Advanced Computing Tools and Models for Accelerator Physics

"We cannot foresee what this kind of creativity in physics will bring…"

Robert D. Ryne

Lawrence Berkeley National Laboratory

EPAC'08

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Genoa, Italy

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Acknowledgements, cont.

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SciDAC Scientific Discovery through Advanced Computing

Office of Science U.S. DEPARTMENT OF ENERGY

Acknowledgements, cont.

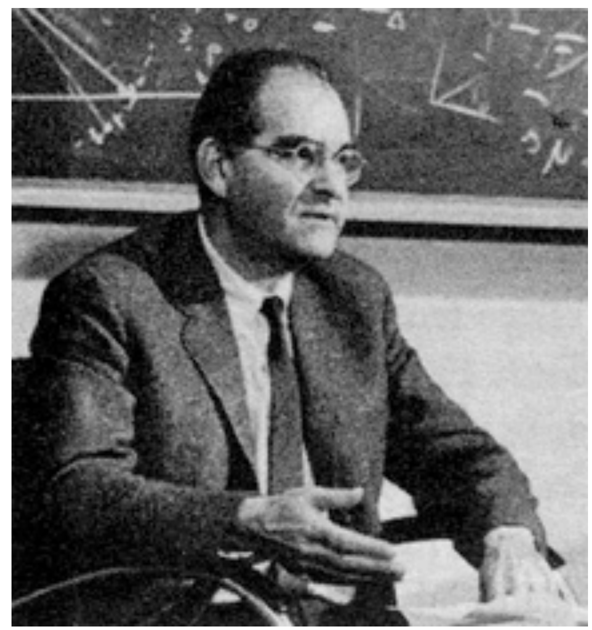
- Many of the results presented here made use of resources of the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory
- Results also made use of the ATLAS cluster at LLNL

From proceedings of 8th Int’l Conf on High Energy Accelerators, Geneva, 1971

- V. Weisskopf’s opening address
- Comment of L. Kowarsky

Weisskopf:

"…something new entered the picture – in this period from the thirties to the fifties, a new type of physicist appeared. No longer do we have only the experimental physicists and the theoretical physicists, but we have a new group which, for lack of a better word, I shall call the machine physicists."



Kowarsky:

"I would like to comment on your three kinds of physicists in a perspective somewhat more extended in time..."

Kowarsky, cont:

"Early experimentalists worked with their hands: Galileo's legendary tossing of stones from the Tower of Pisa, or the alchemists mixing by hand the ingredients in their mixing bowls. In a similar way the theoreticians manipulated their numerical quantities and symbols by their unaided brain-power. Then came the machines to extend the experimenter's manual skill and to open whole new worlds of things to be handled in ways nobody could predict or even imagine before they really got going."

Kowarsky, cont:

"Now we are at the beginning of a new kind of extension by machine: the computer comes to supplement the theoretician's brain. We cannot foresee what this fourth kind of creativity in physics will bring, but we may expect that, just as Ernest Lawrence's contribution was decisive to the development of nuclear machines, the name of John von Neumann will be remembered in connection with the origins of computational physics."

These remarks were made in 1971, when we had:

CDC 7600: From ~1969 - 1975, generally regarded as fastest computer in the world.   Performance ~ 10 Mflops

Two weeks ago, petaflop announcement:

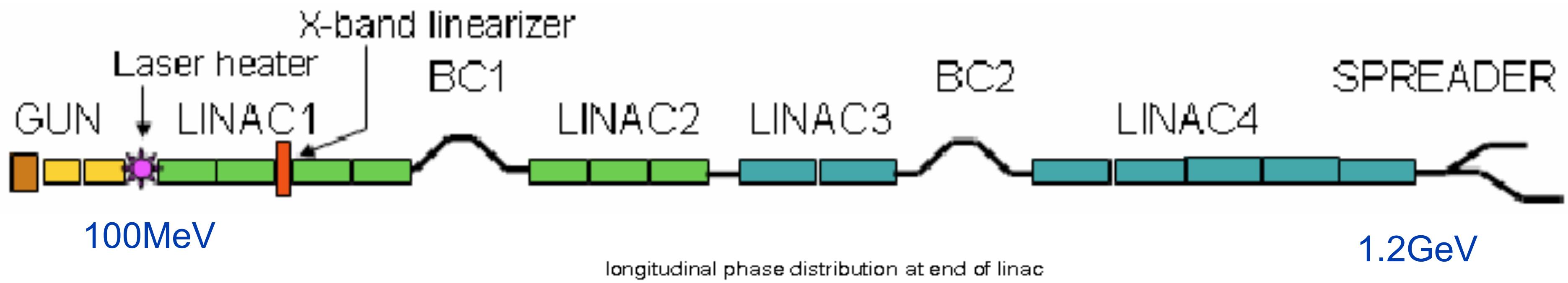
IBM “roadrunner”

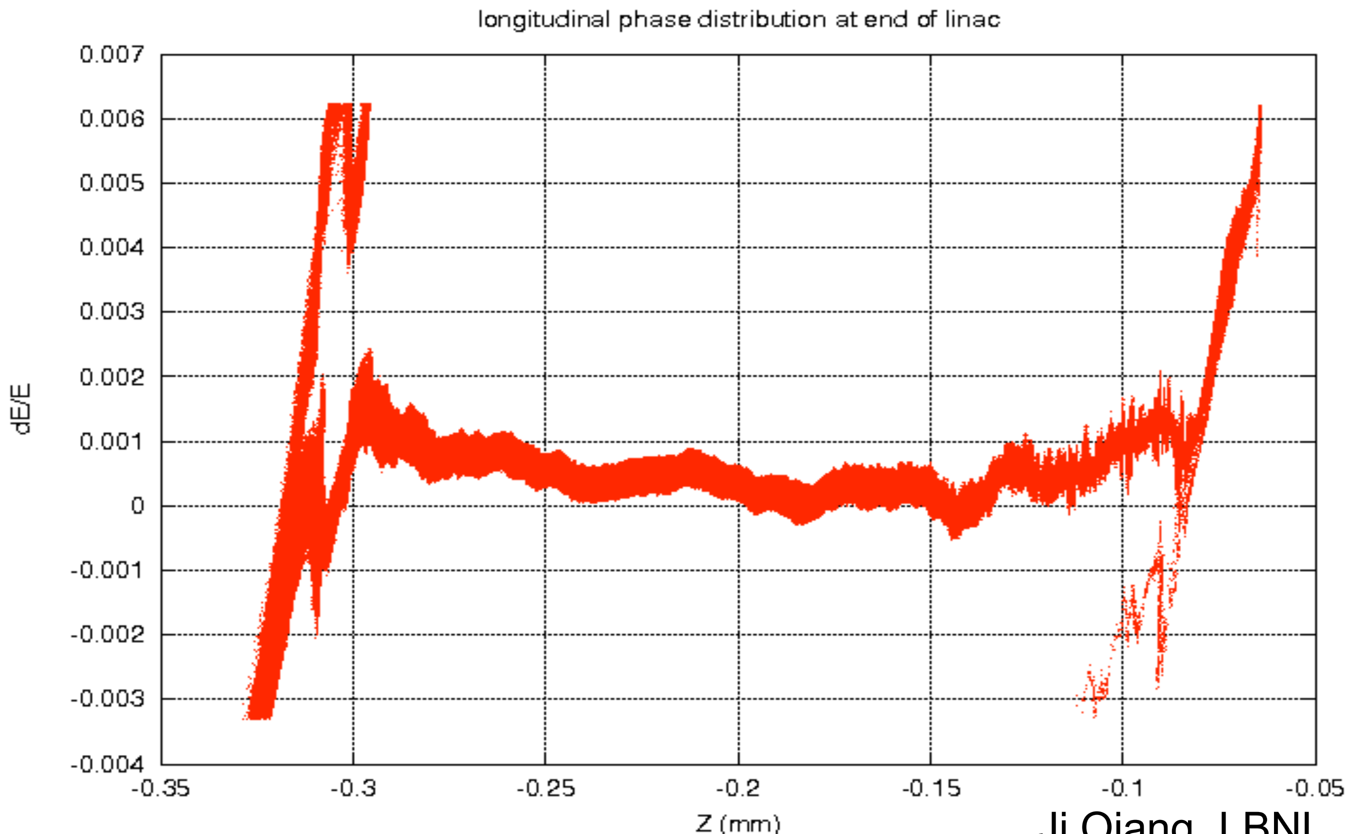
100 million times performance compared with computers at the time of the 1971 High Energy Accelerator Conference!

37 years since Kowarsky’s comments

Let’s see what supercomputing has enabled in accelerator science and technology

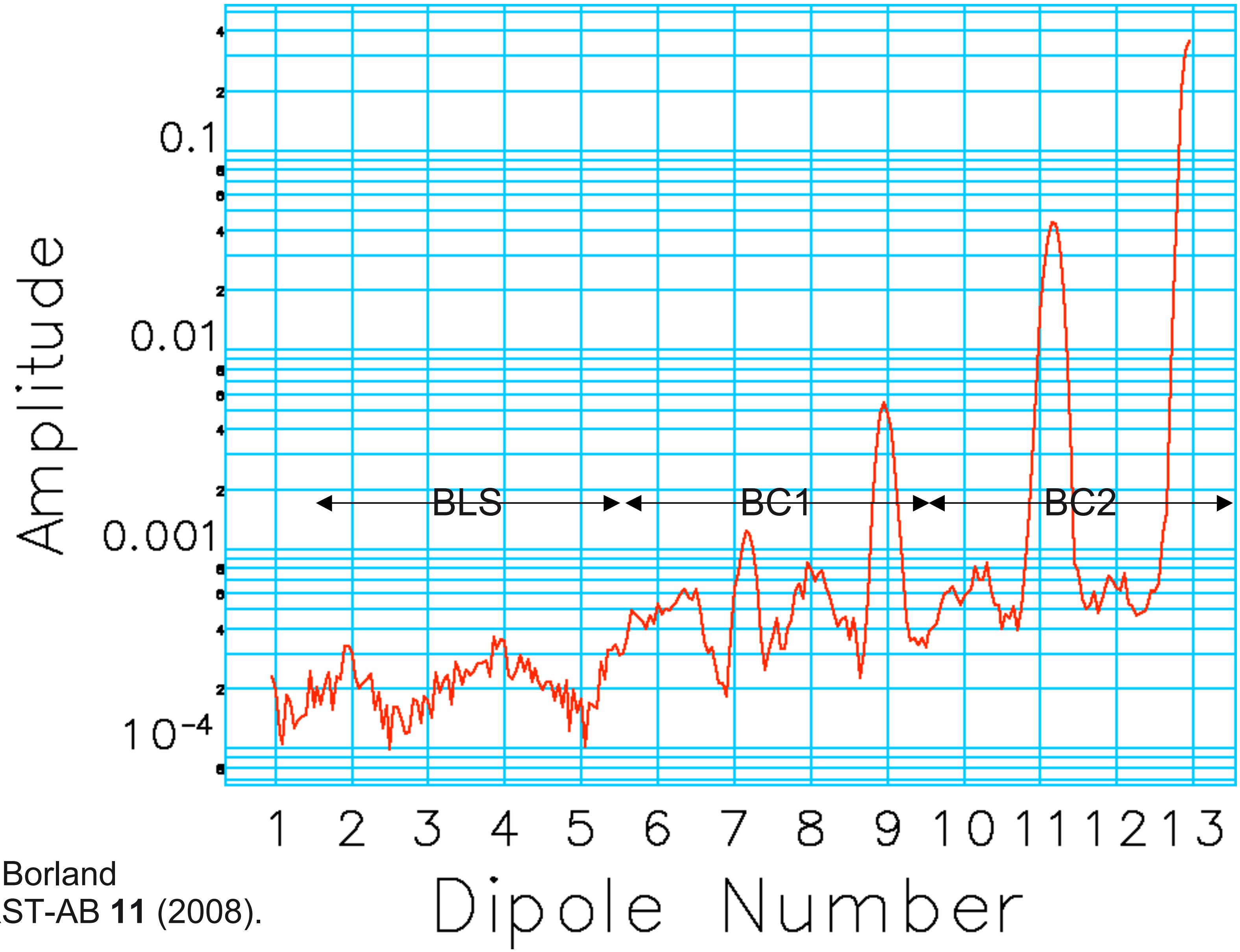
Modeling FERMI@Elettra Linac with IMPACT-Z Using 1 Billion Macroparticles





Ji Qiang, LBNL

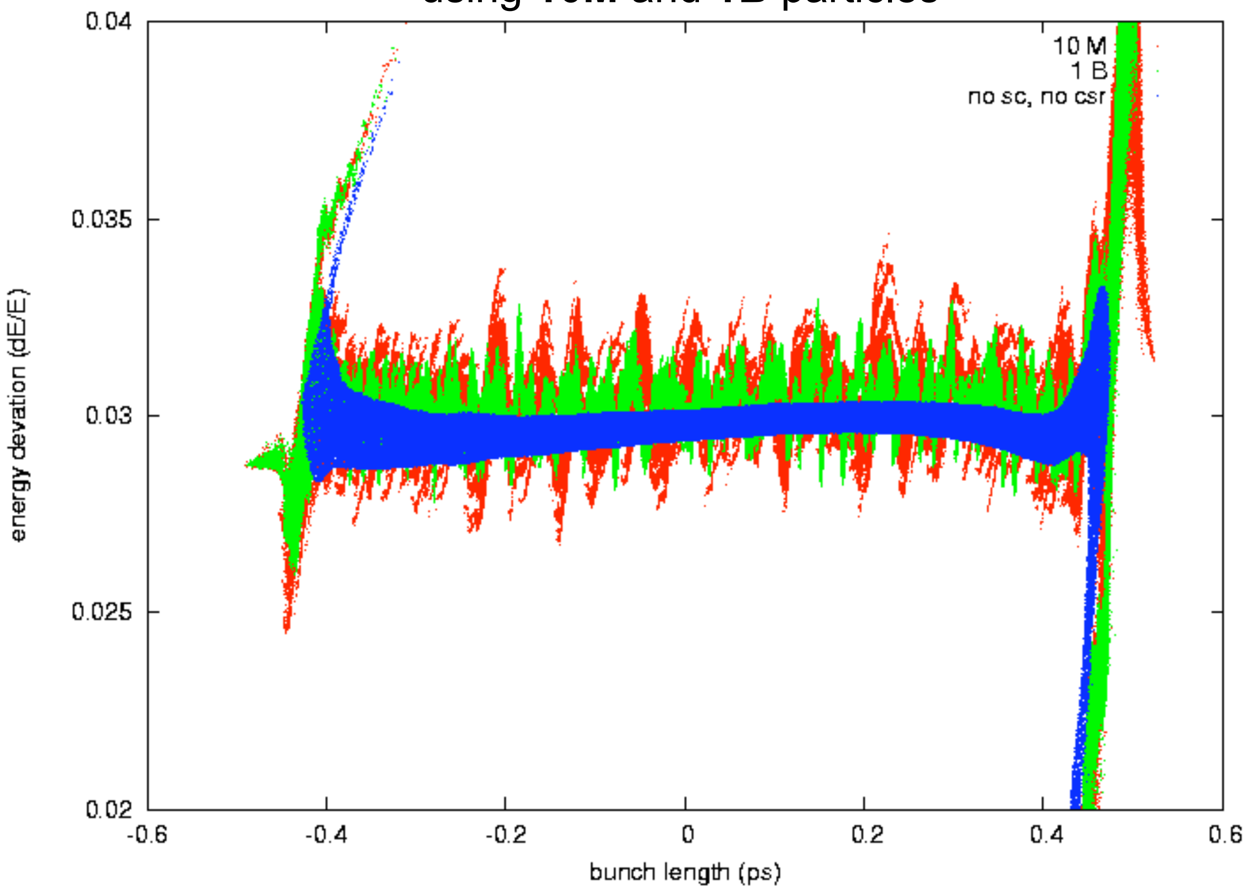
FERMI FEL Microbunching Instability Simulated with ELEGANT



M. Borland
PRST-AB **11** (2008).

Accurate prediction of uncorrelated energy spread in a linac for a future light source

