U.S. Particle Accelerator School
Education in Beam Physics and Accelerator Technology

Simulations of Beam and Plasma Systems

Steven M. Lund, David Bruhwiler, Rémi Lehe, Jean-Luc Vay and Daniel Winklehner

Sponsoring University: Old Dominion University

Hampton, Virginia – January 15-26, 2018

Collaborations

Jean-Luc Vay, Rémi Lehe

Lawrence Berkeley National Laboratory

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Particle accelerators are essential tools in modern life

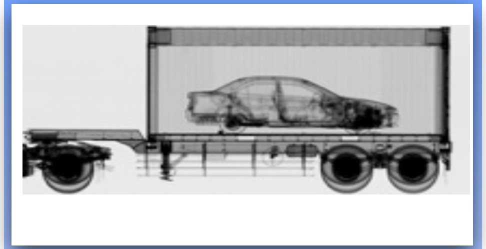
Medicine

- ~9000 medical accelerators in operation worldwide
- 10's of millions of patients treated/yr
- 50 medical isotopes, routinely produced with accelerators

Industry

- ~20,000 industrial accelerators in use
  - Semiconductor manufacturing
  - cross-linking/ polymerization
  - Sterilization/ irradiation
  - Welding/cutting
- Annual value of all products that use accel. Tech.: $500B

National Security



- Cargo scanning
- Active interrogation
- Stockpile stewardship: materials characterization, radiography, support of non-proliferation

Discovery Science

- ~30% of Nobel Prizes in Physics since 1939 enabled by accelerators
- 4 of last 14 Nobel Prizes in Chemistry for research utilizing accelerator facilities

Opportunity for much bigger impact by reducing size and cost.

Problem: size & cost often a limiting factor
Example 1: Proton Therapy Center

New Rochester Mayo Clinic
Proton Therapy Center
- 4 chambers
- $188M

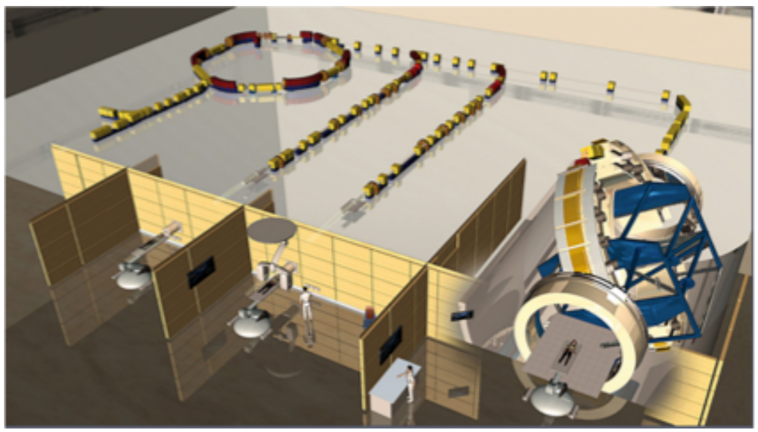
120-ton gantry directs proton beam to appropriate spot on patient by rotating around a three-story chamber.

http://finance-commerce.com/2014/03/status-report-mayo-proton-therapy-facility/#ixzz43DJgnIlA
http://blogs.mprnews.org/statewide/2014/03/mayos-proton-beam-facility-on-track-for-2015-opening/

Problem: size & cost often a limiting factor
Example 2: Carbon Therapy Center

Heidelberg Proton & Carbon Therapy Center

- 2 scans chambers
- one 4π chamber
- €119M

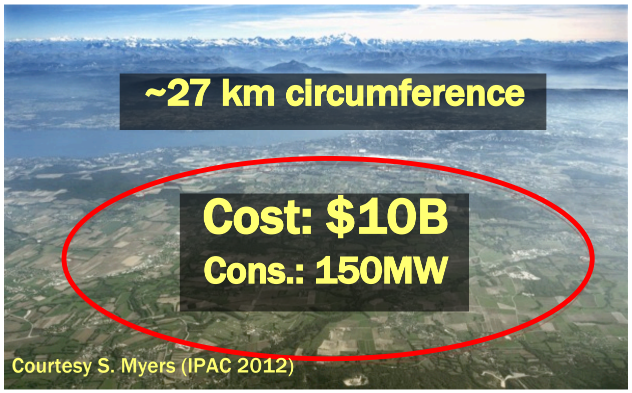


670-ton gantry
~1/10 Eiffel Tower

http://medicalphysicsweb.org/cws/article/research/51684
https://www.klinikum.uni-heidelberg.de/About-us.124447.0.html?&L=1

Problem: size & cost often a limiting factor
Example 3: High-Energy Physics collider

CERN LHC



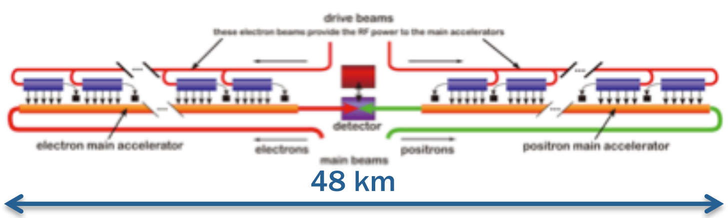
Future colliders?

ILC

Cost: $8B-$20B?

Cons.: 230MW

CLIC



Cost: $?B

Cons.: 415MW

FCC

nature International weekly journal of science

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News & Comment > News > Q&A > 2015 > December > Article

NATURE | NEWS: Q&A

CERN's next director-general on the LHC and her hopes for international particle physics

Fabiola Gianotti talks to *Nature* ahead of taking the helm at Europe's particle-physics laboratory on 1 January.

