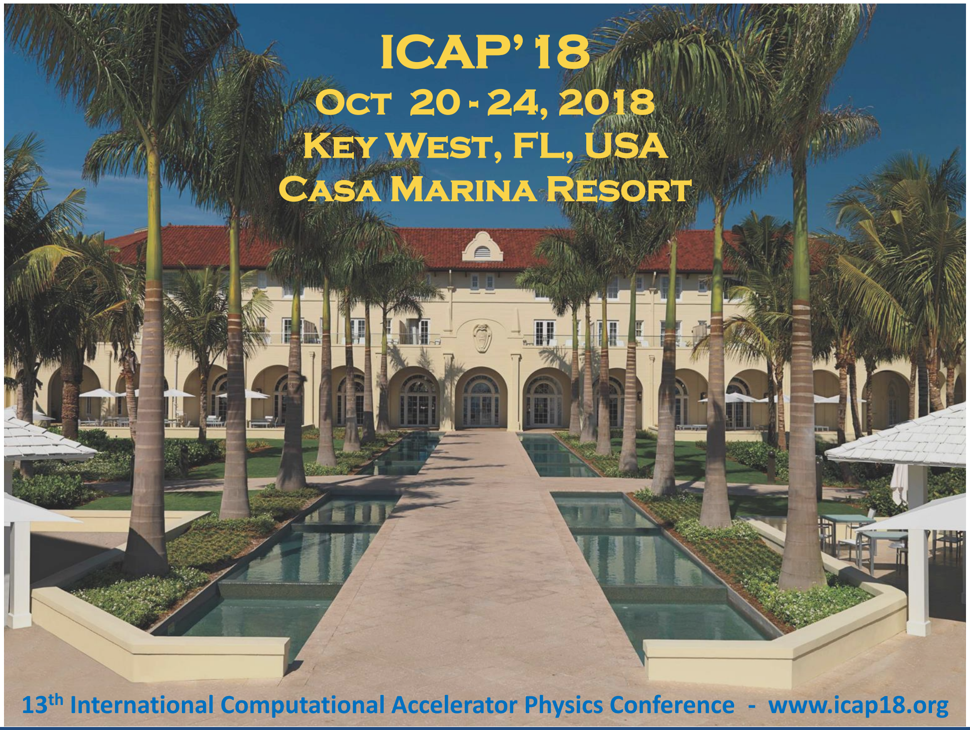
Computation Accelerator Physics: On the Road to Exascale

Robert D. Ryne, Lawrence Berkeley National Laboratory

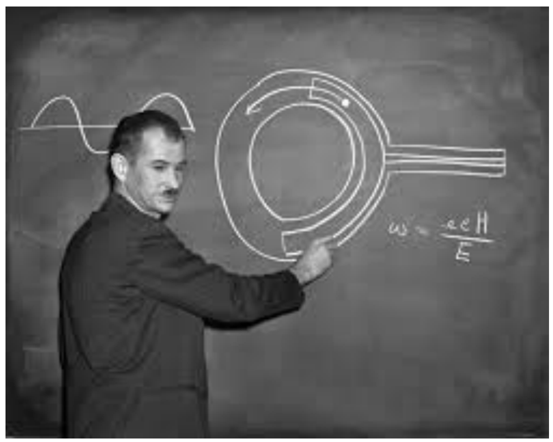


Outline

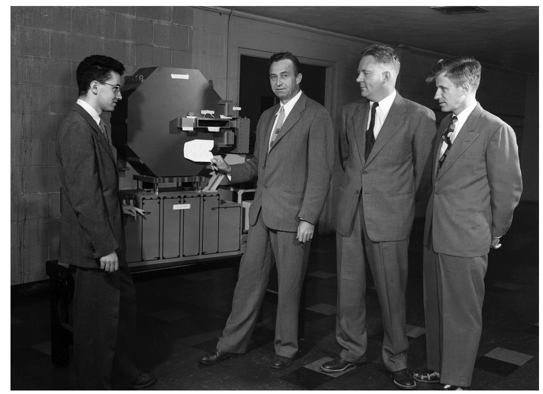
- Introduction
- Early CAP conferences
- 2000’s: Terascale Era
- 2010’s: Petascale Era
- Present and Future: Toward Exascale