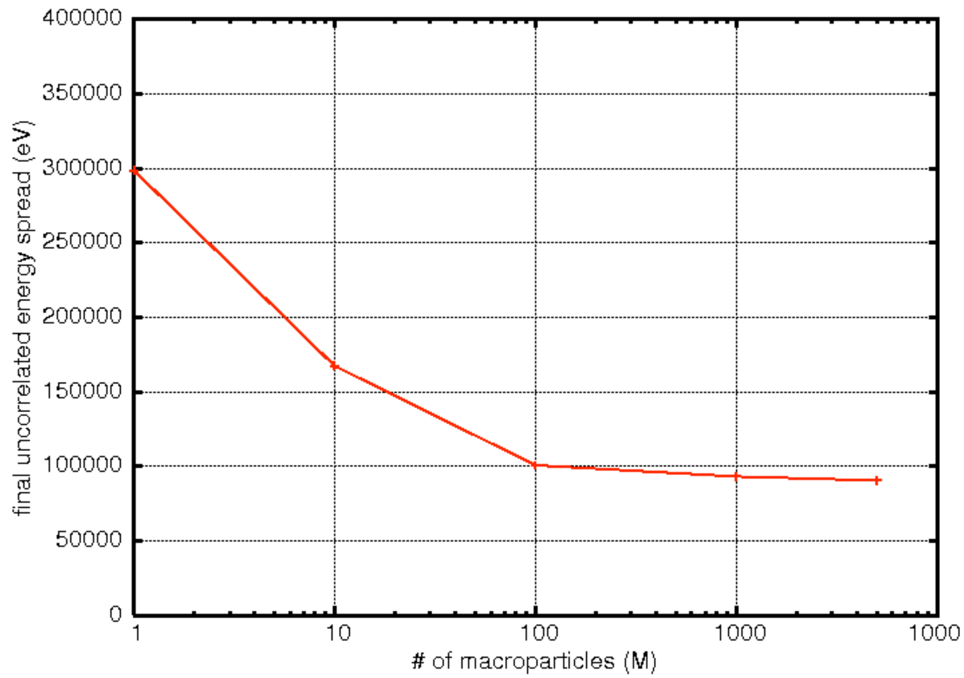
Final longitudinal phase space from IMPACT-Z simulation using **10M** and **1B** particles



Ji Qiang

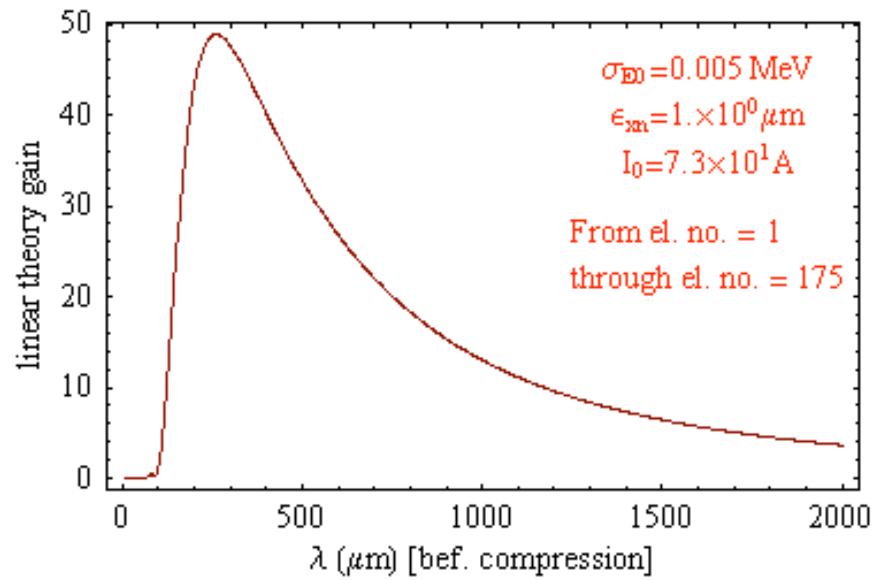
Final Uncorrelated Energy Spread versus # of Macroparticles: 10M, 100M, 1B, 5B

IMPACT-Z results



Ji Qiang

Microbunching instability gain function



M. Venuturini

High Performance Computing has made detailed 3D cavity calculations routine

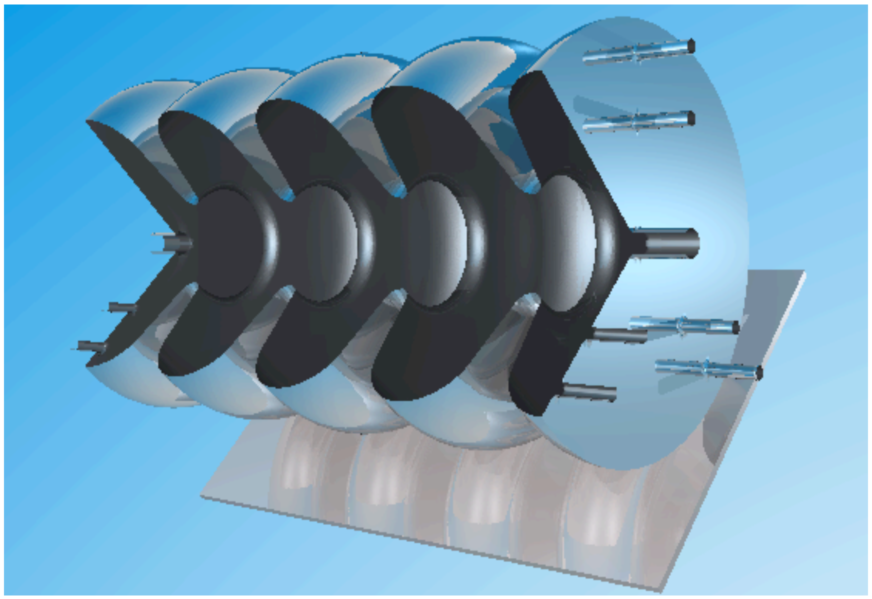
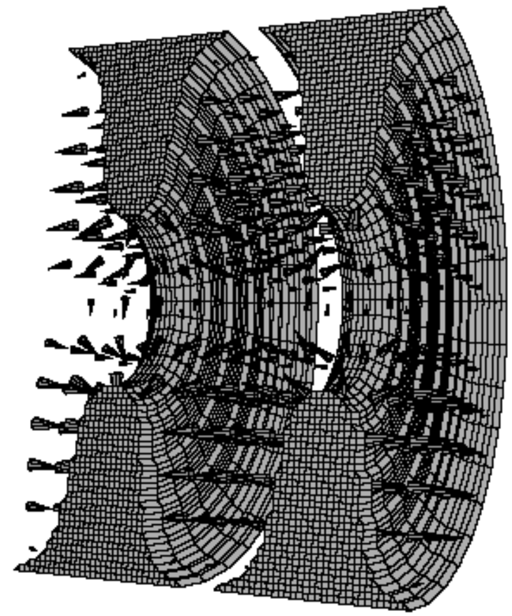


Image of crab cavity from computer model
J. Cary, Tech-X

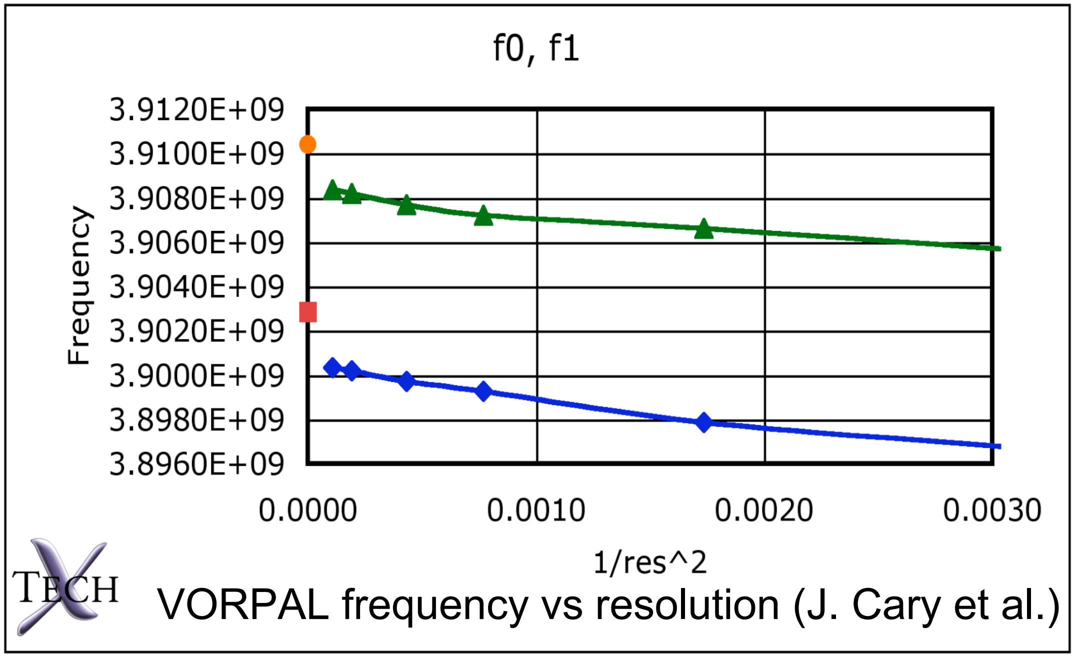


Typical computer model used in 1990's

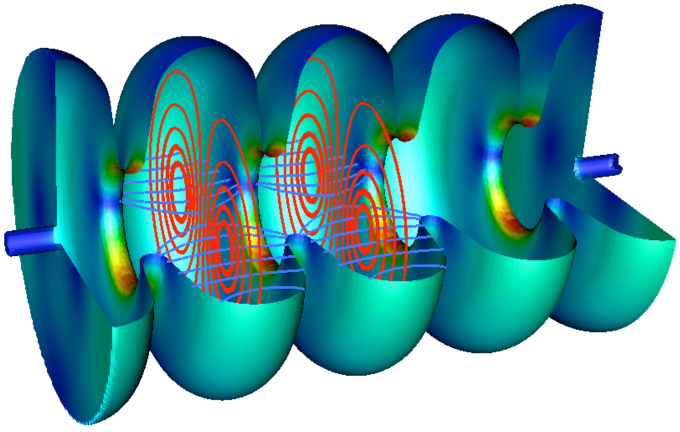
- Less than a decade ago: cylindrical symmetry, stairstep boundaries, accuracy ~0.1%
- Now: fully 3D, realistic boundary geometry, accuracy ~0.001 %

Present-day calculations can be more accurate than cavities can be constructed

- Convergence: accuracy sub-100 kHZ for 3.9 GHz cavity
- 120 M DoF calc can even get 20 kHz splitting of probe holes
- Differ from (air-corrected) measurements by 2 MHz
- But 1 mil = 25 micron difference in waist radius gives 2 MHz shift



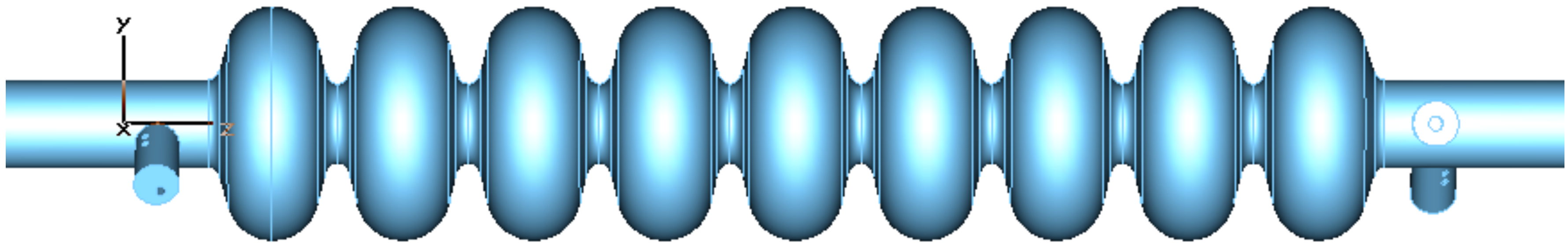
VORPAL frequency vs resolution (J. Cary et al.)

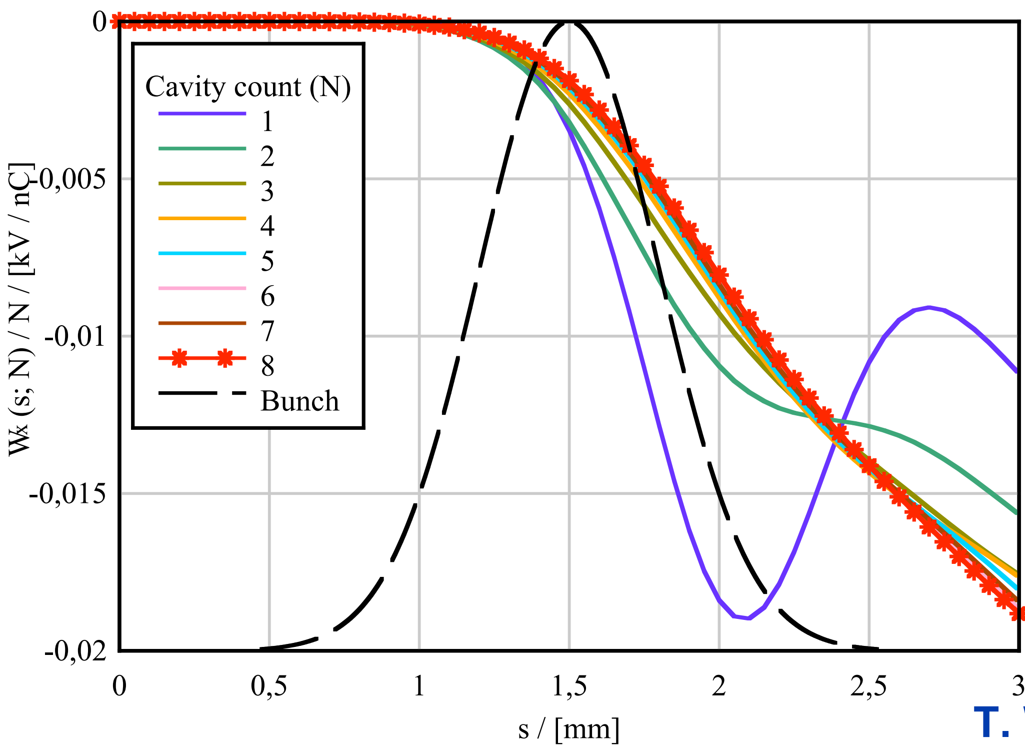


Calculations more accurate than manufacturing tolerances

Application of PBCI

TESLA cavities and couplers





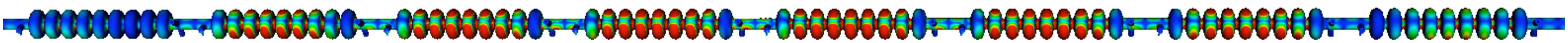
8-cavity simulation

bunch length	**0.3mm**
bunch charge	**1nC**
module length	**~10m**
# of grid points	**~250M**
# of processors	**408**
simulation time	**~7 days**

