Present and Future Computing Requirements for

"Frontiers in Accelerator Design: Advanced Modeling for Next-Generation BES Accelerators" (repo m669)

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NERSC BES Requirements for 2017
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1. Project Description

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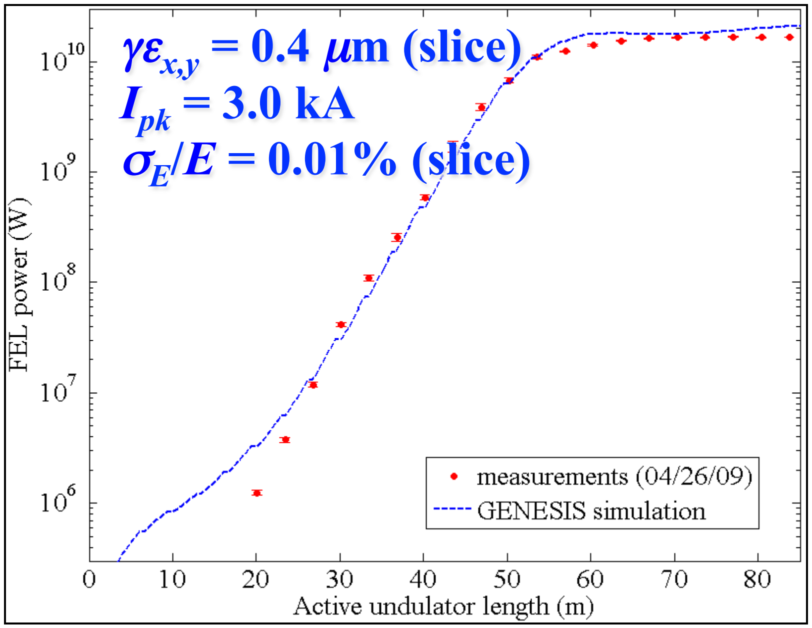
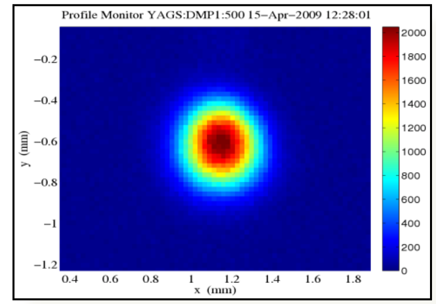
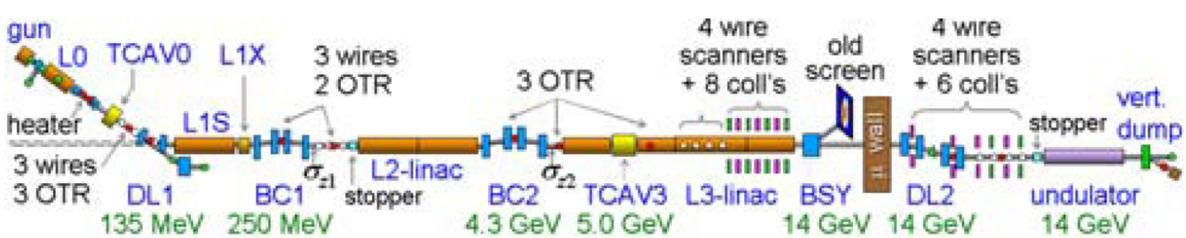
Senior personnel: Ji Qiang (LBNL), Cho Ng (SLAC), Bruce Carlsten (LANL)

- repo m669 supports BES accelerator design
  - concept exploration; accelerator system & accelerator component design; code development
- This presentation focuses on beam dynamics modeling for future light sources, especially X-ray Free Electron Lasers (XFELs)