Brief History
What brought us to the first CAP conference

Earnest Lawrence



Edwin McMillan



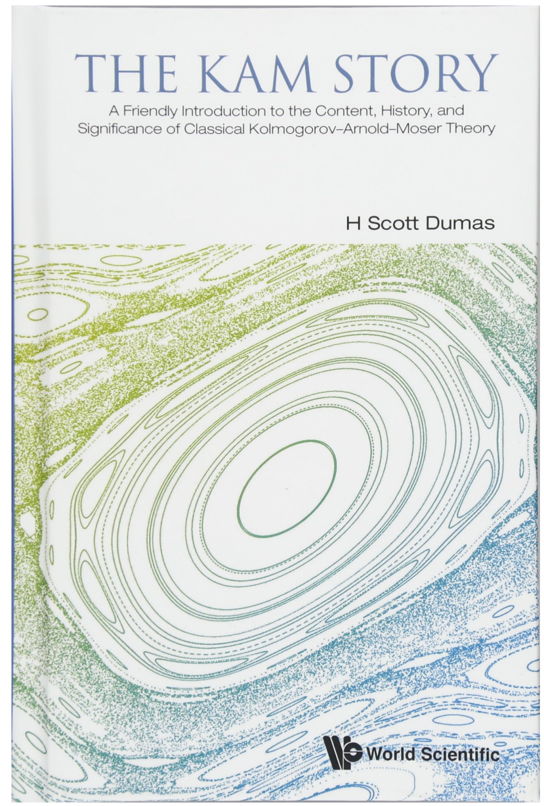
Courant, Snyder,
Livingston, Blewitt

1950's

Digital computation

Jackson Laslett. Observed chaos in calculations using the ILLIAC computer in 1950s

Theory



Kolmogorov's paper published in 1954

Fermi-Pasta-Ulam problem was first studied at LANL in 1955 on MANIAC I

- **Mary Tsingou Menzel was the programmer**
- **Eventually became a member of the Accelerator Technology Division**

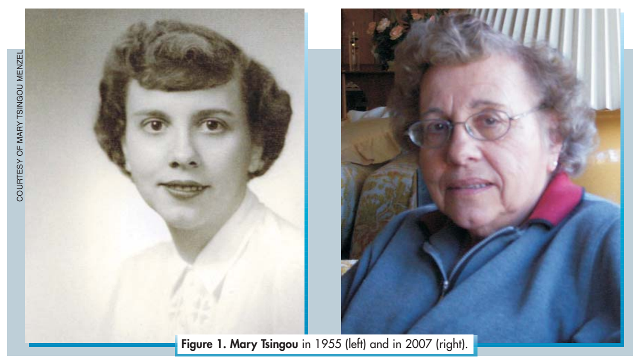


Figure 1. Mary Tsingou in 1955 (left) and in 2007 (right).

From "Fermi, Pasta, Ulam, and a mysterious lady," by Thierry Dauxois, Physics Today, January 2008.

1958: CERN’s first electronic computer

“About the time of the emergence of the bubble chamber technique, and under the influence of Dr. Lew Kowarski's keen awareness of the future need for adequate data-handling facilities when CERN's experimental physics programme would begin, CERN's first electronic computer began operation in the Autumn of 1958.”

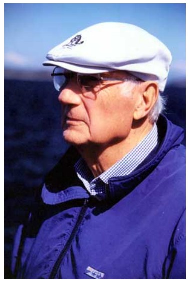
Sept 1967, CERN Courier: "… devoted to the electronic computer and its use at CERN"

The designers of the early computers assumed that programming would be done by small groups of specialists, probably mathematicians, and that it would be undesirable to make the task too easy. For example, von Neumann and Goldstine, who in 1946 proposed what is essentially the modern computer, argued against built-in floating-point arithmetic: "*The floating binary point represents an effort to render a thorough mathematical understanding of at least part of the problem unnecessary, and we feel that this is a step in a doubtful direction*."

Karl Brown, TRANSPORT (1960's)

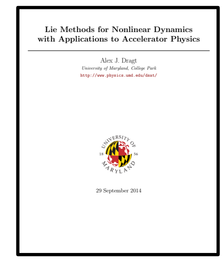
$$\zeta^f = \sum M\zeta^i + \sum\sum T\zeta^i\zeta^i + \sum\sum\sum U\zeta^i\zeta^i\zeta^i + \ldots$$

$$\zeta = (x, px, y, py, t, pt)$$



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

$$\dot{M} = JSM$$
$$\dot{f}_3 = -H_3^{\text{int}}$$
$$\dot{f}_4 = -H_4^{\text{int}} - \frac{1}{2}[f_3, H_3^{\text{int}}]$$
$$\ldots$$



