Computational Challenges in High Intensity and High Brightness Beam Physics

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Lawrence Berkeley National Laboratory

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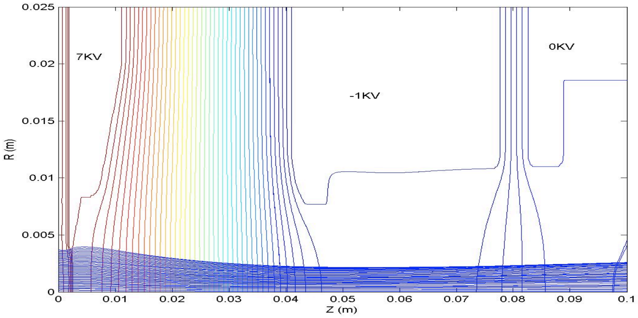
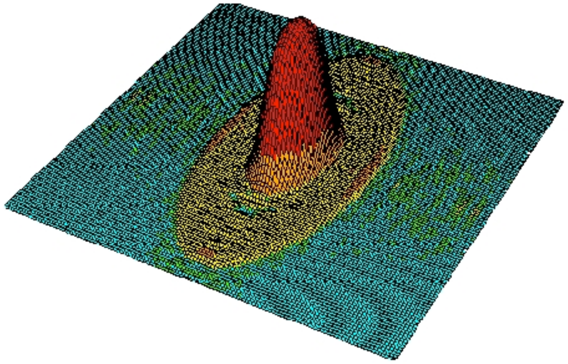
Presented at PAHBEB2005

Erice, Sicily



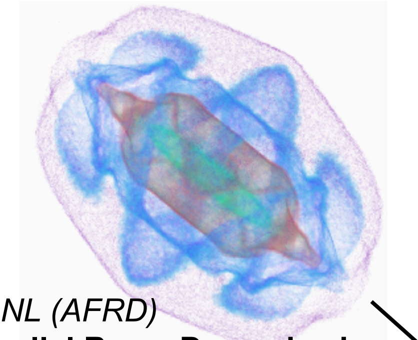


Acknowledgement

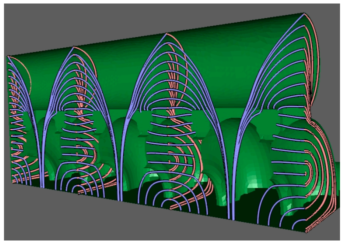
Thanks to

Ji Qiang, LBNL

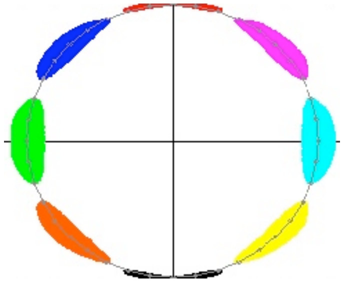
SciDAC AST: A multidisciplinary, multi-institutional effort to produce comprehensive parallel accelerator design tools



LBNL (AFRD)
Parallel Beam Dynamics in Linacs and Rings; Beam-Beam; Space Charge; Collisions



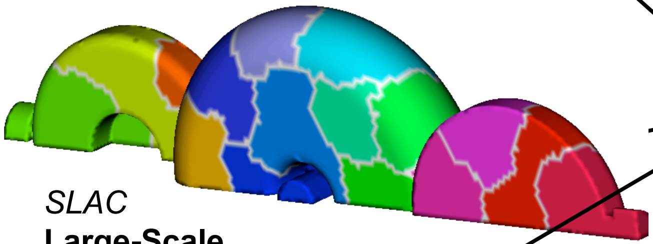
UC Davis
Particle & Mesh Visualization



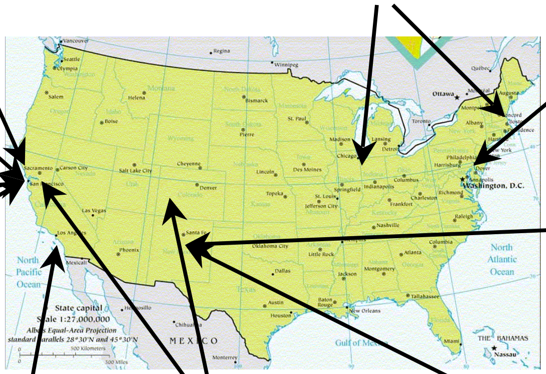
FNAL, BNL
High Intensity Beams in Circular Machines

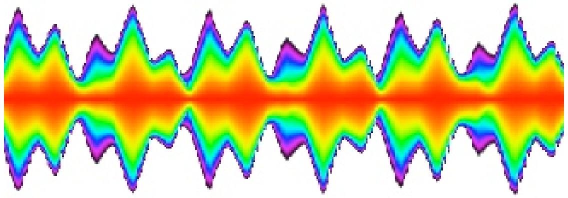
$$M = e^{:f_2:}\, e^{:f_3:}\, e^{:f_4:} \ldots$$
$$N = A^{-1}\, M\, A$$

U. Maryland
Lie Methods in Accelerator Physics

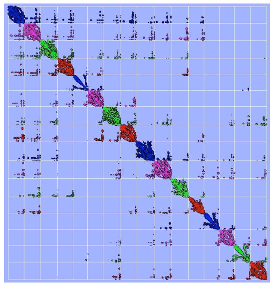


SLAC
Large-Scale Electromagnetic Modeling

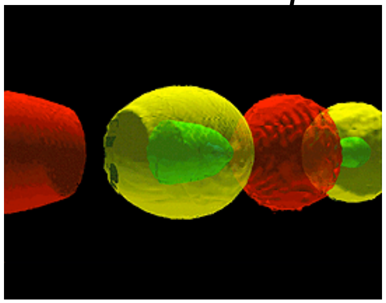


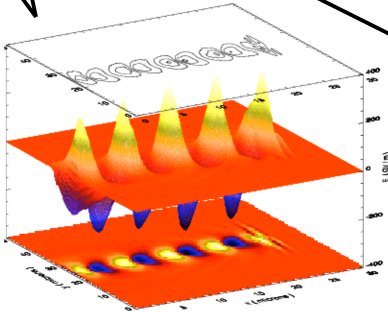


LANL
High Intensity Linacs, Computer Model Evaluation

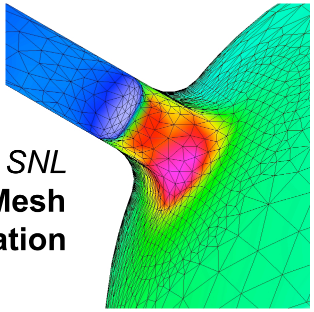


Stanford, LBNL (CRD)
Parallel Linear Solvers & Eigensolvers





UCLA, USC, Tech-X, U. Colorado, LBNL
Plasma-Based Accelerator Modeling



SNL
Mesh Generation

SciDAC Applications

- Beam dynamics codes developed under the SciDAC AST project have been applied to many projects. Some examples
  - —Tevatron, RHIC, PEP-II, LHC
  - —NLC, ILC
  - —FNAL Booster
  - —RIA
  - —SNS, LCLS
  - —CERN SPS benchmark study
  - —CERN SPL design
  - —J-PARC commissioning

Computational beam dynamics: toward higher intensity, higher brightness, and greater precision

- **Modeling challenges for next-generation light sources:**
  - —Photoinjector design and limits to brightness
  - —Emittance preservation in the presence of CSR
  - —Issues for energy recovery linacs
  - —Diagnostics: design of ultrafast streak cameras
  - —…
  - —**Modeling challenges for high intensity rings (e.g. accumulators):**
  - —Predicting halo formation, beam loss,and stability thresholds
- **Modeling challenges for other rings**
  - —Predicting long-term effect of weak space charge + nonlinearities
- **Modeling challenges for colliders**
  - —Maximizing luminosity, predicting lifetime due to b-b effect

Predicting radiation production/consequences

- Sub-ps duration bunches emit "long" wavelength (i.e. $\lambda \sim 100$ nm – 100μm) coherent radiation in bends (i.e. CSR) and in undulators (CUR, or coherent undulator radiation)
- This radiation can cause microbunching instabilities, increased energy spread, and emittance growth --- can strongly reduce the *desired* FEL instability in x-ray devices such as the LCLS
- Some CSR modeling capabilities rely on N^2 algorithms; leads to
  - —numerically noisy simulations
  - —limited spatial & temporal resolution
- Minimal CUR modeling capability when considering interaction with simultaneously growing FEL instability --- vast longitudinal scale length difference. Multiscale/multiresolution techniques needed.

