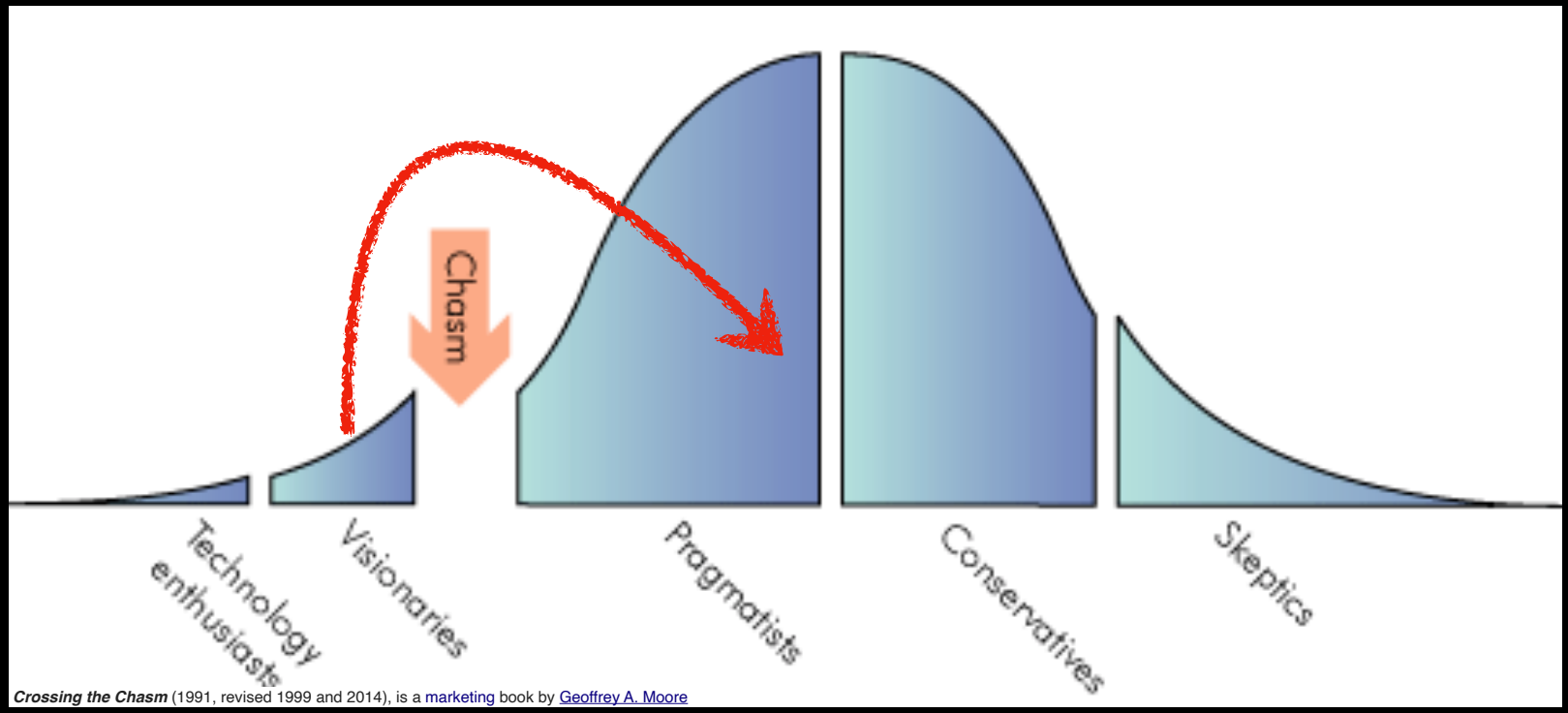
OPAL

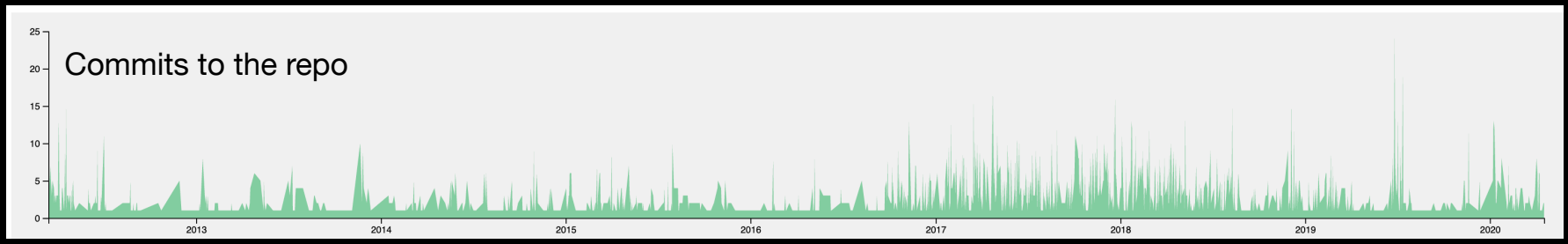
Discussion on integration of features - Physics - CS - HPC

Andreas Adelmann (Paul Scherrer Institut)

We crossed the Chasm



Crossing the Chasm (1991, revised 1999 and 2014), is a marketing book by Geoffrey A. Moore



We crossed the Chasm

- 79 member in the active mailing list (opal@lists.psi.ch)
- 12 active developers
- Sirepo by Radiasoft

Sirepo Public Cloud

The *OPAL* Framework: Version 2.3

Andreas Adelmann (PSI) · Pedro Calvo (CIEMAT) · Matthias Frey (PSI) · Achim Gsell (PSI) · Uldis Locans (PSI) · Christof Metzger-Kraus · Nicole Neveu (SLAC) · Chris Rogers (RAL) · Steve Russell (LANL) · Suzanne Sheehy (Oxford) · Jochem Snuverink (PSI) · Daniel Winklehner (MIT)