Elizabeth Gibney

22 December 2015

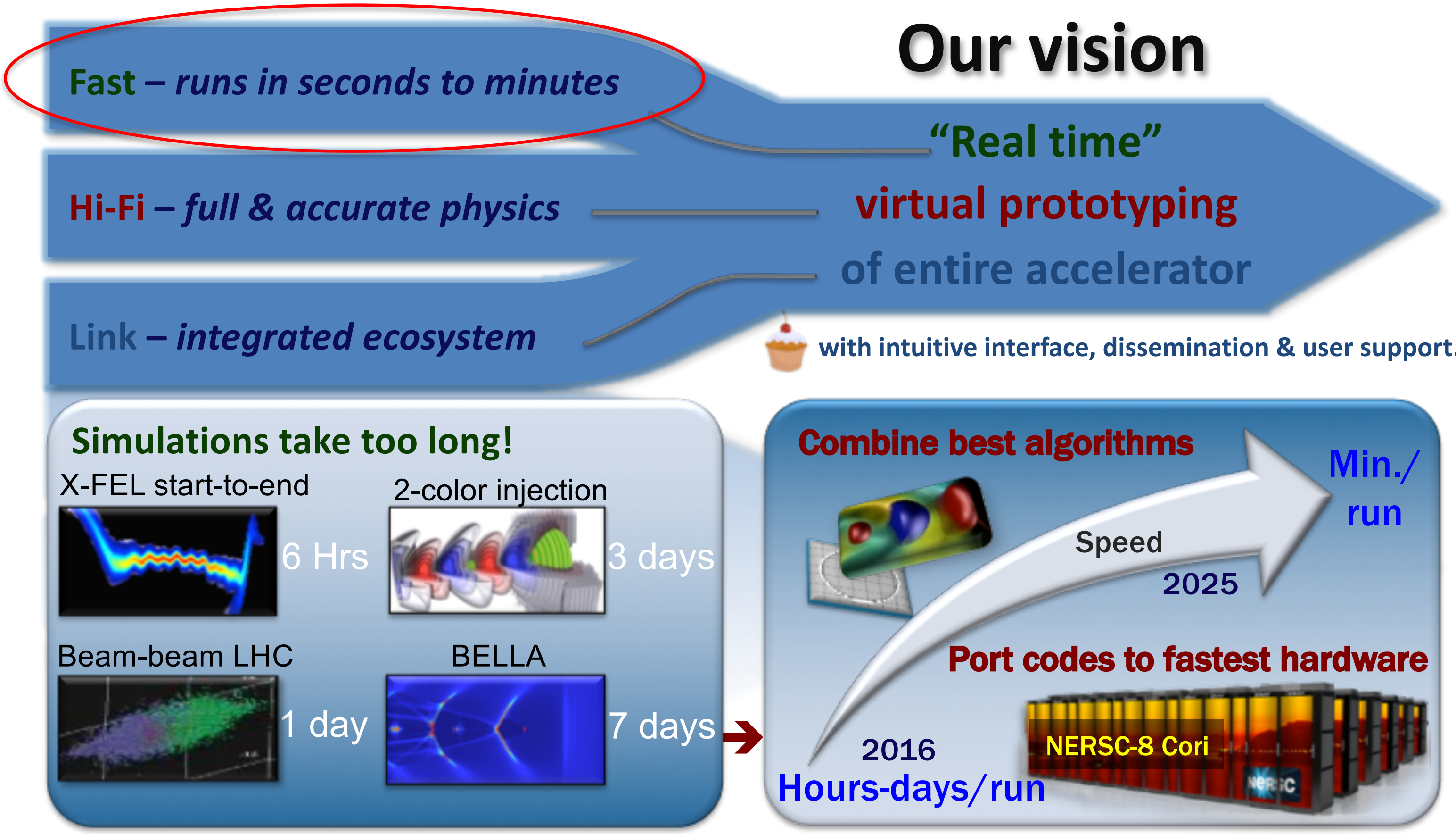
Fabiola Gianotti is the incoming director-general of CERN.

Some people think that future governments will be unwilling to fund larger and more expensive facilities. Do you think a collider bigger than the LHC will ever be built? And will it depend on the LHC finding something new?

