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

Self-Consistent Simulations of Beam and Plasma Systems
Steven M. Lund, Jean-Luc Vay, Rémi Lehe and Daniel Winklehner
Colorado State U., Ft. Collins, CO, 13-17 June, 2016

A5. Collaborations

Jean-Luc Vay, Rémi Lehe
Lawrence Berkeley National Laboratory

Particle accelerators are essential tools in modern life that power scientific discovery, cure cancer, secure our borders, and help create a wide range of products

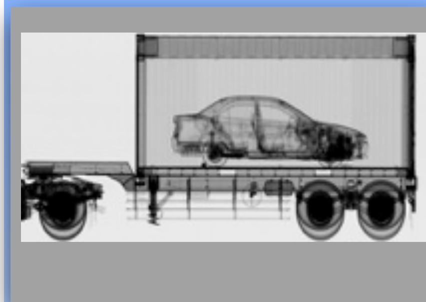
Medicine

- ~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

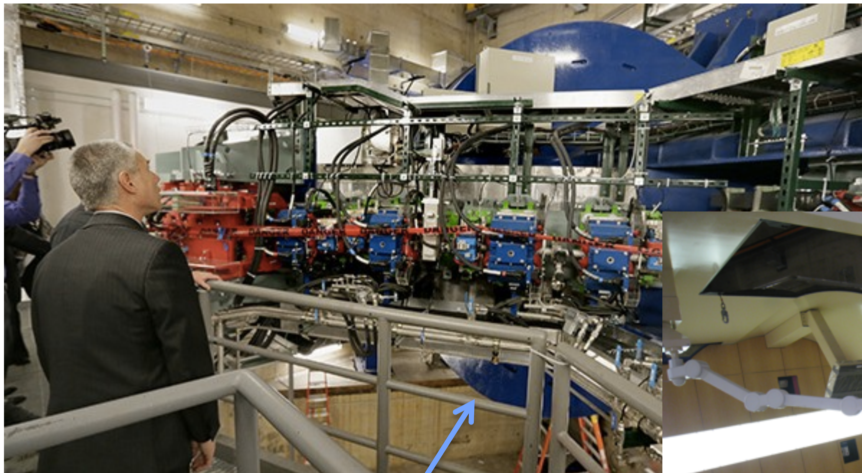
Discovery Science

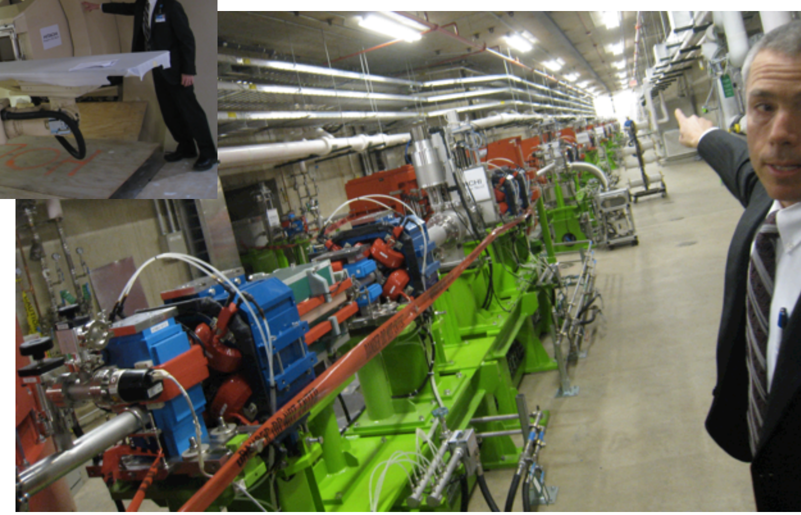
- ~30% of Nobel Prizes in Physics since 1939 enabled by accelerators
- 4 of last 14 Nobel Prizes in Chemistry for research utilizing accelerator facilities

There are 30,000 Particle Accelerators Making an Impact on Our Lives

But often too big and expensive!

