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State of the art of high intensity simulation codes: new algorithms and methods for rings [1] - a personal and biased view

Andreas Adelmann, Accelerator Modelling and Advanced Simulation (AMAS)

26. August 2008 HB2008 - Nashville

[1] incl. Cyclotrons and FFAGs

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Thank you for all the material

G. Franchetti, F.W. Jones,
S. Machida, J.A. Holmes,
J. Qiang, A. Molodozhentsev,
R.D Ryne, J. Amundson,
M. Furman, D. Grothe,
I. Hofmann, C. Prior, S. Panagiotis, J.-L Vay,
F. Zimmermann, S. Cousineau and
F. Méot

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1. Physics Challenges i.e. Drivers for Method & Code Development
2. Overview of Received Contributions
   - Synergia
   - Orbit-ORNL
   - ORBIT-BNL
   - Simpsons
   - PTC/MADX & ORBIT-ORNL
   - Accsim
   - ML/IMPACT - MaryLie Impact
   - Warp
   - OPAL - Object Oriented Parallel Accelerator Library
3. **New** Development
4. Outlook

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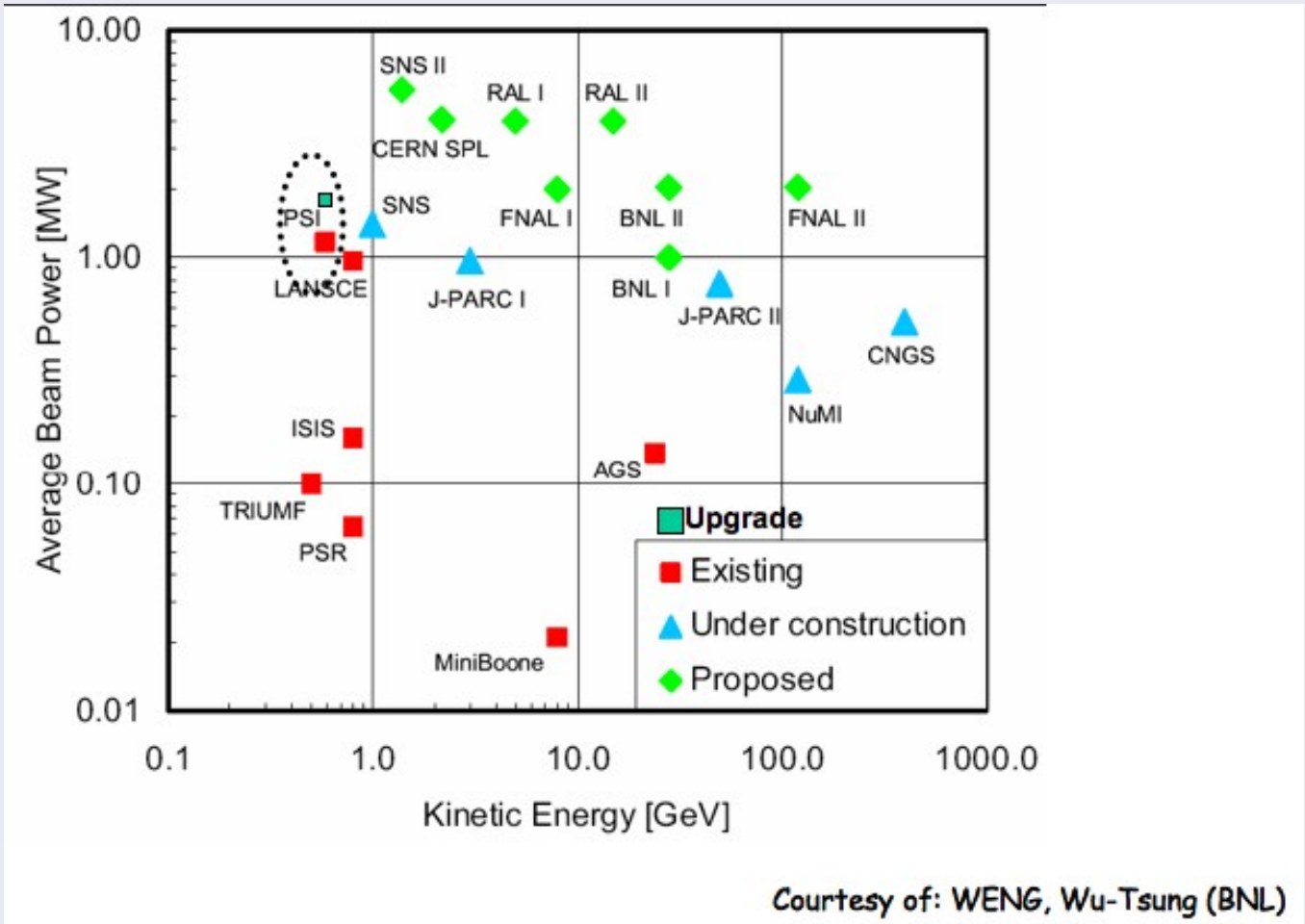
Physics Challenges: Drivers for Method & Code Development



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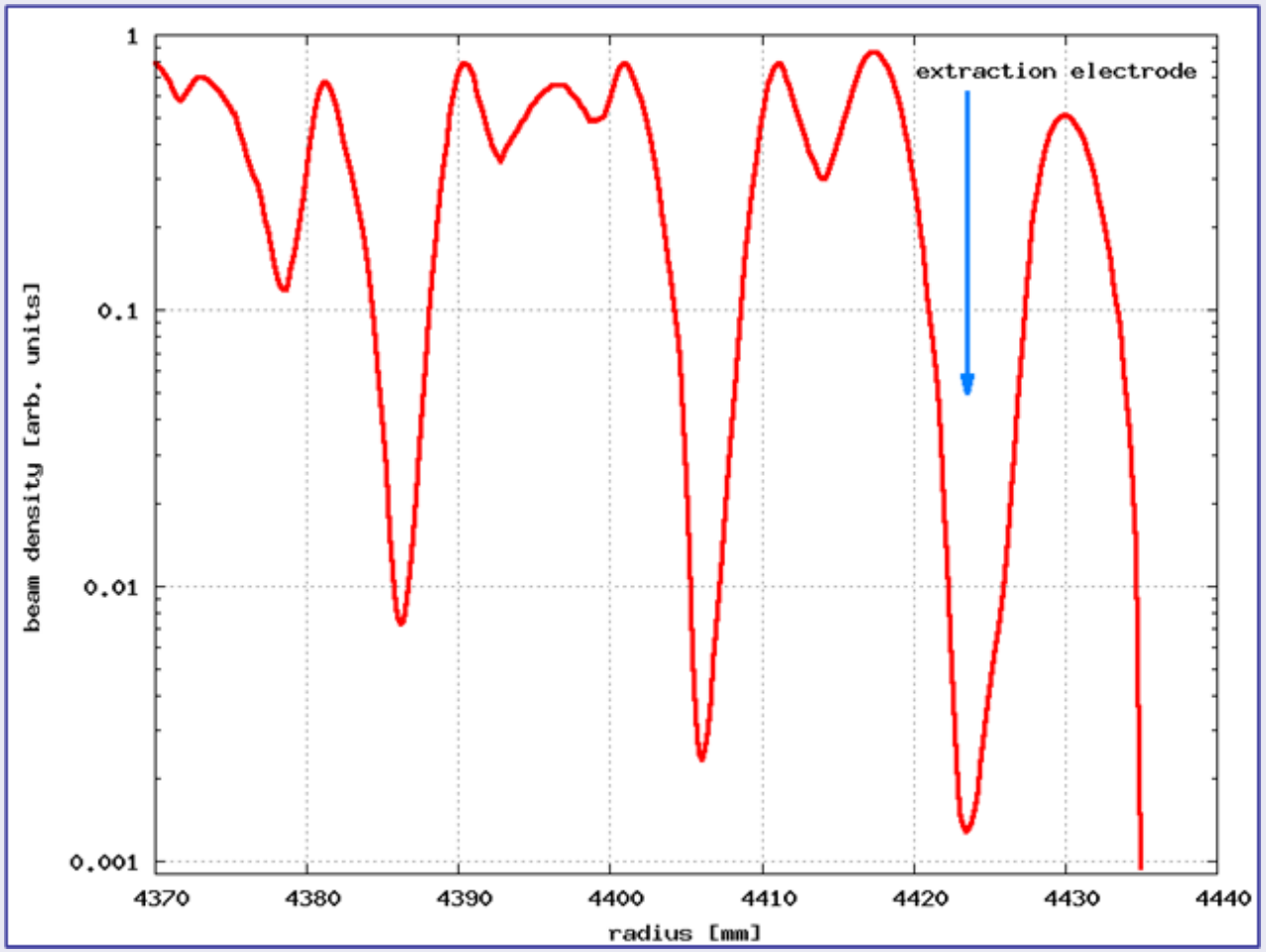
1.2 MW CW at extraction of the PSI Ring Cyclotron