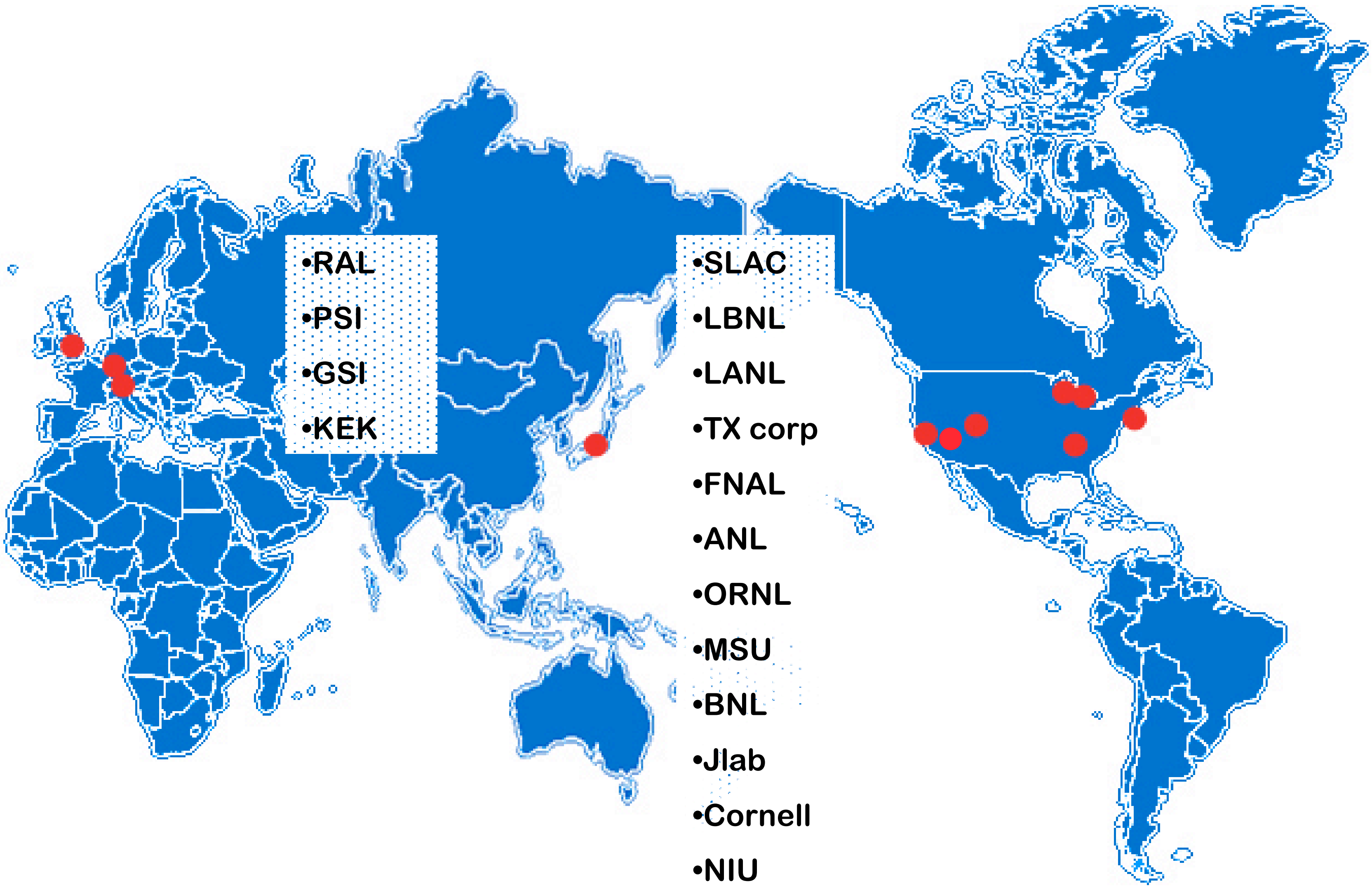
Computational Challenges

- Multi-physics modeling:
  - —Nonlinear optics, space charge, wakes, CSR, collisions
- Multi-scale modeling:
  - —In space and time
- Getting the physics right. For example:
  - —Tools for computing transfer maps from field data
  - —Self-consistent modeling (when needed)
- Using codes to make predictions
  - —Code benchmarking, code calibration, combining simulation and experiment to make predictions
- Visualizing/exploring massive data sets
- Building codes to make use of state-of-the-art platforms
  - —Computers >10K processors here now, >100K soon

IMPACT (Integrated-Map and Particle Accelerator Tracking) code (J. Qiang)

- A code suite (linac design code, 3D rms envelope code, 2 parallel PIC tracking codes)
- Recent enhancements
  - —IMPACT-T: time-based (instead of z-based) version
  - —Cathode emission model
  - —Images from cathode
  - —Poisson solver for high aspect ratio situations
  - —Energy binning for large energy spread
  - —Multi-charge state capability
- These enhancements benefit projects
  - —Modeling rf photoinjectors
  - —Modeling beams w/ large energy spread, as for electron bunches emerging from plasma-based accelerators
  - —Multi-charge state for RIA

Impact User-Map



- RAL
- PSI
- GSI
- KEK

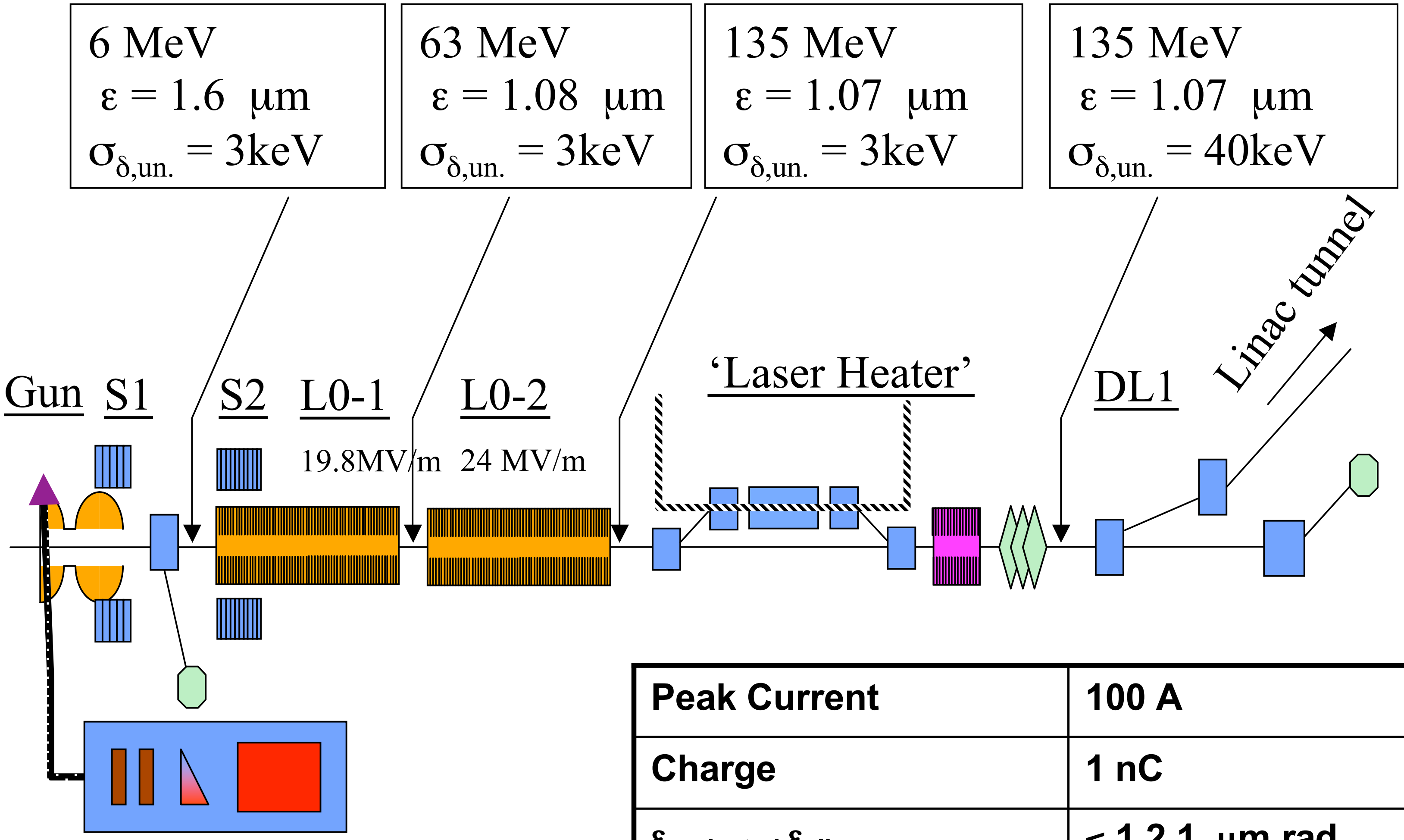
- SLAC
- LBNL
- LANL
- TX corp
- FNAL
- ANL
- ORNL
- MSU
- BNL
- Jlab
- Cornell
- NIU

Photoinjector Modeling

Several groups are using IMPACT-T (or have expressed an interest) for photoinjector studies

- Fermilab RF photoinjector
- LCLS
- Fermi@Elettra project
- Cornell ERL
- ALS streak camera
- BNL electron cooling project
- ANL advanced accelerator project
- JLab

A Schematic Plot of LCLS Injector Layout



6 MeV
$\varepsilon = 1.6\ \mu m$
$\sigma_{\delta,un.} = 3keV$

63 MeV
$\varepsilon = 1.08\ \mu m$
$\sigma_{\delta,un.} = 3keV$

135 MeV
$\varepsilon = 1.07\ \mu m$
$\sigma_{\delta,un.} = 3keV$

135 MeV
$\varepsilon = 1.07\ \mu m$
$\sigma_{\delta,un.} = 40keV$

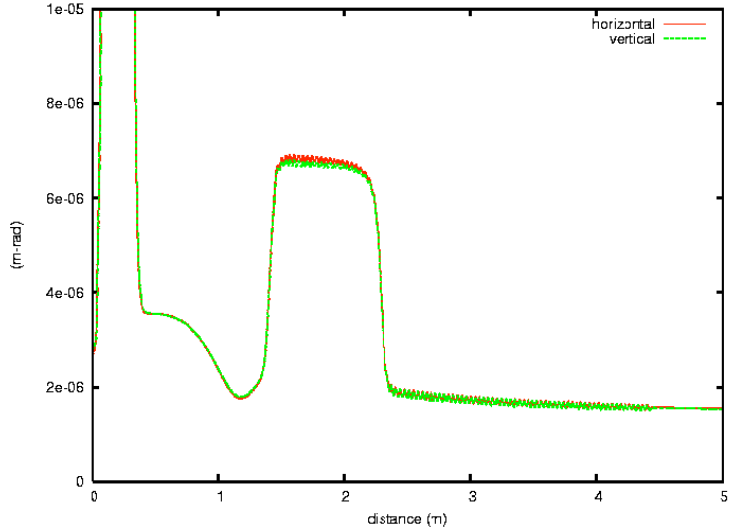
Peak Current	**100 A**
Charge	**1 nC**
$\varepsilon_{projected}, \varepsilon_{slice}$	**≤ 1.2,1 μm.rad**
Repetition rate	**120 Hz**