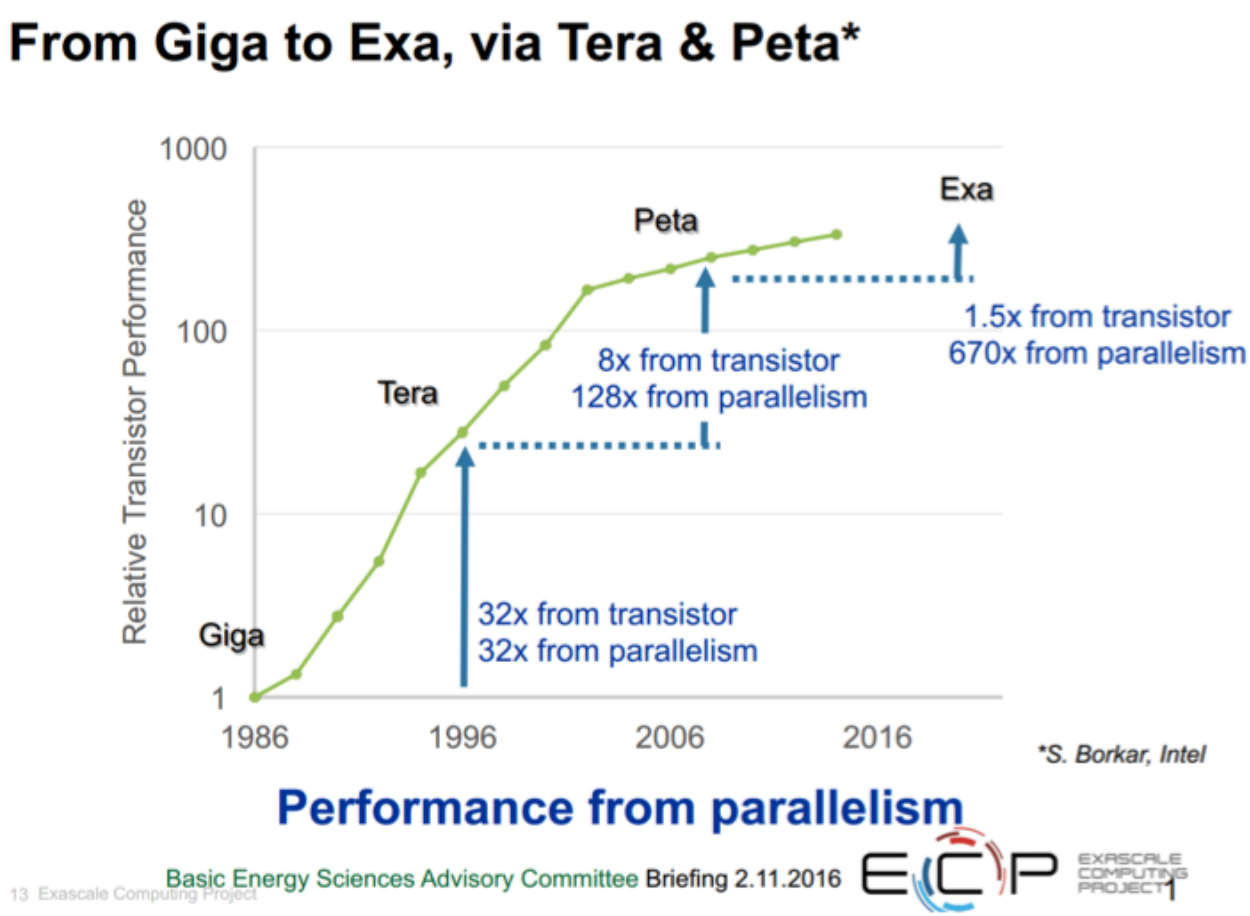
The outstanding questions in physics are important and complex and difficult, and they require the deployment of all the approaches the discipline has developed, from high-energy colliders to precision experiments and cosmic surveys. High-energy accelerators have been our most powerful tools of exploration in particle physics, so we cannot abandon them. What we have to do is push the research and development in accelerator technology, so that we will be able to reach higher energy with compact accelerators.

Computer modeling has unique role to play!

The next generation of accelerators needs the *next generation* of modeling tools



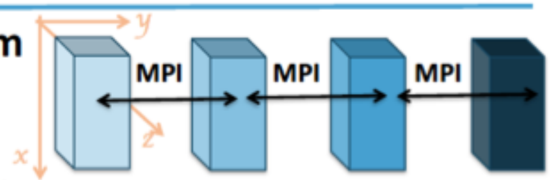
Speedup not from transistors speed anymore, need to increase parallelism

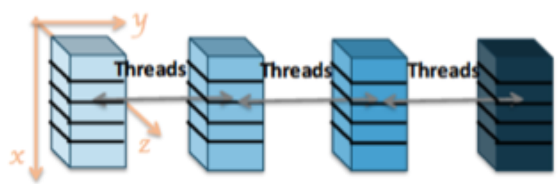


Emerging supercomputing architectures require restructuration with “multi-level parallelism”

To run effectively on future systems

- **Manage Domain Parallelism**
  - independent program units; explicit
- **Increase Thread Parallelism**
  - independent execution units within the program; generally explicit
- **Exploit Data Parallelism**
  - Same operation on multiple elements
- **Improve data locality**
  - Cache blocking; Use on-package memory






```
|--> DO I = 1, N
|       R(I) = B(I) + A(I)
|--> ENDDO
```

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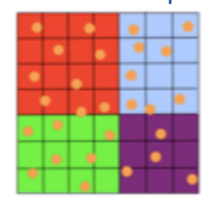
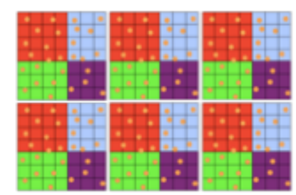
Courtesy Katherine Riley, FES Exascale Review, 2016

Particle-In-Cell

Domain decomposition



Threading + tiling



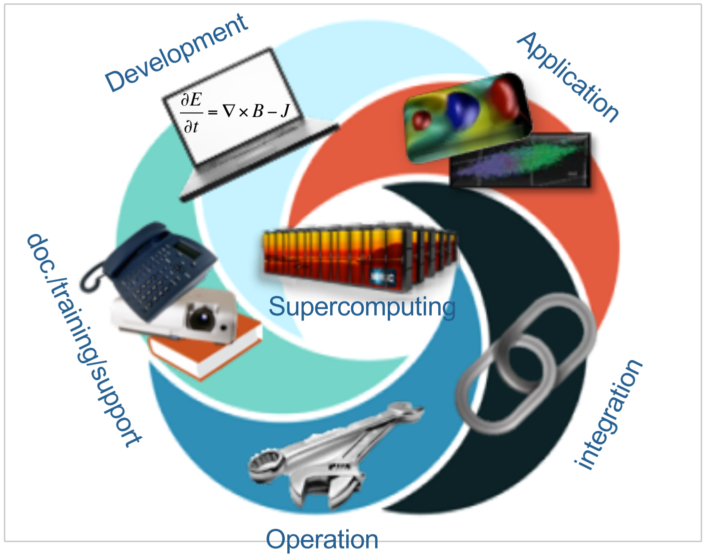
Vecrtorization, …

Supporting community calls for large efforts

Community HPC hardware needs community HPC software

needs:

- Development
- Application
- Integration of multiphysics modules
- Operation
- Doc./training/support
- On laptop/desktop to supercomputers



How is the community doing?