courtesy of M. Sidel (PSI)

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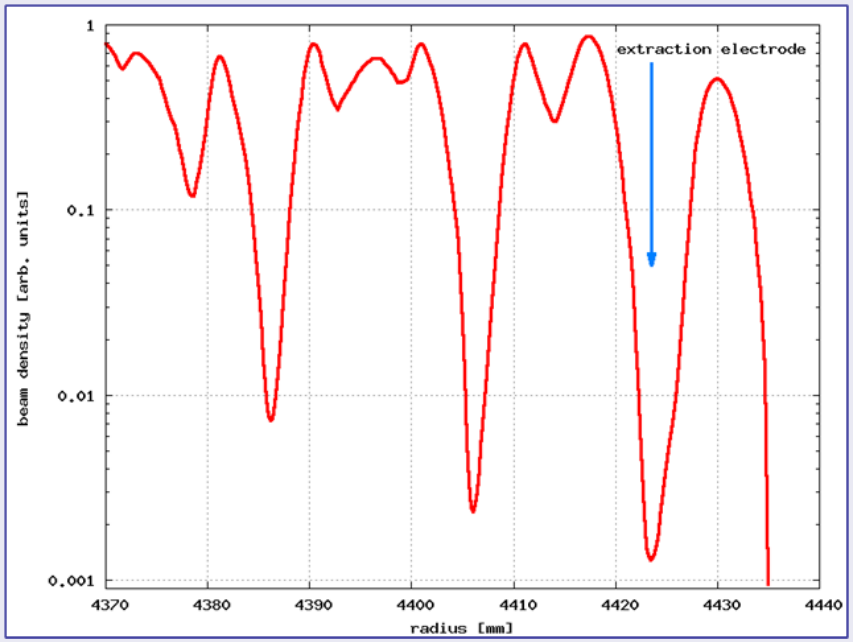

courtesy of M. Sidel (PSI)

In the MW- League

its all towards: Quantitative i.e. precise BD simulation

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Physics Goals - Important Issues Observed

J-PARC Main Ring: study combined effect of the machine imperfections and the collective space charge effects of the low energy beam in order to keep the particle losses below the acceptable level (450W@collimator and <0.5W/m around MR)

SNS: foil, collimator [EPAC08-TUPP042] & uncontrolled losses $\mathcal{O}(10^{-6})\ m^{-1}$

ECL: improve agreement w.t.r. measurements [LBNL CBP TN-387]

GSI/CERN: towards long term self consistent effects in space charge induced resonance trapping [ICAP06-MOA2IS03]

PSI Ring Cyclotron: neighboring turn simulations and towards comparison of beam profiles and simulations [WG-A, Thu 8:30: Jianjun Yang] & controlled and uncontrolled losses

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Overview of Received Contributions

Code	Author (et.al)	Space Charge	Dim	Parallel
Micromap	G. Franchetti	analyt.	2/3	no
Accsim	F.W. Jones	Hyb. FMM	2.5	no
Simpson	S. Machida	PIC	3	(yes)
Orbit	J.A. Holmes	PIC	3	yes
IMPACTx	J. Qiang	PIC	3	yes
PTC/Orbit	A. Molodozhentsev	PIC	3	yes
ML/IMPACT	R.D. Ryne	PIC	3	yes
Synergia2	J. Amundson	PIC	3	yes
OPAL	A. Adelmann	PIC	3	yes
Posinst	M. Furman	analyt. & e-cloud	2	no
Warp	D. Grothe	PIC & e-cloud	3	yes

Oberservation 1: clear trend towards 3D & parallel

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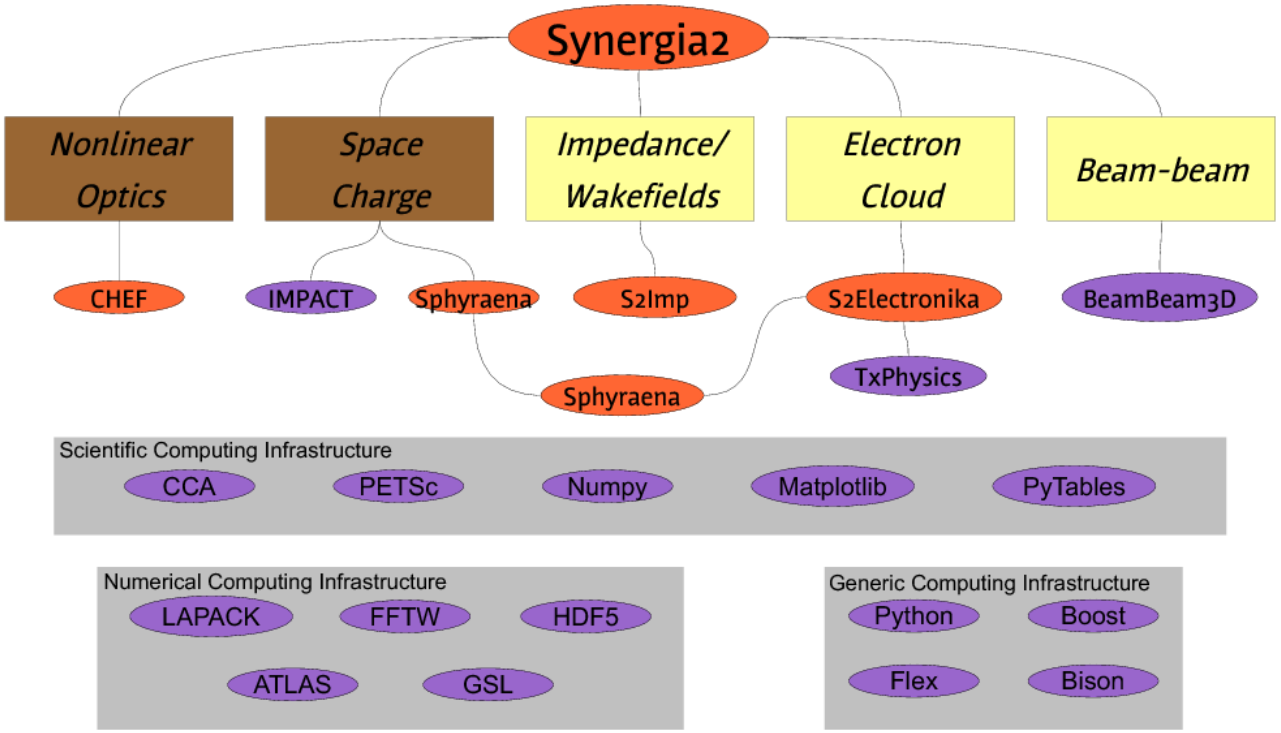
Oberservation 1: clear trend towards 3D & parallel