UV Laser 200 μJ,

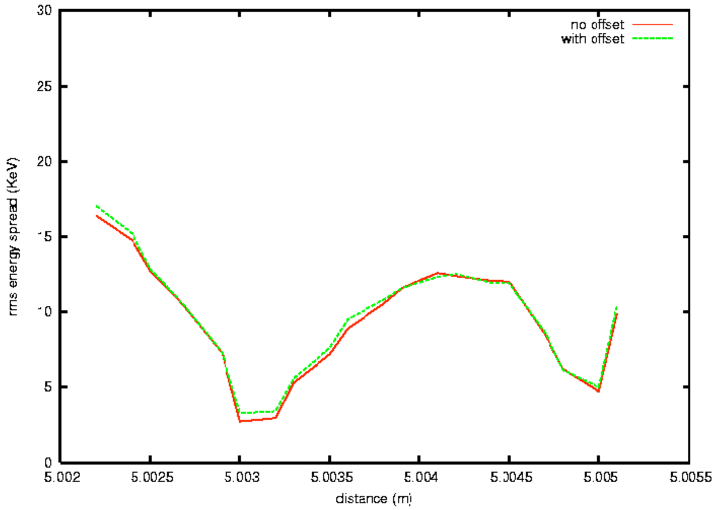
λ = 255 nm, 10ps, r = 1.2 mm

LCLS modeling using IMPACT-T

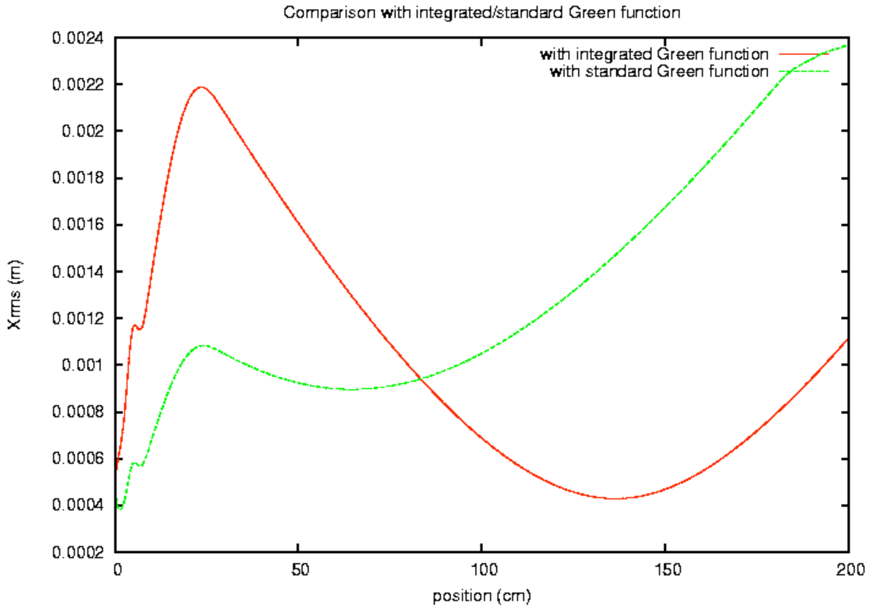
J. Qiang/LBNL and C. Limborg/SLAC



LCLS injector transverse emittance vs distance



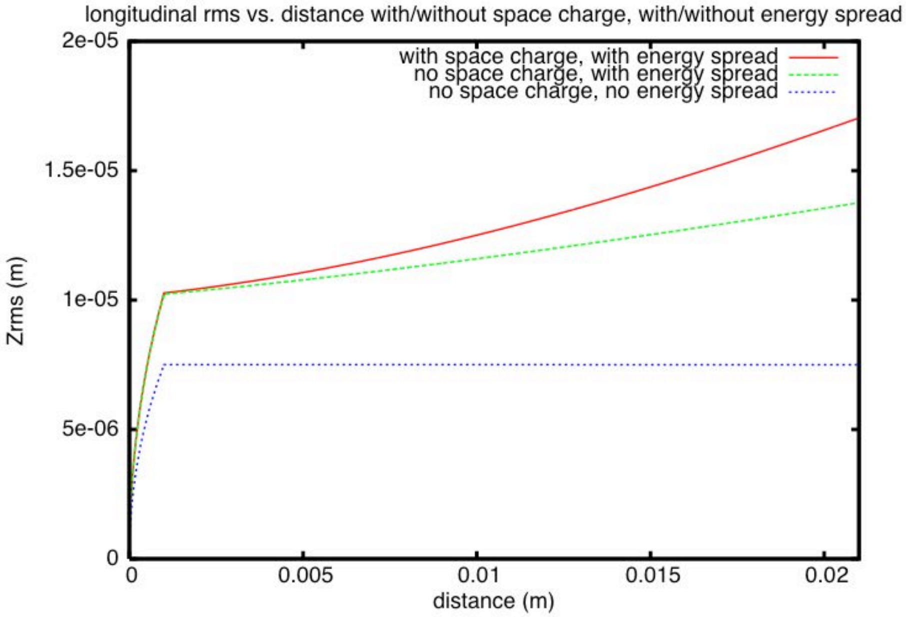
LCLS slice rms energy spread after 1st TW linac (w/ and w/out initial 100μ offset)



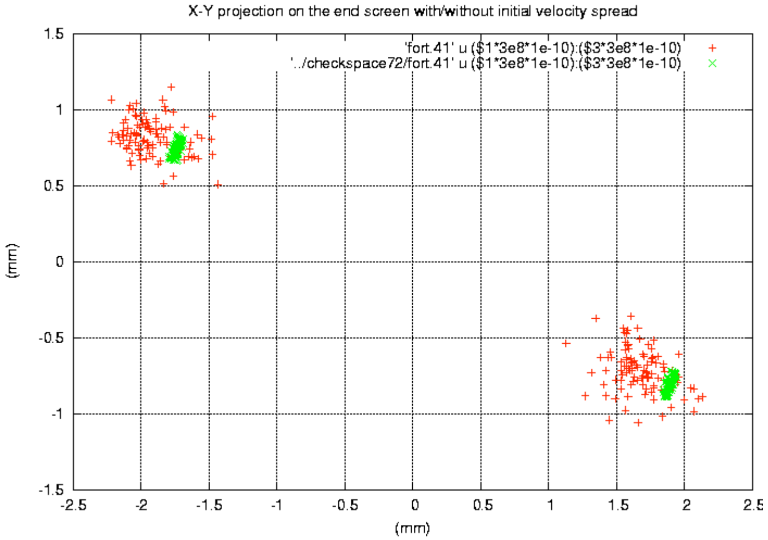
LCLS simulation: Large effect observed when using Integrated Green function compared with standard Green function

Design of ultrafast streak cameras

- **Ultrafast streak cameras being designed for LCLS and ALS**
  - **Simulating LCLS version challenging: space-charge effects**
  - **Simulating ALS version challenging: small # of electrons (N^2 code)**
- **Both currently being modeling using IMPACT-T**



Plot of rms bunch length vs distance in the proposed LCLS streak camera showing the effect of space charge on the bunch length



X-Y projection on the end screen w/ and w/out energy spread in the ALS streak camera (proposed LBNL LDRD)

Algorithmic Advances

- Integrated Green function
  - —Solves the long-standing problem that has plagued certain codes (e.g. PARMELA, original IMPACT) when grid aspect ratios become large
- Shifted Green function
  - —Originally developed to model long-range beam-beam interactions
  - —Same algorithm used to treat cathode image effects
- Wavelet-based methods
- Multi-level gridding, AMR

Integrated Green Function (IGF) addresses a Critical Issue: high aspect ratios

- **Poisson solvers used in static electric and gravitational particle-in-cell simulations often fail when the grid aspect ratio >> 1**
- **Some important problems involve extreme aspect ratios:**
  - **—Long beams in rf accelerators; pancake beams**
  - **—Beams in induction linacs: L~ 10s of meters; R ~ cm**
  - **—Galaxies**
- **Standard grid-based approaches involve using a very large # of grid points in the long dimension, leading to prohibitively long run times**
  - **—As a result, it is *extremely* difficult model high aspect ratio systems accurately using standard grid-based approaches**

IGF recognizes that certain physical quantities may vary on vastly different scales

- **The Green function, G, and source density, ρ, may change over different scales**
- **G is known apriori; ρ is not**

We should use all the information available regarding G so that the numerical solution is only limited by our approximate knowledge of ρ

- **Example: 2D Poisson equation in free space**

$$\phi(x,y) = \int G(x-x',y-y')\rho(x',y')dx'dy'$$

Standard Approach (Hockney and Eastwood)

$$\phi_{i,j} = \sum G_{i-i',j-j'} \rho_{i',j'}$$

- **This approach is equivalent to using the trapezoidal rule (modulo treatment of boundary terms) to approximate the convolution integral**
- **This approach makes use of only partial knowledge of G**
- **The error depends on how rapidly the integrand, ρG, varies over an elemental volume**
  - **—If ρ changes slowly we might try to use a large grid spacing; but this can introduce huge errors due to the change in G over a grid length**

IGF Algorithm

- Assume the charge density, ρ, varies in a prescribed way in each cell
- Use the analytic form of the Green function to perform the convolution integral exactly in each cell, then sum over cells
- Example: linear basis functions to approximate ρ in a cell:

$$\phi(x_i, y_j) = \sum_{i',j'} \rho_{i,j} \int_0^{h_x} dx' \int_0^{h_x} dy'(h_x - x')(h_y - y')G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\sum_{i',j'} \rho_{i+1,j} \int_0^{h_x} dx' \int_0^{h_x} dy'\, x'(h_y - y')G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\sum_{i',j'} \rho_{i,j+1} \int_0^{h_x} dx' \int_0^{h_x} dy'(h_x - x')y' G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\sum_{i',j'} \rho_{i+1,j+1} \int_0^{h_x} dx' \int_0^{h_x} dy' x' y' G(x_i - x_{i'} - x', y_j - y_{j'} - y')$$