The LCLS XFEL is a spectacular success

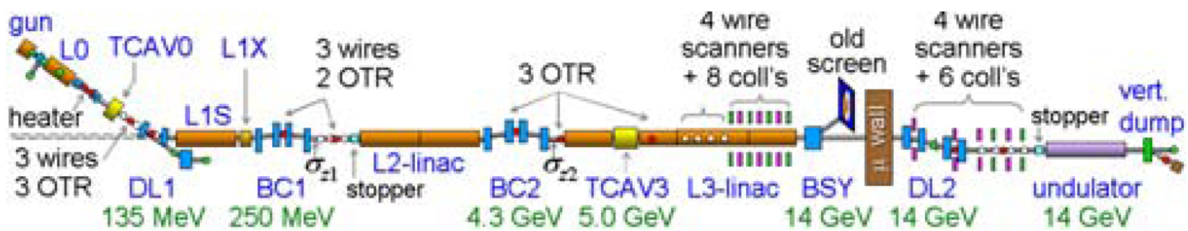




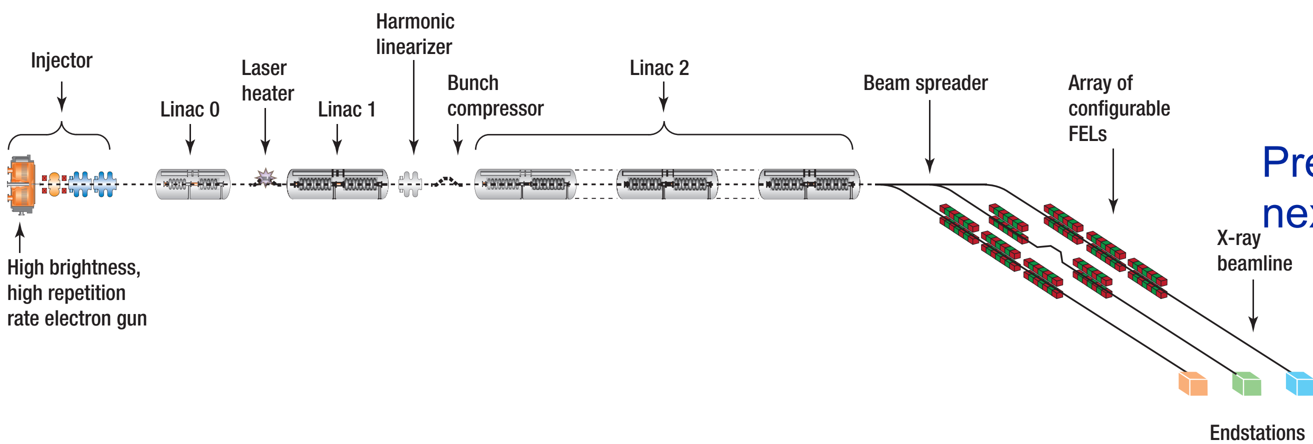


What is so challenging about future XFEL modeling?

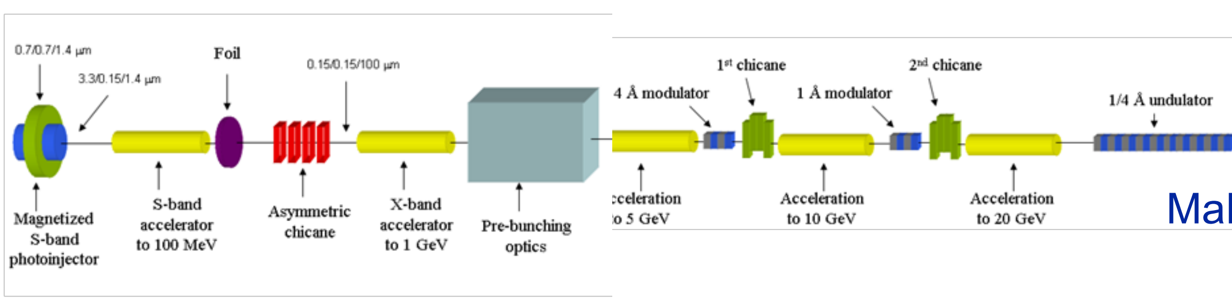
- To answer this, need to see what's in an XFEL:



LCLS



Pre-conceptual design of a next-generation light source



MaRIE (pre-conceptual design)

Components of an XFEL accelerator

- High brightness injector
  - e^- gun + systems to shape & accelerate the beam in the first ~100 MeV
- Complex “beam gymnastics” in the beam delivery system to accelerate up to final energy, and to prepare the beam before entering the FEL undulator
  - flat beam transformers, emittance exchangers, chicanes, bunch compressors,…
  - seeding sections
  - beam deflection systems
- The FEL itself

Leads to new regime of high resolution, multi-physics, beam dynamics modeling

- Requires
  - nonlinear optics
  - space charge
  - structure wakes
  - radiation
  - e^- beam/laser interaction

under control thanks to programs like SciDAC (nonlinear optics, space charge, structure wakes)

very challening, extremely important! (radiation, e^- beam/laser interaction)

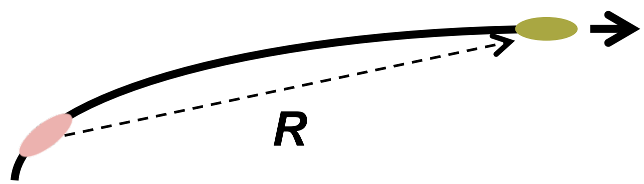
- Extreme resolution and/or multi-scale modeling needed to simulate e^- beam/laser interaction (seeding) – included in BES Accelerator R&D project

Light source milestone (2013, Ji Qiang et al)

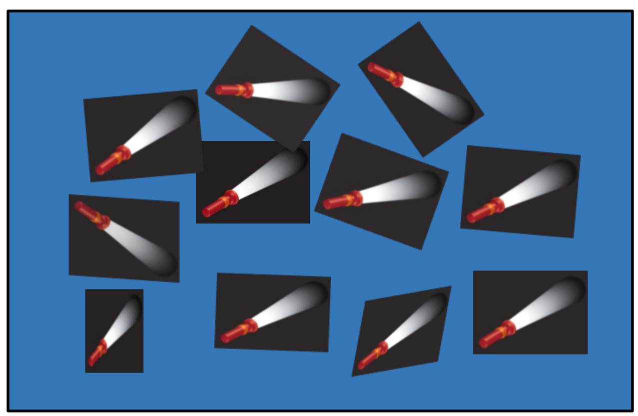
- start-to-end parallel simulation of future light source
- real-world # of simulation particles (2 billion)
- interfaced/combined 3 key codes into a single executable:
  - IMPACT-T, IMPACT-Z, GENESIS
- included beam optics, 3D space-charge, wakes, 1D CSR
- 14 hrs on 2048 cores of Hopper