Lie Methods for Nonlinear Dynamics with Applications to Accelerator Physics

Alex J. Dragt

University of Maryland, College Park

http://www.physics.umd.edu/dsat/

29 September 2014

1976: Dragt-Finn factored product of Lie transformations

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

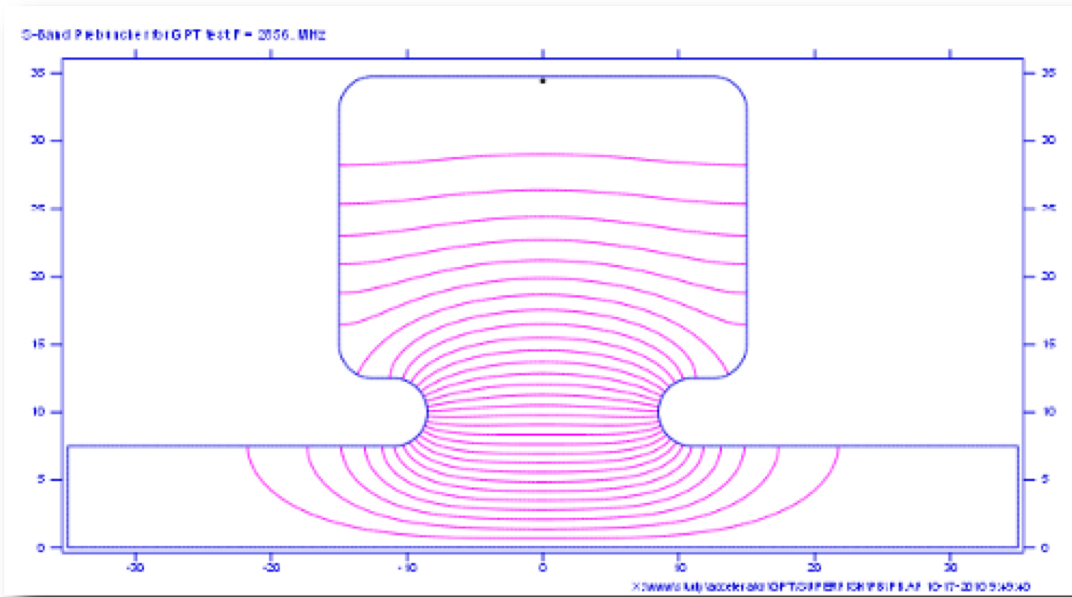
$$\zeta^f = \mathcal{M}\zeta^i = e^{:f_2:}\underbrace{(1 + :f_3: + \frac{1}{2}:f_3:^2 \ldots)(1 + :f_4: + \ldots)}\zeta^i$$

CERN Courier, March 1972: Special Issue on Computers
Opening article by Lew Kowarski: "Computers: Why?"

We are only beginning to discover and explore the new ways of acquiring scientific knowledge which have been opened by the advent of computers…

Modes of application:
(1) Numerical mathematics, (2) Data processing, (3) Symbolic calculations,
(4) Computer graphics, (5) Simulation, (6) File management and retrieval,
(7) Pattern recognition, (8) Process control

1976: Halbach & Holsinger -- SUPERFISH



1982, Keil, “Computer Programs in Accelerator Physics”

1987, LAACG, First Edition of LAACG Compendium of “Computer Programs used in Particle Accelerator Design”

1983: Equations of motion for the matrix and Lie polynomials in the Dragt-Finn facorization

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

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

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

$\ldots$

A. J. Dragt and E. Forest, "Computation of nonlinear behavior of Hamiltonian systems using Lie algebraic methods," J.Math.Phys. 24 (1983) 2734-2744

Numerically integrate these equations to compute transfer maps for beams with realistic fringe fields

The equations involve generalized gradients that can be computed using surface methods (papers of Dragt, Mitchell, Venturini, Abell, Walstrom,...)

1987: Berz, Differential Algebra

- The method of power series tracking for the mathematical description of beam dynamics (1987)
- Differential algebraic description of beam dynamics to very high orders (1988)

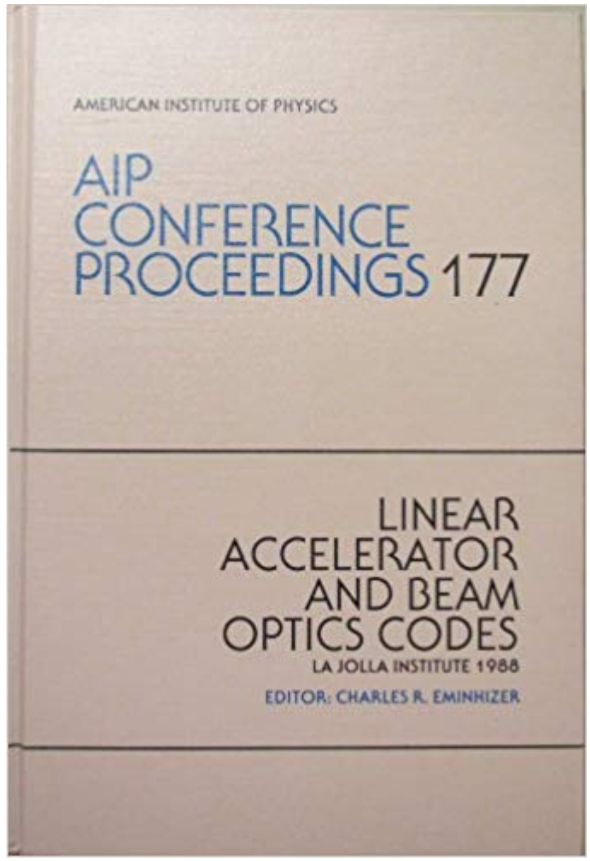
Sympectic Integration

- Ruth (1983), Forest & Ruth (1989), Yoshida (1990), Forest/Bengtsson/Reusch (1991),…