Beam dynamics codes

Beam Dynamics Codes:

Codes section from Accelerator Handbook (A. Chao, 2013)

(Below, PIC refers to codes with particle-in-cell space-charge capability.)

Code	URL or Contact	Description/Comments
ASTRA	tesla.desy.de/~meykopff	3D parallel, general charged particle beams incl. space charge
AT	sourceforge.net/projects/atcollab/	Accelerator Toolbox
BETACOOL	betacool.jinr.ru	Long term beam dynamics: ECOOL, IBS, internal target
Bmad, Tao	www.lns.cornell.edu/~dcs/bmad/	General purpose toolbox library + driver program
COSY INFINITY	www.cosyinfinity.org	Arbitrary-order beam optics code
CSRTrack	www.desy.de/xfel-beam/csrtrack	3D parallel PIC; includes CSR; mainly for e^- dynamics
Elegant/SDDS suite	aps.anl.gov/elegant.html	parallel; track, optimize; errors; wakes; CSR
ESME	www-ap.fnal.gov/ESME	Longitudinal tracking in rings
HOMDYN	Massimo.Ferrario@LNF.INFN.IT	Envelope equations, analytic space charge and wake fields
IMPACT code suite	amac.lbl.gov	3D parallel multi-charge PIC for linacs and rings
LAACG code suite	laacg.lanl.gov	Includes PARMILA, PARMELA, PARMTEQ, TRACE2D/3D
LiTrack	www.slac.stanford.edu/~emma/	Longitudinal linac dynamics; wakes; GUI-based; error studies
LOCO	safranek@slac.stanford.edu	Analysis of optics of storage rings; runs under matlab
LUCRETIA	www.slac.stanford.edu/accel/ilc/codes	Matlab-based toolbox for simulation of single-pass e^- systems
MaryLie	www.physics.umd.edu/dsat	Lie algebraic code for maps, orbits, moments, fitting, analysis
MaryLie/IMPACT	amac.lbl.gov	3D parallel PIC; MaryLie optics + IMPACT space charge
MAD-X	mad.web.cern.ch/mad	General purpose beam optics
MERLIN	www.desy.de/~merlin	C++ class library for charged particle accelerator simulation
OPAL	amas.web.psi.ch	3D parallel PIC; cyclotrons, FFAGs, linacs; particle-matter int.
ORBIT	jzh@ornl.gov	Collective beam dynamics in rings and transport lines
PATH	Alessandra.Lombardi@cern.ch	3D PIC; linacs and transfer lines; matching and error studies
SAD	acc-physics.kek.jp/SAD/sad.html	Design, simulation, online modeling & control
SIMBAD	agsrhichome.bnl.gov/People/luccio	3D parallel PIC; mainly for hadron synchrotrons, storage rings
SIXTRACK	frs.home.cern.ch/frs/	Single particle optics; long term tracking in LHC
STRUCT	www-ap.fnal.gov/users/drozhdin	Long term tracking w/ emphasis on collimators
Synergia	https://compacc.fnal.gov/projects	3d parallel PIC; space charge, nonlinear tracking and wakes
TESLA	lyyang@bnl.gov	Parallel; tracking; analysis; optimization
TRACK	www.phy.anl.gov/atlas/TRACK	3D parallel PIC; mainly for ion or electron linacs
LIBTRACY	libtracy.sourceforge.net/	Library for beam dynamics simulation
TREDI	www.tredi.enea.it	3D parallel PIC; point-to-point Lienard-Wiechert
UAL	code.google.com/p/ual/	Unified Accelerator Libraries
WARP	DPGrote@lbl.gov	3D parallel ES and EM PIC with accelerator models
ZGOUBI	sourceforge.net/projects/zgoubi/	Magnetic optics; spin; sync radiation; in-flight decay

Beam/plasma codes

Table 1. List of simulation PIC codes for the modeling of plasma accelerators.

Code	Type	Website/reference	Availability/license
ALaDyn/PICCANTE	EM-PIC 3D	http://aladyn.github.io/piccante	Open/GPLv3+
Architect	EM-PIC RZ	https://github.com/albz/Architect	Open/GPL
Calder	EM-PIC 3D	http://iopscience.iop.org/article/10.1088/0029-5515/43/7/317	Collaborators/Proprietary
Calder-Circ	EM-PIC RZ^+	http://dx.doi.org/10.1016/j.jcp.2008.11.017	Upon Request/Proprietary
CHIMERA	EM-PIC RZ+	https://github.com/hightower8083/chimera	Open/GPLv3
ELMIS	EM-PIC 3D	http://www.diva-portal.org/smash/record.jsf?pid=diva2%3A681092&dswid=-8610	Collaborators/Proprietary
EPOCH	EM-PIC 3D	http://www.ccpp.ac.uk/codes.html	Collaborators/GPL
FBPIC	EM-PIC RZ^+	https://fbpic.github.io	Open/modified BSD
HiPACE	QS-PIC 3D	http://dx.doi.org/10.1088/0741-3335/56/8/084012	Collaborators/Proprietary
INF&RNO	QS/EM-PIC RZ	http://dx.doi.org/10.1063/1.3520323	Collaborators/Proprietary
LCODE	QS-PIC RZ	http://www.inp.nsk.su/~lotov/lcode	Open/None
LSP	EM-PIC 3D/RZ	http://www.lspsuite.com/LSP/index.html	Commercial/Proprietary
MAGIC	EM-PIC 3D	http://www.mrcwdc.com/magic/index.html	Commercial/Proprietary
Osiris	EM-PIC 3D/RZ^+	http://picksc.idre.ucla.edu/software/software-production-codes/osiris	Collaborators/Proprietary
PHOTON-PLASMA	EM-PIC 3D	https://bitbucket.org/thaugboelle/ppcode	Open/GPLv2
PICADOR	EM-PIC 3D	http://hpc-education.unn.ru/en/research/overview/laser-plasma	Collaborators/Proprietary
PIConGPU	EM-PIC 3D	http://picongpu.hzdr.de	Open/GPLv3+
PICLS	EM-PIC 3D	http://dx.doi.org/10.1016/j.jcp.2008.03.043	Collaborators/Proprietary
PSC	EM-PIC 3D	http://www.sciencedirect.com/science/article/pii/S0021999116301413	Open/GPLv3
QuickPIC	QS-PIC 3D	http://picksc.idre.ucla.edu/software/software-production-codes/quickpic	Collaborators/Proprietary
REMP	EM-PIC 3D	http://dx.doi.org/10.1016/S0010-4655(00)00228-9	Collaborators/Proprietary
Smilei	EM-PIC 2D	http://www.maisondelasimulation.fr/projects/Smilei/html/licence.html	Open/CeCILL
TurboWave	EM-PIC 3D/RZ	http://dx.doi.org/10.1109/27.893300	Collaborators/Proprietary
UPIC-EMMA	EM-PIC 3D	http://picksc.idre.ucla.edu/software/software-production-codes/upic-emma	Collaborators/Proprietary
VLPL	EM/QS-PIC 3D	http://www.tp1.hhu.de/~pukhov/	Collaborators/Proprietary
VPIC	EM-PIC 3D	http://github.com/losalamos/vpic	Open/BSD clause-3 license
VSim (Vorpal)	EM-PIC 3D	https://txcorp.com/vsim	Commercial/Proprietary
Wake	QS-PIC RZ	http://dx.doi.org/10.1063/1.872134	Collaborators/Proprietary
Warp	EM-PIC 3D/RZ^+	http://warp.lbl.gov	Open/modified BSD