T. Weiland et al., TEMF

Large-Scale Simulation for International Linear Collider

1 hour CPU time, 1024 processors, 300 GB memory at NERSC



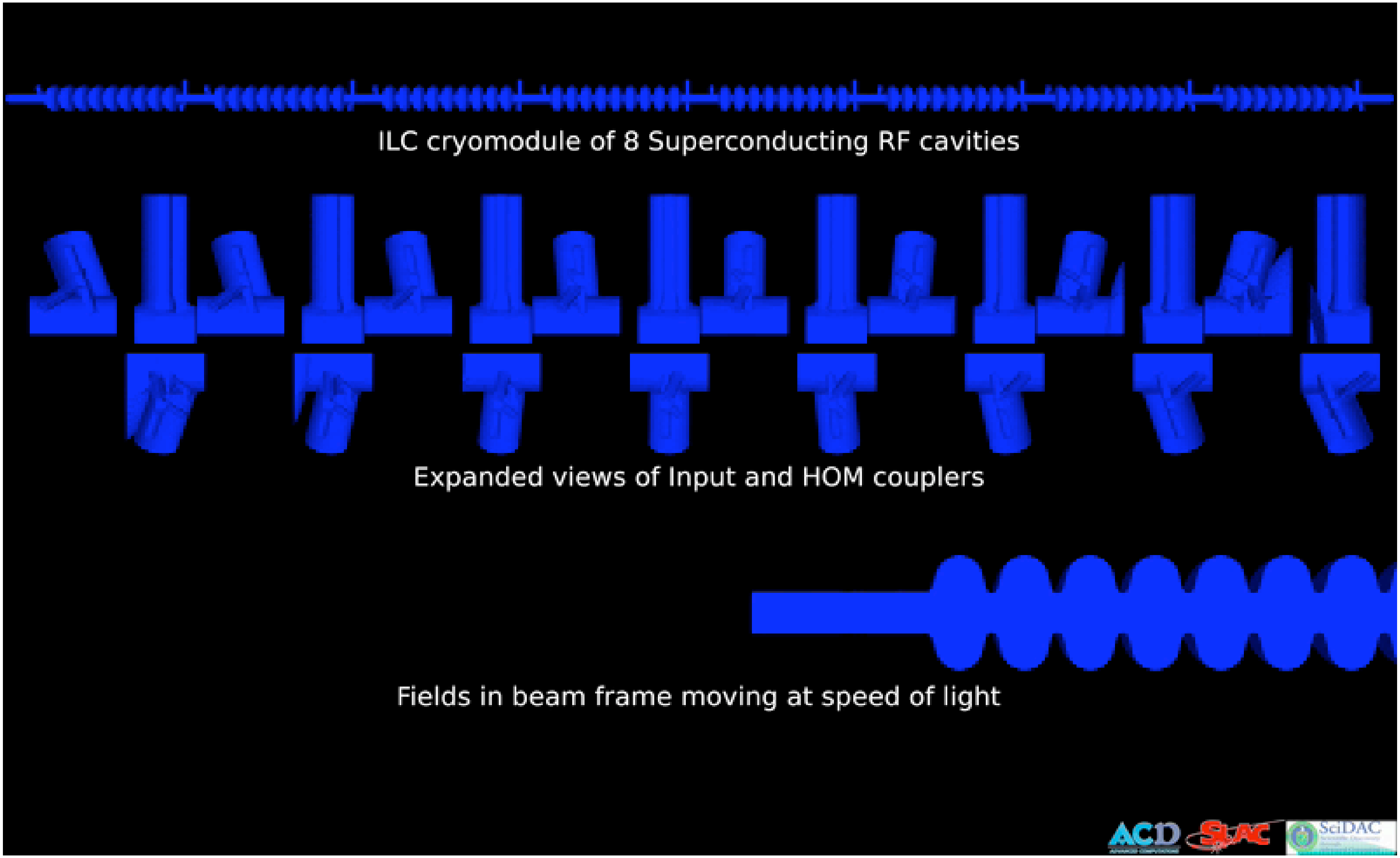
Field distribution of a resonant mode in cryomodule

ILC cryomodule of 8 superconducting RF cavities

Expanded views of input and HOM couplers

Fields in beam frame moving at speed of light

Rich Lee, Zenghai Li, Greg Schussman, Ravi Uplenchwar, Liling Xiao, Cho Ng, and Kwok Ko, SLAC


ILC cryomodule of 8 Superconducting RF cavities
Expanded views of Input and HOM couplers
Fields in beam frame moving at speed of light

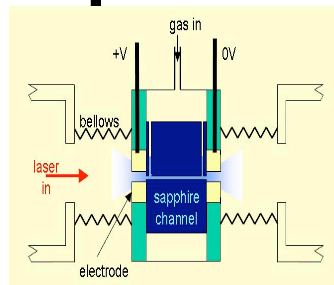
Progress in laser/plasma based concepts has accelerated significantly in recent years

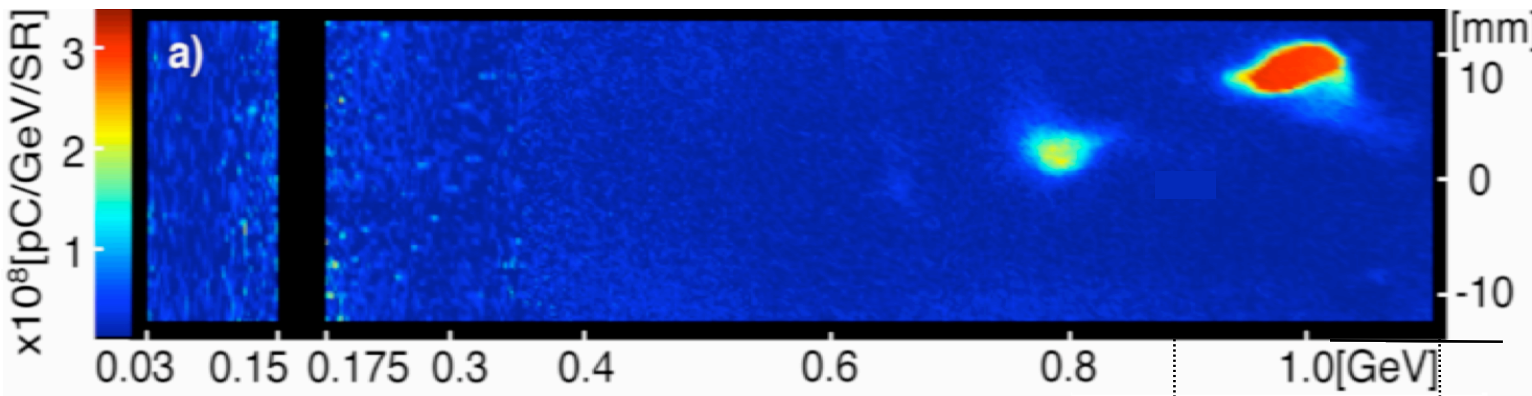
- 3 Key breakthroughs
  - Observation of low-energy spread bunches from LWFA
  - Production of 100 MeV beam from LWFA
  - Doubling of a 28.5 GeV beam in a PWFA

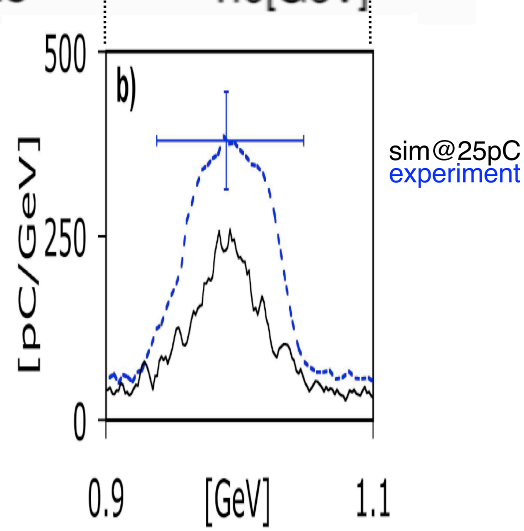
Physics behind these breakthroughs understood (in some cases, predicted) through large-scale PIC codes including OSIRIS, VORPAL ,QuickPIC

GeV acceleration in capillary waveguides: Simulation feedback to experiments

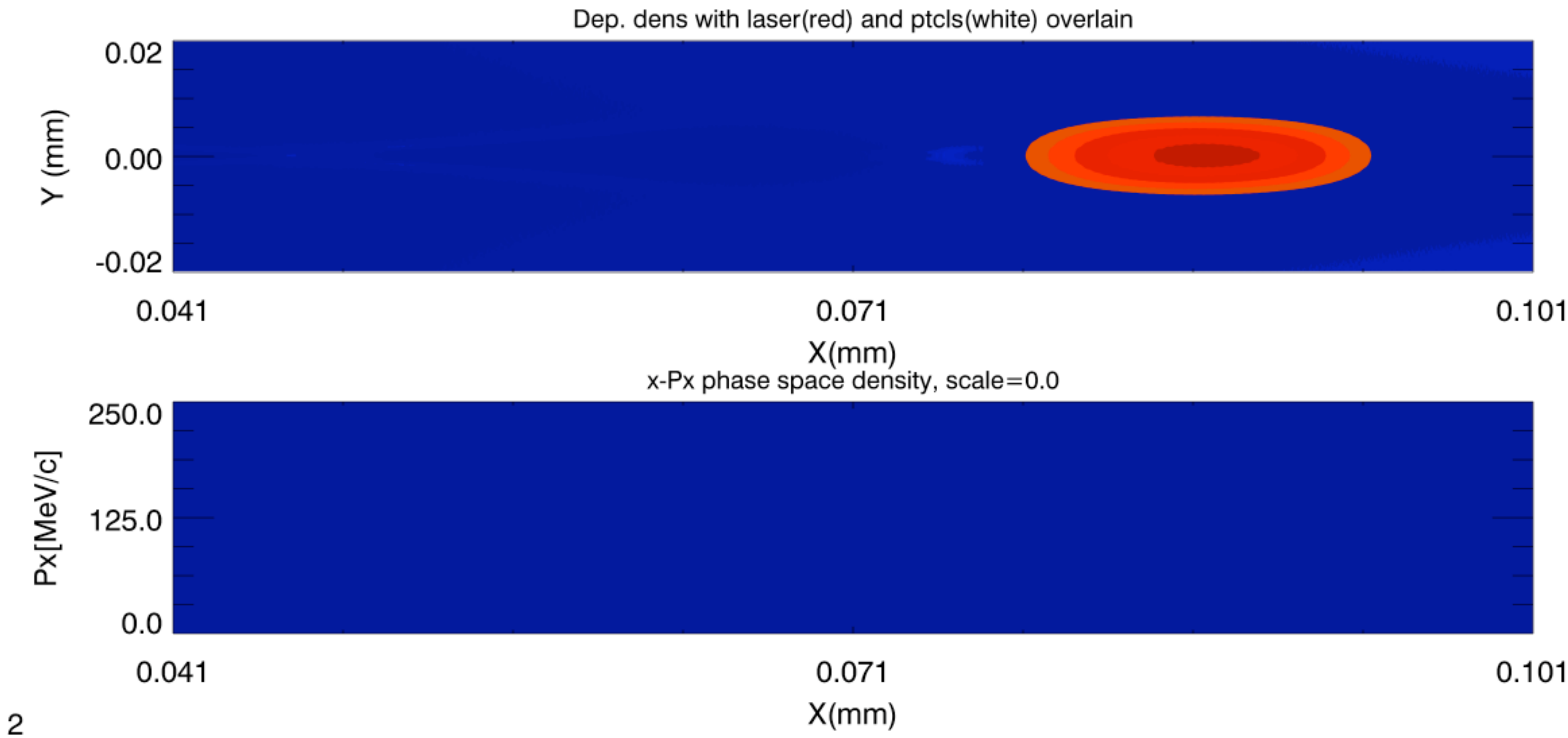
- **LOASIS 3.3 cm capillary experiment at reduced density produced GeV bunches**







- **2D VORPAL simulations close to experimental results for energy gain**



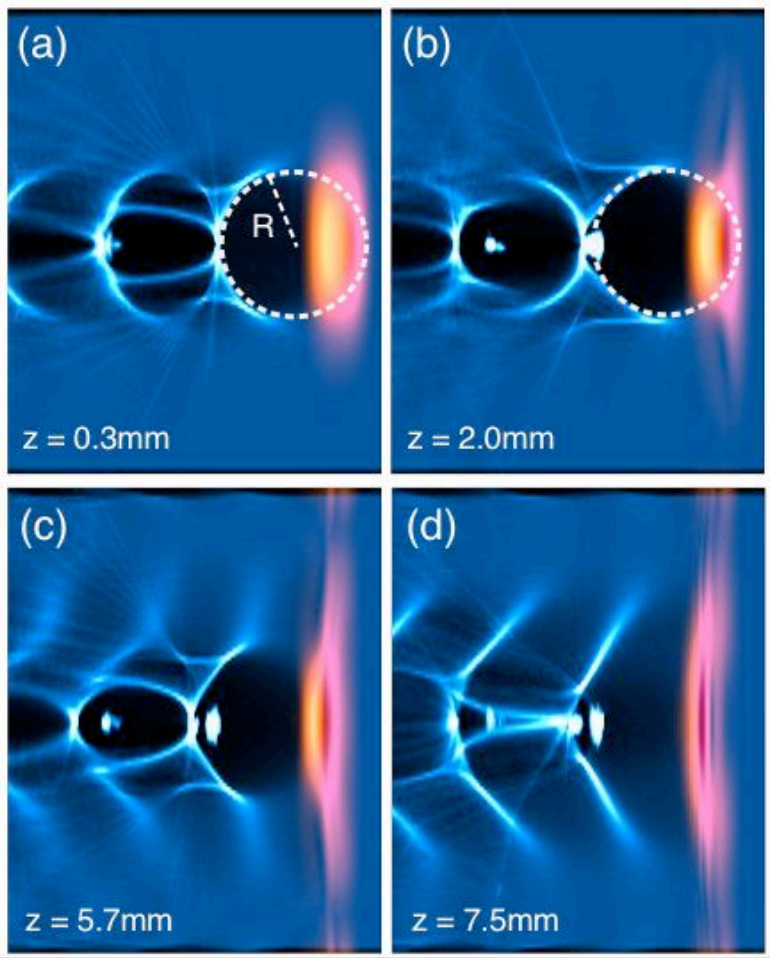
VORPAL simulation: 125M cells, 1920 procs
D. Bruhwiler, Tech-X

Large scale modeling is being used to unravel the physics of LWFA in the Bubble or blowout regime (W. Mori et al.)

UCLA

- **dev stable high-quality accelerators**
- $4000\times256\times256$ grids, and 4×10^5 time-steps

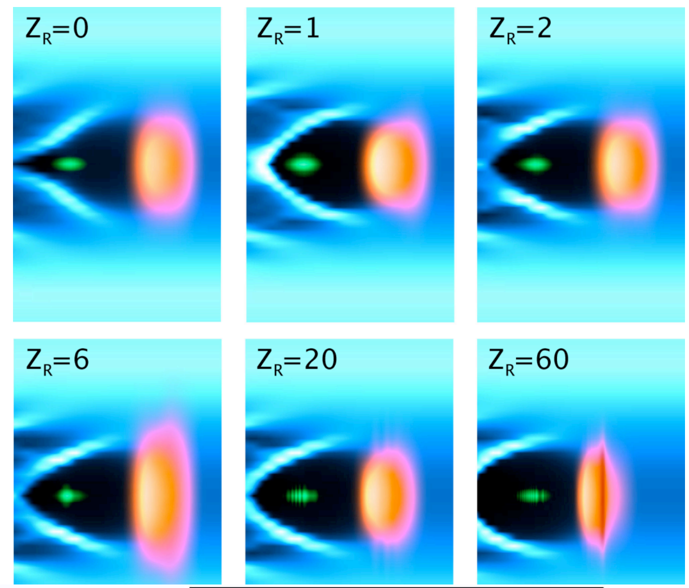
OSIRIS

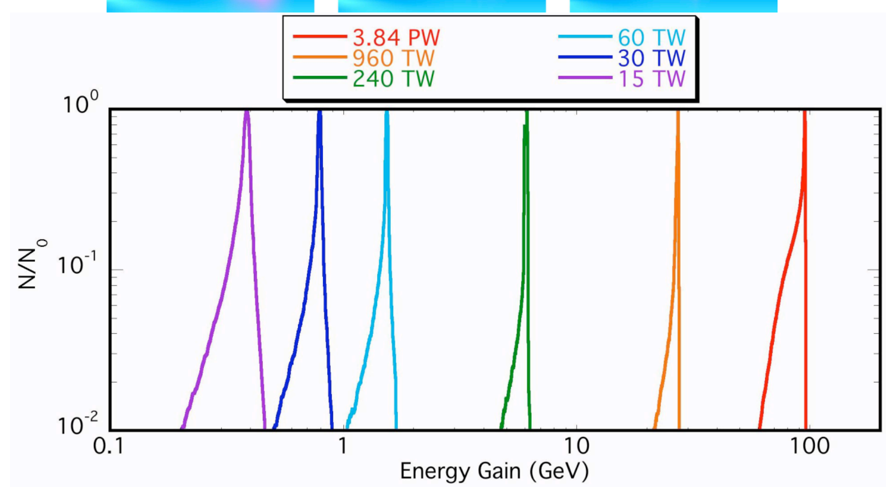


0.3nC accelerated to 1GeV by a 200TW laser

- **LWFA stages designed to 100GeV**
- $2048\times128\times128$ grids and 7,200 time-steps