Normal Form Techniques

First Conference in ICAP series: 1988

Kona Kai Beach and Tennis Resort, San Diego, California



Some excerpts from the CAP 1988 Proceedings

- “The problem shown required 22 seconds on the IBM 3080 and 23 minutes on a machine with 8 MHz clock… The PC had the Intel 80287 Math co-processor and 1.1 Mbyte storage…”
- “This code, under the tentative name COSY INFINITY, will work to arbitrary order…”
- “…the beam transport designer’s world is richer and probably evolving faster than at any time since Karl Brown first put finger to keypunch”

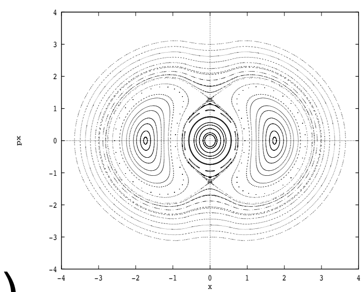
1990’s

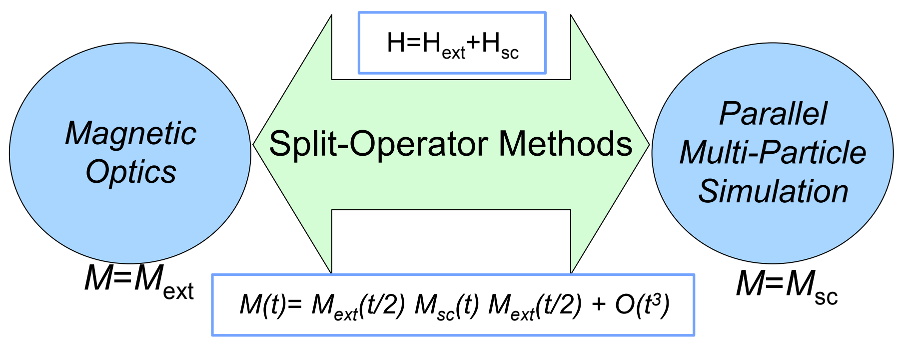
- 1990: Conference on Computer Codes in the Accelerator Community (Santa Fe, NM)
- 1993: Computational Accelerator Physics Conference (Pleasanton, CA)
- 1996: Computational Accelerator Physics Conference (Williamsburg, VA)
- 1997: DOE Grand Challenge in Comp. Acc. Physics
- 1997: First teraflop computer
- 1998: ICAP’98 (Monterey)

WAKEFIELD CALCULATIONS ON PARALLEL COMPUTERS

Paul Schoessow+
High Energy Physics Division
Argonne National Laboratory

Abstract: The use of parallelism in the solution of wakefield problems is illustrated for two different computer architectures (SIMD and MIMD). Results are given for finite difference codes which have been implemented on a Connection Machine and an Alliant FX/8 and which are used to compute wakefields in dielectric loaded structures. Benchmarks on code performance are presented for both cases.





2000’s: Terascale Era

- ICAP 2000 (Darmstadt)
- 2001: 1D CSR (Borland)
- ICAP 2002 (East Lansing)
- 2002: SciDAC
- ICAP 2004 (St. Petersburg)
- 2004: First million particle strong-strong beam-beam (Qiang)
- ICAP 2006 (Chamonix)
- 2008: First billion particle linac simulations (Qiang et al)
- 2008: First petaflop computer
- ICAP 2009 (San Francisco)

2010’s: Petascale Era

- Design optimization
- ICAP 2012 (Rostock-Warnemünde)
- ICAP 2015 (Shanghai)
- Themes:
  - Big Data
  - Increased heterogeneity (MPI+X, GPUs,…)
  - Machine Learning
- ICAP 2018 (Key West)

Present Day, Moving Forward: On to Exascale

- 3D Lienard-Wiechert modeling
- Exascale modeling of advanced particle accelerators
- Cosmology

Lienard-Wiechert Particle-Mesh (LWPM) Method

- Widely used space-charge technique:

$$\int \rho(\vec{x}\,')\vec{G}(\vec{x}-\vec{x}\,')\,d\vec{x}\,' \Rightarrow \sum \rho_j G_{i-j}$$

- FFTs to perform the discrete convolution
  - turns $O(N^2)$ problem into $O(N \log N)$
  - This is a mathematical trick (not a spectral algorithm)

Choice of Green function

$$\frac{1}{\sqrt{x^2+y^2+z^2}}$$

Ordinary Green function

$$\iiint \frac{1}{\sqrt{x^2+y^2+z^2}}dxdydz \doteq -\frac{z^2}{2}\arctan\left(\frac{xy}{z\sqrt{x^2+y^2+z^2}}\right)-\frac{y^2}{2}\arctan\left(\frac{xz}{y\sqrt{x^2+y^2+z^2}}\right)-\frac{x^2}{2}\arctan\left(\frac{yz}{x\sqrt{x^2+y^2+z^2}}\right)$$
$$+yz\ln(x+\sqrt{x^2+y^2+z^2})+xz\ln(y+\sqrt{x^2+y^2+z^2})+xy\ln(z+\sqrt{x^2+y^2+z^2}). \quad (2)$$