- Shifting the indices results in a single convolution involving an integrated effective Green function:

$$\phi_{i,j} = \sum G^{eff}_{i-i',j-j'} \rho_{i',j'}$$

Cost and Accuracy of IGF; Improvement over Standard Approach

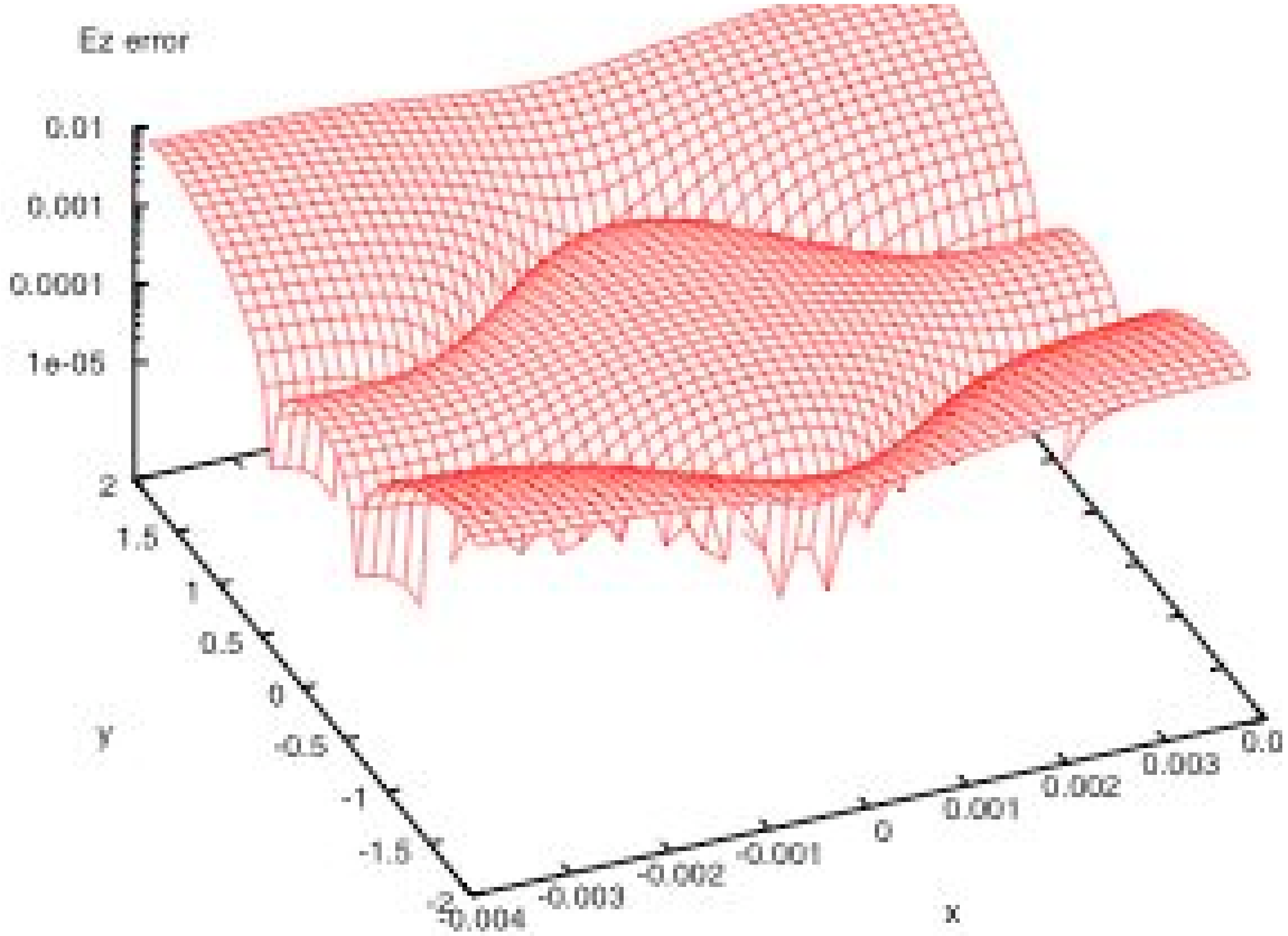
- Cost: IGF elemental integrals can be done analytically; formulas are very lengthy
  - —Requires more FLOPS than simply using G_{ij} but…
  - —In situations where the grid is fixed, this only needs to be done once at the start of a run. Amortized over many time steps, this does not significantly impact run time.
- Accuracy: Method works as long as the elemental integrals are computed accurately and as long as the grid and # of macroparticles are sufficient to resolve variation in ρ
- IGF maintains accuracy even for extreme aspect ratios (>1000:1)

As a result, IGF performs orders of magnitude better than the standard convolution algorithm for realistic problems involving large aspect ratios

Example: 2D gaussian ellipse

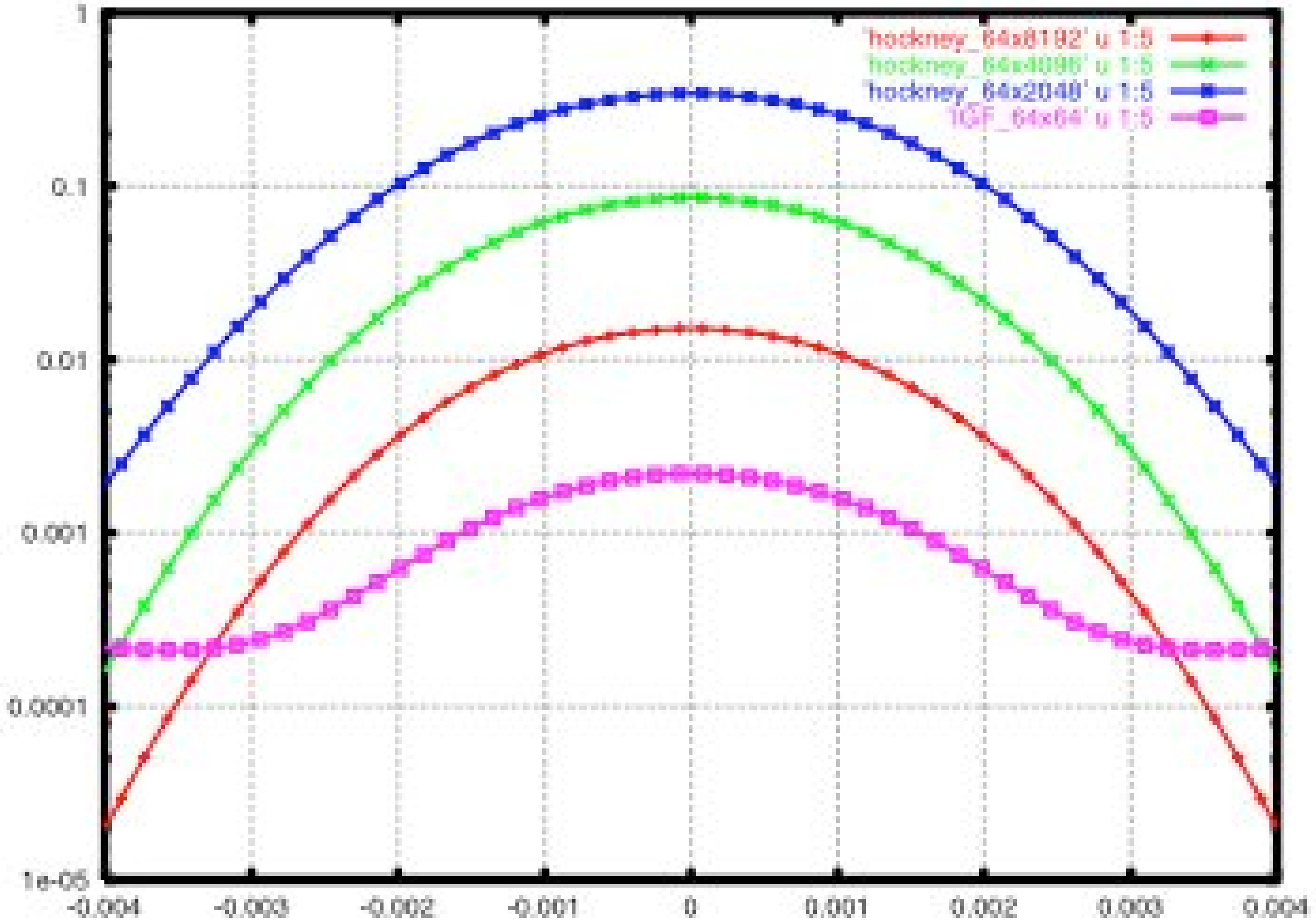
- Aspect ratio is 1:500 -- x_{max}=0.002, y_{max}=1
- Calculation of fields using (1) standard Hockney algorithm and (2) IGF approach
  - In both cases, performed convolutions for the fields directly (rather than calculating the potential and using finite differences to obtain fields)
- Calculation performed using a mesh of size
  - Hockney: 64x64, 64x128, 64x256,…, 64x16384
  - IGF: 64x64

IGF field error



Electric field error using IGF is below 1% using a 64x64 grid.

Comparison of IGF vs standard Hockney approach



Simulation of a high-aspect ratio bunch using an integrated Green Function (IGF) and a conventional algorithm (Hockney). IGF on a 64x64 grid (purple) is more accurate than a standard calculation using 64x2048 (blue), 64x4096 (green), and 64x8192 (red).