QuickPIC

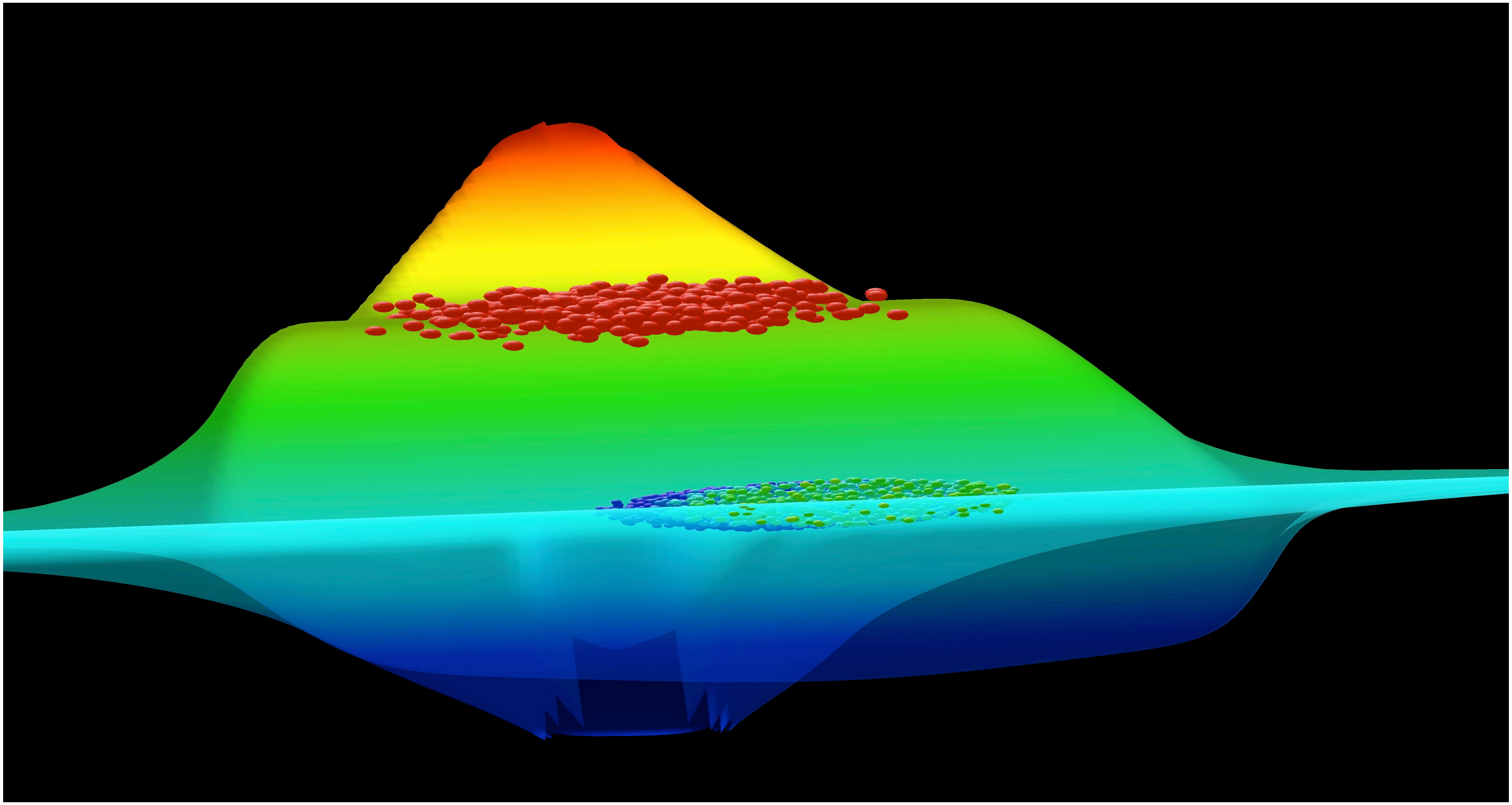




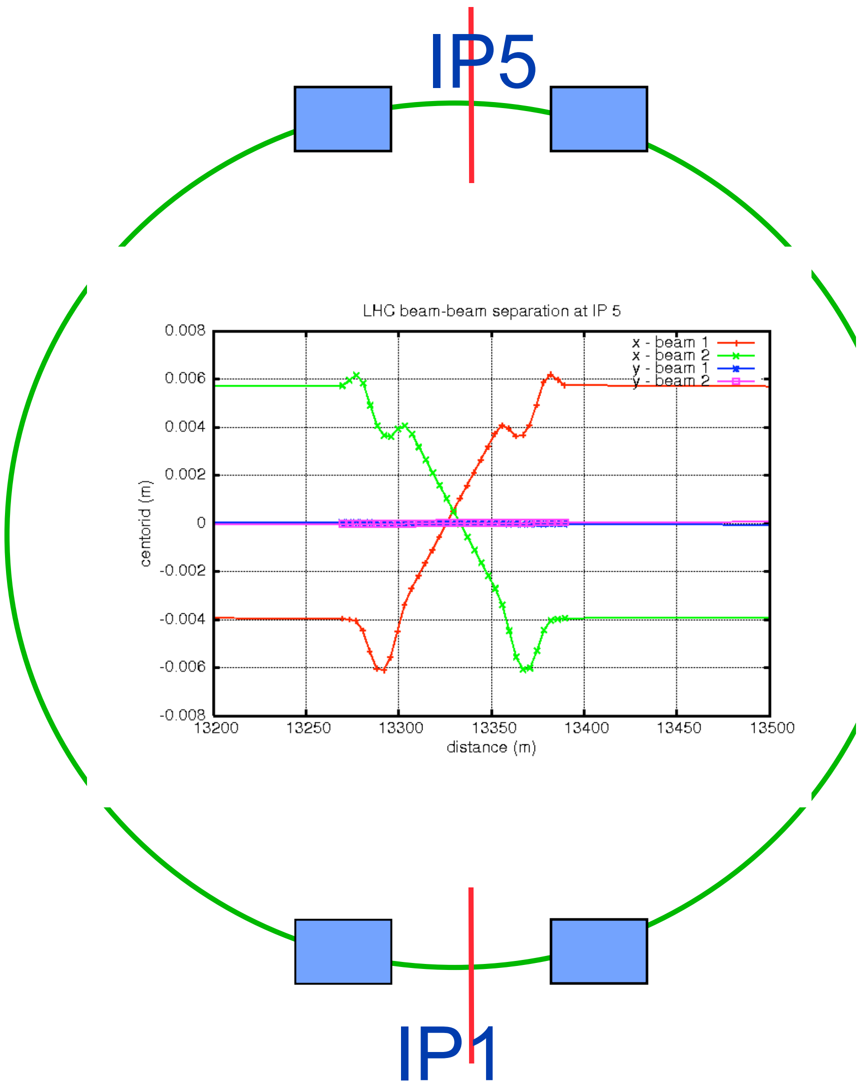
Design 25 GeV PWFA stage w/ QuickPIC

Simulations w/ 512x512x265 to 2048x2048x256 grids
Initial beam energy 25 GeV; ~25 GeV energy gain in 0.7m
0.46% energy spread for witness beam

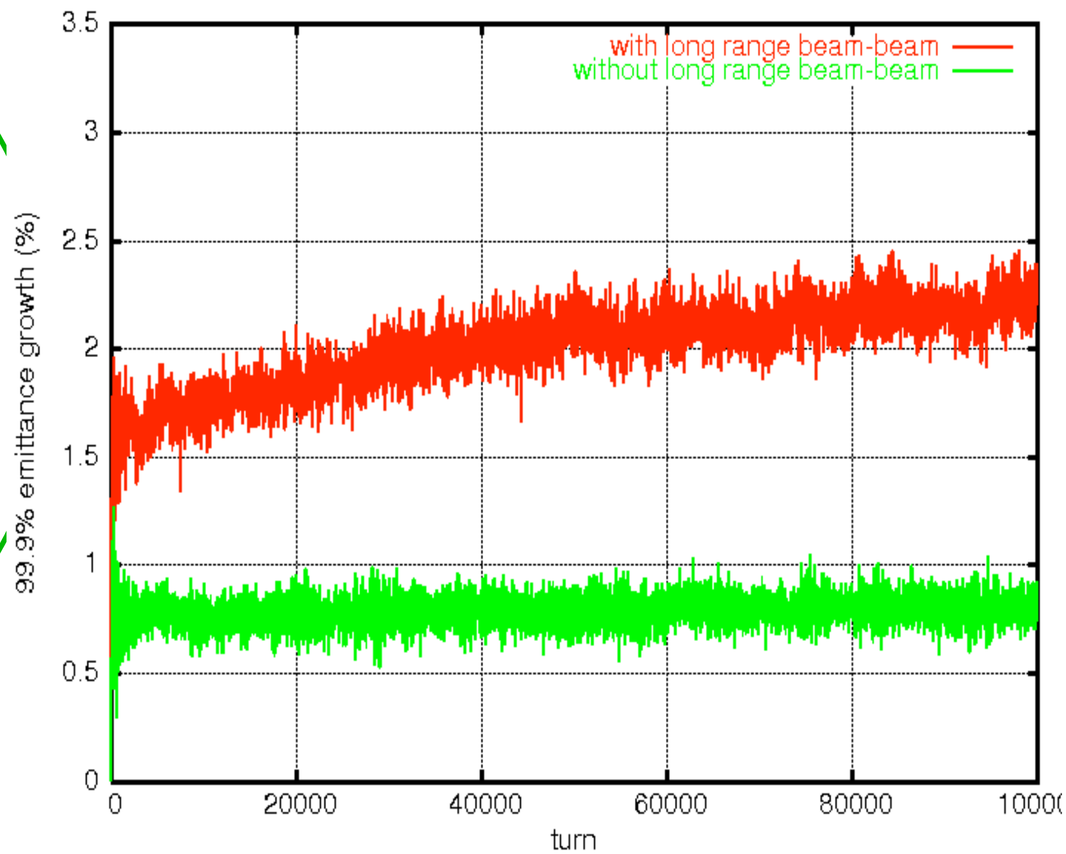
W. Mori et al.



Strong-Strong Simulation LHC Collisions using the BeamBeam3D code (2 Head-On + 64 Long Range)

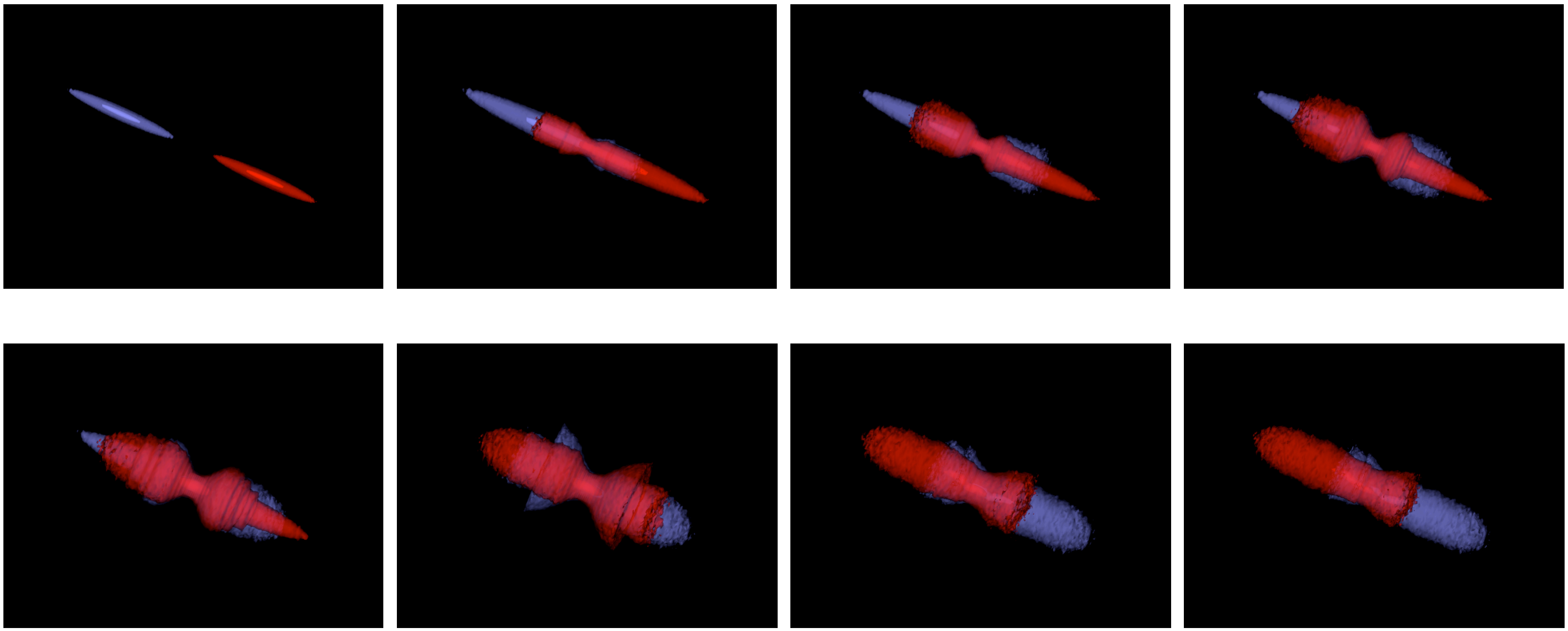


BeamBeam3D results

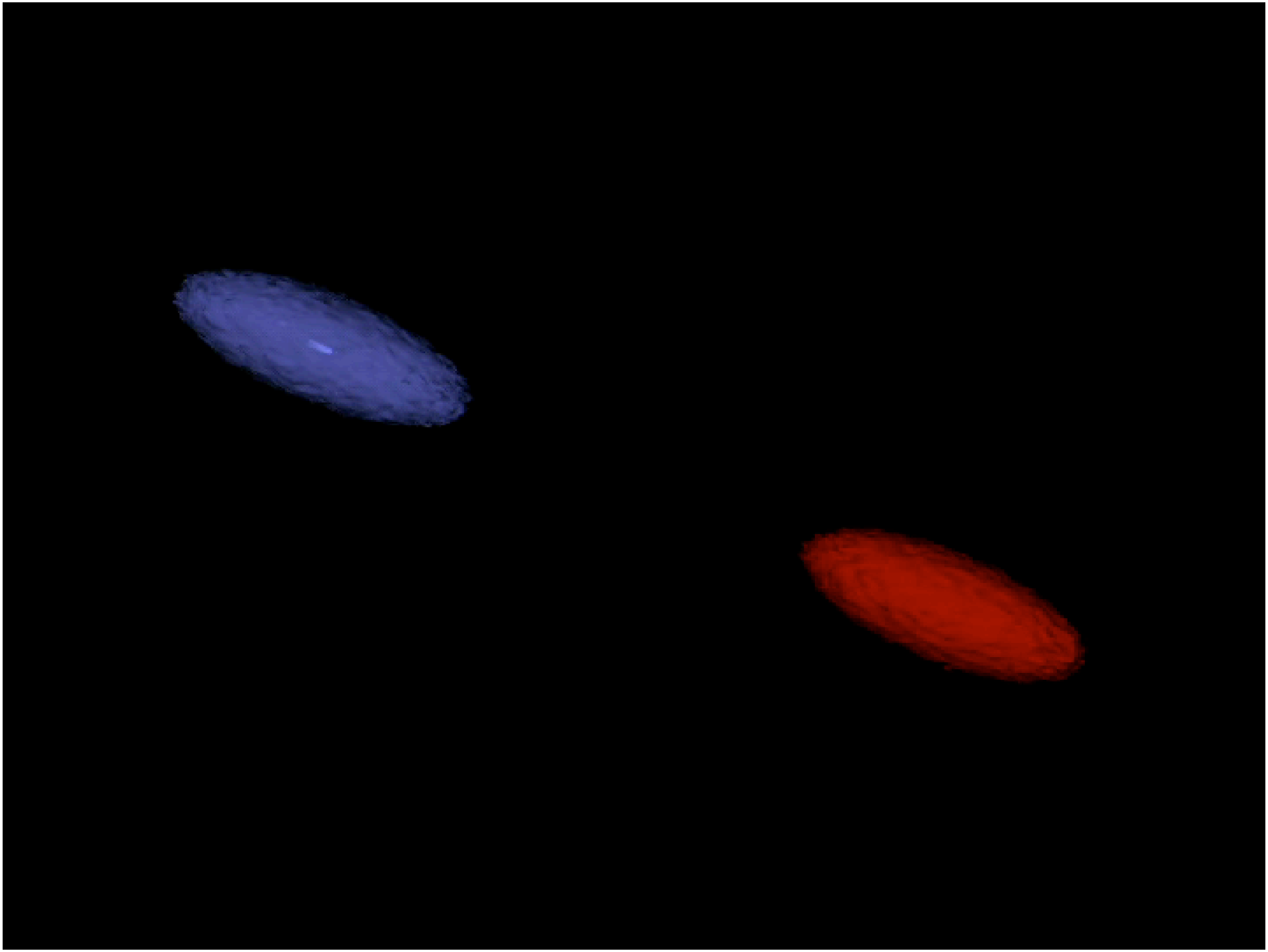


Ji Qiang

BeamBeam3D simulation and visualization of beam-beam interaction at Tevatron 400 times usual intensity