3D simulation of synchrotron radiation has remained a major challenge

- Synchrotron radiation: arguably the least well modeled physical phenomenon in e^- linacs for future light sources
  - most codes use a simplified 1D model
- Highly important to beam quality and beam stability:
  - emittance degradation
  - microbunching instability



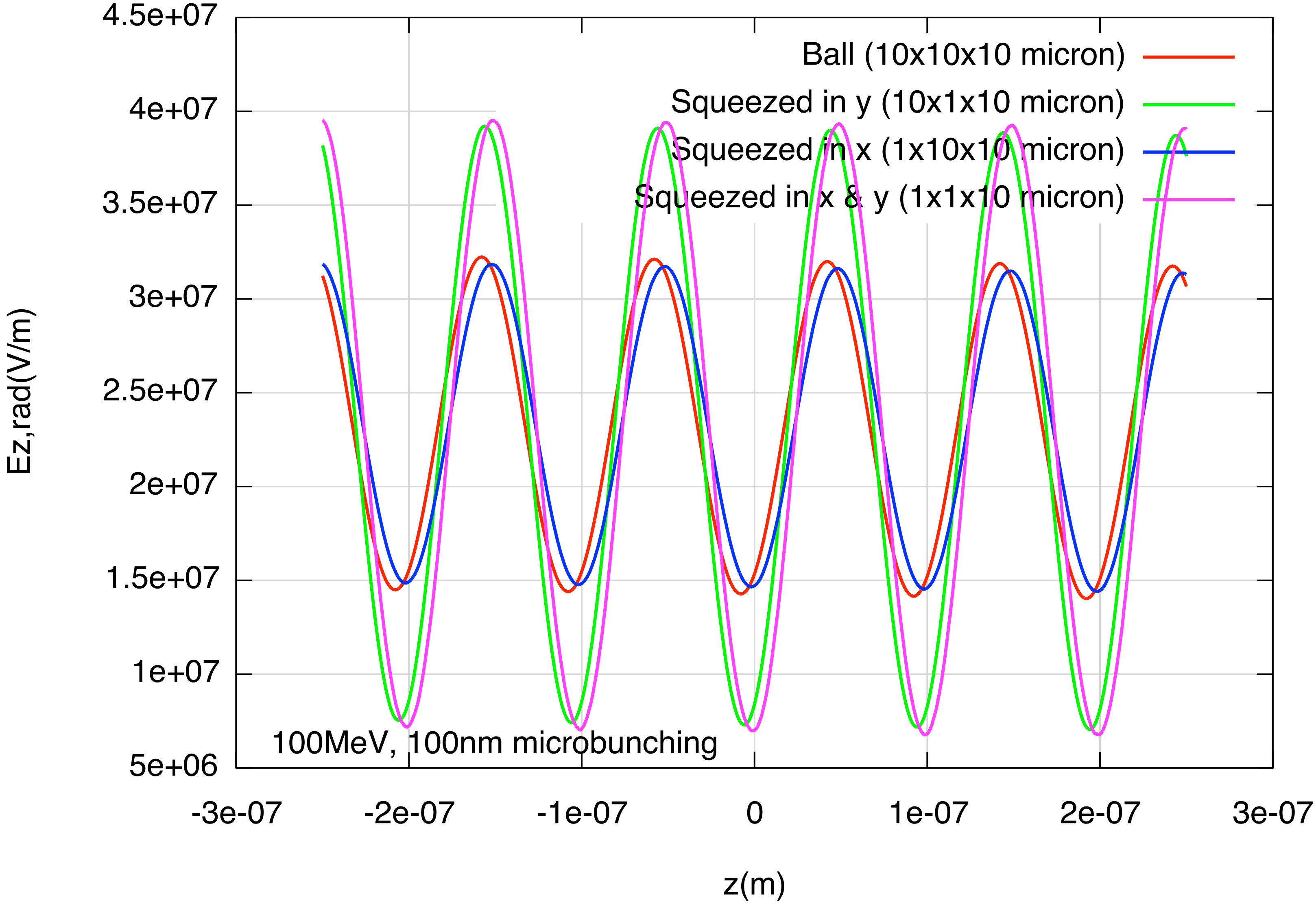
- challenging spatial dependence: radiation confined to very tiny cone angle ($\sim 1/\gamma$)