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





New Rochester Mayo Clinic
Proton Therapy Center

- 4 chambers
- $188M

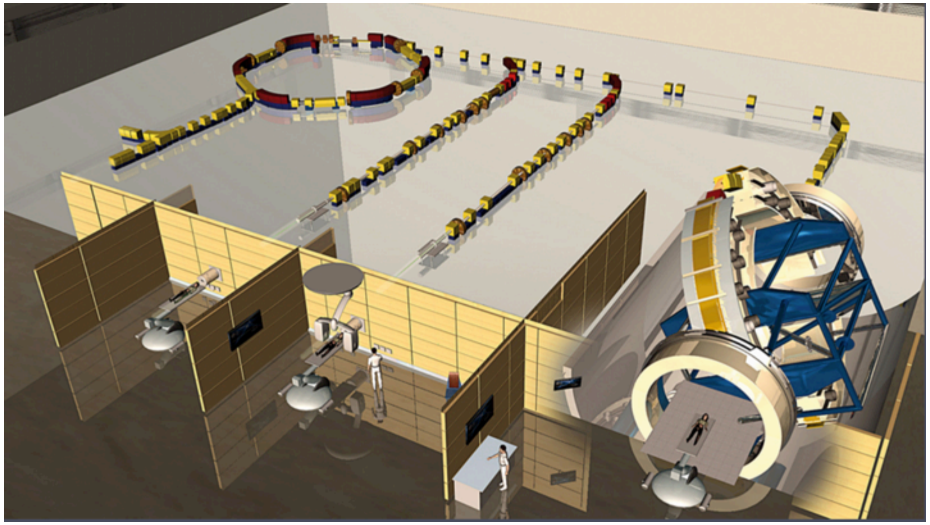
120-ton gantry directs proton beam to appropriate spot on patient by rotating around a three-story chamber.

http://finance-commerce.com/2014/03/status-report-mayo-proton-therapy-facility/#ixzz43DJgnIIA
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

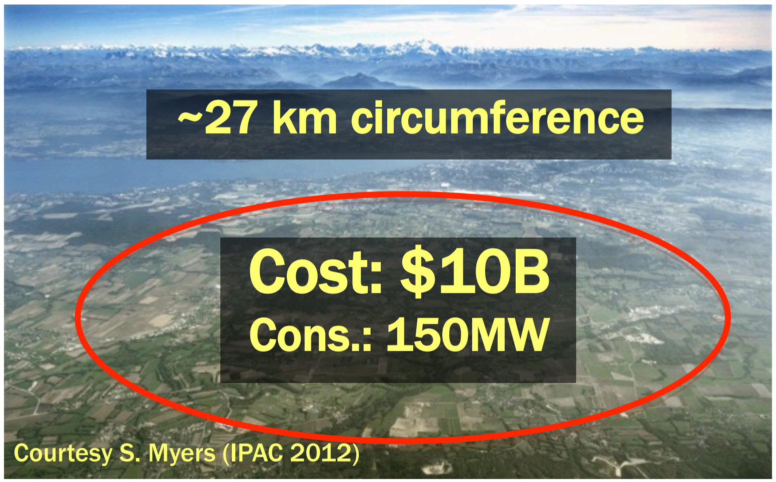


670-ton gantry
~1/10 Eiffel Tower

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



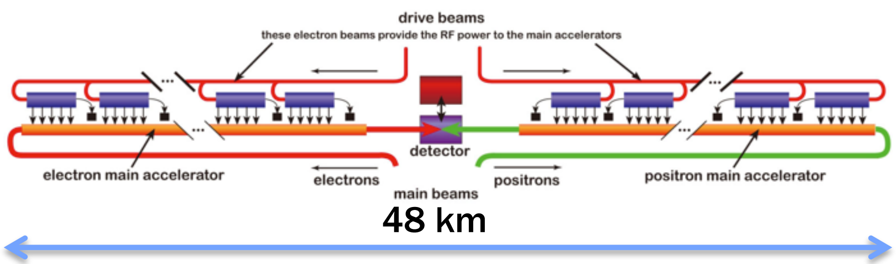
Future colliders?

ILC

Cost: $8B-$20B?

Cons.: 230MW

CLIC



Cost: $?B

Cons.: 415MW

FCC

nature International weekly journal of science

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!

Next generation of accelerators *needs* next generation of modeling tools

Our vision

Fast – *runs in seconds to minutes*

Hi-Fi – *full & accurate physics*

Link – *integrated ecosystem*

Real-time virtual prototyping of entire accelerator

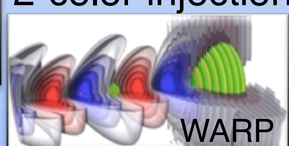
with intuitive interface, dissemination & user support.