Synergia



Synergia2 framework development includes multiple advanced accelerator physics topics. Development is aided by relying on both internally- (orange) and externally- (magenta) developed state-of-the-art packages. New physics modules (yellow) are currently under development.

PTC/MADX & ORBIT-ORNL

'Virtual' accelerator code

Polymorphic Tracking Code (PTC)
Etienne Forest (KEK)

Module structure

+ Splitting of magnets

Symplectic 6D Tracker

Taylor Map & DA analysis

Normal Form analysis

Acceleration

TOSCA field data

Fringe field of magnets

Misalignment

Many other things ... on demand

Lattice analysis
Single particle dynamics

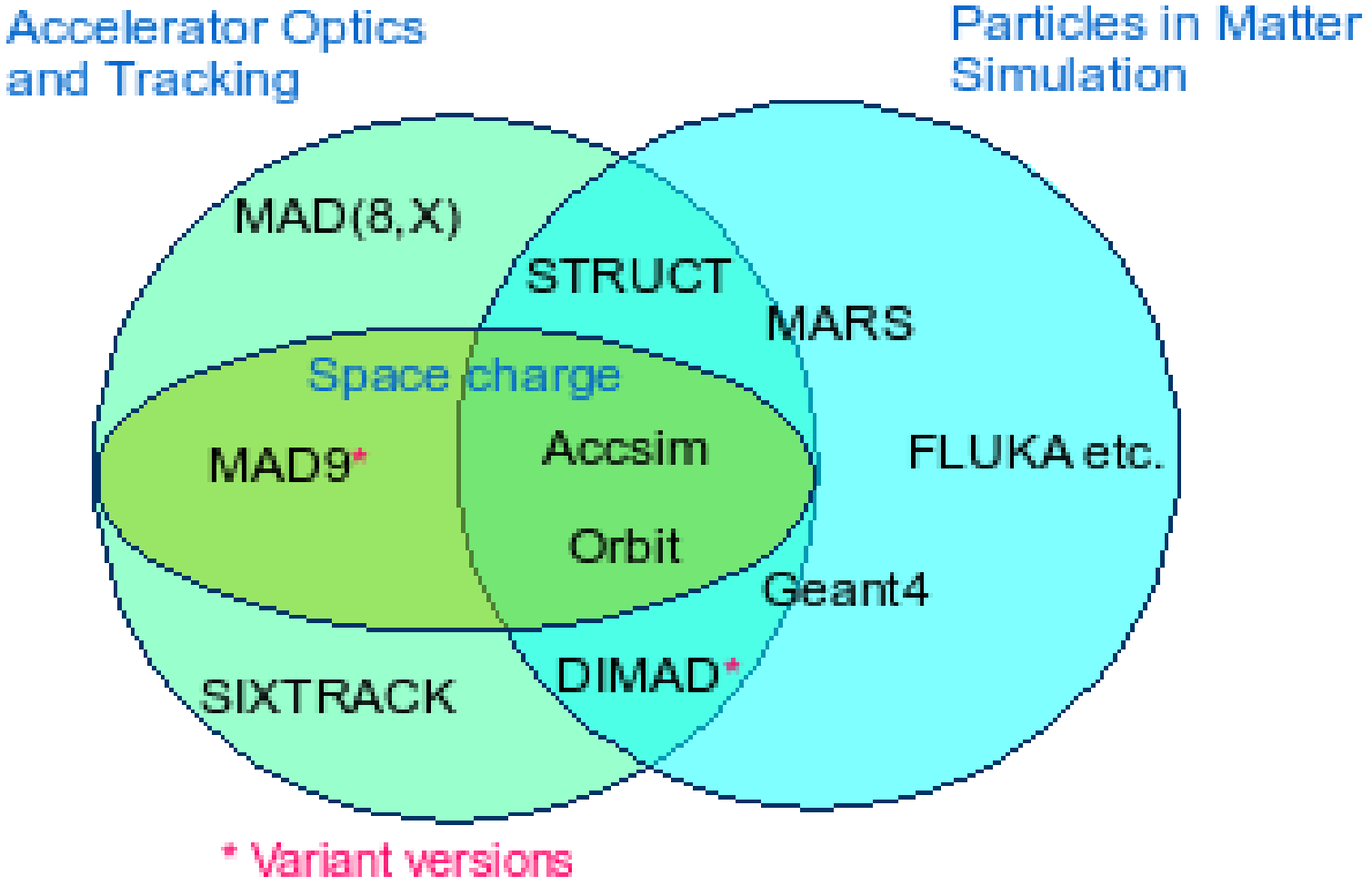
Multi particle dynamics...
Collective effects