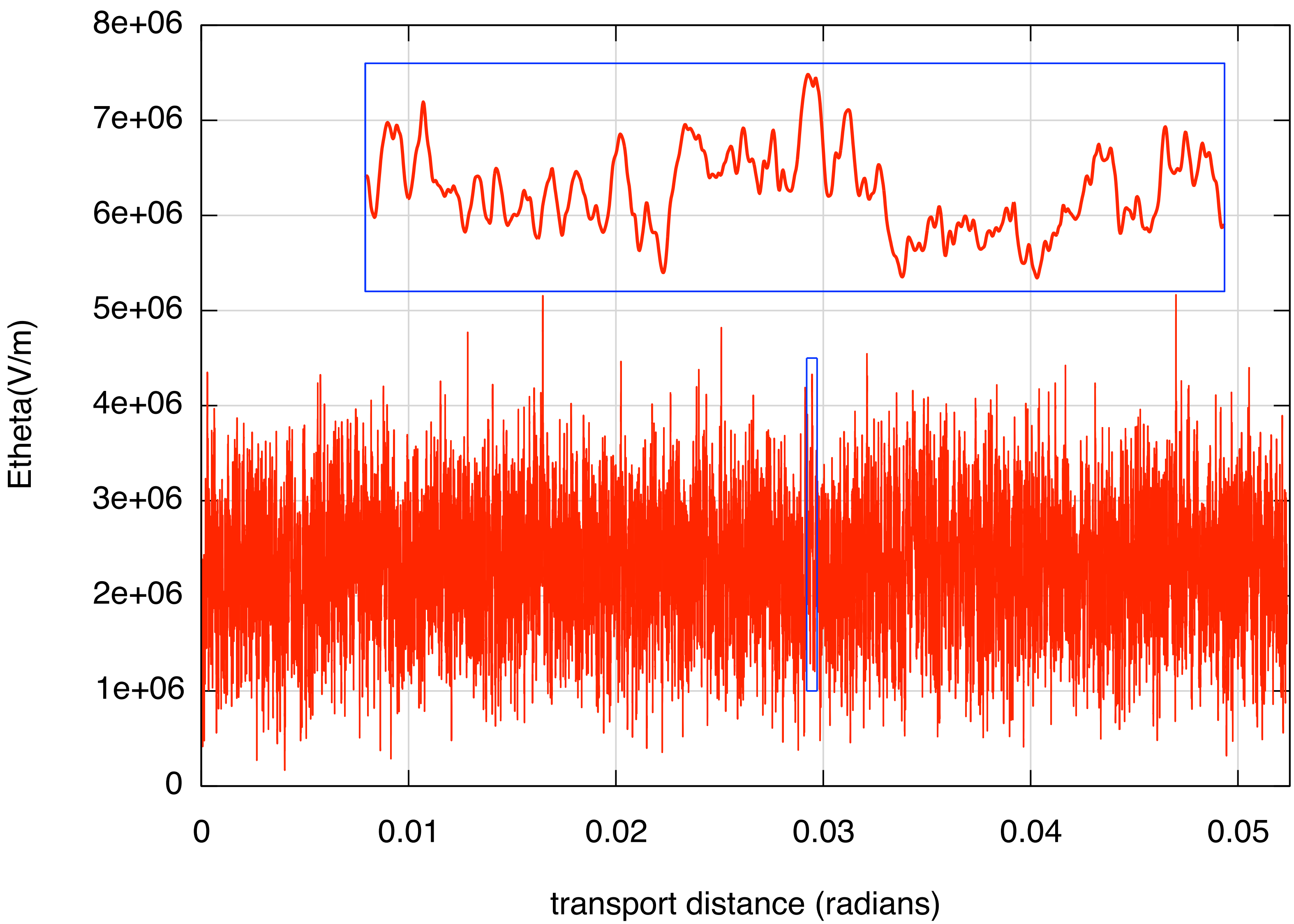
imagine a billion ultra-narrow flashlight beams shining on each other

besides difficult-to-model spatial dependence, also need to take into account finite speed of light