Simulations take too long!

BELLA

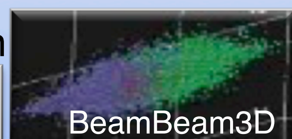
~1 week

2-color injection



~3 days

Beam-beam LHC

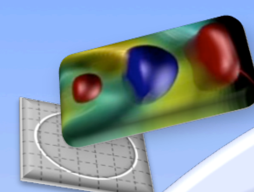


~1 day

Need to speedup by $\times 10^n$

→

Combine best algorithms

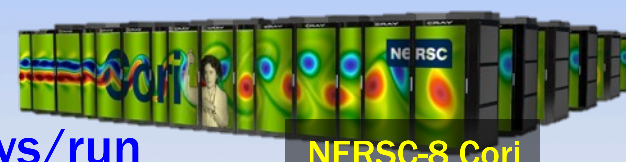


Speed

2016 Hours-days/run

2025 Min./run

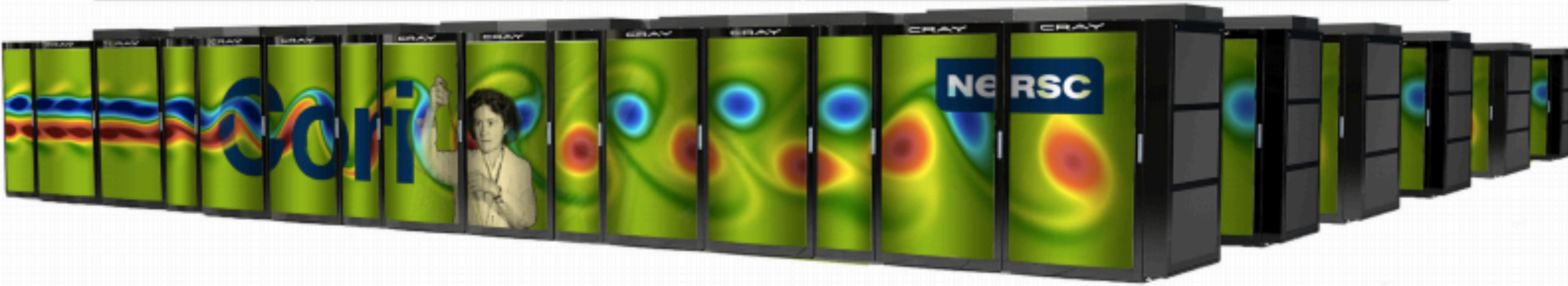
Port codes to fastest hardware



NERSC systems to reach 1 ExaFlops by 2024

NERSC Systems Timeline

2007/2009	NERSC-5	Franklin	Cray XT4	102/352 TF
2010	NERSC-6	Hopper	Cray XE6	1.28 PF
2014	NERSC-7	Edison	Cray XC30	2.57 PF
2016	NERSC-8	Cori	Cray XC	30 PF
2020	NERSC-9			100PF-300PF
2024	NERSC-10			1EF
2028	NERSC-11			5-10EF