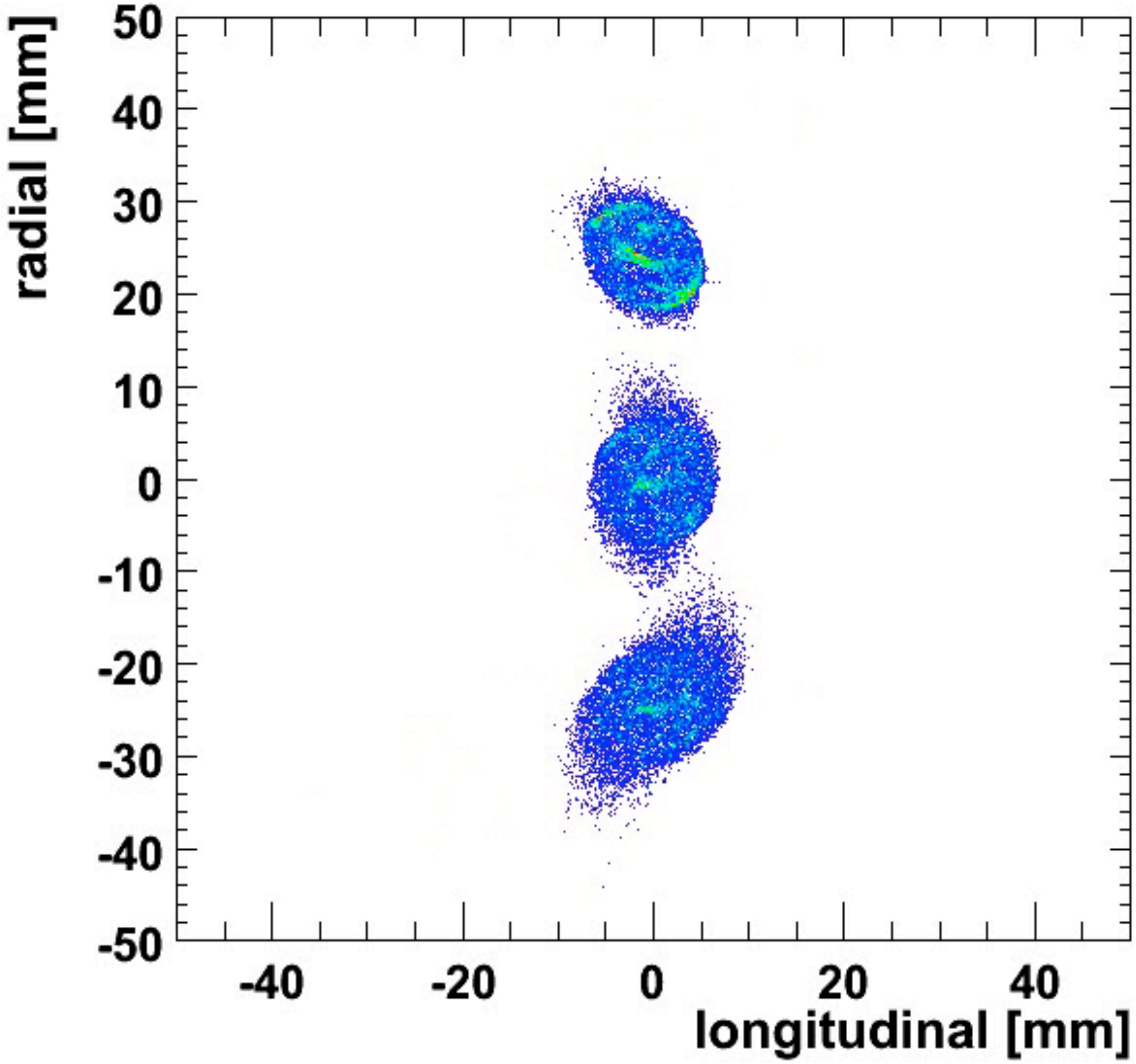
Eric Stern et al., FNAL



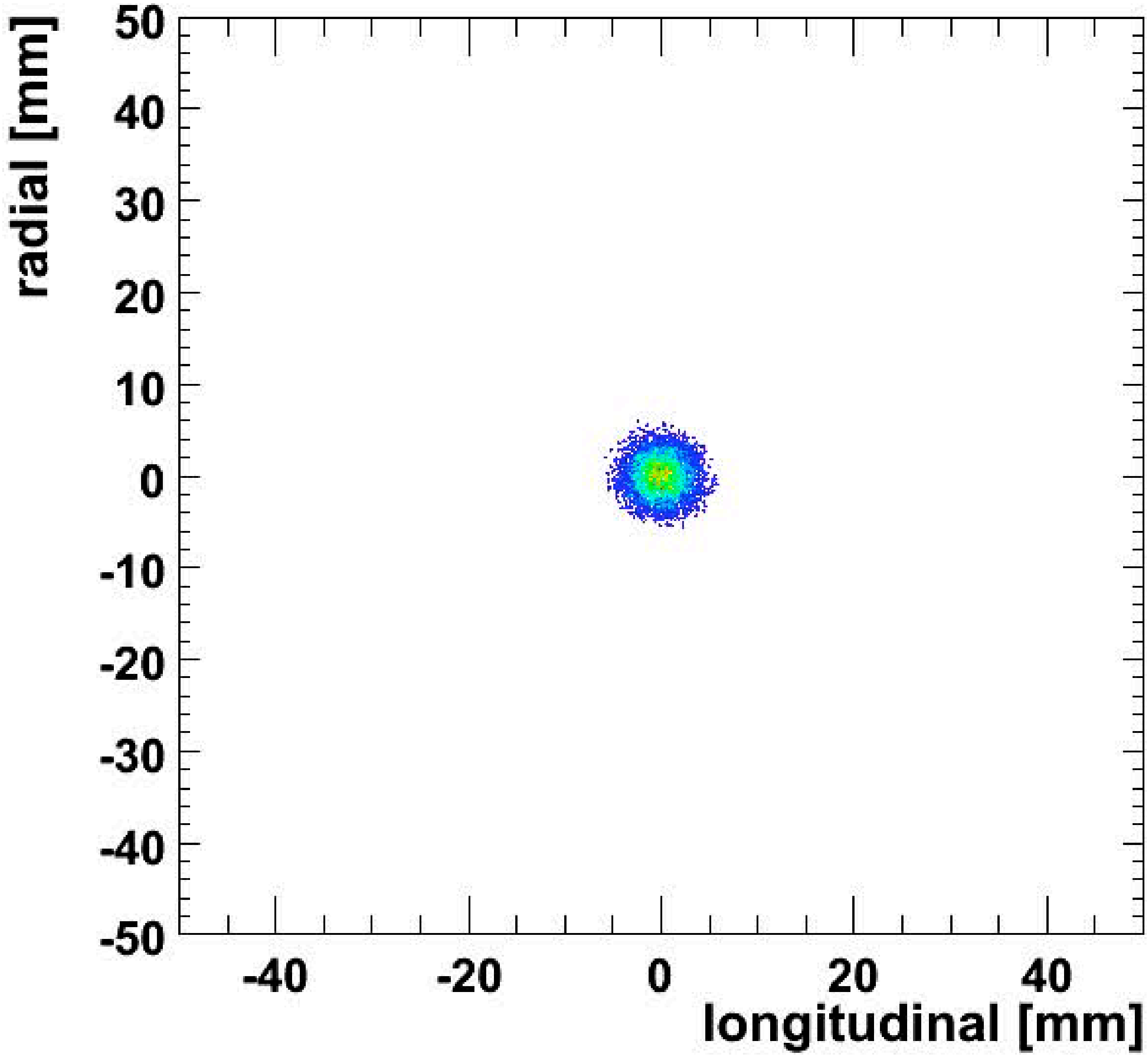
BeamBeam3D simulation of the Tevatron: 36-on-36 bunch run for 50,000 turns -- Comparison of simulation and experiment

Eric Stern et al., FNAL

Cyclotron modeling using OPAL-cycl: 3D space-charge, neighboring bunches



Andreas Adelmann et al., PSI



Andreas Adelmann et al., PSI

Parallel VORPAL simulations accurately calculate friction force on relativistic Au^{+79} ions in support of electron cooling designs

TECH-X BROOKHAVEN NATIONAL LABORATORY

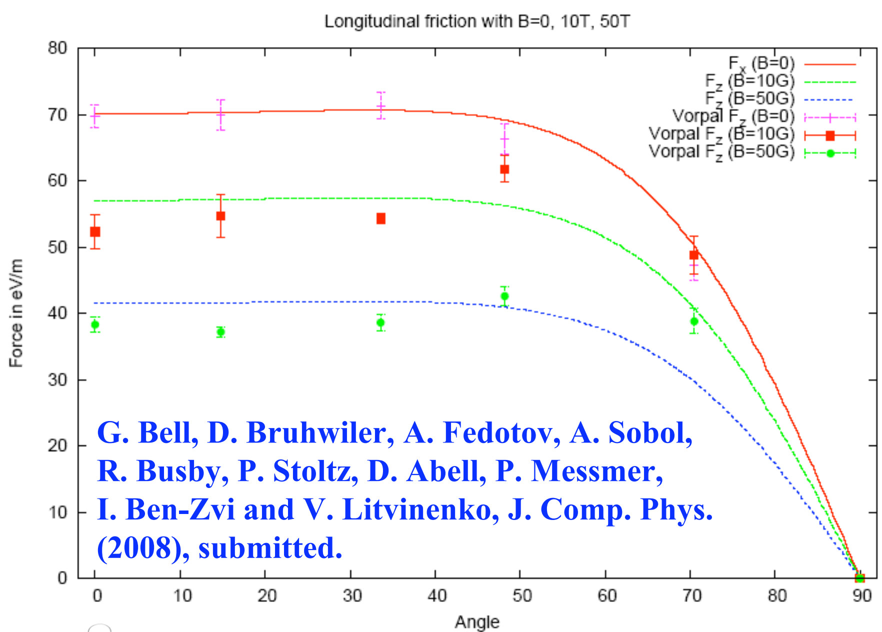
- **Electron cooling required for high luminosities of electron-ion collider (EIC) concepts**
  - **in the mid-term, RHIC luminosity could be increased ~10x**
  - **conventional wiggler could replace expensive solenoid**
    - **friction force should be reduced only by $\rho_{min} \rightarrow \rho_w$ in Coulomb log**

$$\rho_w = \frac{\Omega_{gyro}}{k_w^2 v_{beam}} \sim 1.4x10^{-3} \lambda_w^2 [m] B_w [G] / \gamma$$

– suggested independently by V. Litvinenko and Ya. Derbenev

– confirmed via VORPAL simulations

I. Ben-Zvi *et al.*, "Status of the R&D towards electron cooling of RHIC," Part. Accel. Conf. (2007).



G. Bell, D. Bruhwiler, A. Fedotov, A. Sobol, R. Busby, P. Stoltz, D. Abell, P. Messmer, I. Ben-Zvi and V. Litvinenko, J. Comp. Phys. (2008), submitted.

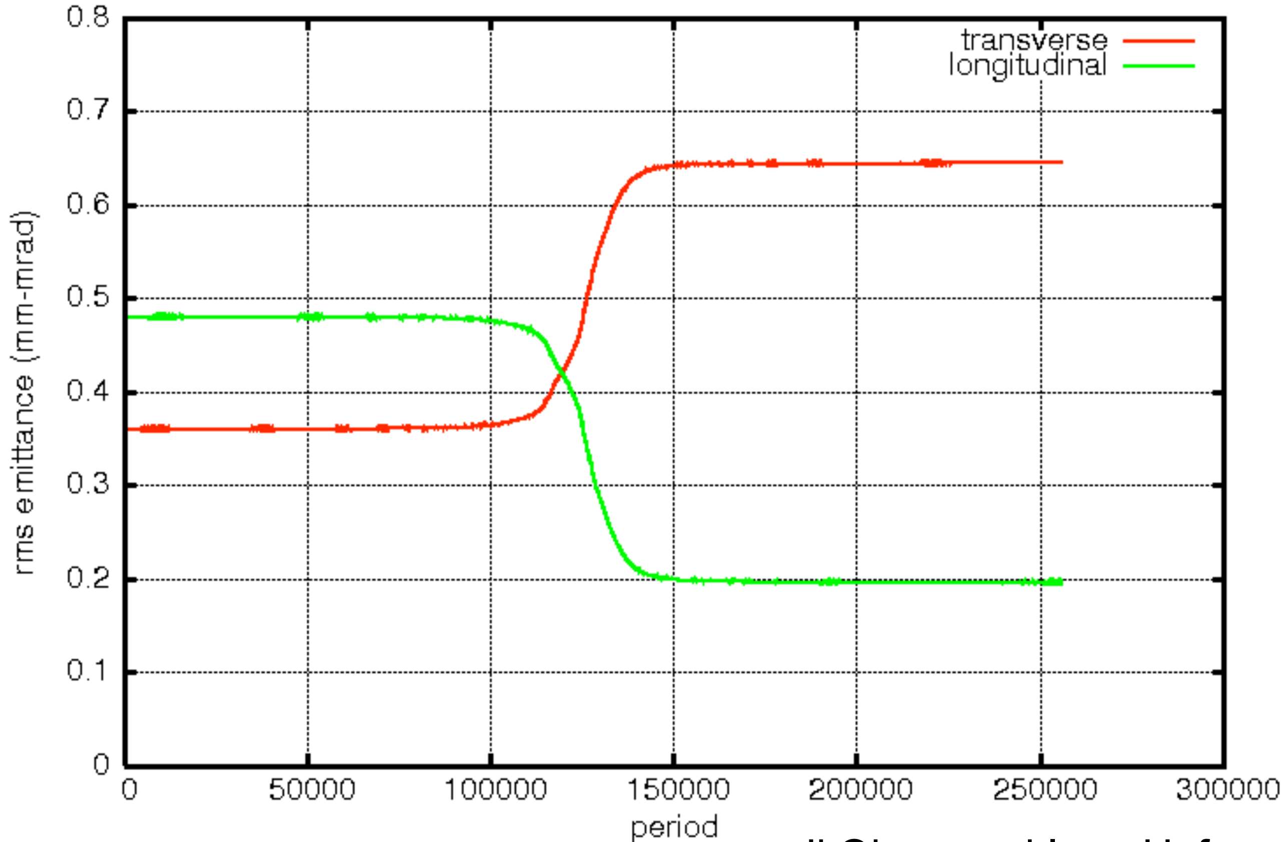
Office of Nuclear Physics — Exploring Nuclear Matter - Quarks to Stars