EM = electromagnetic; QS = quasistatic; PIC = particle-in-cell; 3D = three-dimensional; RZ = axisymmetric; RZ^+ = axisymmetric with azimuthal Fourier decomposition.

J.-L. Vay and R. Lehe, "Simulations for Plasma and Laser Acceleration", Reviews of Accelerator Science and Technology **9**, 165 (2016).

Need of solutions for non-disruptive coordination

Significant investments into existing pool of codes:

- essential to **minimize disruptions** to developers and users,
- while **enabling interoperability** and **expandability**.

Challenges:

Technical

- programming languages
- data formats, parallelism
- code architectures
- open vs proprietary sources
- keep creativity

Human

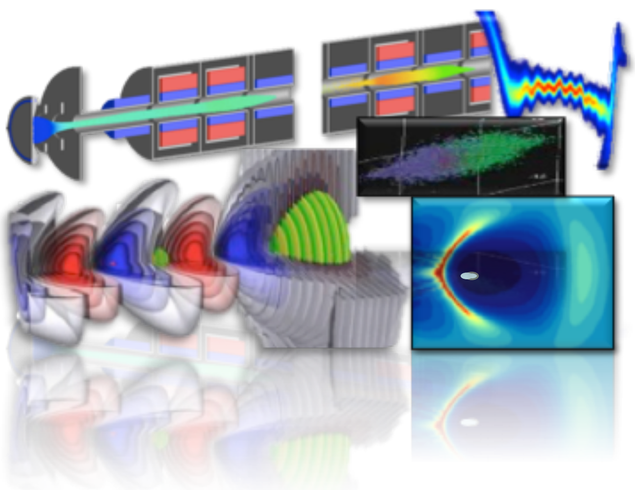
- changing habits is hard
- different visions
- recognition
- distance
- corporatism/rivalry
- (re)build trust

LBNL codes assembled in "BLAST" simulation toolset

blast.lbl.gov

BLAST

BERKELEY LAB ACCELERATOR SIMULATION TOOLKIT



Advanced simulation toolset:

(For conventional & advanced concept accelerators)

- ***Multi-physics frameworks***: IMPACT, Warp, WarpX.
- ***Specialized codes***: BeamBeam3D, CSR3D, FBPIC, HiPACE, INF&RNO, POSINST.
- ***Libraries***: PICSAR.

Wide set of physics & components:

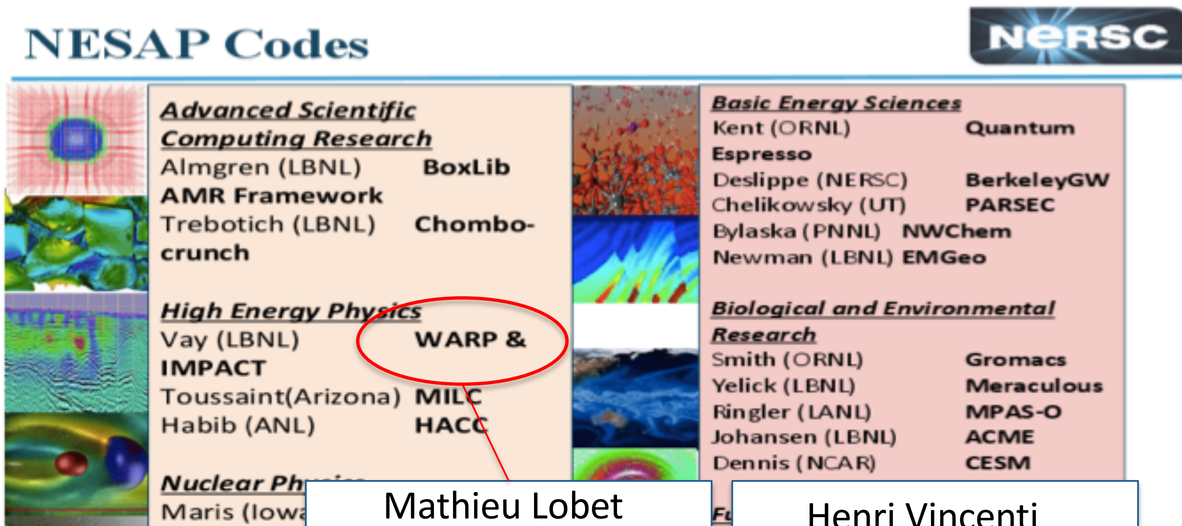
- beams, plasmas, lasers, structures, beam-beam, e^- clouds, ...
- linacs, rings, injectors, traps, ...

