$$\underline{\varepsilon}_i^f = \underline{\varepsilon}_i \quad \textit{(i=1,...,3)}$$

The eigen-emittances are invariant under linear symplectic transformations

* See E. Courant, "Conservation of Phase Space in Hamiltonian Systems and Particle Beams," (1966)

END OF EXTRA MATERIAL