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Computing Sciences Area

Courtesy Sudip Dosanjh, IXPUG 2015

Next DOE supercomputers based on manycore and GPUs

ASCR Computing Upgrades At a Glance

System attributes	NERSC Now	OLCF Now	ALCF Now	NERSC Upgrade	OLCF Upgrade	ALCF Upgrades	
Name Planned Installation	Edison	TITAN	MIRA	Cori 2016	Summit 2017-2018	Theta 2016	Aurora 2018-2019
System peak (PF)	2.6	27	10	> 30	150	>8.5	180
Peak Power (MW)	2	9	4.8	< 3.7	10	1.7	13
Total system memory	357 TB	710TB	768TB	~1 PB DDR4 + High Bandwidth Memory (HBM) +1.5PB persistent memory	> 1.74 PB DDR4 + HBM + 2.8 PB persistent memory	>676 TB DDR4 + High Bandwidth Memory (HBM)	> 7 PB High Bandwidth On-Package Memory Local Memory and Persistent Memory
Node performance (TF)	0.460	1.452	0.204	> 3	> 40	> 3	> 17 times Mira
Node processors	Intel Ivy Bridge	AMD Opteron Nvidia Kepler	64-bit PowerPC A2	Intel Knights Landing many core CPUs Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Voltas GPUS	Intel Knights Landing Xeon Phi many core CPUs	Knights Hill Xeon Phi many core CPUs
System size (nodes)	5,600 nodes	18,688 nodes	49,152	9,300 nodes 1,900 nodes in data partition	~3,500 nodes	>3,200 nodes	>50,000 nodes
System Interconnect	Aries	Gemini	5D Torus	Aries	Dual Rail EDR-IB	Aries	2nd Generation Intel Omni-Path Architecture
File System	7.6 PB 168 GB/s, Lustre®	32 PB 1 TB/s, Lustre®	26 PB 300 GB/s GPFS™	28 PB 744 GB/s Lustre®	120 PB 1 TB/s GPFS™	10PB, 210 GB/s Lustre initial	150 PB 1 TB/s Lustre®

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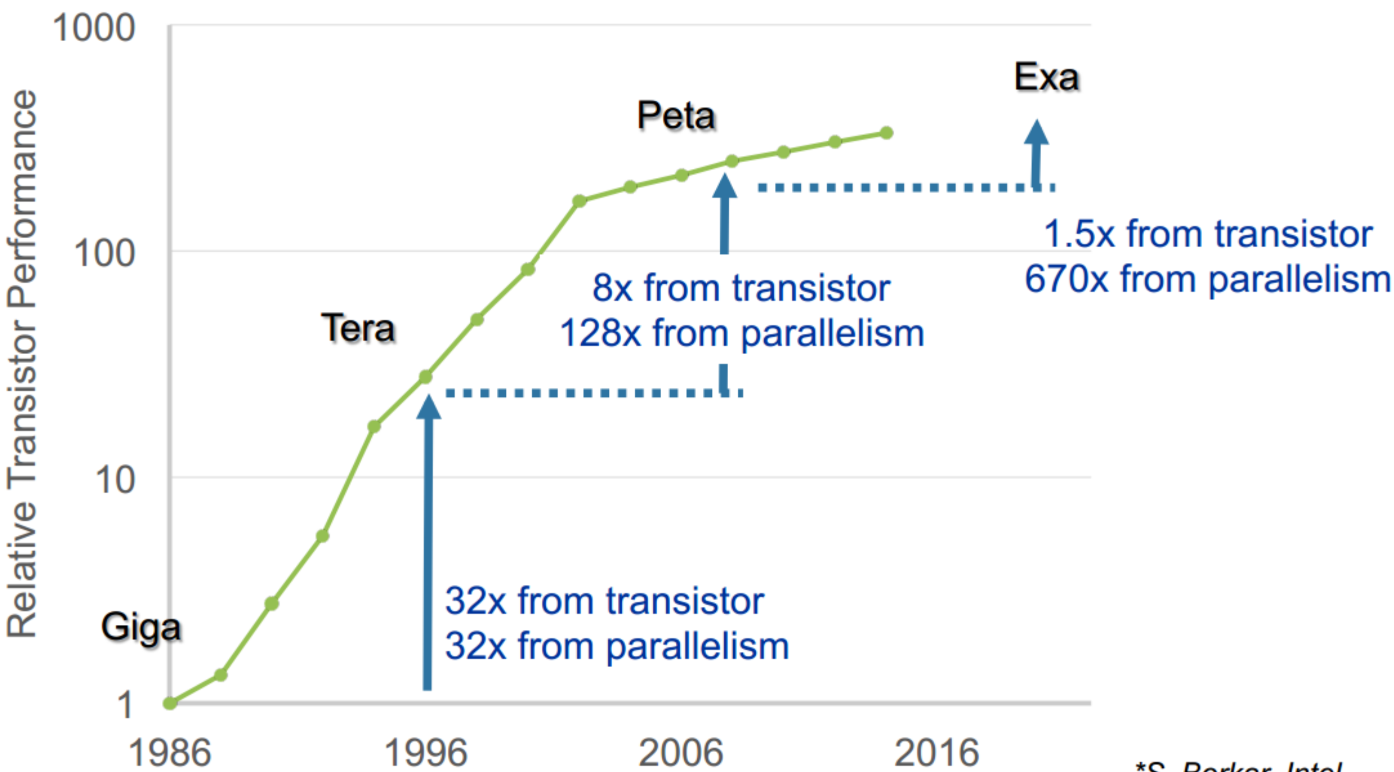
Exascale Requirements Gathering -- FES 1/27/2016 4