Conclusion: 2D Gaussian example

- **For this test problem, the standard Hockney algorithm would require ~500 times more computational effort to achieve the same worst-case accuracy as a simulation using the IGF approach.**
- **IGF works whether the aspect ratio is large, small, or near unity, i.e. it is generally applicable.**
- **Verified in 2D and 3D**
  - **3D might require quad precision**

Extension of IGF to Beams in Pipes

- IGF is especially useful when applied to beams in pipes, since the Green function falls off exponentially in z, though $\rho(z)$ may change slowly over meters
- Due to shielding in beampipe, sum can be truncated in the “long” direction:

$$\phi_{i,j} = \sum_{i'=1}^{N_x} \sum_{j'=j}^{j \pm j_{cutoff}} G^{eff}_{i-i',j-j'} \rho_{i',j'}$$

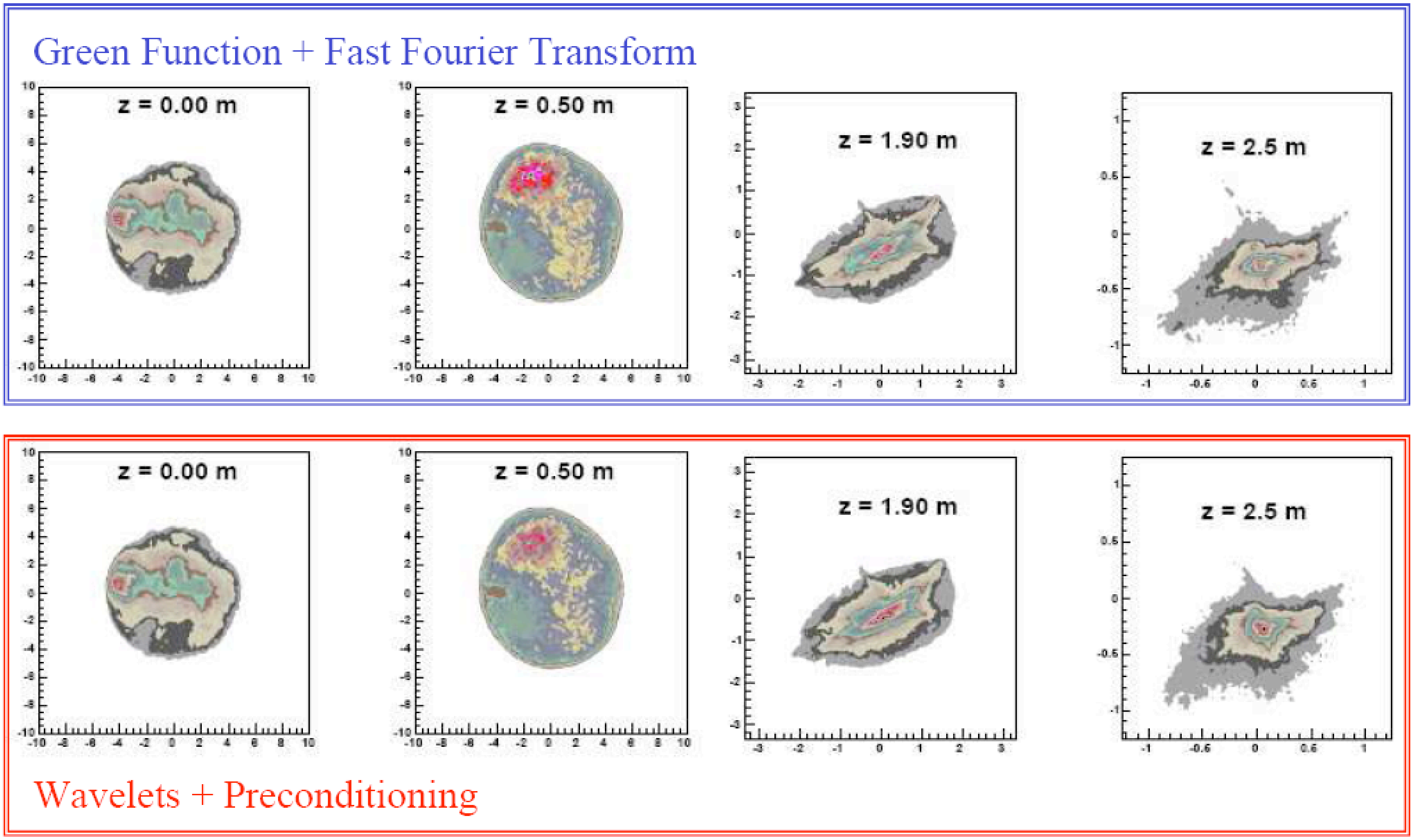
- If grid length in z is >> pipe radius, can truncate at nearest neighbors:

$$\phi_{i,j} = \sum_{i'=1}^{N_x} \left(G^{eff}_{i-i',j-1} \rho_{i',j-1} + G^{eff}_{i-i',j} \rho_{i',j} + G^{eff}_{i-i',j+1} \rho_{i',j+1} \right)$$

- For a rectangular pipe, can rewrite Green function as a sum of convolutions and correlations; can still use FFT-based approach to sum over elements
- Applicability to circular pipes is still an open problem

Toward multiscale/multiresolution modeling:

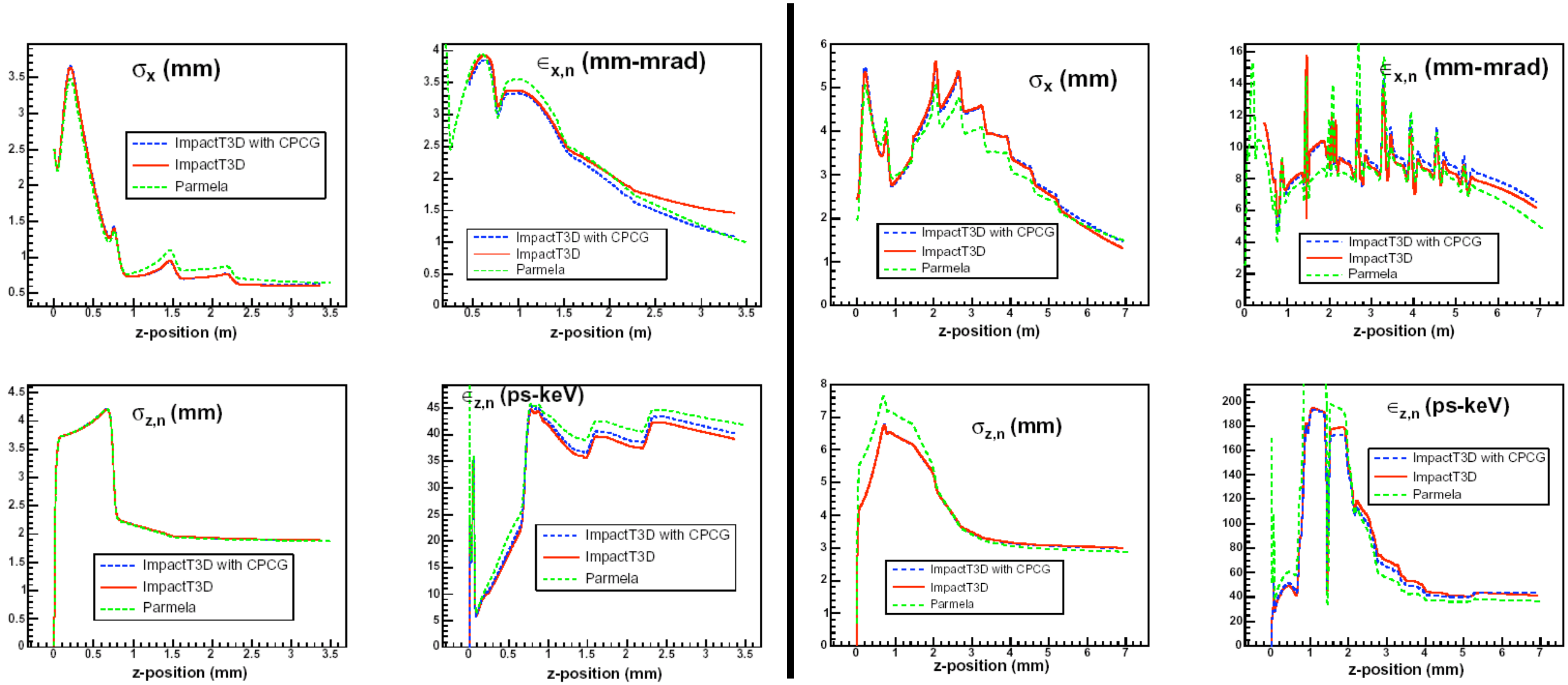
high level of spatial resolution maintained by wavelet-based solver



Comparison between IMPACT-T (upper plots), IMPACT-T w/ wavelet-based Poisson solver (lower plots) for transverse distributions at different z-locations in the AES/Jlab low-charge photoinjector. Wavelet solver is already as fast as standard solver in IMPACT-T; significant speedup will follow implementation of wavelet thresholding.Also investigating more effective preconditioner.

Simulation of AES/Jlab photoinjector

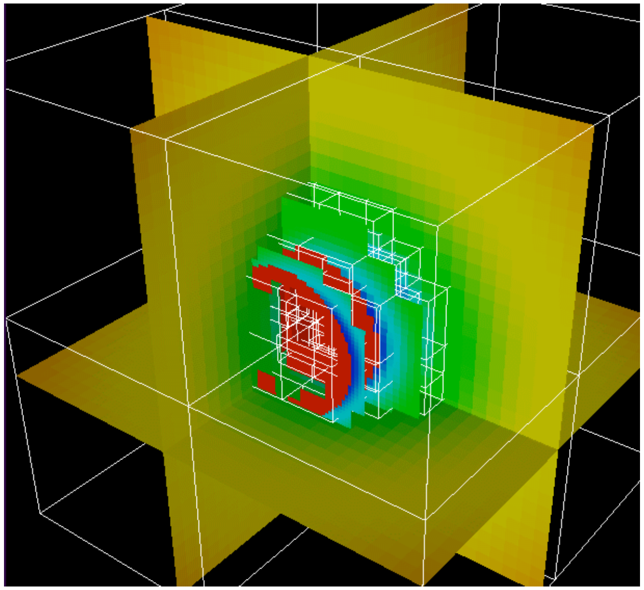
I. Pogorelov/LBNL and B. Terzek/Northern Ilinois Univ.

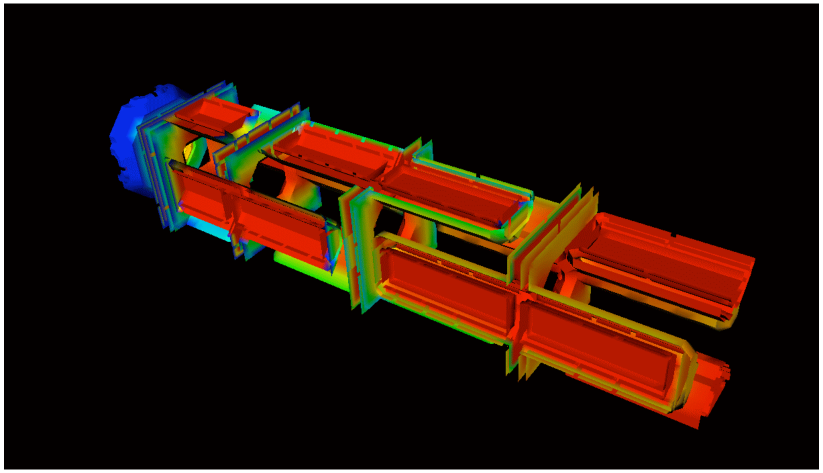


Comparison of IMPACT-T, IMPACT-T w/ iterative wavelet-based Poisson solver, and PARMELA for the AES/Jlab low-charge photoinjector (left 4 plots) and high-charge photoinjector (right 4 plots)

Particle-In-Cell AMR: Highly challenging!