3D CSR effect: sensitivity to vertical bunch size



Influence of shot noise on energy

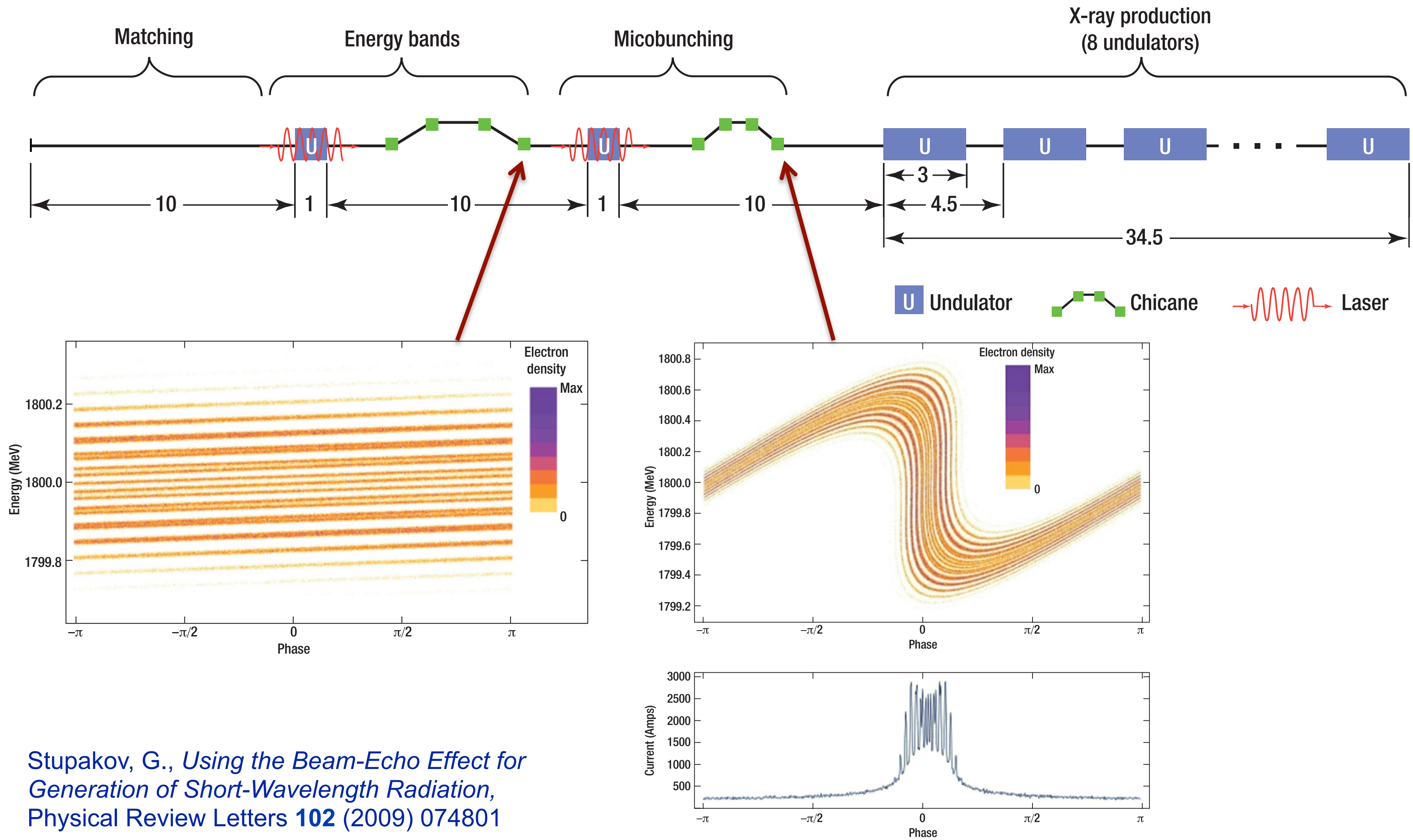


E_θ at the center of Gaussian bunch w/ 6 billion particles

Exploring seeding schemes through simulation is extremely challenging

- Seeding: Impressing short λ modulation on a beam so that radiation grows from the impressed modulation, not from spontaneous emission
  - higher power, increased coherence, potentially shorter undulators & reduced cost
- Length scales: laser λ is ~10-100 nm, bunch length ~0.1 mm
- Resolution required: need to resolve features 10,000x times smaller than the bunch length
- Compounding the challenge: beam transport schemes under study *mix* the transverse and longitudinal phase spaces. So the transverse dimensions might also require high resolution!

Seeding imparts fine structure on the beam longitudinal phase space



Stupakov, G., *Using the Beam-Echo Effect for Generation of Short-Wavelength Radiation,* Physical Review Letters **102** (2009) 074801

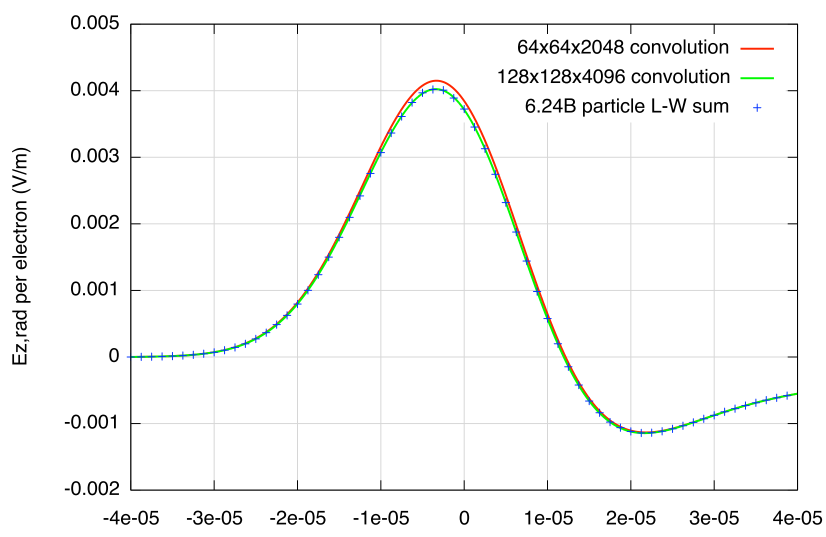
1. Project Description, cont.

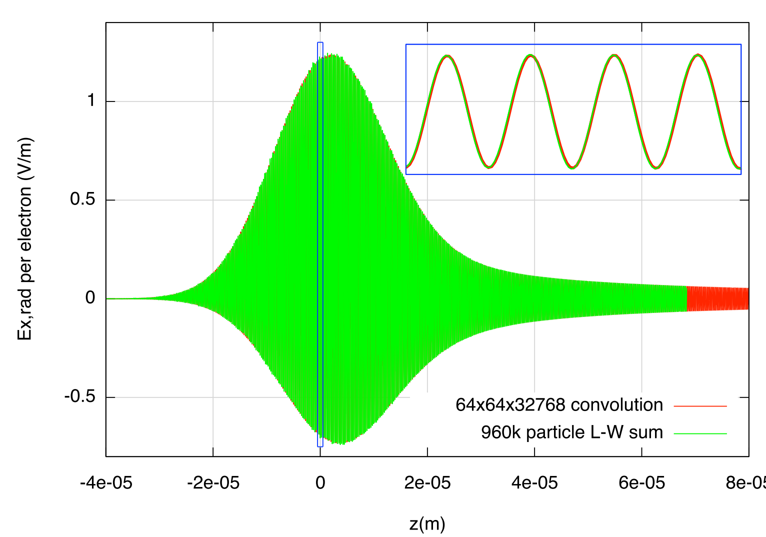
- Scientific objectives through 2017:
  - develop scalable, parallel beam dynamics capabilities for BES light source design
    - including high-resolution modeling of radiative phenomena in 3D
  - seeding
  - shot noise effects
  - parallel design optimization
  - applications to BES light source projects
  - distribute & deploy capabilities to the community