Keeping up at the forefront of computing:

- ***novel algorithms:*** boosted frame, particle pushers, etc.
- SciDAC, INCITE, NESAP, DOE Exascale.

*Most codes open source, available at blast.lbl.gov or upon request.

PICSAR created as part of
NERSC Exascale Applications Program (NESAP)



Mathieu Lobet

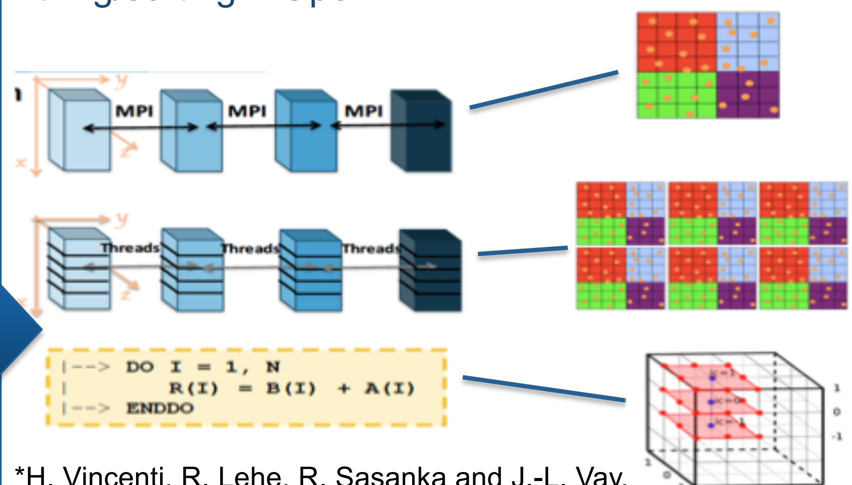
Ex-NESAP postdoc
(now at CEA, Saclay, France)

Henri Vincenti

Marie Curie postdoc fellowship
(now at CEA, Saclay, France)

Warp EM-PIC kernel extracted
➔ Particle-In-Cell Scalable Architecture Resources (PICSAR) library + miniapp

Optimized with new vectorization algo.* + tiling/sorting + OpenMP + MPI



*H. Vincenti, R. Lehe, R. Sasanka and J.-L. Vay, *Comp. Phys. Comm.* , 210, 145-154 (2017).

PICSAR is now open source: https://picsar.net
Used in Warp, WarpX & SMILEI.

Now developed within DOE ECP project and CEA Saclay.

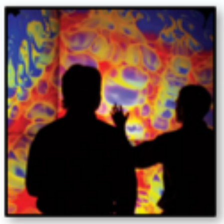
U.S. DOE Exascale Computing Project (ECP)

- As part of the National Strategic Computing initiative, ECP was established to accelerate delivery of a **capable exascale** computing system that integrates hardware and software capability to deliver approximately 50 times more performance than today's 20-petaflops machines on mission critical applications.
  - DOE is a lead agency within NSCI, along with DoD and NSF
  - Deployment agencies: NASA, FBI, NIH, DHS, NOAA
- ECP's work encompasses
  - applications,
  - system software,
  - hardware technologies and architectures, and
  - workforce development to meet scientific and national security mission needs.

Capable Exascale System Applications Will Deliver Broad Coverage of 6 Strategic Pillars

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

Plasma-based acceleration has the potential to make accelerators small (again), and cut cost dramatically

First
cyclotron
~0.1 MeV

Plasma
accelerator
1 GeV

Tens of plasma accelerator stages needed for a 1 TeV e^-e^+ collider.

BUT: simulations in 2-D can take days for 1 stage (even at insufficient resolution for collider beam quality).

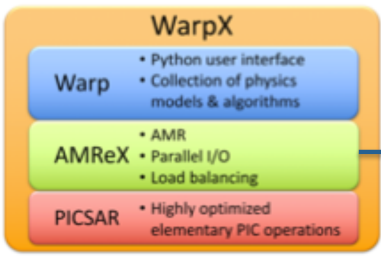
➔ ***Full 3-D modeling of tens of stages intractable without Exascale computing.***

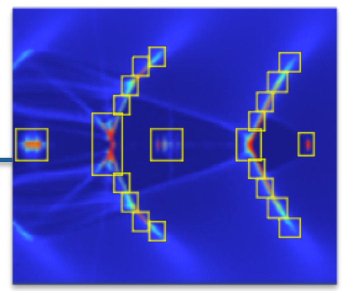
ECP Project WarpX: "Exascale Modeling of Advanced Particle Accelerators"

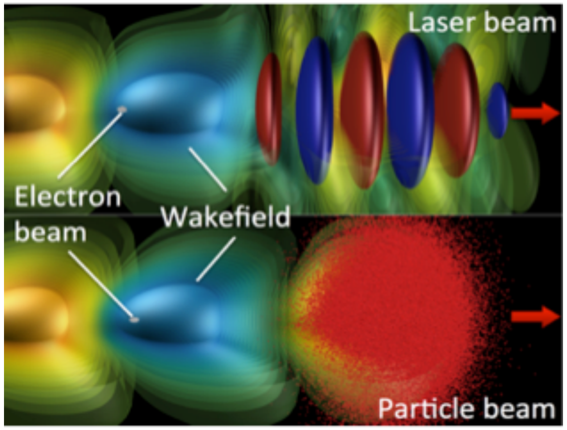
Goal (4 years): Convergence study in 3-D of 10 consecutive multi-GeV stages in linear and bubble regime, for laser- & beam-driven plasma accelerators.