SciDAC — Scientific Discovery through Advanced Computing

VORPAL

Long-Term Simulation of Space-Charge Driven Dynamic Emittance Exchange

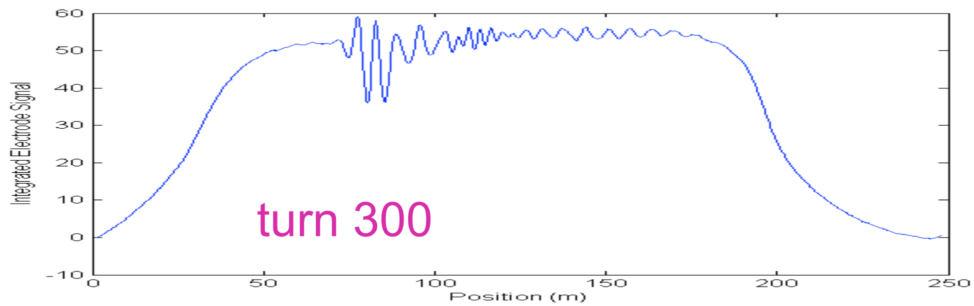
- Not large scale, but time-to-solution unacceptable w/out parallel computing
- IMPACT-Z simulation used 1.3 million space-charge kicks, 32 hrs on 64 procs of IBM/SP5



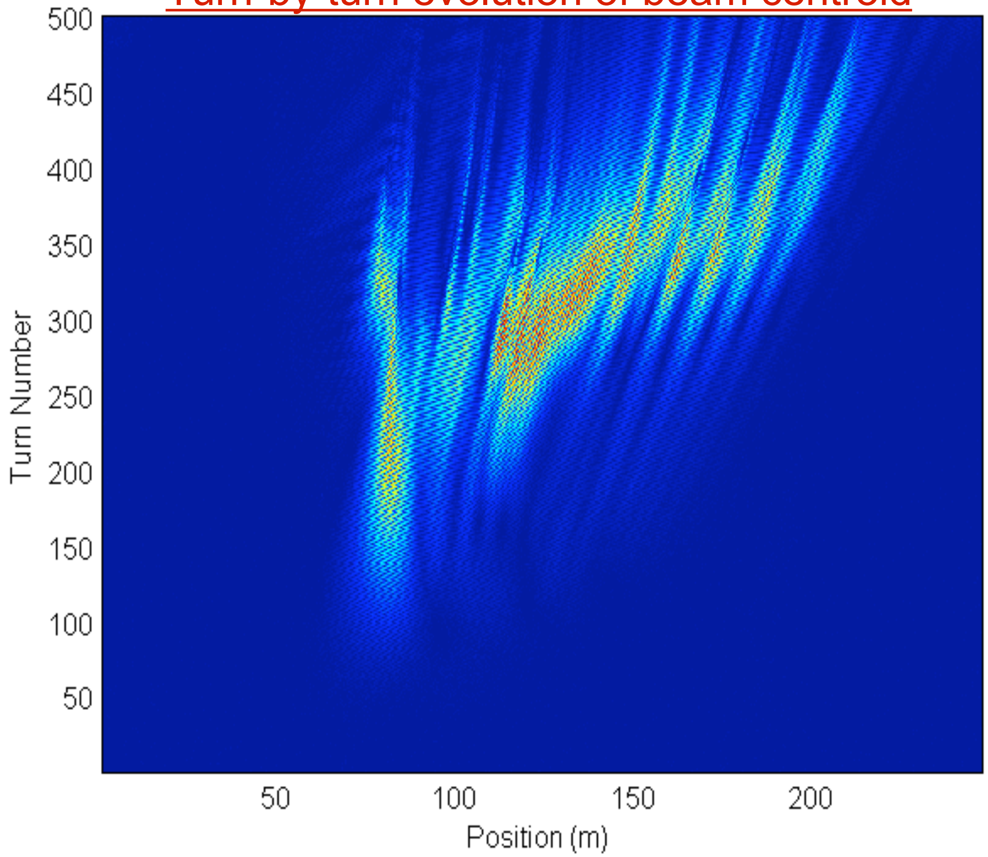
Ji Qiang and Ingo Hofmann

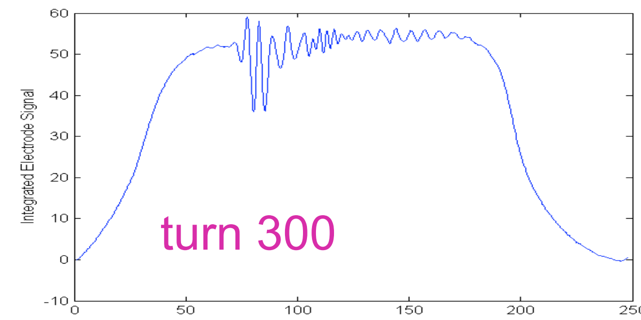
Electron-Proton Instability at SNS

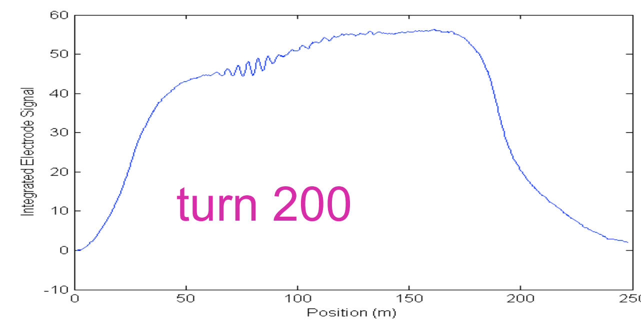
Instability occurs at flat top, closer to front of the beam, and moves backwards.

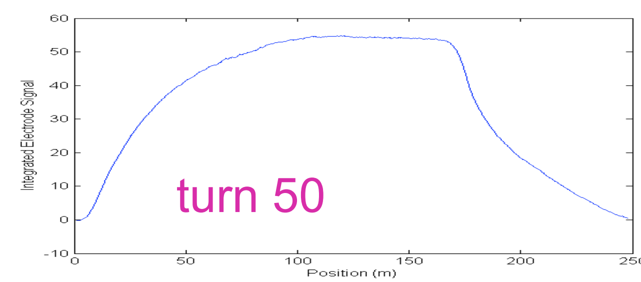


Turn-by-turn evolution of beam centroid







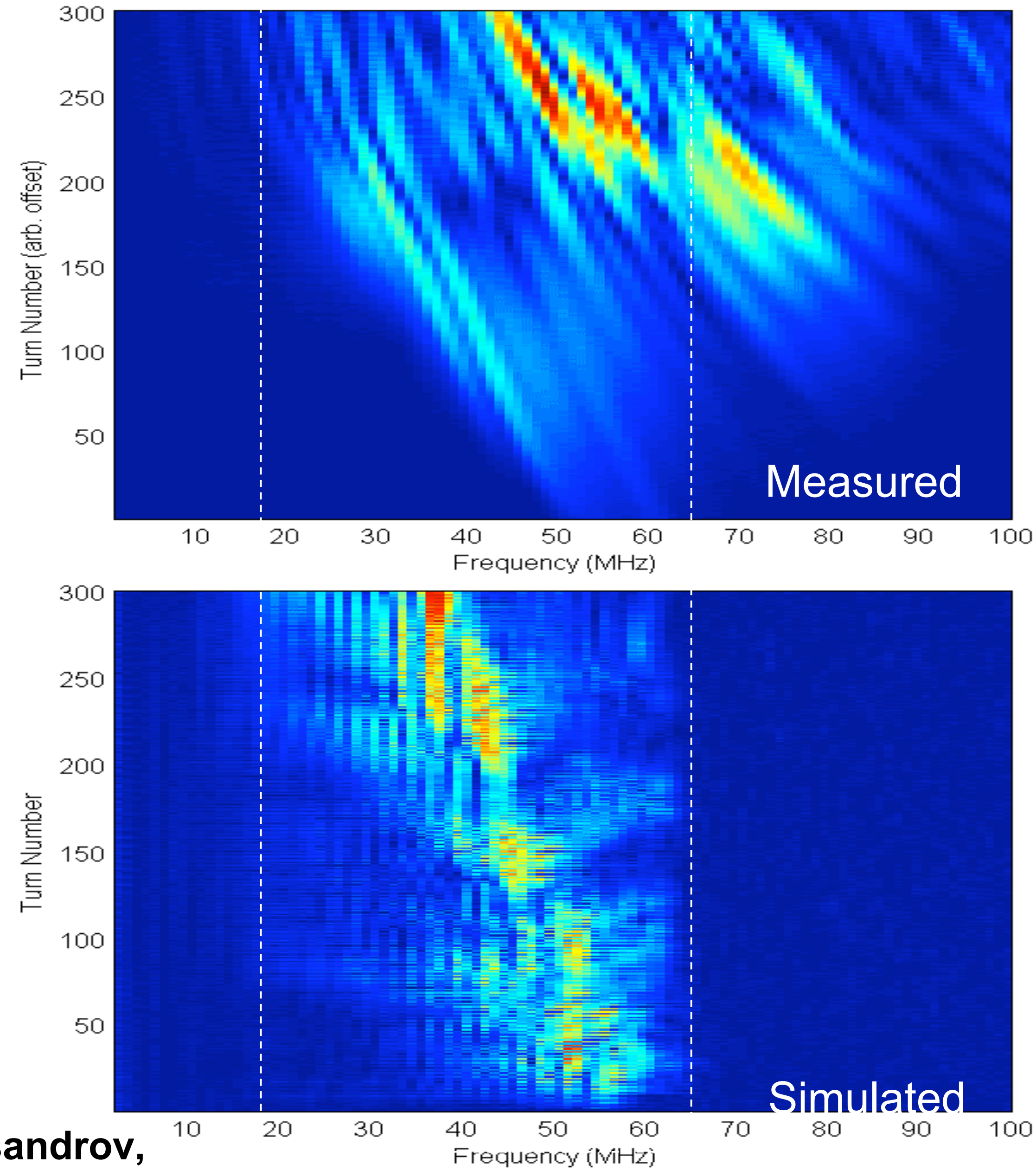


SNS e-P instability: simulation & measurement

We see narrower excitation frequency in the simulation: 20 – 65 MHz.

Excitation frequency content and extent is likely due the position and localization of the two ECloud nodes.

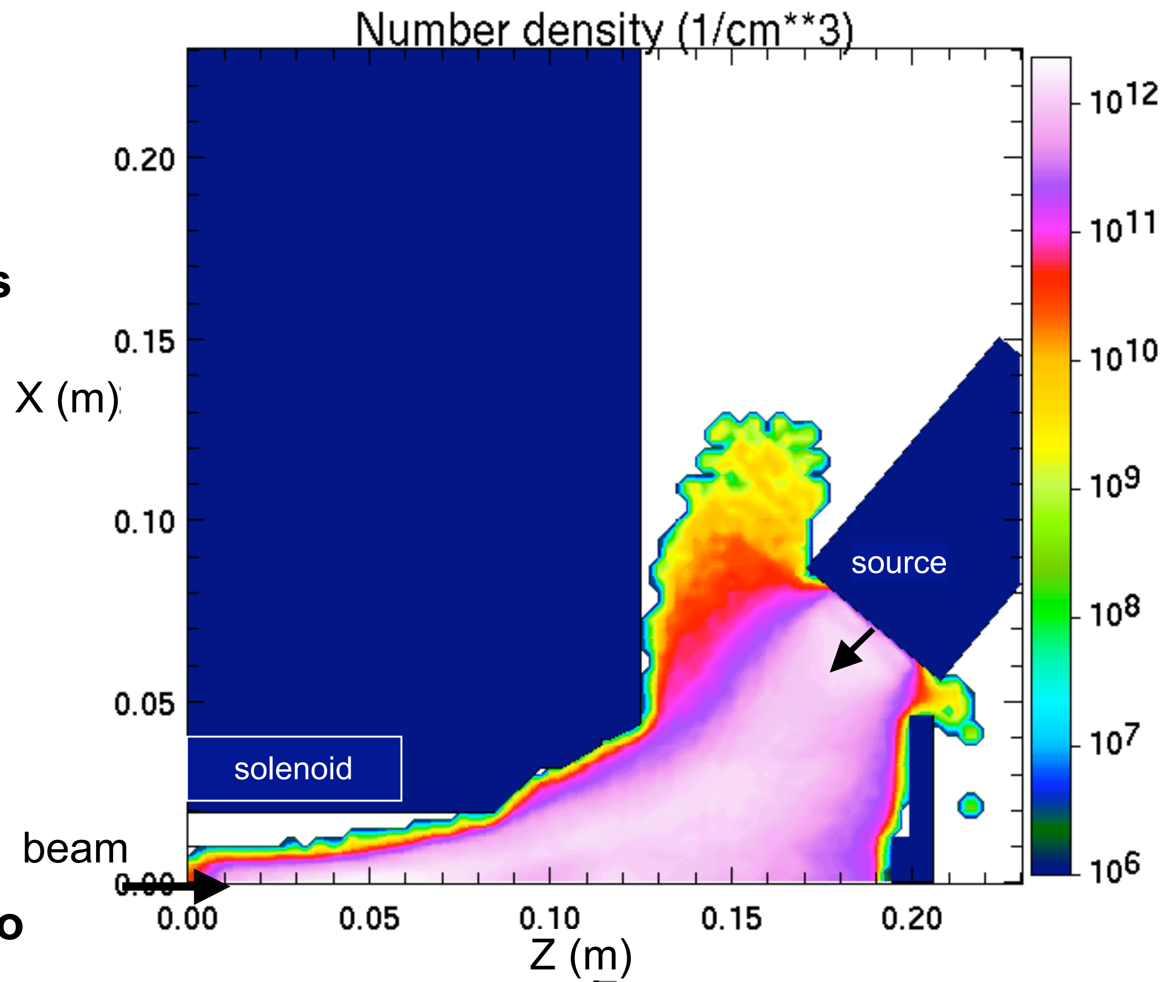
We see the same drift of excitation bands to lower frequency in both simulation and experiment.



S. Cousineau, A. Shishlo, A. Aleksandrov, S. Assadi, V. Danilov, C. Deibele, M. Plum

HIFS-VNL: 3-D simulation of plasma formation in NDCX experiment at LBNL

- **Plasma injected upstream from angled sources to neutralize high current ion beam during pulse compression and focusing onto a target**
- **High density plasma oscillates w/ a high fundamental freq; this constrains timestep size**
- **Simulations of existing expt require ~10 days on 16 procs**
- **Upcoming NDCX-II cases will be more challenging with higher plasma densities**
- **Future simulations expected to require ~1 day on 1600 procs**