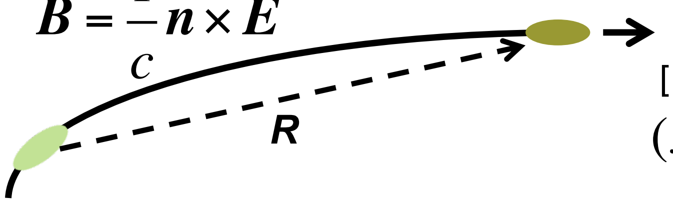
Integrated Green function

Qiang et al., Phys. Rev. ST Accel. Beams 9, 044204 (2006)

Lienard-Wiechert Green function

$$\boldsymbol{E}=\frac{1}{4\pi\varepsilon_0}\left[\frac{q}{\gamma^2\kappa^3R^2}(\boldsymbol{n}-\boldsymbol{\beta})+\frac{q}{\kappa^3Rc}\boldsymbol{n}\times\left((\boldsymbol{n}-\boldsymbol{\beta})\times\frac{\partial\boldsymbol{\beta}}{\partial t}\right)\right]$$

$$\boldsymbol{B}=\frac{1}{c}\boldsymbol{n}\times\boldsymbol{E}$$



[…] denotes quantities evaluated at the retarded time,

$$(x-x_r)^2+(y-y_r)^2+(z-z_r)^2=c^2(t-t_r)^2$$

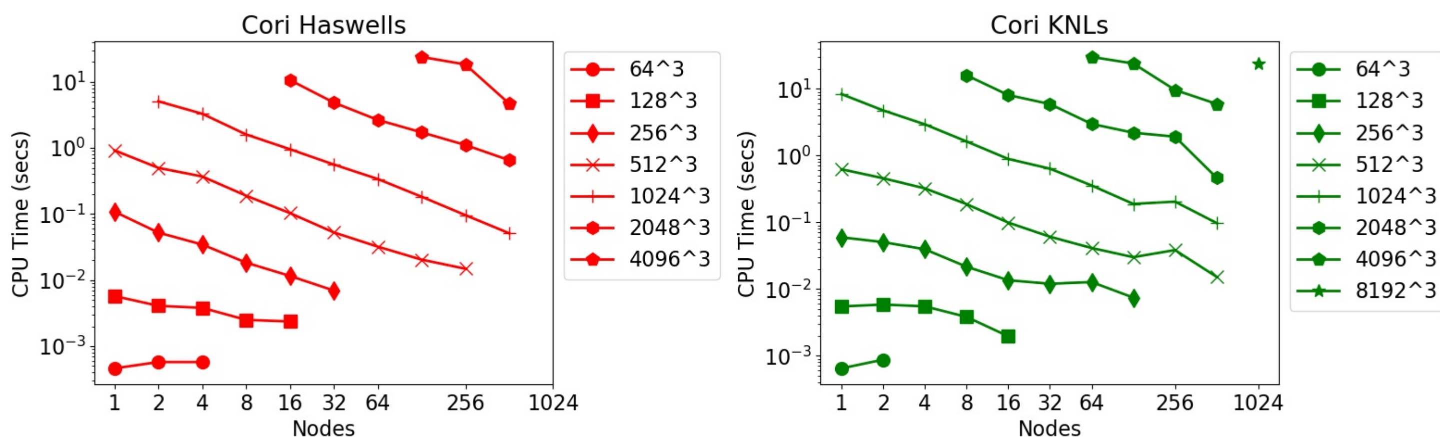
$$\boldsymbol{\beta}=\mathbf{v}/c$$

$$\boldsymbol{n}=\boldsymbol{R}/|\boldsymbol{R}|$$

$$\kappa=1-\boldsymbol{n}\cdot\boldsymbol{\beta}$$

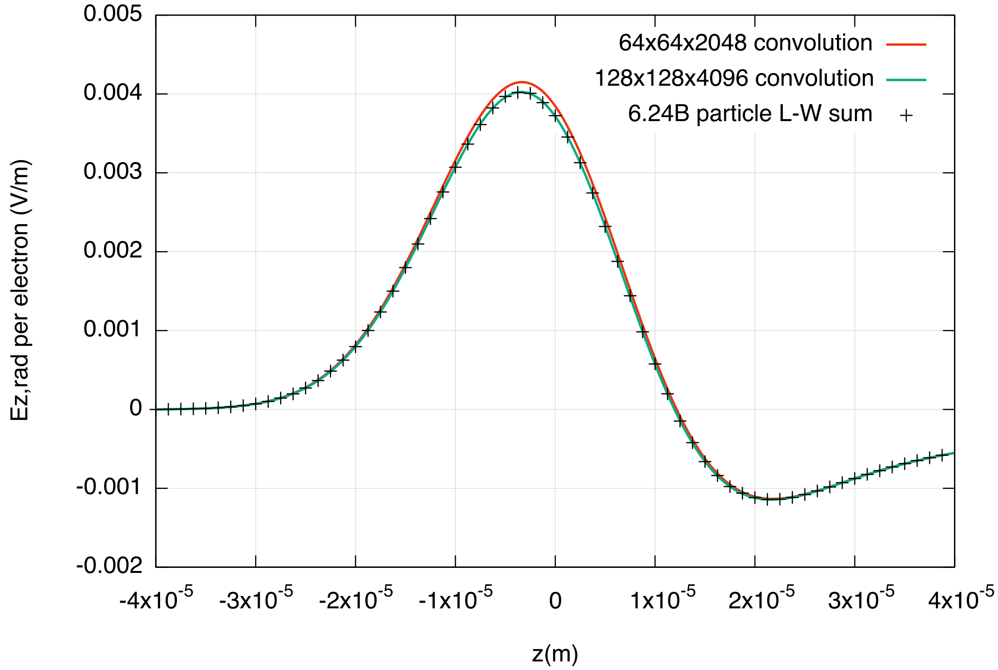
Parallel FFTs

- CPU time for single 3d FFT (non-convolution)
- Tune() method for pencil/brick and point/all2all options
- Using 32 MPI/node on Haswell, 64 MPI/node on KNL

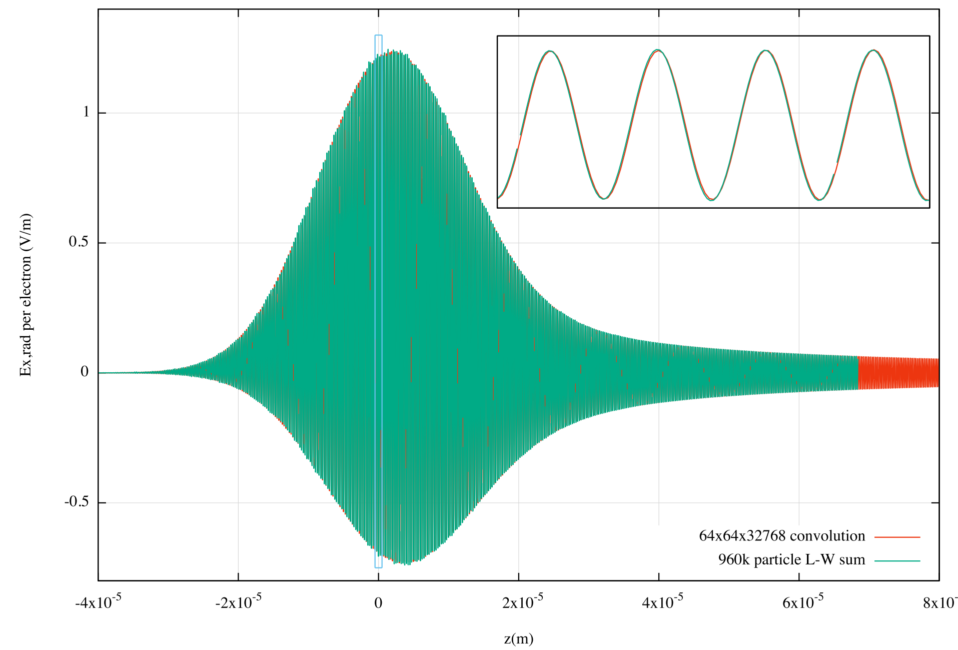


Courtesy Steve Plimpton

A sample of LW3D results



3D convolution vs LW sum: Steady-state dipole radiation

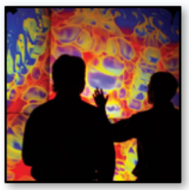


3D convolution vs LW sum: Undulator radiation

R. Ryne et al., “Large Scale Simulation of Synchrotron Radiation using a Lienard-Wiechert Approach,” Proc IPAC 2012
R. Ryne et al., “Using a Lienard-Wiechert Solver to Study Coherent Synchrotron Radiation Effects,” Proc FEL 2013
B. Garcia, T. Raubenheimer, and R. Ryne, “Stochastic Effects from Classical 3D Synchrotron Radiation,” Proc FEL 2017
R. Ryne et al., “Self-Consistent Modeling using a Lienard-Wiechert Particle-Mesh Method,” Proc PAC 2018

DOE Exascale Computing Project

National security
Stockpile stewardship



Energy security
Turbine wind plant efficiency

Design and commercialization of SMRs

Nuclear fission and fusion reactor materials design

Subsurface use for carbon capture, petro extraction, waste disposal

High-efficiency, low-emission combustion engine and gas turbine design

Carbon capture and sequestration scaleup

Biofuel catalyst design

Economic security
Additive manufacturing of qualifiable metal parts

Urban planning

Reliable and efficient planning of the power grid

Seismic hazard risk assessment

Scientific discovery
Cosmological probe of the standard model of particle physics