- One approach uses capability originally developed for the combustion community
    - —Chombo framework for block-structured AMR
- Issues/Goals
    - —Eliminating numerical self-forces in nonuniform grids
    - —Fast infinite-domain boundary conditions.
    - —Flexible specification of interaction between grid and particle data.
    - —Accurate representation of complex geometries.





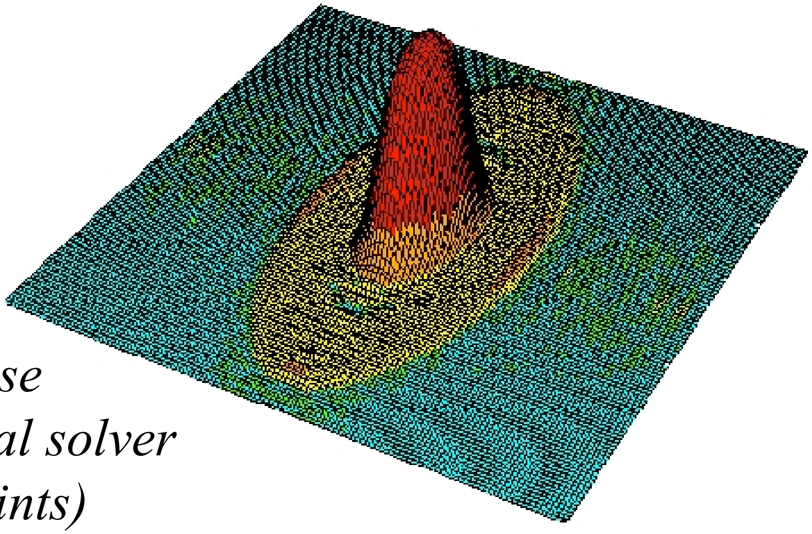
Direct Solvers: A future alternative to particle-based methods?

$$\frac{\partial f}{\partial t} + (\boldsymbol{p}\cdot\partial_{\boldsymbol{q}})f - (\nabla\Phi\cdot\partial_{\boldsymbol{p}})f = 0.$$

Vlasov equation

$$f(\boldsymbol{q},\boldsymbol{p},t) = \exp(-\frac{t}{2}\boldsymbol{p}\cdot\partial_{\boldsymbol{q}})\exp(t\nabla\Phi\cdot\partial_{\boldsymbol{p}})\exp(-\frac{t}{2}\boldsymbol{p}\cdot\partial_{\boldsymbol{q}})f(\boldsymbol{q},\boldsymbol{p},0) + O(t^3)$$

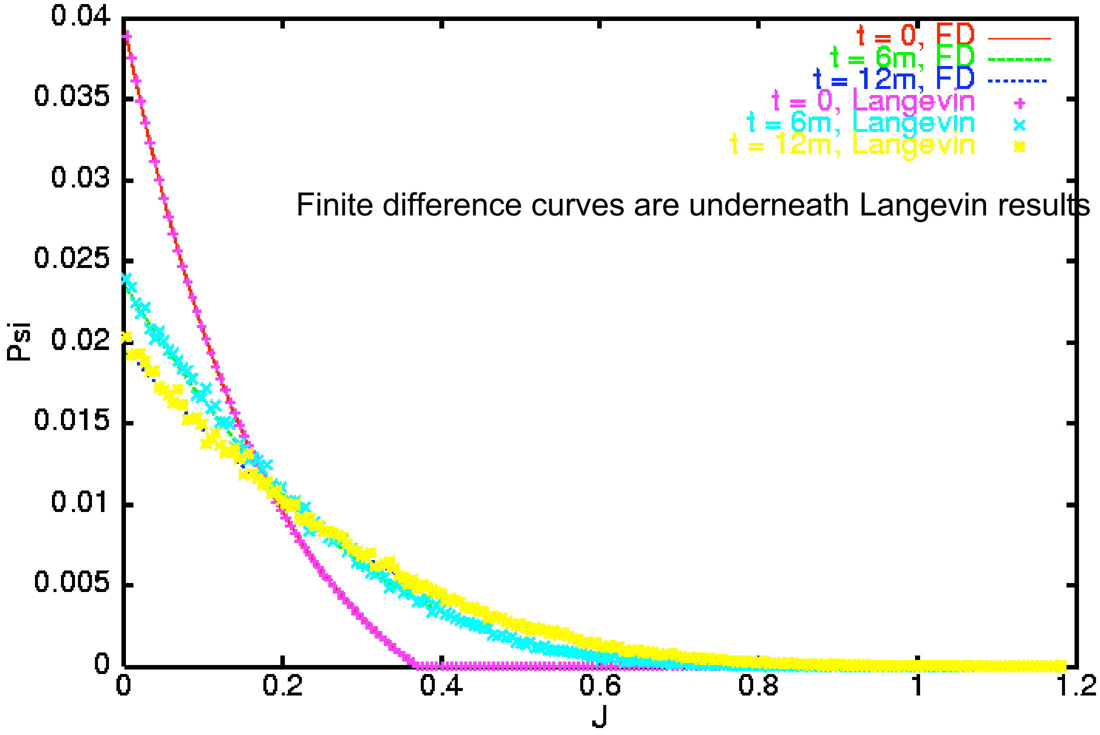
Split-operator stepping algorithm



Density plot from a 2D simulation of an intense beam in a quadrupole channel using a spectral solver with a 128^4 phase-space grid (268M mesh points)

Modeling Additional Effects: Collisional Effects

- In collaboration w/ BNL (J. Wei), have performed comparisons of the self-consistent Langevin approach with a finite difference model
  - —Langevin results and FD results are in excellent agreement, but Langevin does not have instability problem present in FD method

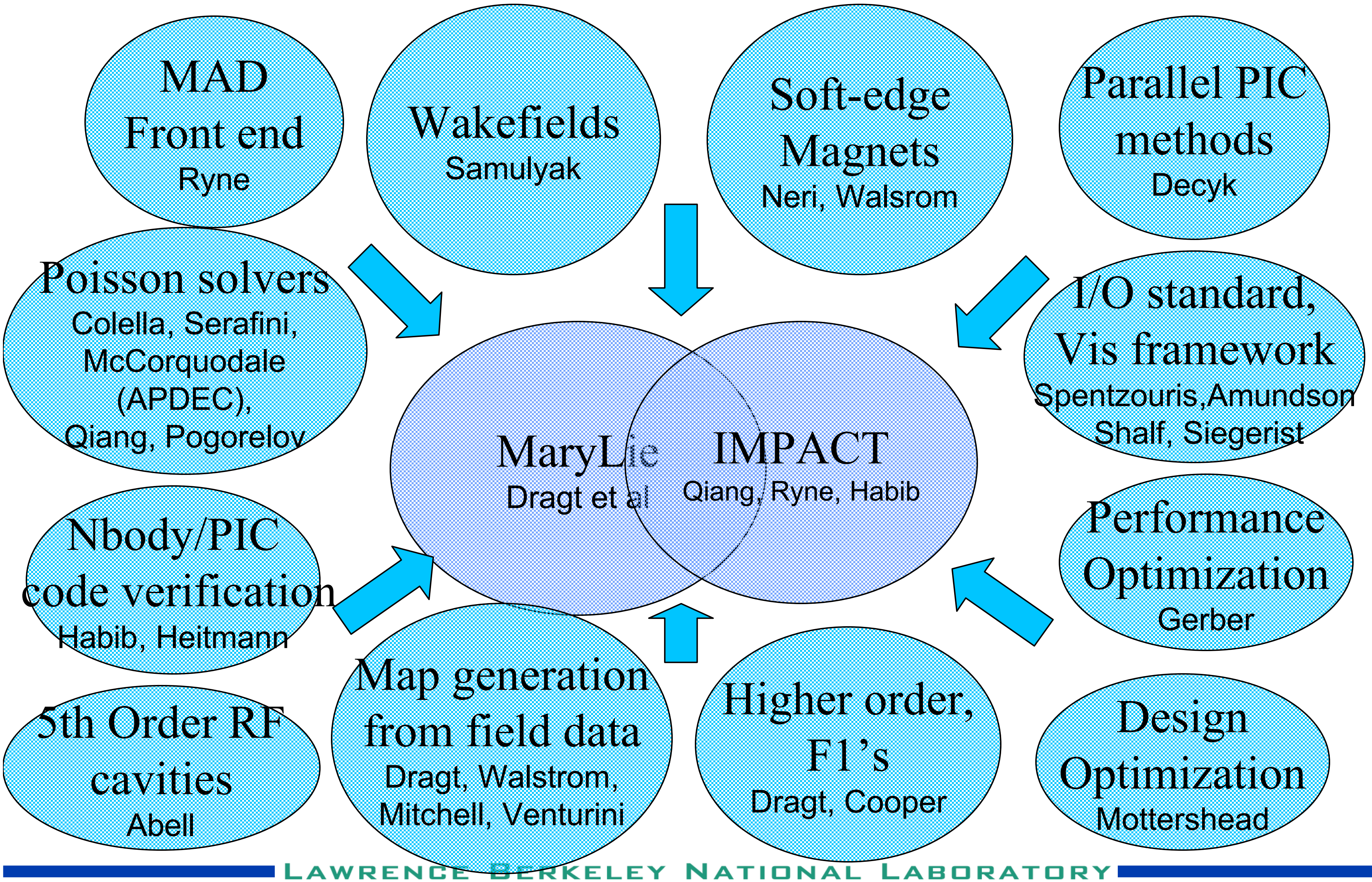


Finite difference curves are underneath Langevin results

Code Componentization and Reuse

- SciDAC model emphasizes large multidisciplinary teams; code componentization and reuse; involvement of applications scientists, computer scientists, mathematicians, visualization experts…
- Examples:
  - —Incorporation of Poisson solvers (P. Colella (APDEC), Chombo)
  - —Incorporation of PIC code parallelization strategies (V. Decyk, UPIC)
  - —Incorporation of parallel PIC data handling & viz (PARTVIEW,H5PART; J. Shalf,C. Siegerist, A. Adelmann)