How: ➔ Combination of most advanced algorithms

➔ Coupling of Warp+AMReX+PICSAR







➔ Port to emerging architectures (Intel KNL, GPU, ...)

Team: LBNL ATAP (accelerators) + LBNL CRD (computing science) + SLAC + LLNL

Ultimate goal: enable modeling of 100 stages by 2025 for 1 TeV collider design!

WarpX team

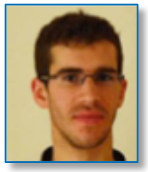
Time on WarpX varies between 5% to 80%

Main topics

LBNL ATAP

Jean-Luc Vay (PI)

Rémi Lehe



Jaehong Park

Robert Ryne

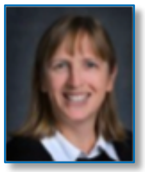
Olga Shapoval

Maxence Thevenet

Main topics:
- Management
- Algorithms
- Optimization
- Visualization & I/O
- LWFA

LBNL CRD

Ann Almgren (coPI)



John Bell

Andrew Myers

Weiqun Zhang

Main topics:
- AMR
- MPI, OpenMP
- Visualization & I/O

SLAC

Marc Hogan (coPI)

Lixin Ge

Cho Ng

Oleksiy Kononenko

Main topics:
- Optimization
- Visualization
- PWFA

LLNL

David Grote (coPI)

Main topics:
- Python interface

Consortium for accelerator modeling provides the foundations for community software

Consortium for
Advanced
Modeling of
Particles
Accelerators

CAMPA

BLAST (Warp, IMPACT, BB3D, FBPIC, PICSAR, Posinst)

ACE3P (Omega3P, S3P, Track3P, T3P, PIC3P, TEM3P)

SYNERGIA (space-charge, wakes, e-cloud, beam-beam…)

PICKSC (Osiris, QuickPIC, UPIC, UPIC-EMMA, Oshun)

Points of contact:
- **LBNL:** J.-L. Vay
- **SLAC:** C.-K. Ng
- **FNAL:** J. Amundson
- **UCLA:** W. Mori

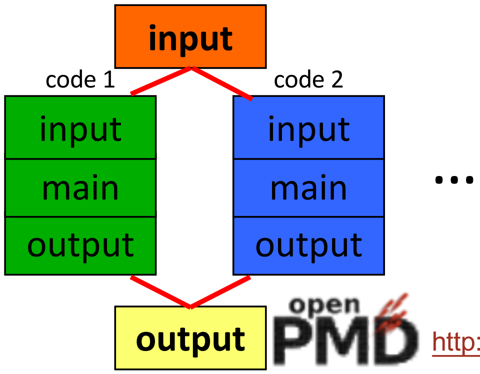
Activities:

- Coordination/integration of codes & modules, user interfaces and data formats.
- Maintenance, dissemination, support & training.
- High Performance Computing (not covered by SciDAC/ECP).

Common input/output standards to ease usage of multiple codes

- Currently, each code has own input script & output format

  ➔ user needs 1 input script/code & different data reader or software



http://www.openpmd.org

Bridge codes to enable:

- **unified** input/output interface
- **separation** of description/resolution/analysis

- In the process of defining standard for common input

  ➔ translate to individual code "language"

  - **PICMI**: Particle-In-Cell Modeling Interface
  - **AMI**: Accelerator Modeling Interface (aim to compatibility with MAD8/MAD-X)

OpenPMD: a common data standard for particles & meshes

Initiated and led by Axel Huebl (HZDR, Germany)

Common output data standard

Adopted by several PIC codes use HDF5:

- Warp
- PIConGPU
- FBPIC

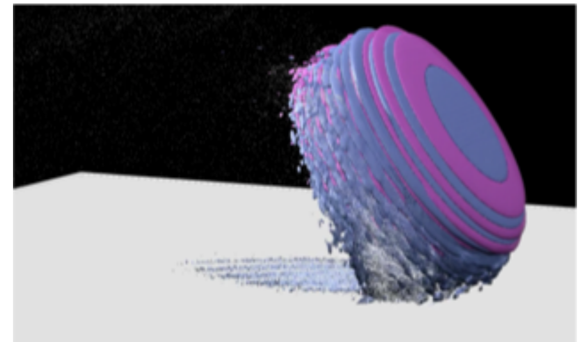
Fully open-source
Hosted on Github: https://github.com/openPMD

Implementation in progress in a number of other codes (QuickPIC, …).

C++ & FORTRAN reader/writer in development.

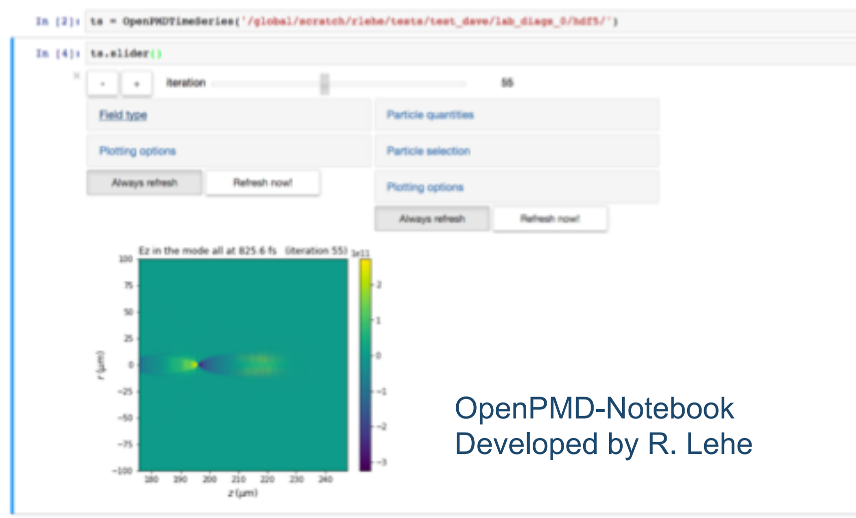
Accelerator extension in development.