Courtesy Barbar Helland, FES Exascale Review, 2016

Cannot wait for speedup from transistors anymore

From Giga to Exa, via Tera & Peta*



**S. Borkar, Intel*

Performance from parallelism

Basic Energy Sciences Advisory Committee Briefing 2.11.2016

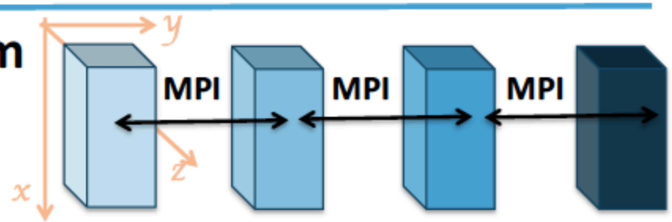
13 Exascale Computing Project

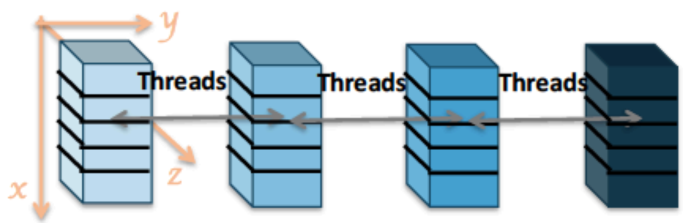
EXASCALE COMPUTING PROJECT

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





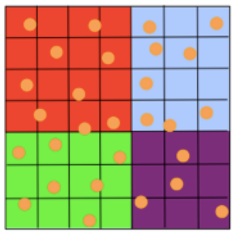

```
|--> DO I = 1, N
|        R(I) = B(I) + A(I)
|--> ENDDO
```

- 12 -

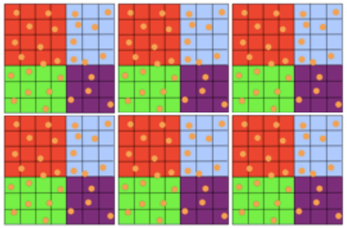
Courtesy Katherine Riley, FES Exascale Review, 2016

Particle-In-Cell

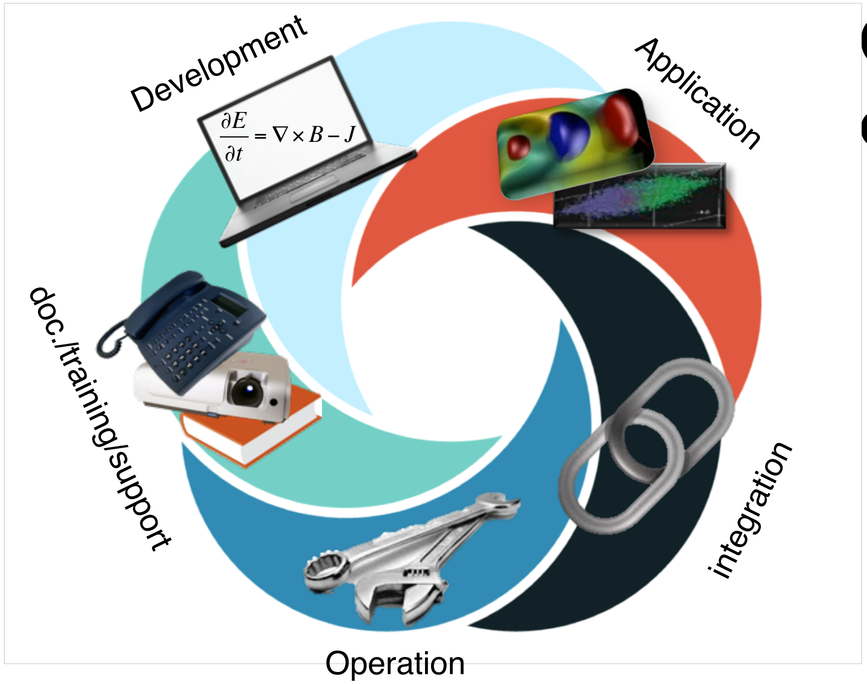
Domain decomposition



Domain decomposition + tiling



Supporting community calls for large efforts



Community HPC hardware needs community HPC software

- **needs:** development + application + integration intra/inter community + operation + doc./training/support