PTC UNIVERSE
F90 compiler

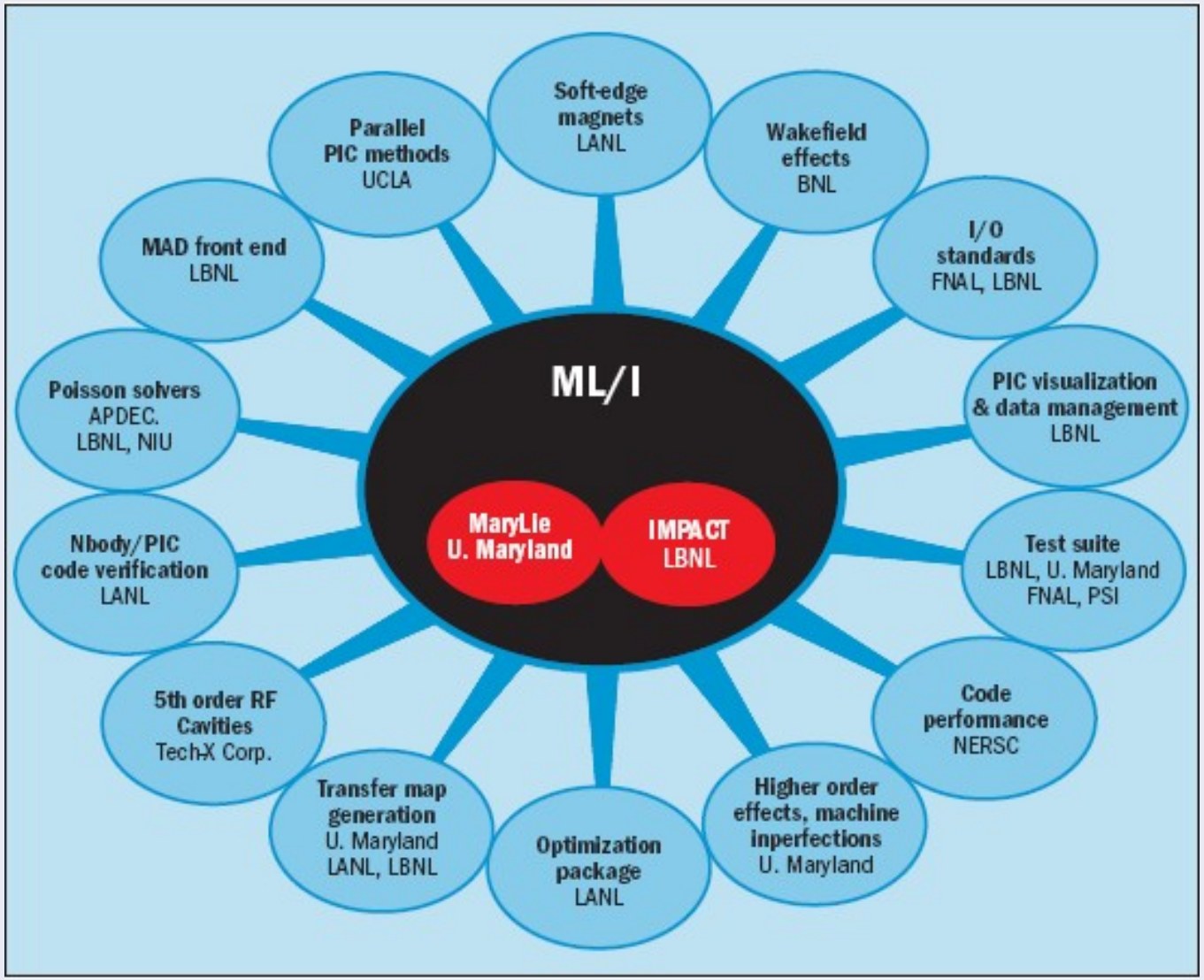
ORBIT UNIVERSE
GCC compiler

What we need in is some "GLUEING" Bridge between PTC and ORBIT acceptable for Multi Processor simulations (KEK Super Computer) !

Accsim


Accelerator Optics and Tracking
Particles in Matter Simulation
MAD(8,X)
STRUCT
MARS
Space charge
MAD9*
Accsim
FLUKA etc.
Orbit
Geant4
SIXTRACK
DIMAD*
* Variant versions

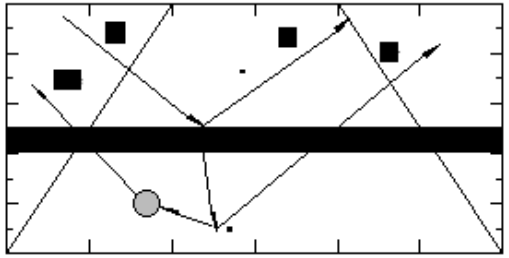
ML/IMPACT - MaryLie Impact

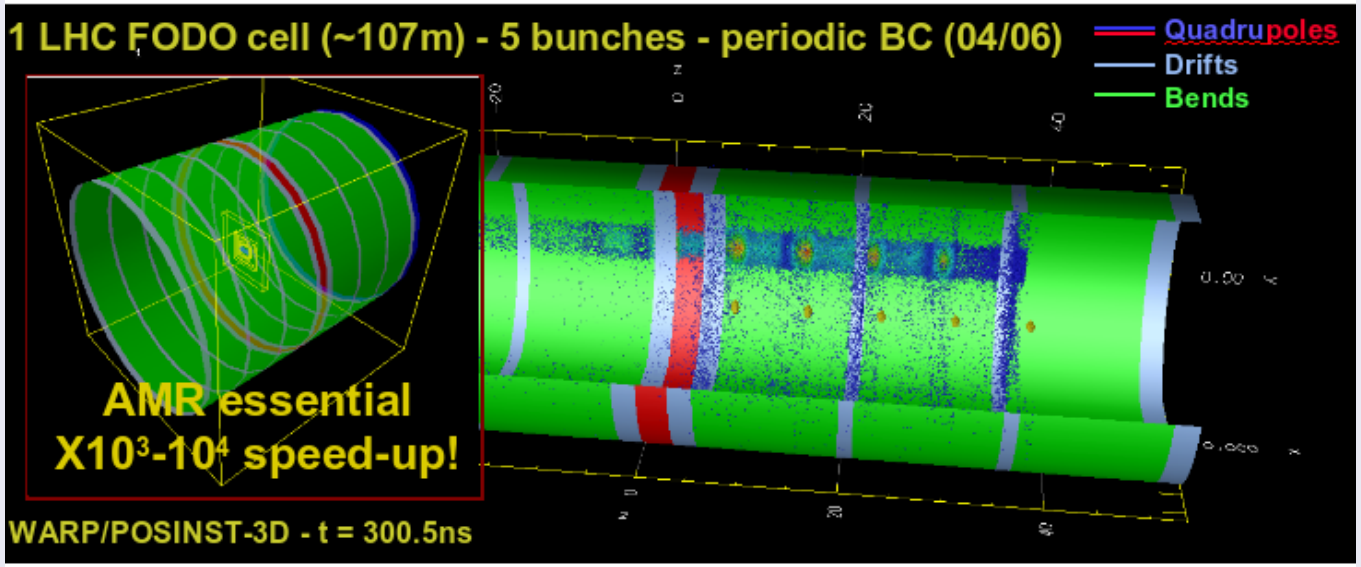


Warp

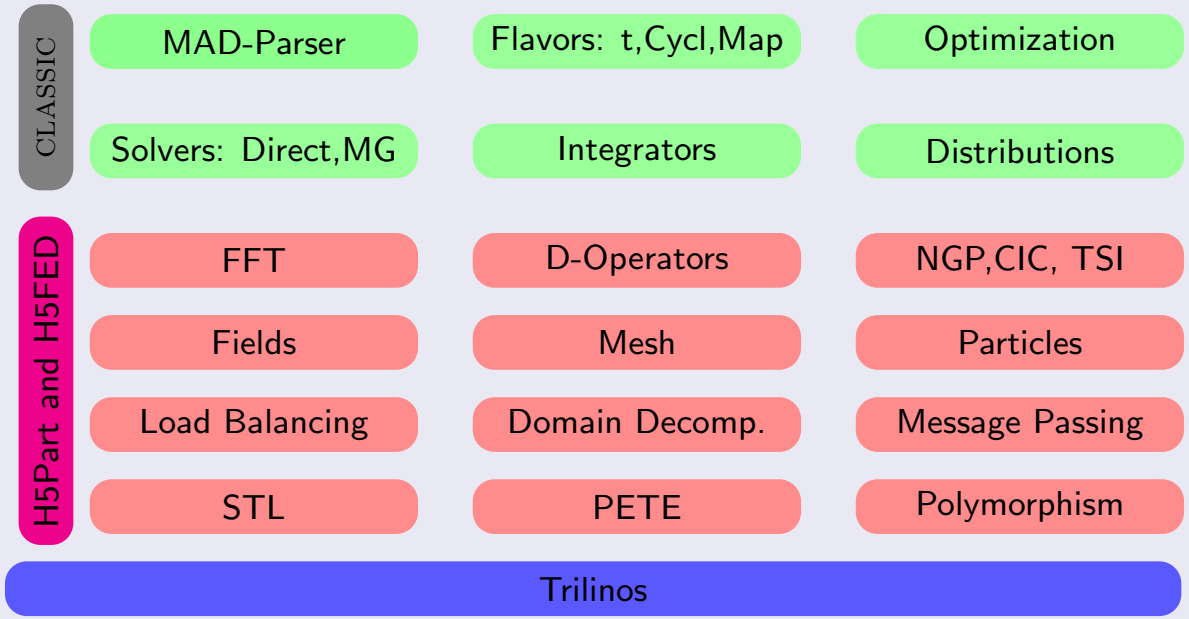
Proof of principle simulation of beam interaction with e-cloud in LHC