Open-source plugins for visualization with Matplotlib, Visit, yt



3D viz with VisIt
Simulation by G. Blaclard
with Warp+PICSAR

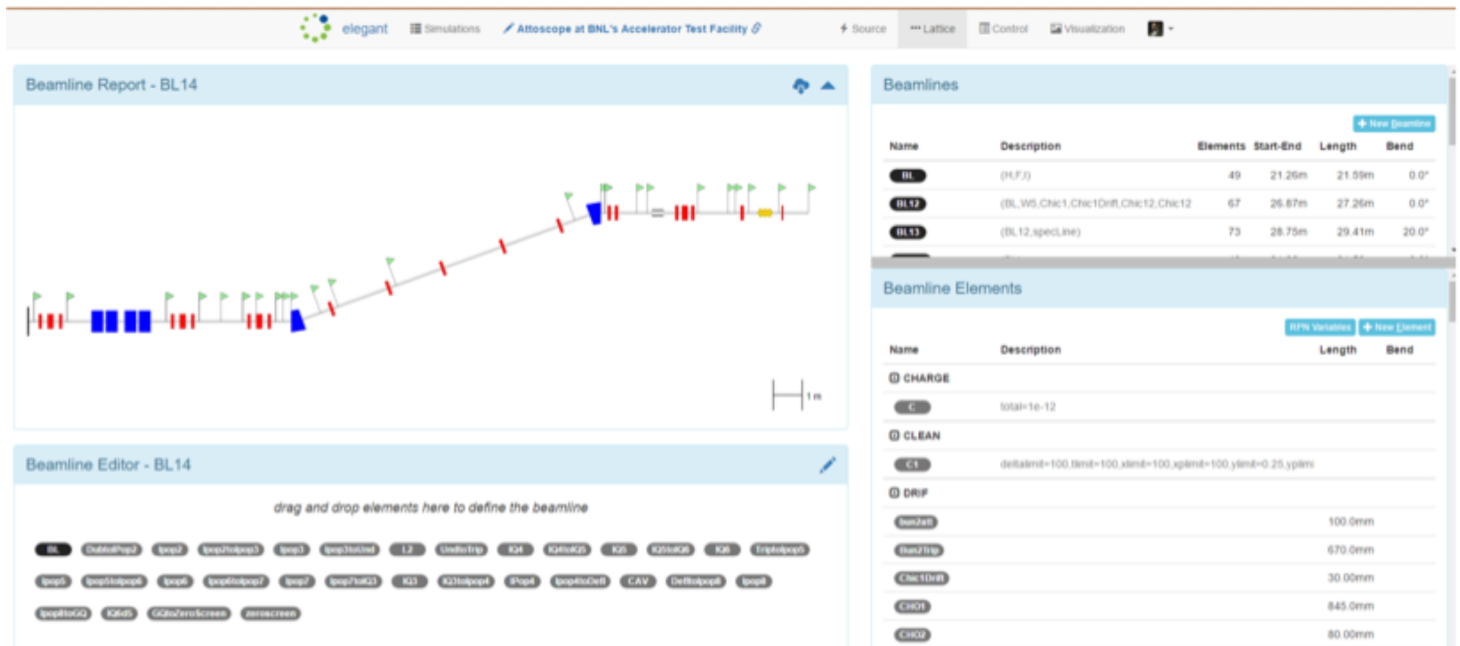
Open-source tools for interactive analysis in Jupyter



OpenPMD-Notebook
Developed by R. Lehe

Radiasoft Sirepo: a cloud computing framework solution

- Open source, https://github.com/radiasoft/sirepo
- Freely available in open beta, https://sirepo.com
- Growing number of codes
  - X-ray optics: SRW, Shadow
  - Particle accelerators:
    - **Elegant**
    - **Warp (special cases)**
    - **more on the way**
- Growing number of users
  - independent servers at
    - **BNL/NSLS-II**
    - **LBNL/ALS**
    - **PSI/ETH Zurich**
  - about 100 users visit the open beta site



Summary

- Computer modeling can play a key role in the development of more compact & cheaper accelerators

- Increasing complexity of computer architectures and codes calls for collaborations

- Efforts are underway for non-disruptive solutions toward increased collaborative code developments

BLAST Workshop 2018 (7-9 May, LBNL, Berkeley, California, US)

7-9 May 2018
59
US/Pacific timezone

Workshop informations: conferences.lbl.gov/e/BLAST-2018

- Overview
- BLAST
- Timetable
- Contribution List
- Author List
- Registration

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The Accelerator Modeling Program at Lawrence Berkeley National Laboratory is pleased to announce the first workshop on the Berkeley Lab Accelerator Simulation Toolkit (blast.lbl.gov), to be held on May 7-9, 2018.

- Intro to codes (IMPACT, WARP, BB3D, CSR3D, FBPIC, POSINST).
- Hands-on sessions
- Flash talks from users on experience with codes
- Ample time for group and one-on-one discussions

Goals:

- Foster a community of users & developers of BLAST codes
- Share users experiences & highlights
- Introduce new users to code & existing users to latest features
- Discuss ideas & needs from the users community
- Plan & prioritize future code features & developments

The venue will be Shyh Wang Hall (Building 59), home of the U.S. Department of Energy National Energy Research Supercomputer Center (nersc.gov) at Lawrence Berkeley National Laboratory, overlooking San Francisco Bay.

A visit of the supercomputer rooms is scheduled.