2. Computational Strategies

- We approach this problem computationally at a high level via parallel particle-in-cell codes
- The beam dynamics codes we currently use are primarily in the IMPACT suite
- IMPACT PIC codes are characterized by these algorithms:
  - particle advance via maps and via numerical integration for a wide variety of accelerator systems
  - parallel Poisson solvers
  - solvers for other phenomena (1D CSR, structure wakes,...)
- Our biggest computational challenges are:
  - communication associated w/ 3D space-charge solver
    - charge deposition, field solution, field interpolation
- Our parallel scaling is limited by communication
  - some PIC codes scale well by using large # of particles; in our case, we use the real-world # of particles, no more.

- We expect our computational approach and/or codes to change significantly by 2017 (actually sooner)
- We have demonstrated on Hopper and Edison that a new approach allows accurate calculation of 3D radiative effects using a single-particle Lienard-Wiechert Green function





Comparison of two methods -- brute-force Lienard-Wiechert (L-W) summation and L-W convolution with a retarded Green function -- for two test problems. Left: z-component of the radiation electric field of a 1 GeV Gaussian bunch inside a dipole magnet. Right: x-component of the radiation electric field of a 125 MeV modulated Gaussian bunch inside an undulator of a free electron laser. The two methods are in excellent agreement for both test problems. The narrow blue rectangle on the right figure shows the domain of the inset, and demonstrates excellent agreement even at the level of the radiation wavelength (250 nm in this example).

Parallel optimization

- Besides individual simulations to evaluate a specific design, we also have tools for parallel design optimization
- We use a 2-level parallelization strategy
  - 1 level for individual simulations of a single point in parameter space
  - 1 level for the optimizer
    - e.g., use differential evolutionary optimizers with ~100 population members

3. Current HPC Usage

- Machines currently using: Hopper, Edison
- Hours used in 2013: 10M
- Typical parallel concurrency and run time:
    - few thousand to 10K cores, 10+ hrs
- Largest runs to date: ~100K cores

4. HPC Requirements for 2017

(Key point is to directly link NERSC requirements to science goals)

- Compute hours needed (in units of Hopper hours): >100M
- Changes to parallel concurrency, run time
  - Our Lienard-Wiechert codes will scale to ~100K cores for a "point" simulation, ~1M cores for design optimization
    - usage for "typical" runs will depend on queue wait times
- Scratch space: ~100 TB
- Aggregate bandwidth: 0.5 -1 TB/sec

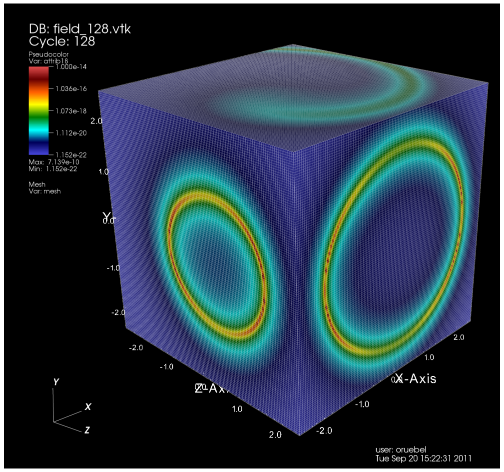
5. Strategies for New Architectures

- Our strategy for running on new many-core technologies (GPUs or MIC) is:
  - if NERSC plans to acquire a GPU-based system, we will adapt the Lienard-Wiechert solver to make use of it
    - many FLOPs, but not much data movement

- To date we have prepared for many core by:
  - exploration of using MPI+OpenMP

Collaboration w/ ASCR researchers has been, and will continue to be, essential

- ExaHDF5 team: parallel I/O, analysis, vis.
    - Chou, Wu, Rubel, Howison, Qiang, Prabhat, Austin, Bethel, Ryne, Shoshani, *Parallel Index and Query for Large Scale Data Analysis*, to appear in SuperComputing 2011.
- E. Wes Bethel et al (VACET):
    - O. Rubel, C. G. R. Geddes, E. Cormier-Michel, K. Wu, Prabhat , G. H. Weber, D. M. Ushizima, P. Messmer, H. Hagen, B. Hamann, E. W. Bethel, *Automatic beam path analysis of laser wakefield particle acceleration data*, Computational Science & Discovery, vol. 2, 015005 (2009)
    - O. Rubel and R. Ryne, CSR visualization using VisIt
- H. Shan et al: code performance optimization
    - H. Shan, E. Strohmaier, J. Qiang, D. Bailey, K. Yelik, *Performance Modeling and Optimization of a high energy colliding beam simulation code*, Proc. Supercomputing' 06
- D. Higdon et al: statistical methods for inference, forecasting
    - D. Higdon et. al, *Combining Field Data and Computer Simulations for Calibration and Prediction*, SIAM J. Sci. Comput. Vol. 26, No. 2, pp. 448-466 (2004).
- X. Li: multi-core performance optimization