Warp uses the phenomenological model from Furman and Pivi for the modeling of secondary electrons.

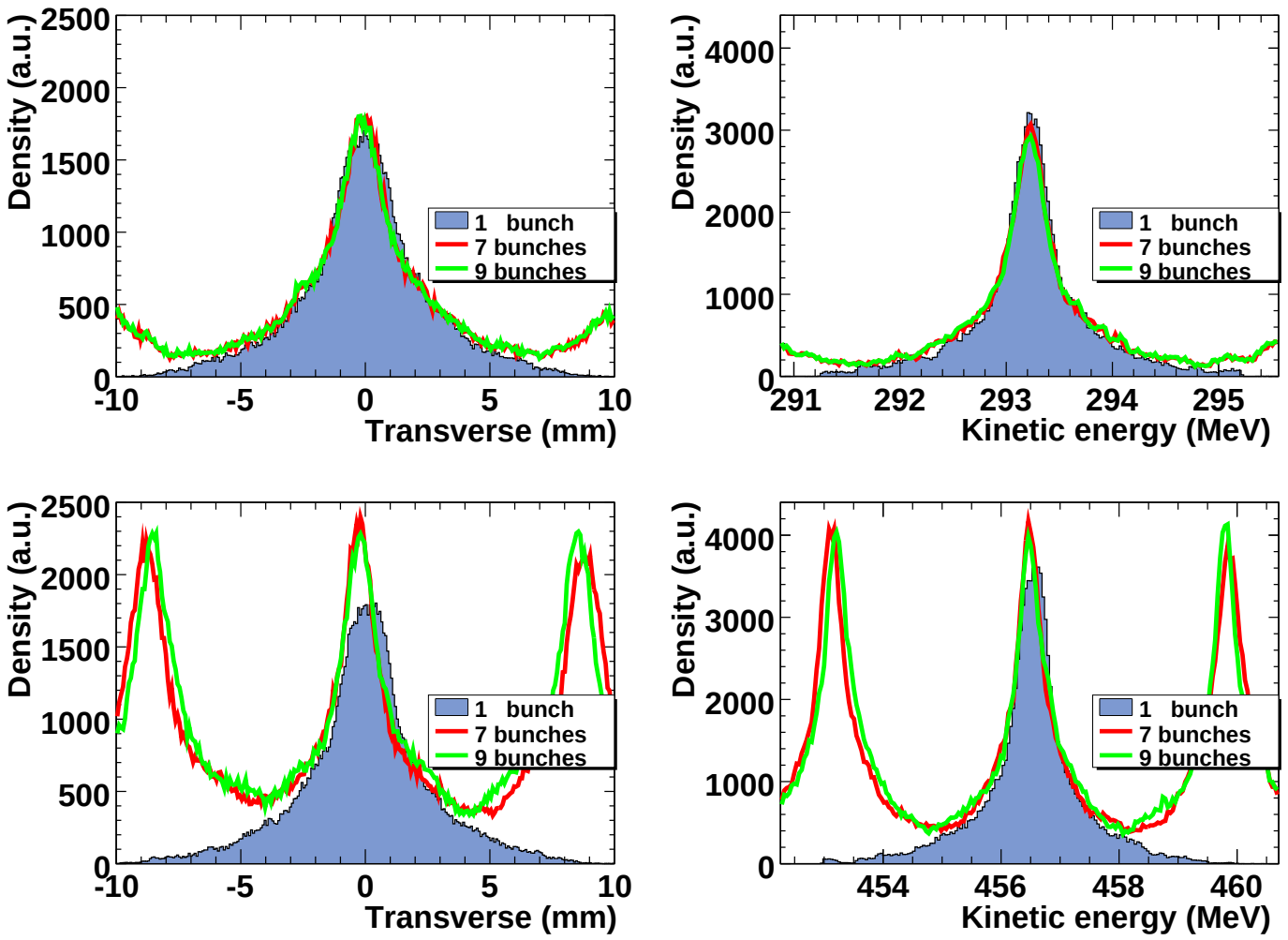




OPAL Object Oriented Parallel Accelerator Library



- OPAL is built from the ground up as a parallel application exemplifying the fact that HPC (High Performance Computing) is the third leg of science, complementing theory and the experiment
- OPAL runs on your laptop as well as on the largest HPC clusters
- OPAL uses the MAD language with extensions
- $\mathcal{O}$(real number of protons) in our Cyclotrons incl. neighboring turns.



[WG-A, Thu 8:30: Jianjun Yang]

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Oberservation 2:

- trend towards complex/multiphysics codes
  - high resolution
  - large amount of date
- *community effort* - loosely coupled set of individuals
- usage of external frameworks and libraries (standalone is out!)
- no SC FFAG code but checkout: [WG-A, Thu 9.10, D. Abell]