Any overlap in 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

Need of solution for non-disruptive integration

Significant investments into existing pool of codes:

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

Challenges:

Technical

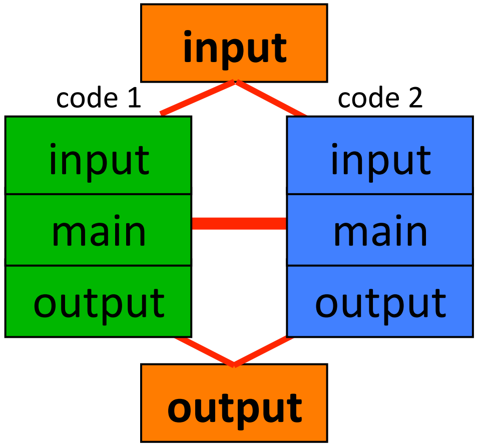
- programming languages
- data formats, parallelism
- code architectures
- open vs proprietary sources
- keep creativity

Human

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

Mitigation of difficulties through adiabatic transition

Existing set of separate codes ➔ **ecosystem** of **interconnected codes**



…

Bridge codes to enable:

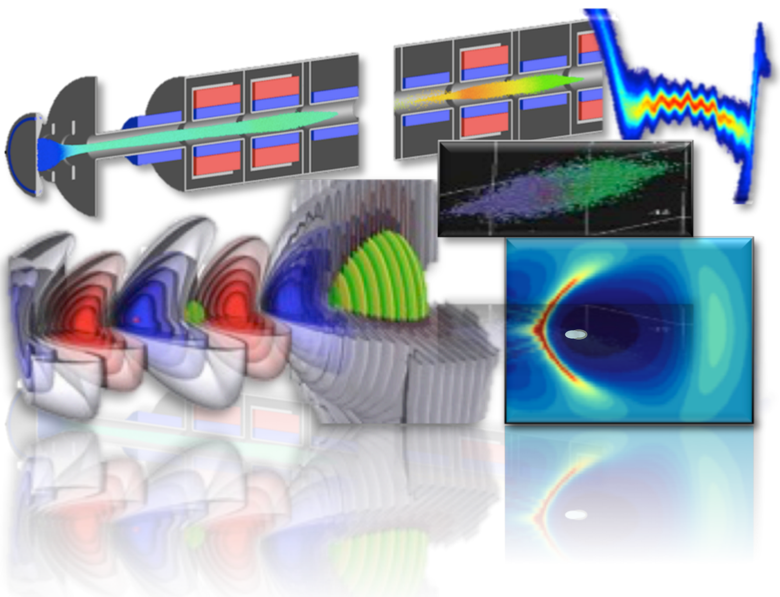
- **common** user input/output interface
- **sharing** of functionalities
- **collaborative** development of common units

Common data format enables separation between user I/O interfaces and "kernels".

Assess of kernels as Python modules enables tighter coupling.

Berkeley Lab Accelerator Simulation Toolkit

BLAST
BERKELEY LAB ACCELERATOR SIMULATION TOOLKIT



Suite of state-of-the-art codes:

- BEAMBEAM3D, IMPACT, WARP/PICSAR, INF&RNO, POSINST, FBPIC, ...

Large set of physics & components:

- beams, plasmas, lasers, structures...
- linacs, rings, injectors, traps, ...

Supporting many accelerators:

- across DOE (HEP, BES, NP, FES, DNN) and beyond (CERN, DESY, KEK, ...).

http://blast.lbl.gov

Emerging national consortium for accelerator modeling

x

Consortium for
Advanced
Modeling of
Particle
Accelerators

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

CAMPA

BERKELEY LAB
BLAST
(Warp, IMPACT, BeamBeam3D, Posinst)

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

Fermilab
SYNERGIA
(space-charge, wakes, e-cloud, beam-beam...)

Activities:
- High Performance Computing (beyond SciDAC),
- coordination/integration of codes/modules, user interfaces, data formats, ...
- dissemination, support & training.