Validate fundamental laws of nature

Plasma wakefield accelerator design

Light source-enabled analysis of protein and molecular structure and design

Find, predict, and control materials and properties

Predict and control stable ITER operational performance

Demystify origin of chemical elements

Earth system
Accurate regional impact assessments in Earth system models

Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols

Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation

Health care
Accelerate and translate cancer research

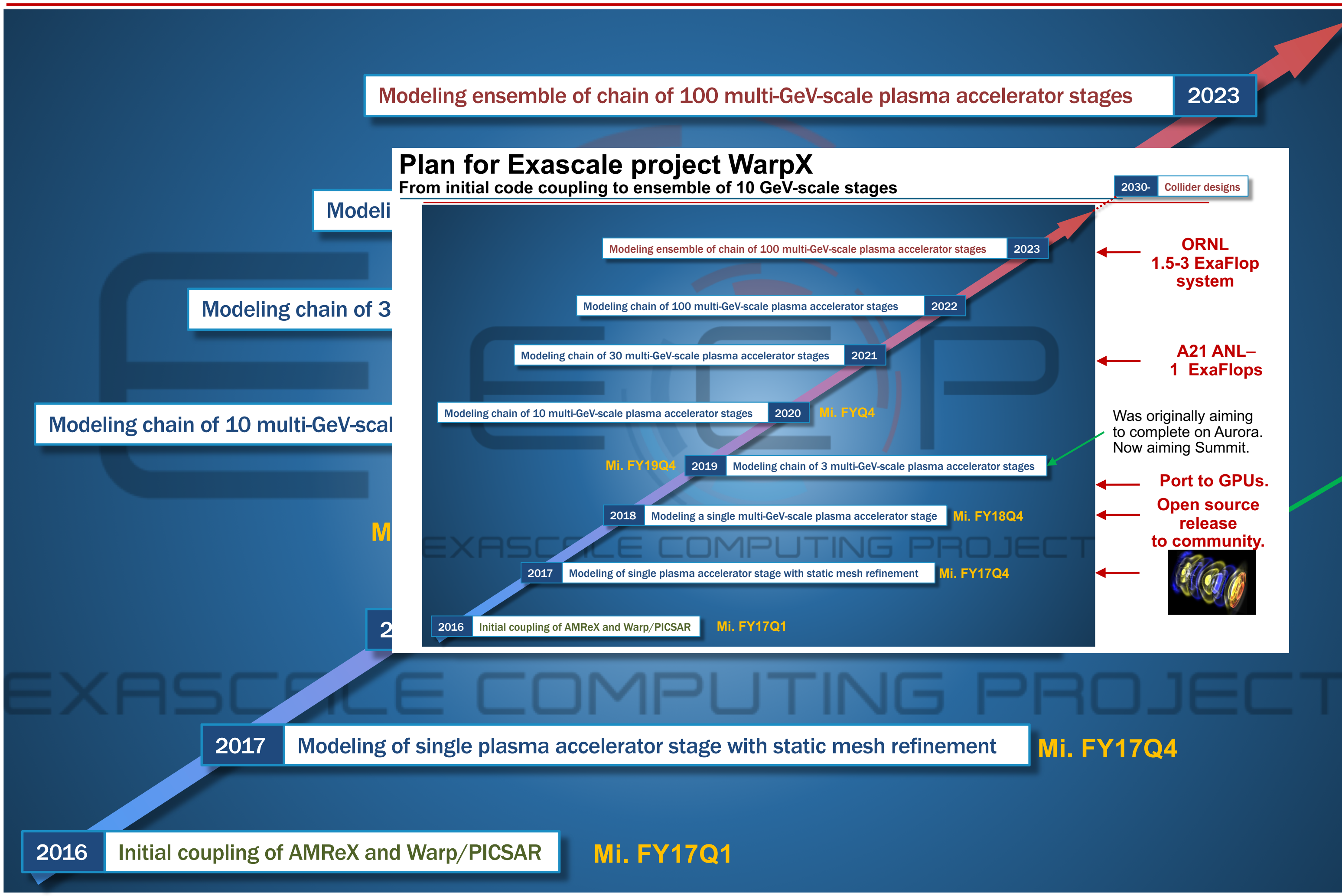
ECP EXASCALE COMPUTING PROJECT

For details on Plasma accelerator ECP see the talk by R. Lehi

Plan for Exascale project WarpX

From initial code coupling to ensemble of 10 GeV-scale stages

2030- Collider designs



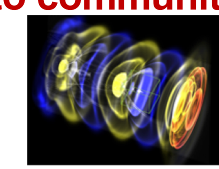
ORNL
1.5-3 ExaFlop
system

A21 ANL–
1 ExaFlops

Was originally aiming
to complete on Aurora.
Now aiming Summit.