Dipole CSR (O. Ruebel and R. Ryne, LBNL)

ExaHDF5 plans

- Parallel I/O in IMPACT, CSR3D, Warp
  - scale up to 130K cores on Edison
  - Benefit from ExaHDF5 performance scaling in other areas such as plasma physics
    - VPIC 2 Trillion particle simulation on 120,000 cores on Hopper
    - VPIC next-generation runs involving 10 Trillion particles are being planned

Conclusion

- The future of beam dynamics codes for light source design & simulation...

CODES, CAPABILITIES & METHODOLOGIES FOR BEAM DYNAMICS SIMULATION IN ACCELERATORS

IMPACT-Z
IMPACT-T
ML/I
Synergia
ORBIT
BeamBeam3D

PARMTEQ

WARP

PARMELA

PARMILA

SIMPSONS

IMPACT

2D space charge

rms eqns

3D space charge

GCPIC

MAD-X/PTC

DA

Freq maps

Symp Integ

Normal Forms

Integrated Maps

COSY-INF

MXYZPTLK

Partial list only;
Many codes
not shown

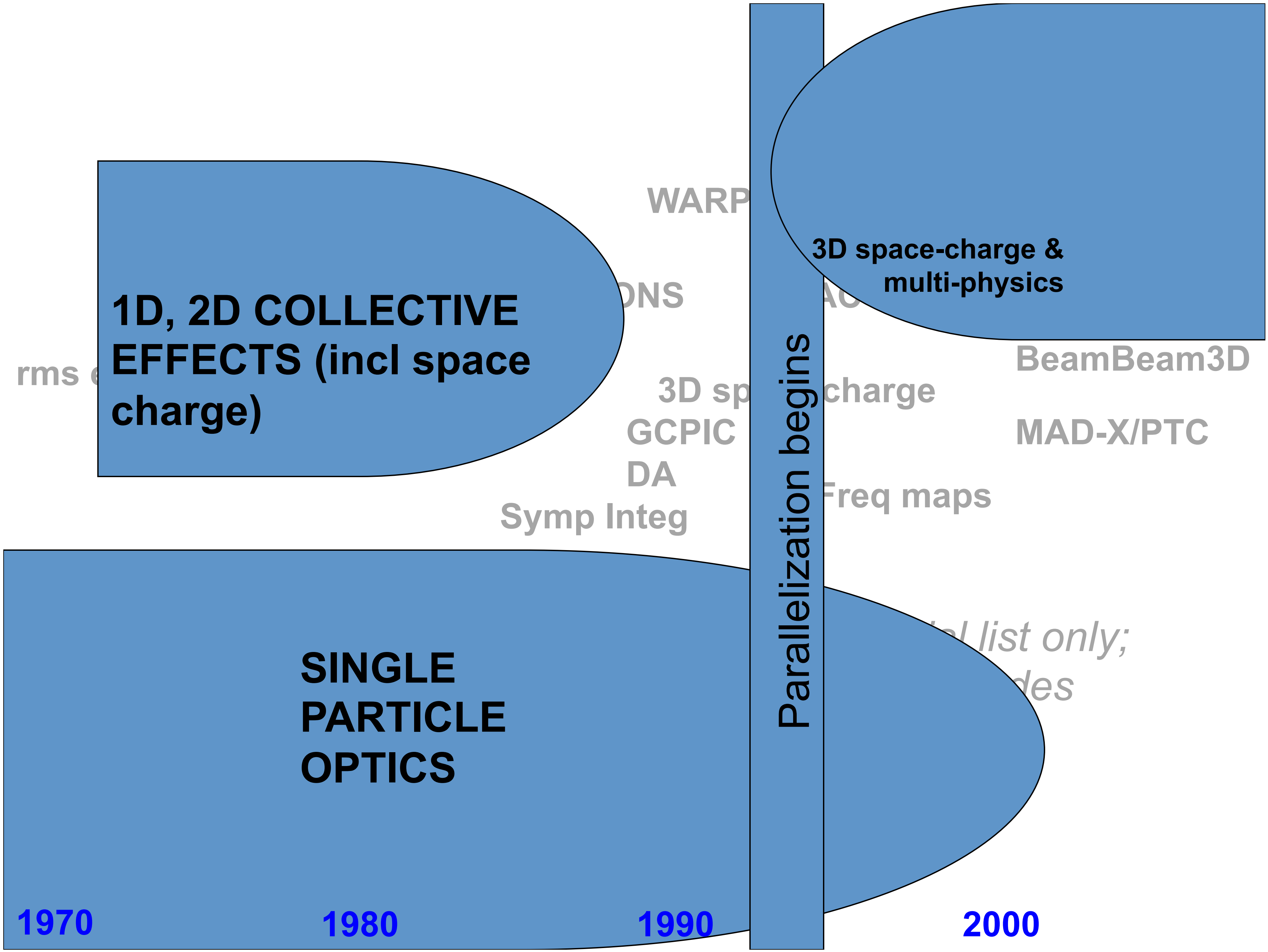
MaryLie

Dragt-Finn

MAD

Transport

1970 1980 1990 2000



1D, 2D COLLECTIVE EFFECTS (incl space charge)
3D space-charge & multi-physics
Parallelization begins
SINGLE PARTICLE OPTICS
WARP
rms
GCPIC
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Symp Integ
charge
Freq maps
BeamBeam3D
MAD-X/PTC