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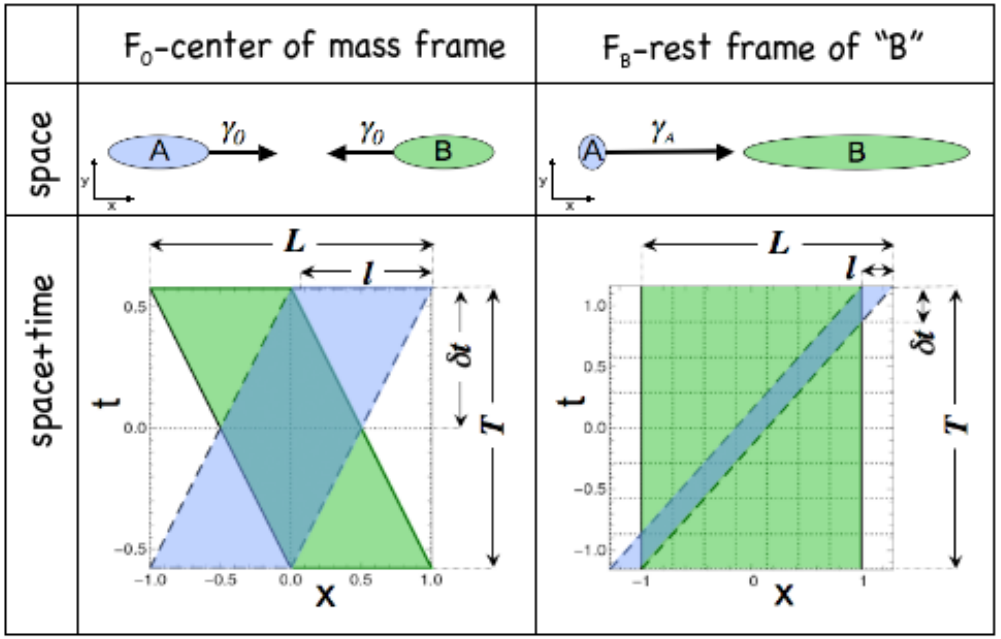
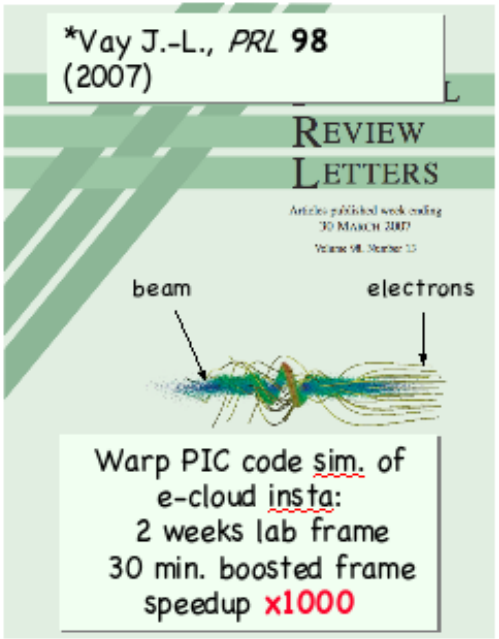
New Development

- Physics inside: tremendous increase in the efficiency of the simulation
  - J.-L. Vay - Warp
- 3D semi-analytic space charge model (ellipsoidal symmetry)
  - G. Franchetti et.al - MICROMAP
- Iterative Methods and exact Geometry
  - J. Amundson et.al - Synergia
  - A. Adelmann et.al - OPAL
- High Performance Computing (& CS)
  - go parallel - or go massively parallel: pain or fun?

Physics inside: increase in the efficiency of the simulation

First-principle (PIC) sim. of beam interacting with e-cloud is orders of magnitude faster in a Lorentz boosted frame*





- Uses novel particle pusher* (Boris pusher fails with relativistic species),
- if resolving beam betatron oscillations: runtime similar to "quasistatic" codes (Headtail, Quickpic) but without requiring quasistatic approximation,
- ability to push beam particles with maps being added to allow time steps > betatron period

Vay J.-L., *Phys. Plasmas* **15 (2008)

3D semi-analytic space charge model (ellipsoidal symmetry)

PRST-AB-**6**, 124201 *Space Charge and octupole driven resonance trapping observed at the CERN PS* : "The failure of 2D simulation to describe ...."

Assume ellipsoidal symmetry: $\rho(t) = \frac{Q}{4\pi abc} n(t)$ with $t = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}$ and n proper normalized:

$$E_x = \frac{Qx}{2} \int_0^\infty \frac{n(T)ds}{(a^2+s)^{2/3}(b^2+s)^{1/3}(c^2+s)^{1/3}} \tag{1}$$

$$T = \frac{x^2}{a^2+s} + \frac{y^2}{b^2+s} + \frac{z^2}{c^2+s}. \tag{2}$$

Fine for constant 3D focusing!

3D semi-analytic space charge model (ellipsoidal symmetry)

Take the long bunch Ansatz for AG focussing:

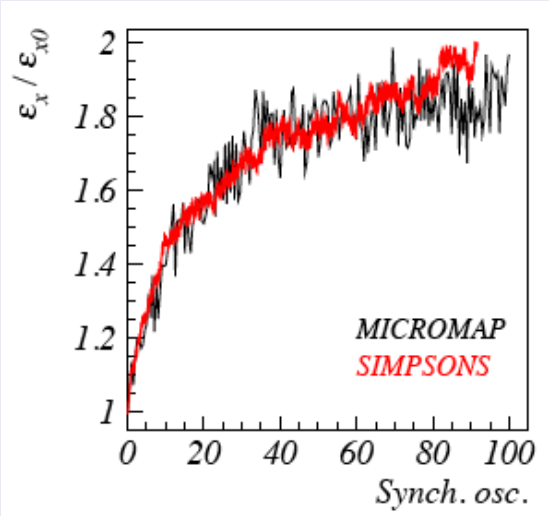
$$\rho = \frac{\lambda(z)}{4\pi a(z)b(z)} n\left(\frac{x^2}{a^2(z)} + \frac{y^2}{b^2(z)}\right)$$

$$a(z) = \sqrt{\varepsilon_x \beta_x(z)} \text{ and } b(z) = \sqrt{\varepsilon_y \beta_y(z)}$$

do a series expansion of $n(t)$ and inserted into (1) [ICAP06 TUPPP06 & MOA2IS03] $\rightarrow$ $\mathbf{E}(\mathbf{x}, \mathbf{y}, \mathbf{z})$.

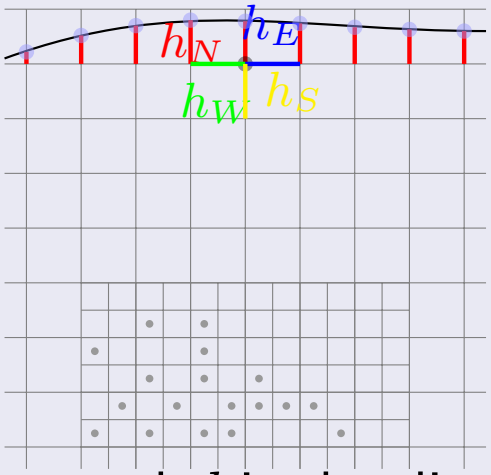
Remarks:

- long term tracking & SC
- choice of integration scheme
  10 fold decrease in T_{sol}



Iterative Methods and exact Geometry

Lets denote $\Omega \subset \mathbb{R}^3$ the simply connected computational domain and $\Gamma = \Gamma_1 \cup \Gamma_2$, the boundary of Ω ($\Gamma_1 \cap \Gamma_2 = \emptyset$):



$$\nabla^2 \phi = -\frac{\rho}{\varepsilon_0}, \text{ in } \Omega \subset \mathbb{R}^3,$$

$$\phi = 0, \text{ on } \Gamma_1$$

$$\frac{\partial \phi}{\partial \mathbf{n}} + \frac{1}{d}\phi = 0, \text{ on } \Gamma_2,$$

with ε_0 denotes the dielectric constant and d is the distance of the bunches centroid to the boundary. We apply a second order finite difference scheme which leads to a set of linear equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}.$$

Using a parallel **CG** or **BiCGSTAB** with a multigrid preconditioner shows very promising results, $\mathcal{O}(2 \ldots 10)$ fold decrease in T_{sol}.