Code dev. involves large multidisciplinary teams. Example: MaryLie/IMPACT beam dynamics code



MAD Front end
Ryne

Wakefields
Samulyak

Soft-edge Magnets
Neri, Walsrom

Parallel PIC methods
Decyk

Poisson solvers
Colella, Serafini, McCorquodale (APDEC), Qiang, Pogorelov

MaryLie
Dragt et al

IMPACT
Qiang, Ryne, Habib

I/O standard, Vis framework
Spentzouris, Amundson Shalf, Siegerist

Nbody/PIC code verification
Habib, Heitmann

Performance Optimization
Gerber

5th Order RF cavities
Abell

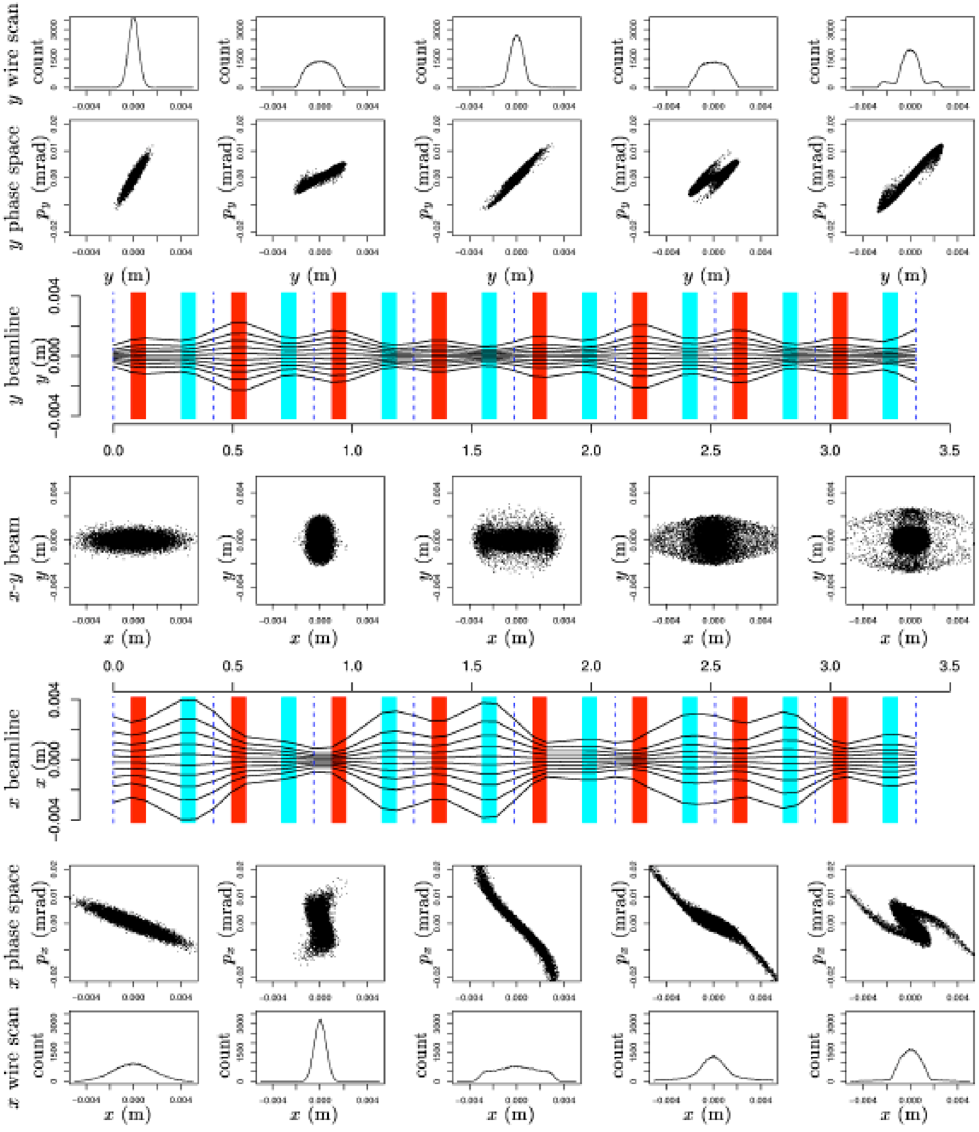
Map generation from field data
Dragt, Walstrom, Mitchell, Venturini

Higher order, F1's
Dragt, Cooper

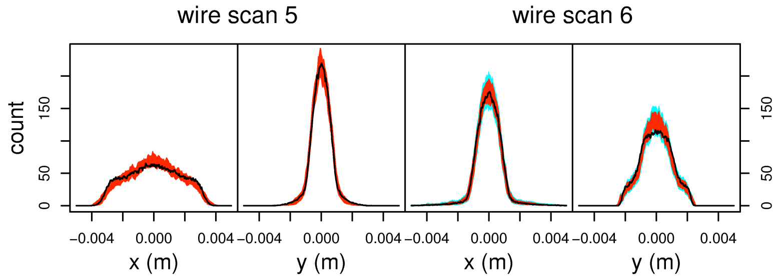
Design Optimization
Mottershead

Predictability; Uncertainty Quantification; Code Verification and Validation

Statistical Methods for Calibration & Forcasting (D. Higdon et al, LANL)



- **Determining initial phase space distribution from 1D wire scan data.**



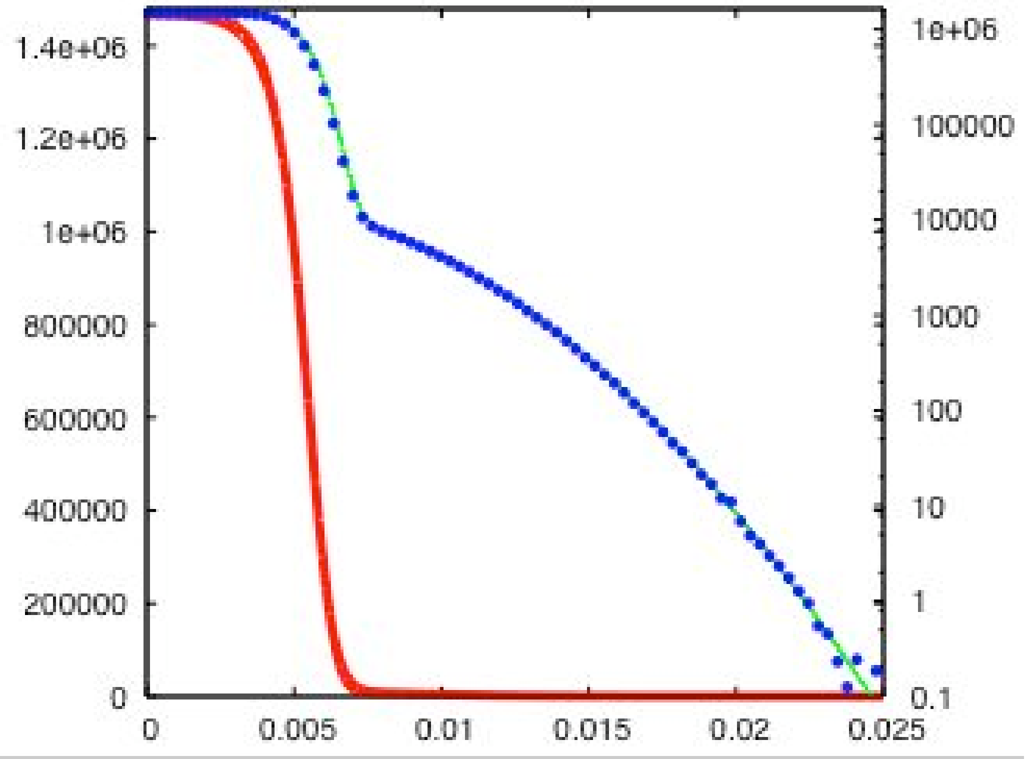
Simulation of a high intensity proton beam through a series of quadrupole magnets. Statistical techniques were used to combine 1D profile monitor data with simulations to infer the 4D beam distribution. The figure shows the 90% intervals for the predicted profile at scanner #6 (shaded regions), and, for comparison, the observed data (black line). Only data from the odd numbered scanners were used to make the prediction.

Code Test Suite

(dev in collab w/ A. Adelmann, J. Amundson, P. Spentzouris)

- KV beam in a FODO channel
- Free expansion of a cold, uniform density bunch
- Cold beam in a FODO channel with RF cavities
- Thermal beam in a constant focusing channel
- Bi-thermal beam in a constant focusing channel

Bithermal distribution: A self-consistent 3D beam w/ a pronounced halo



ML/I simulation of bithermal distribution: 95% charge in core, 5% charge in halo. Note 6 order of magnitude resolution in simulated wirescan.