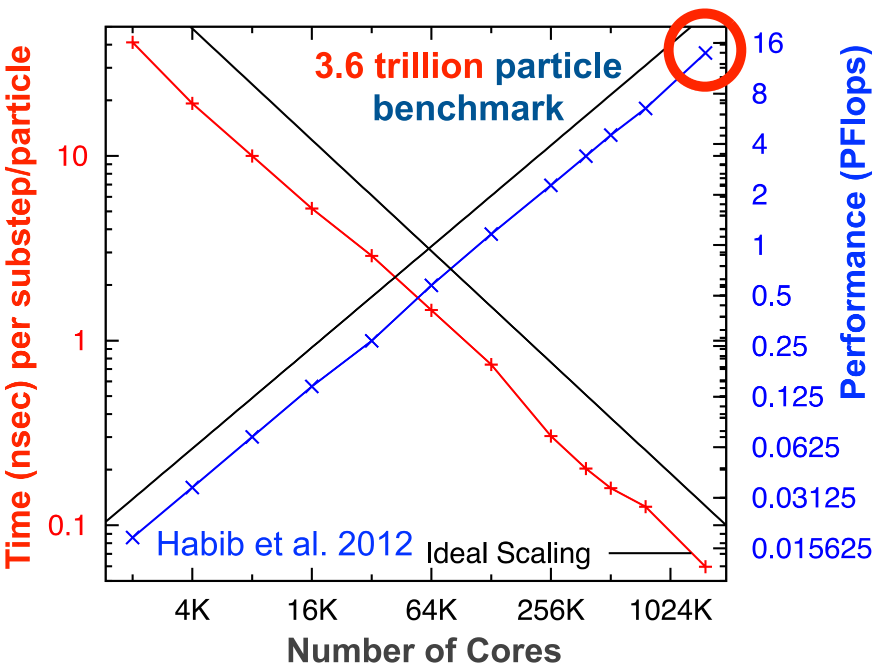
Port to GPUs.

Open source
release
to community.

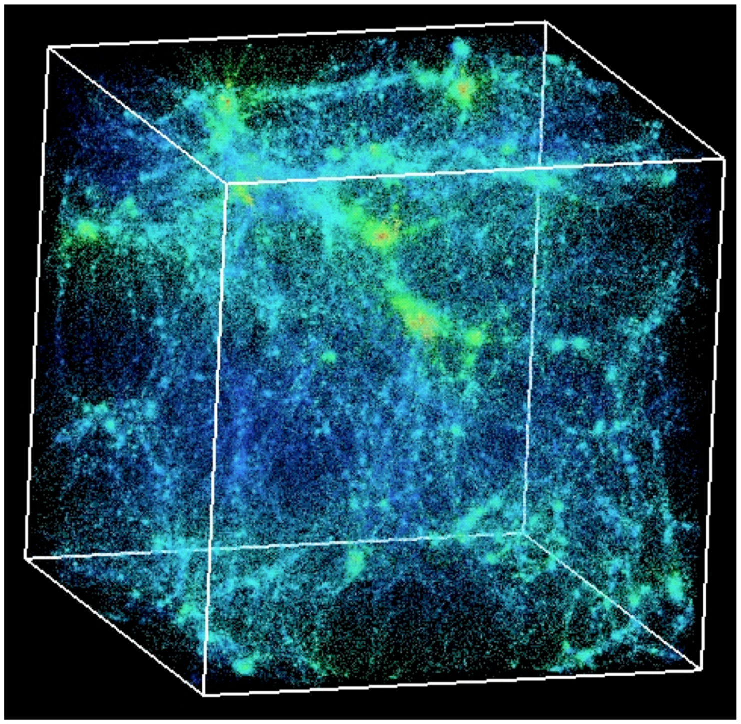


Courtesy J.-L. Vay

ExaSky project (Computational Cosmology, Habib et al.)



HACC on Sequoia (2012): 13.94 PFlops, 69.2% peak, 90% parallel efficiency on 1,572,864 cores/MPI ranks, 6.3M-way concurrency



Courtesy S. Habib

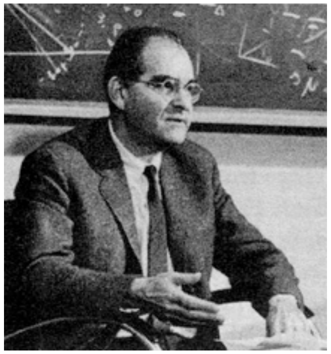
Conclusion

- What projects will we apply these advanced computing tools to?
  - Advanced accelerator concepts for stages
  - Advanced accelerator concepts for multi-stage systems – colliders
  - Advanced schemes for future light sources
  - Novel concepts like IOTA
  - …

To conclude, let's look back (almost 50 years) to the International Conference on High Energy Accelerators (1971)

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

By the time of ICAP 2021 we will be on the doorstep of the Exascale era

0.1 Trillion times the performance of the CDC 7600 !!

1 Billion times the performance of the Cray YMP at the time of the first CAP conference in 1988!

What breakthroughs will this "4^{th} kind of creativity in physics" bring?

END OF PRESENTATION