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1970
1980
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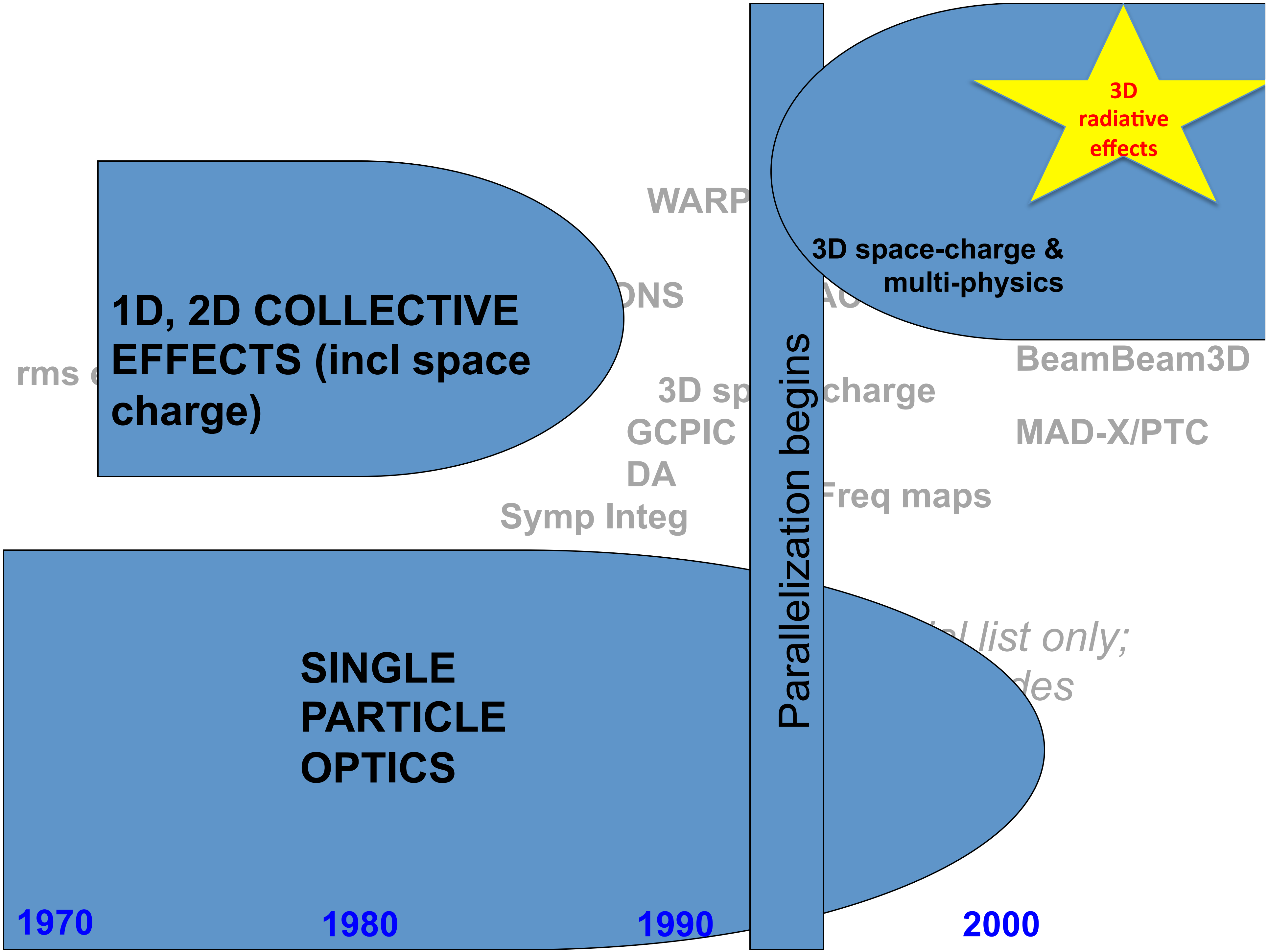
3D radiative effects
3D space-charge & multi-physics
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5. Summary

- We are on the verge of a new era in light source design & simulation
  - New algorithms and high-end HPC will enable Lienard-Wiechert particle-mesh simulations that include 3D radiative phenomena
    - new tools to explore concepts such as seeding
    - high resolution to accurately predict performance at very short wavelengths
    - shot noise effects
    - parallel design optimization including 3D CSR effects
- We are already seeing improved performance on Edison
- 3D modeling of radiative effects (vs 1D as is done now) will place significantly greater demands on our simulations
  - will easily use 10x allocation increase, possibly much more
  - use of GPUs if available would likely be very beneficial

Acknowledgments

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- LANL LDRD
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- VACET
- NERSC
- LANL Institutional Computing