A. Friedman (LLNL), D. Grote (LBNL)

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

Partial list only;
Many codes
not shown

COSY-INF

MXYZPTLK

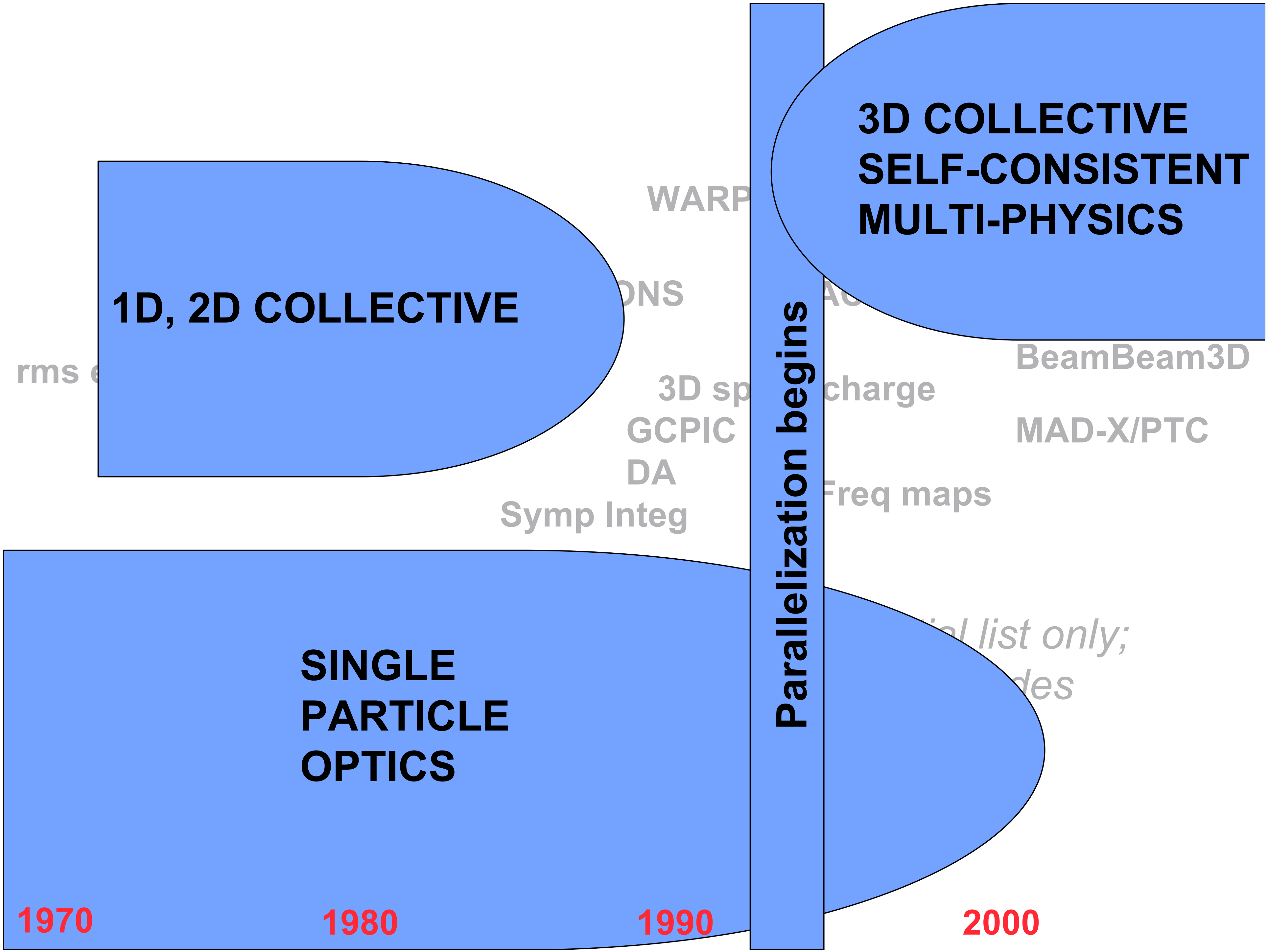
MaryLie

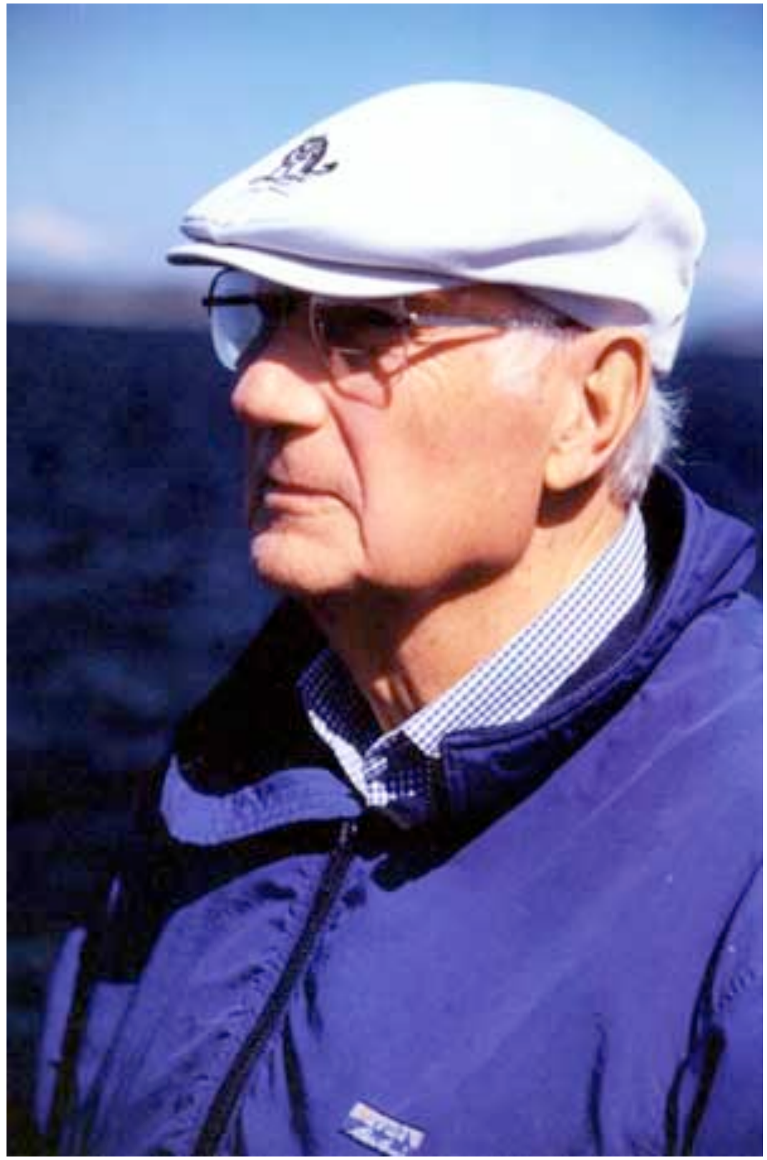
Dragt-Finn

MAD

Transport

1970 **1980** **1990** **2000**

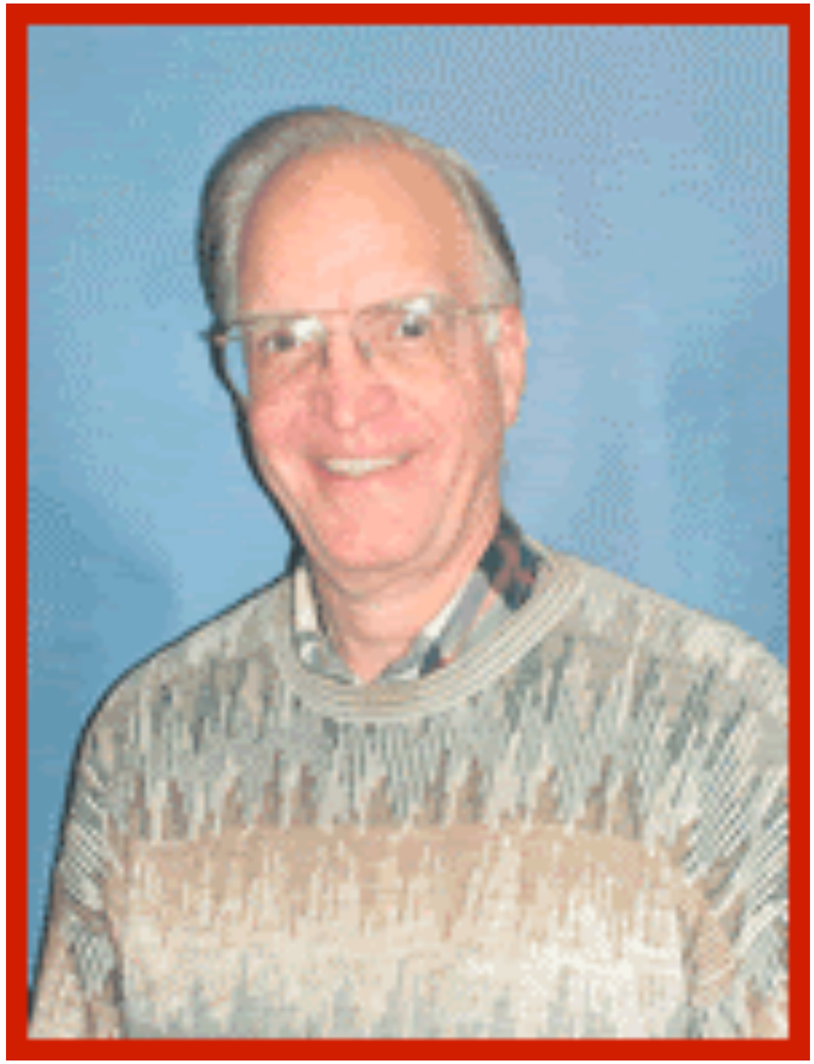

3D COLLECTIVE
SELF-CONSISTENT
MULTI-PHYSICS
WARP
1D, 2D COLLECTIVE
BeamBeam3D
charge
GCPIC
MAD-X/PTC
DA
Freq maps
Symp Integ
Parallelization begins
SINGLE
PARTICLE
OPTICS
1970
1980
1990
2000



$$\zeta^{f} = \sum M\zeta^{i} + \sum\sum T\zeta^{i}\zeta^{i} + \sum\sum\sum U\zeta^{i}\zeta^{i}\zeta^{i} + \ldots$$

$$\zeta^{fin} = M\zeta^{in}$$

Google Images result for “MAD CERN”



$$\mathcal{M} = e^{:f_2:} e^{:f_3:} e^{:f_4:} \ldots$$

$$\zeta^f = \mathcal{M}\zeta^i = e^{:f_2:}(1 + :f_3: + \frac{1}{2}:f_3:^2 \ldots)(1 + :f_4: + \ldots)\zeta^i$$

$$\zeta^f = \sum M\zeta^i + \sum\sum T\zeta^i\zeta^i + \sum\sum\sum U\zeta^i\zeta^i\zeta^i + \ldots$$

$$\mathcal{M} = e^{:f_2:}e^{:f_3:}e^{:f_4:}\ldots$$

$$\zeta^f = \mathcal{M}\zeta^i = e^{:f_2:}(1 + :f_3: + \frac{1}{2}:f_3:^2 \ldots)(1 + :f_4: + \ldots)\zeta^i$$

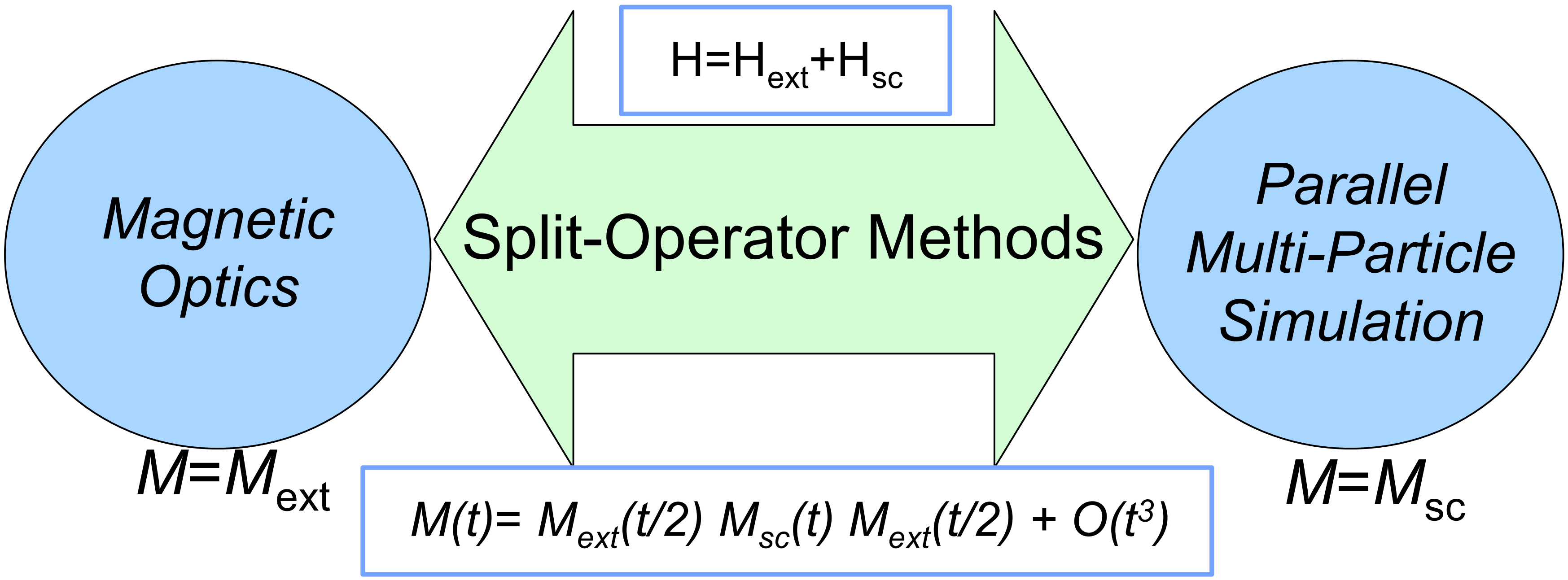
$$\frac{d}{dt}M = JSM$$

$$\frac{d}{dt}f_3 = -H_3^{\text{int}}$$

$$\frac{d}{dt}f_4 = -H_4^{\text{int}} - \frac{1}{2}[f_3, H_3^{\text{int}}]$$

$$\dots$$

IMPACT (Integrated Map and Particle Accelerator Tracking code) used Split-operator approach to combining high-order optics with parallel PIC



- **Note that the rapidly varying s-dependence of external fields is decoupled from slowly varying space charge fields**
- **Leads to extremely efficient particle advance:**
  - **Do not take tiny steps to push ~100M particles**
  - **Do take tiny steps to compute maps; then push particles w/ maps**

R. Ryne, LBNL

Selected beam dynamics algorithms currently the subject of significant R&D

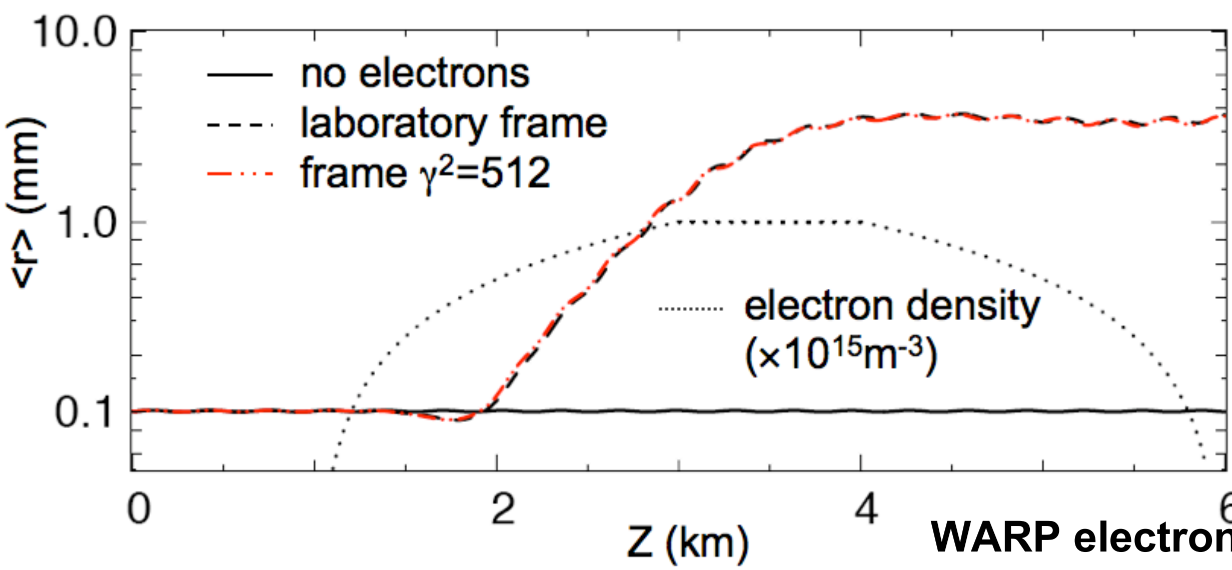
Noninvariance of space- and time-scale ranges under a Lorentz transformation (J.-L. Vay)

Key observation: ***range*** of space and time scales is ***not*** a Lorentz invariant; the ***optimum*** frame to minimize the range is ***not necessarily*** the lab frame

Choosing optimum frame of reference to minimize range can lead to dramatic speed-up for relativistic matter-matter or light-matter interactions.

speedup (PIC in boosted frame vs PIC in lab frame) reported so far:

x1000 3-D e-cloud driven beam instability (LBNL),
x45,000 2-D free electron laser toy problem (LBNL),
x1,500 1-D laser-plasma acceleration (Tech-X),
x150 2-D, x75 3-D laser-plasma acceleration (IST, Portugal).