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High Performance Computing (& CS) - Go parallel ?

typ	Procs.	Mesh	Particles	I-Steps	T_{sol} [h]	Code
typ	80	256^3	8×10^4	54×10^4	$\frac{1}{3}$	ORBIT-SNS
typ	1	4096	2×10^4	7×10^4	10	POSINST
max	1	65536	10^5	25×10^4		POSINST
typ	1	8×10^4	2×10^5			SIMPSONS
typ	16	8×10^6	2×10^5		2.7	PTC/ORBIT
max	256	8×10^6	2×10^5		2.7	PTC/ORBIT
typ	10	10^6	10^6	$\times 10^3$	$\times 1$	WARP
max	100	10^6	10^6	$\times 10^3$	$\times 1$	WARP
typ	48	$32^2 \times 256$	10^6	10^5	$\times 1$	SYNERGIA
max	1024	256^3	5×10^7	5×10^5	$\times 24$	SYNERGIA
typ	128	64^3	10^6	10^5	4	OPAL
max	4096	4096^3	$\times 10^9$	5×10^5	$\times 24$	OPAL

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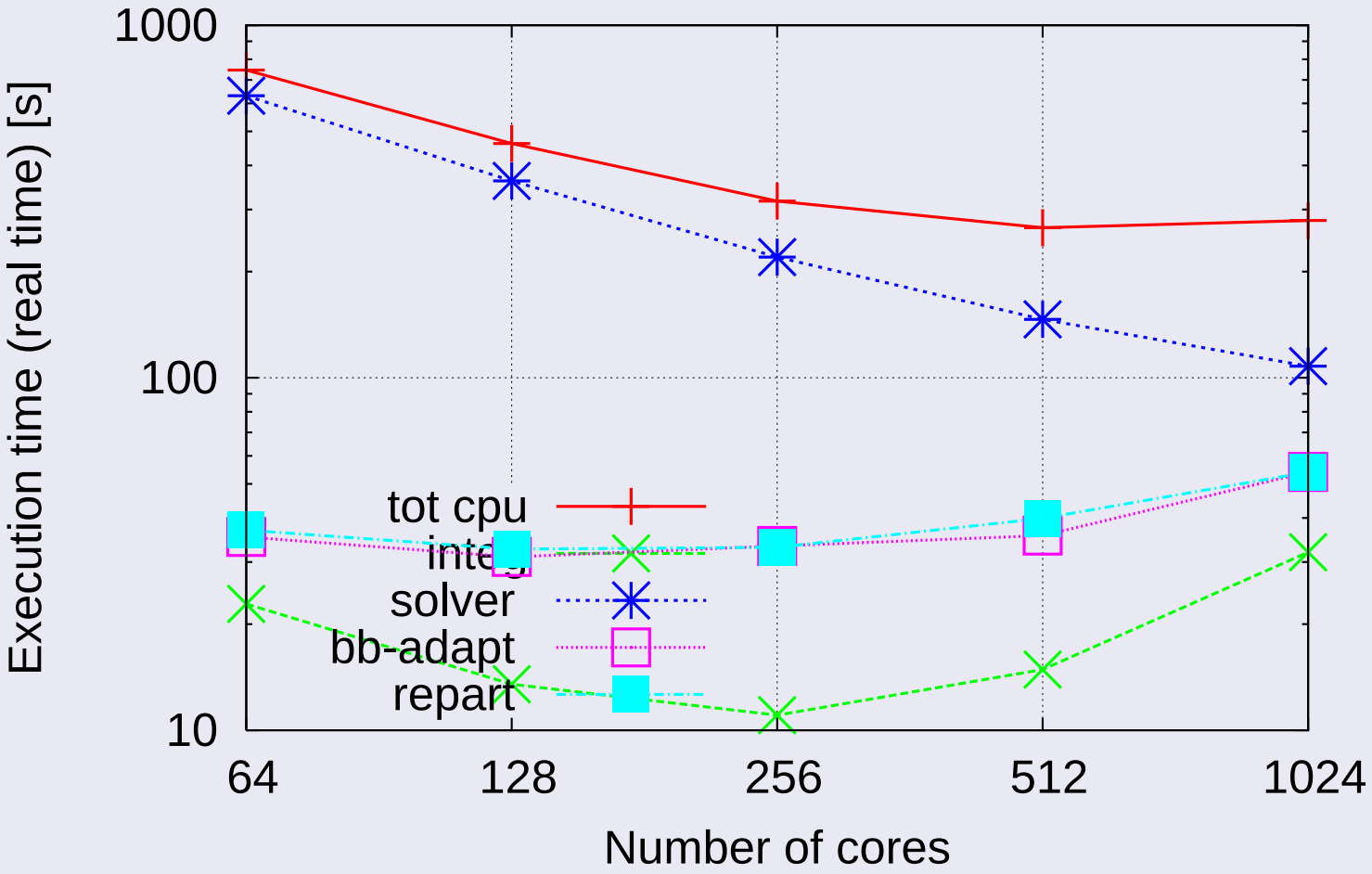
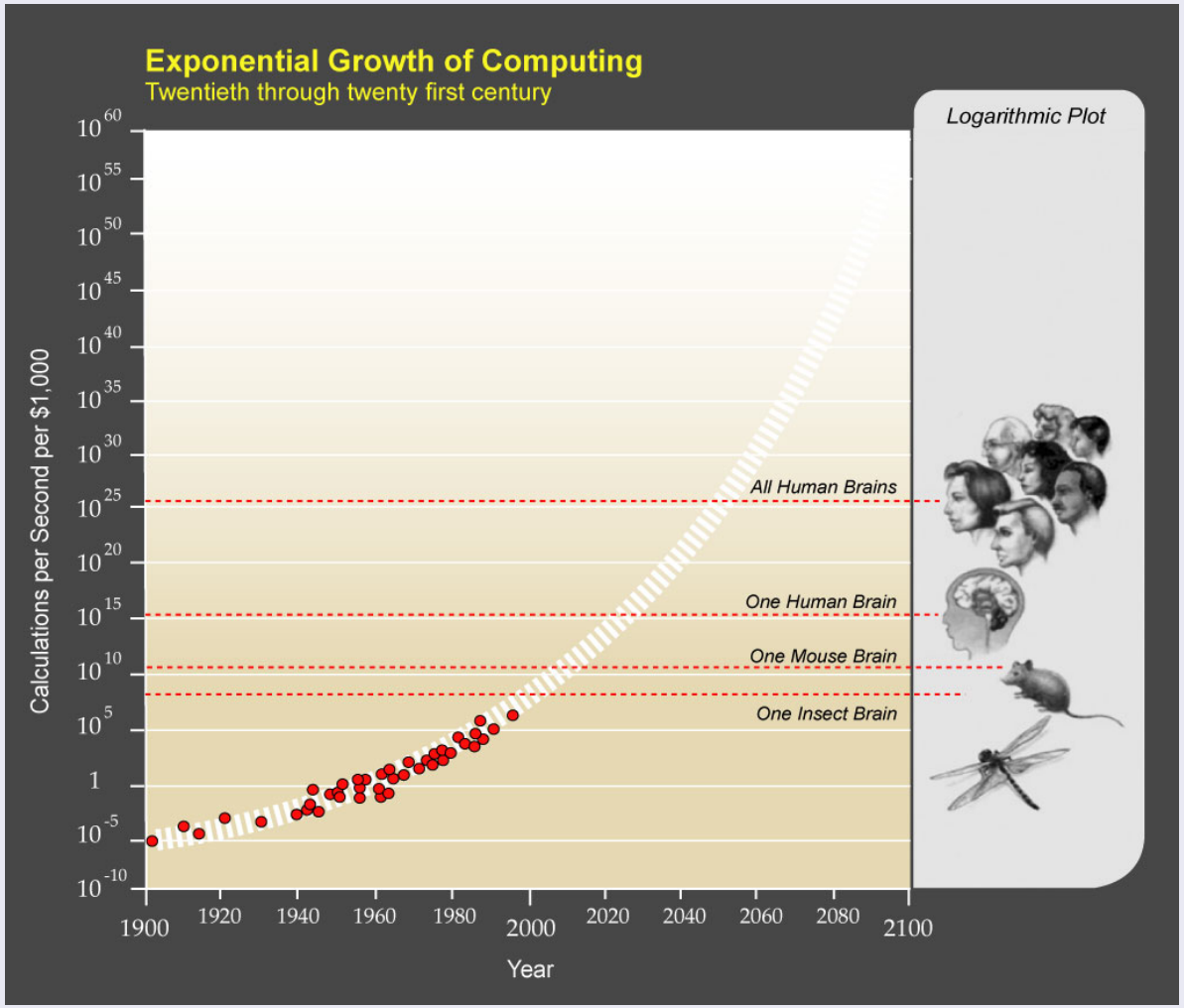
OPAL production run: go massive parallel ..... pain or fun?