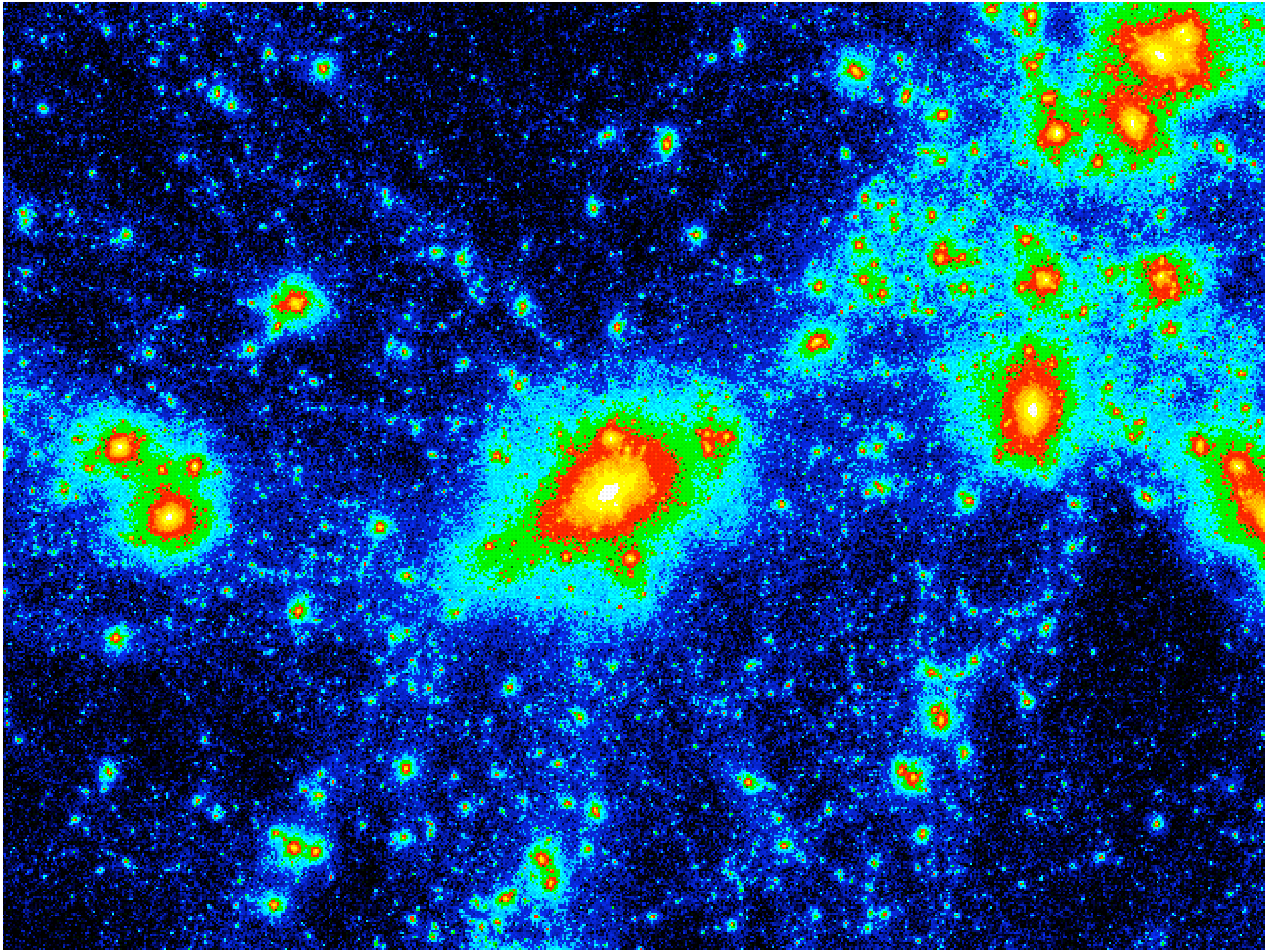
Question: Which accelerator physicist said this about N-body Simulations?

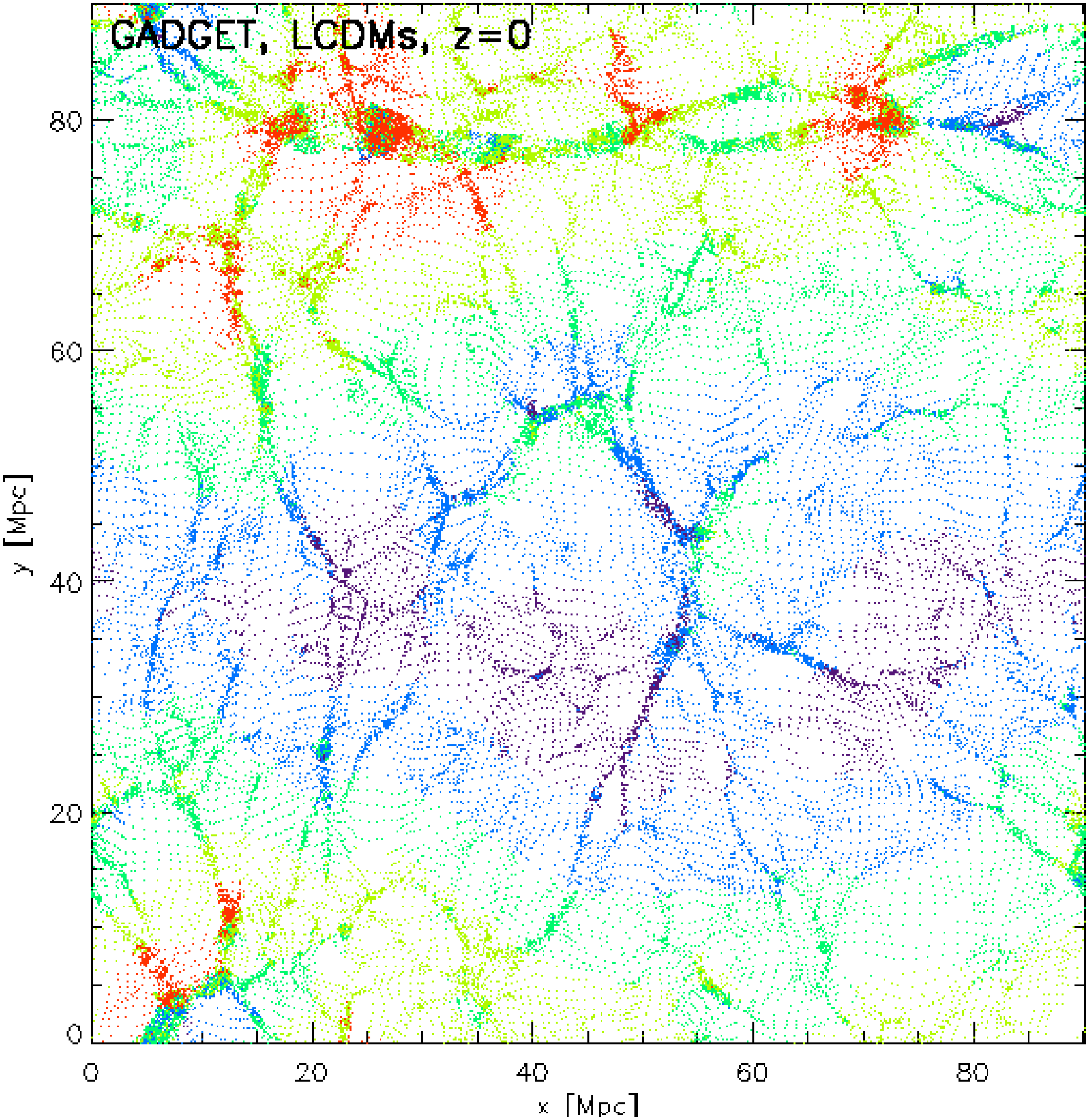
- Task: solve collisionless Vlasov-Poisson equation; problems: 6-dim partial differential equation; because of nonlinearity ever smaller substructure is generated, instabilities occur as structure is generated on sub-resolution scales
- N-body approach: sample phase space distribution with tracer particles and evolve them by computing inter-particle forces -- N^2 problem
- further approximation techniques reduce force calculation to ~O(N) or ~O(NlogN); grid-based or multipole expansions or combination of both
- Klypin/Shandarin (1983): 32,768 particles; now: 1 billion !!

Answer: Not an accelerator physicist. Previous comments from a study on cosmology simulations

- “Robustness of cosmological simulations I: Large-scale structure,” Heitmann, Ricker, Warren, Habib (astro-ph/0411795)
- Goal: test & compare 6 different N-body codes
- Uses 4 test problems
- Every code starts from exactly the same initial conditions
- Results are analyzed with the same set of analysis codes
- Investigation of particle 2-point functions, velocity statistics, halo catalogues

Given the commonality of issues, close collaboration among computational cosmologists, plasma physicists, and accelerator physicists is natural & highly beneficial.

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Signpost System 1985

A CRAY RESEARCH, INC. PUBLICATION

CRAY CHANNELS

Summer 1985

ANNOUNCEMENT!

FEATURE ARTICLES:

Introducing the CRAY-2 Computer System

Computer simulation and nuclear safety

Multitasking at Cray

Migration of seismic source records

CUG grows to meet user needs

DEPARTMENTS:

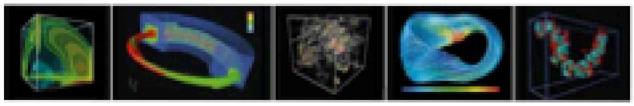
Corporate register

Applications in depth

User news

Cray-2

- 244 MHz (4.1 nsec)
- 4 processors
- 1.95 Gflop/s peak
- 2 GB memory (256 MW)
- 1.2 Gflop/s LINPACK R_max
- 1.6 m^2 floor space
- 0.2 MW power

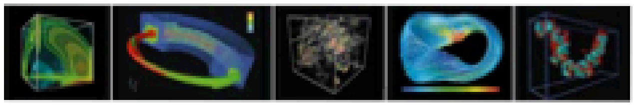


Signpost System in 2005

Artist's rendition of Blue Gene, a full-scale BG/L with 360 Tflop/s peak scheduled to become fully operational in early 2005. The computer's name is derived from its principle intended purpose — to model the folding of human proteins.

IBM BG/L @ LLNL

- 700 MHz (x 2.86)
- 65,536 nodes (x 16,384)
- 180 (360) Tflop/s peak (x 92,307)
- 32 TB memory (x 16,000)
- 135 Tflop/s LINPACK (x 110,000)
- 250 m² floor space (x 156)
- 1.8 MW power (x 9)



Preparing for the future

- High end platforms w/ 10’s of thousands of procs are here now
  - Access to platforms w/ 100’s of thousands of procs is coming
  - Petascale by the end of the decade
- The accelerator community needs to continue to foster close ties with the applied math/comp sci communities. Needs include:
  - Scalable solvers
  - Multiscale/multiresolution solvers
  - Optimization tools
  - Large-scale viz tools
  - Tools for managing massive amounts of data
  - High speed networks
  - Collaborative tools
  - And many others
- Using in concert with theory and expt, petascale computing will open new doors to understanding the physics of intense beams, designing EM structures, and developing new methods of particle acceleration.