The tools of collaboration: git, Github, Bitbucket

x

Github (github.com) and Bitbucket (bitbucket.org):

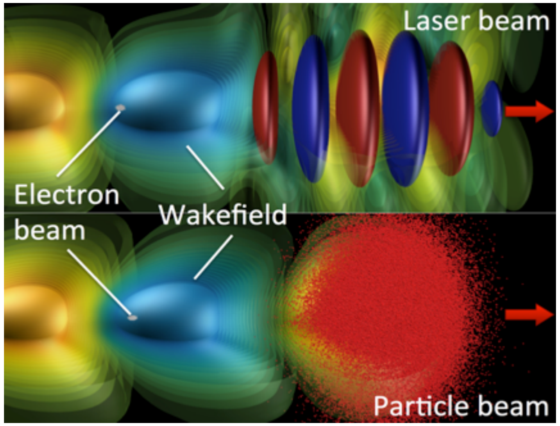
- Websites that allow to **store code**, and make it **available for download**
- Contain many tools for developers to communicate and discuss the code

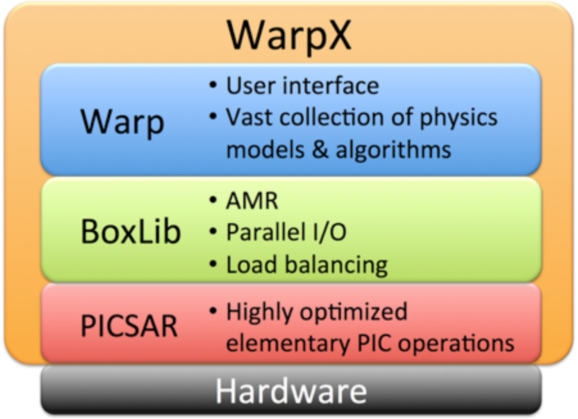
git:

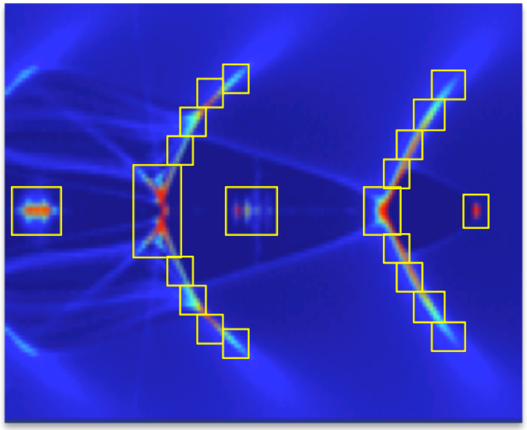
- **Download/upload** code to the websites like Github or Bitbucket
  - git clone (+URL): download code
  - git pull: update code (get latest changes from website)
  - git push: upload local changes to website
- Enables **version control**
  - git commit: save a snapshot of the code

Git tutorial: https://www.atlassian.com/git/tutorials/

We are developing the next generation of Warp







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 best algorithms (boosted frame+spectral+AMR+…) via coupling of Warp+BoxLib+PICSAR and port to emerging architectures (Xeon Phi, GPU).

PICSAR: highly optimized elementary PIC operations (based on Warp kernel).

BoxLib: advanced adaptive mesh refinement library.

Proposal submitted for collaboration LBNL+SLAC+LLNL.

PICSAR and Boxlib libraries will be available for other codes.

Developing common modules/data format is beneficial

- **PICSAR (Particle-In-Cell Scalable Application Resource):**
  - Collection of PIC kernel subroutines (current deposition, field gather, field solve, particle pusher, …)
  - Toward collaborative development of multi-level parallel implementations (vectorization+OpenMP+MPI+GPU+…)
  - For testing, comparing, distributing production-level PIC functionalities
  - To be available with open source license to wider community soon

- **OpenPMD (A. Huebl et al., doi: 10.5281/zenodo.3362):**
  - a common I/O format for simulations with particles and meshes
  - standardized layout of data in file (using hdf5, netcdf, ADIOS, ..)
  - for easy comparisons between codes, common visualization tools
  - OpenPMD Viewer based on IPython+Matplotlib available, Visit reader in dev.
  - implemented in Warp, PIConGPU, FBPIC, …
  - More at https://github.com/openPMD at http://www.openpmd.org

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