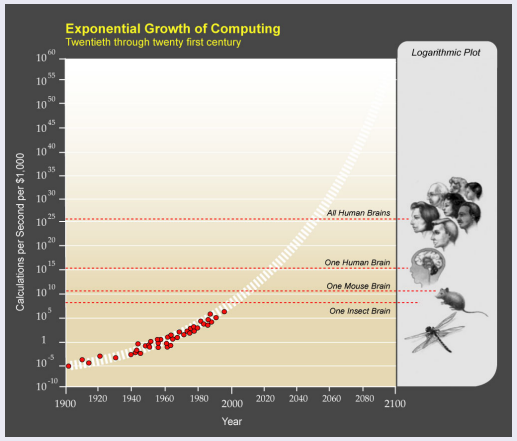
Be aware of: strong scaling and no I/O

Parallel Issues - Reality or Fiction?



Kurzweil - from The Age of Spiritual Machines

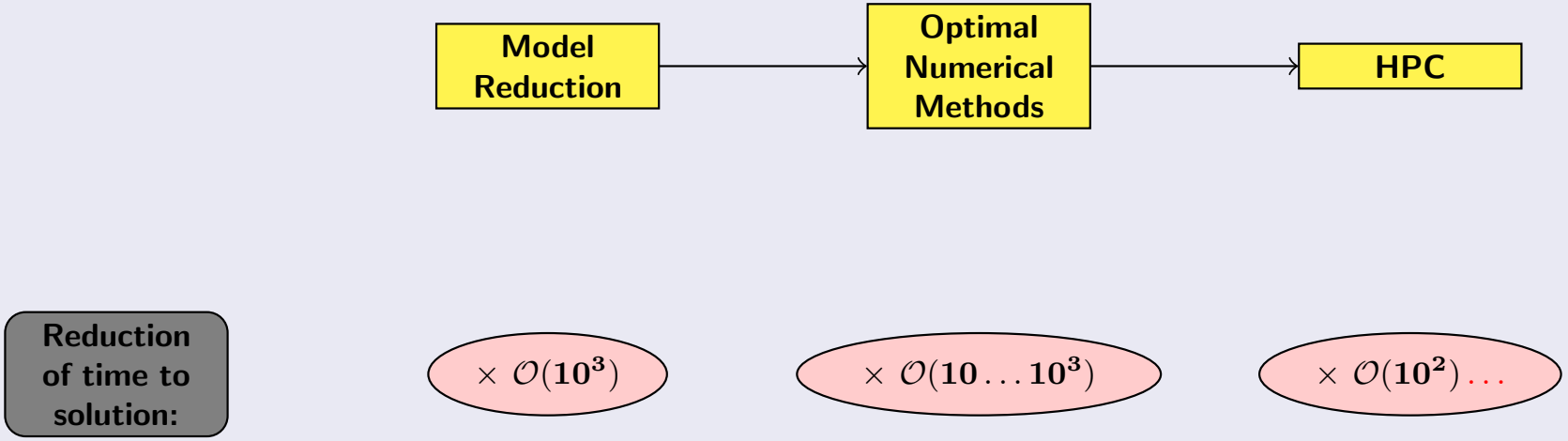
Parallel Issues - Reality or Fiction?



However we only scale weakly!

New Development

Oberservation 3:



- HPC trend: more cores (heterogenous arch.) less clock
- efficient parallelizing of one component of the code is not enough + the whole is more than the sum of its parts

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Outlook

In the MW- League it is all about *quantitative* i.e. *precise* BD simulation

1. The more precise our simulations are the more difficult and important are proper initial conditions
2. Obtain measurements (profiles) with a dynamical range of several orders of magnitude is non trivial but vital in order to fully profit from our precise simulations
3. HPC helps but we have to work hard on the weak scaling

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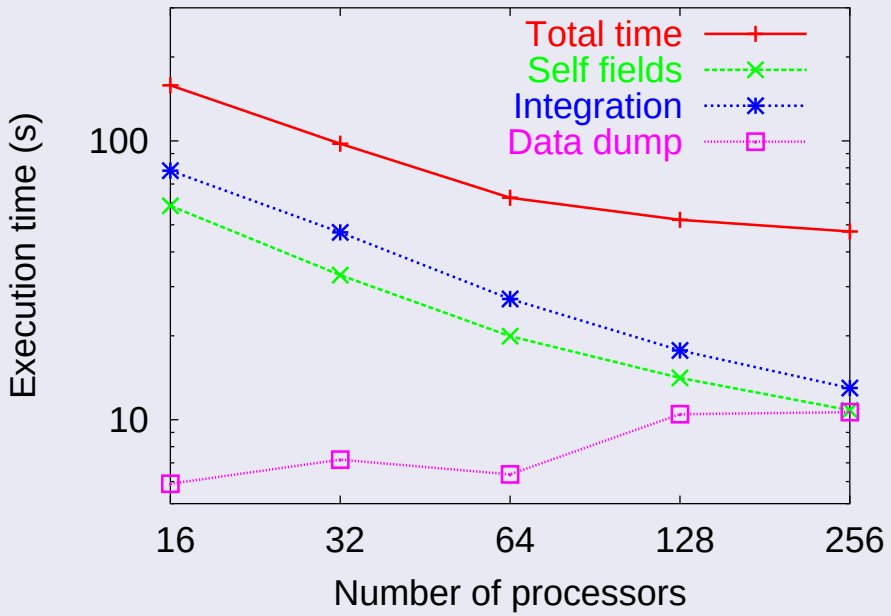
Setup

- 10^6 particles,
- 3D FFT on a 64^3 grid,
- 2D domain decomposition
- Track 200 time steps
- Gaussian distribution
- Dump data into single H5Part file every 10 steps

Observations

- The code scales well
- Good load-balancing
- Dumping time increased