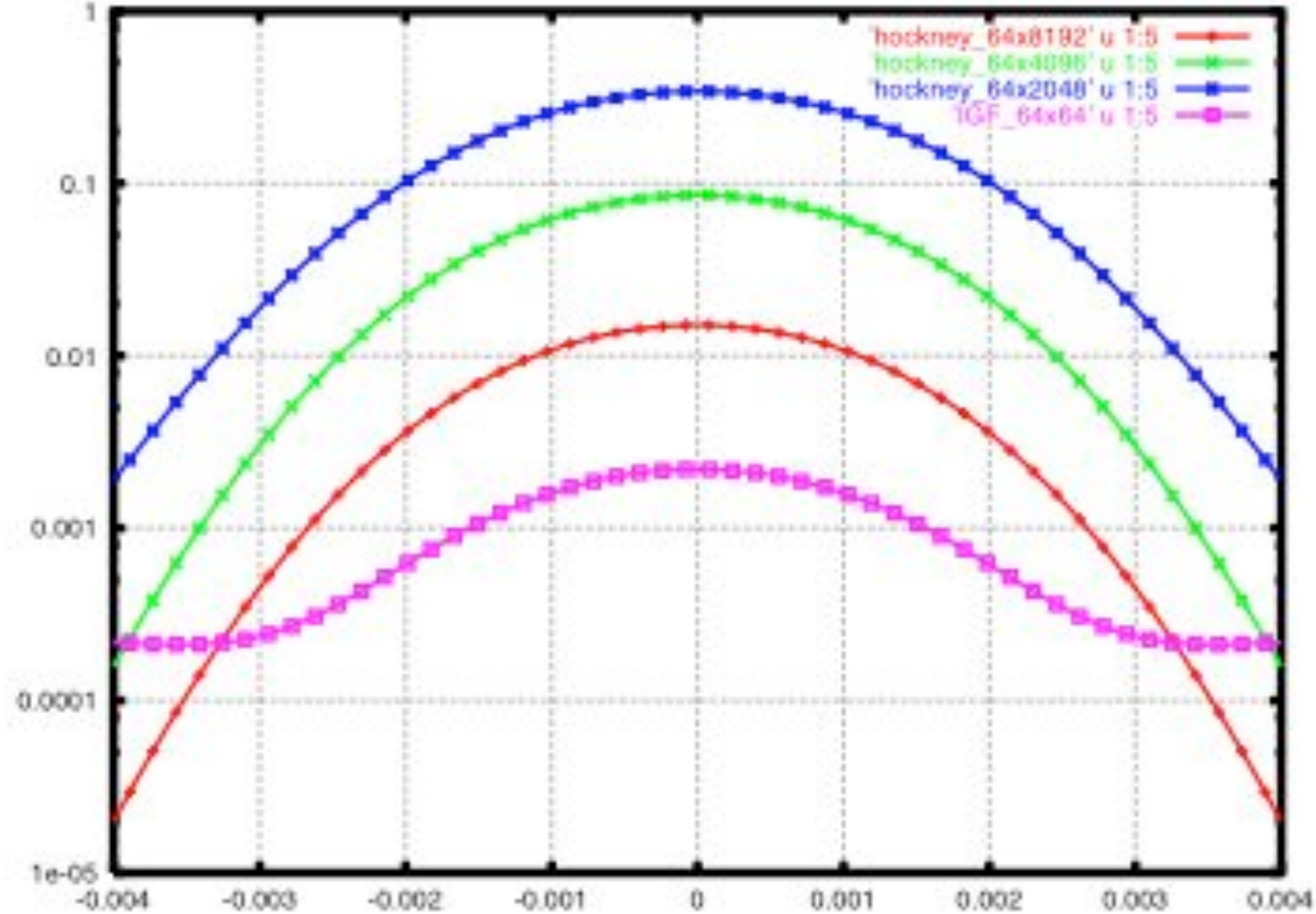


CPU time (8 procs):
- lab frame: >2 weeks
- frame γ^2=512: <30 min

Speedup x1000

WARP electron-cloud instability simulation

Integrated Green Functions in Beam Dynamics

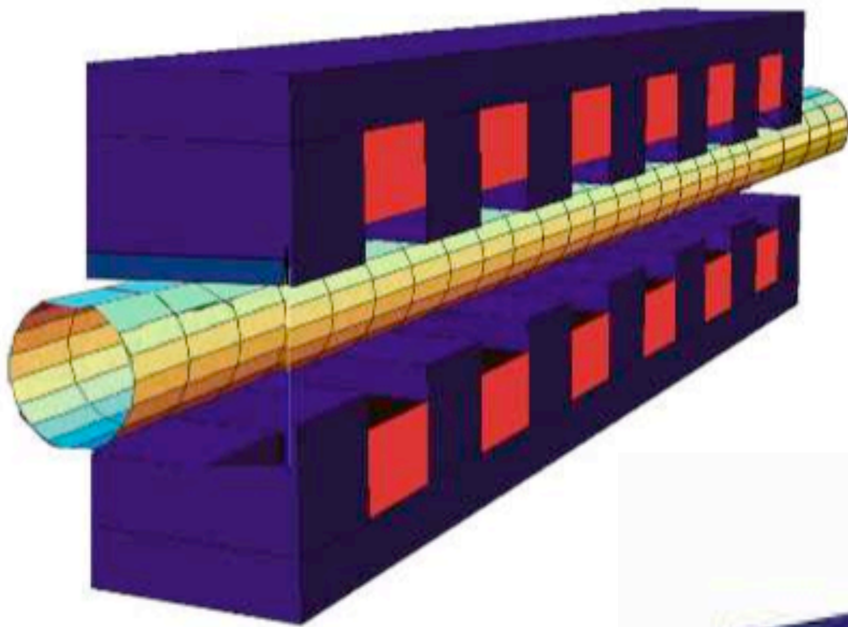


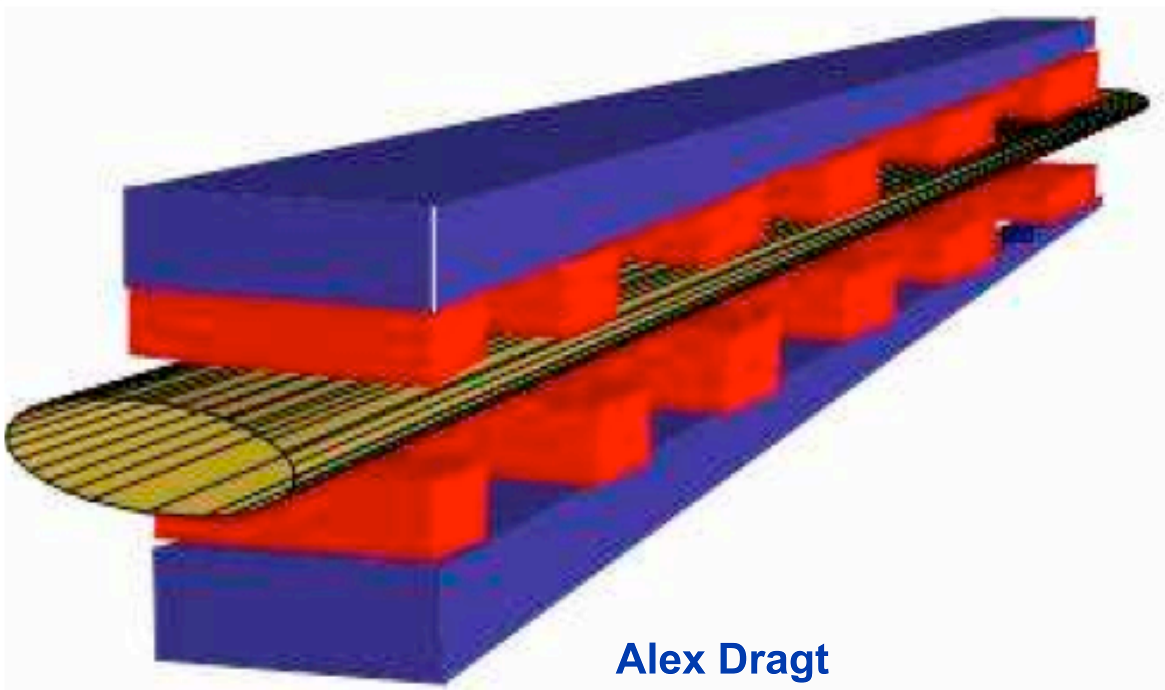
R. Ryne, LBNL

Old: 64x2048, 64x4096, 64x8192

New: 64x64

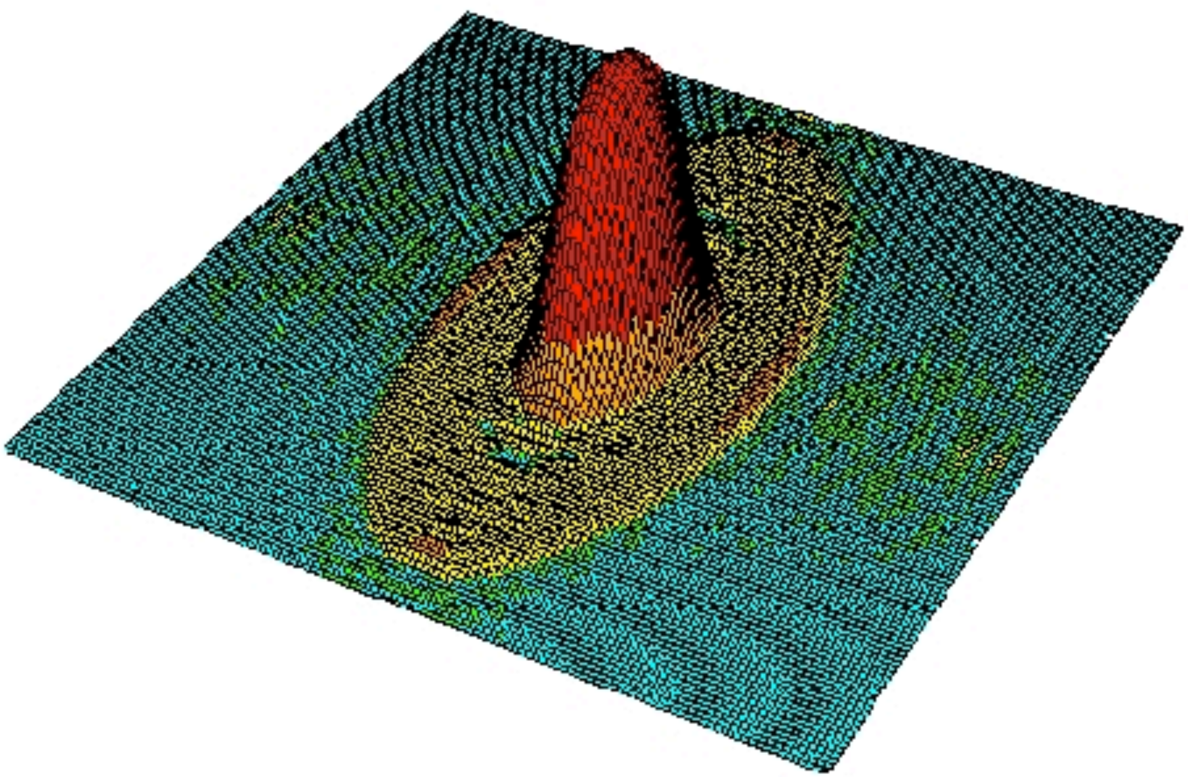
Map production from surface data
(A. Dragt, M. Venturini, P. Walstrom, D. Abell,…)





Direct Vlasov Solvers

- **4D, 5D direct Vlasov already possible**
- **What about 6D in the future?**
  - **$128^6 = 4.4 \times 10^{12}$**



Concluding remarks; Looking to the future

Fastest computers (from TOP500 list)

- 1998: Intel ASCI Red, 1.3 Tflops
- 2000: IBM ASCI White, 5 Tflops
- 2002: Earth Simulator, 35 Tflops
- 2004: IBM BlueGene/L, 70 Tflops
  - —June 2005: 137 Tflops
  - —Nov 2005: 280 Tflops (131K cores)
  - —2007: 478 Tflops (213K cores)
- 2008: IBM/DOE “Roadrunner” : 1 petaflop

Two weeks ago, this headline appeared in ComputerWorld magazine:

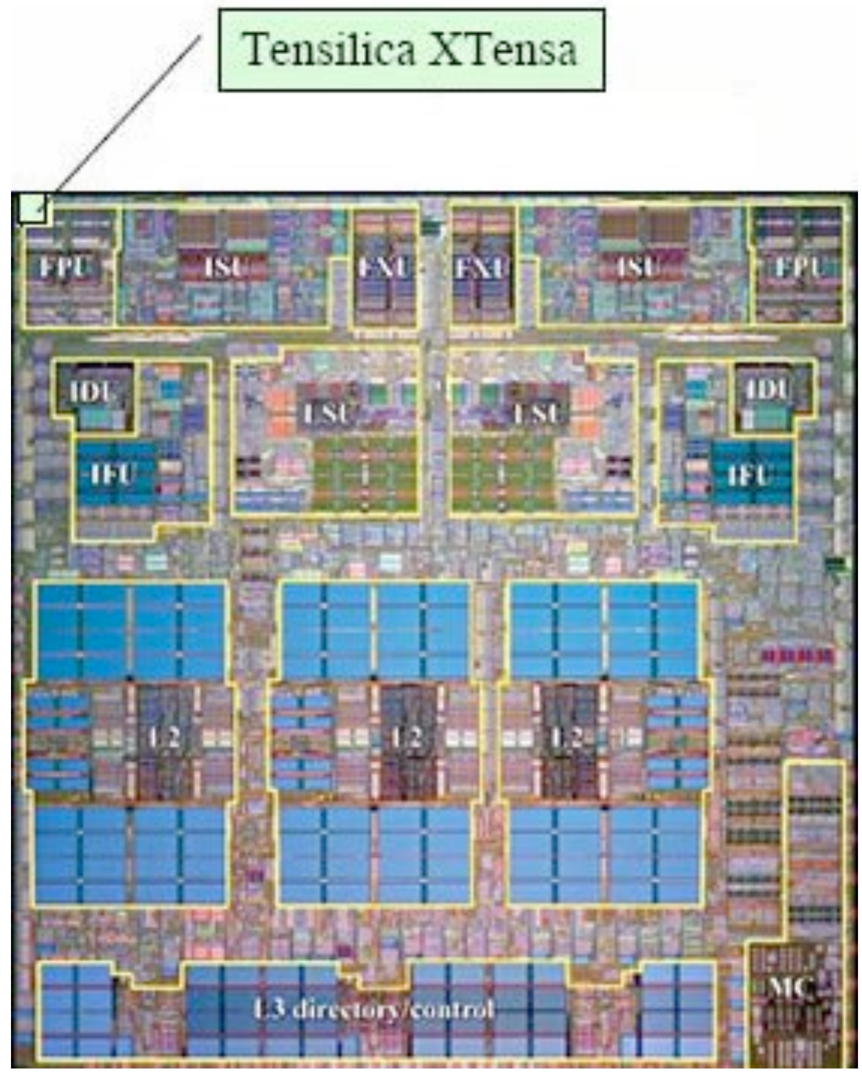
"All hail Roadrunner's petaflop record; now, what about the exaflop?"

prefix	symbol	multiplier
tera	T	10^12
peta	P	10^15
exa	E	10^18
zetta	Z	10^21
yotta	Y	10^24

prefix	symbol	multiplier	EPAC
tera	T	10^12	1998
peta	P	10^15	2008
exa	E	10^18	2018 ?
zetta	Z	10^21	
yotta	Y	10^24	

LBNL and CSU scientists working with Tensilica propose "climate computer" with 20M cores

- **Small size**
- **Low power**
- **4 MW, 200 petaflops**



GPU's gaining popularity

- **1 teraflop**
- **4 GB**
- **1.4 billion transistors**
- **240 cores**
- **$1700**

For comparison:
Photo shown at PAC 2001
3.4 Tflops!

Future Directions (speculation)

- Increased emphasis on parameter scans & optimization on large (>100K proc) computers
  - —Multi-level parallelism
- Increased emphasis on multi-physics and multiple capabilities in a single package
- New modeling approaches will become tractable
  - —New CSR models
  - —6D Direct Vlasov
- New opportunities for modeling in control rooms

It won’t be easy

- **“I know how to get 4 horses to pull a cart, but I don’t know how to make 1024 chickens do it.”**
  Enrico Clementi

- **Looking at a machine like Roadrunner:**
  - **12,240 horses (PowerXCell 8i processors)**
  - **6,120 chickens (dual-core opterons)**

Announcement

2009 International Computational Accelerator Physics Conference (ICAP09)

Aug 30 - Sept 4, 2009

Mark Hopkins Intercontinental Hotel in the heart of San Francisco

Organized by LBNL and SLAC

We hope to see you there!