PAUL SCHERRER INSTITUT PSI · Ciemat · SLAC NATIONAL ACCELERATOR LABORATORY · UKRI Science and Technology Facilities Council · Massachusetts Institute of Technology

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- OPAL-t: improved stability & doc, a few nice papers

  A Parallel General Purpose Multi-Objective Optimization Framework, with Application to Beam Dynamics, N Neveu et al., Phys Rev AB (2019)

  https://link.aps.org/doi/10.1103/PhysRevAccelBeams.22.054602

- OPAL-cycl: FFA capabilities, trim coils, AMR, a few nice papers

  Application of multi-objective optimisation to match turn pattern measurements for cyclotrons, M Frey et al., Phys Rev AB (2019)

  https://journals.aps.org/prab/pdf/10.1103/PhysRevAccelBeams.22.064602

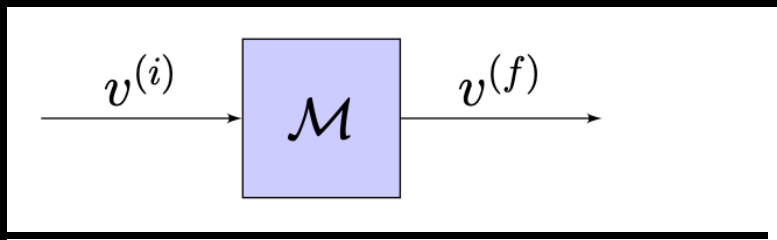
- Checkout the Wiki page https://gitlab.psi.ch/OPAL/src/wikis/home

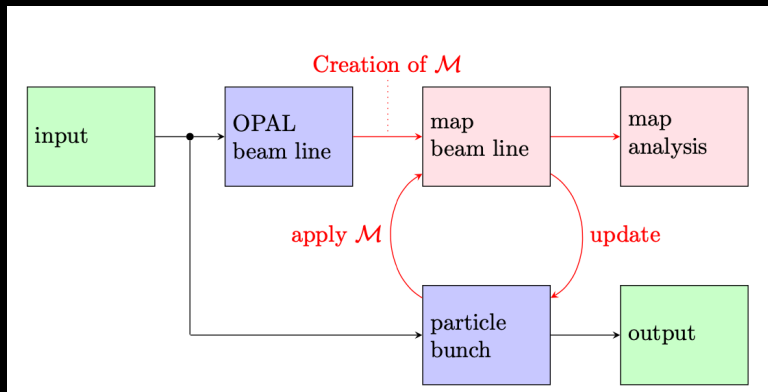
New Developments

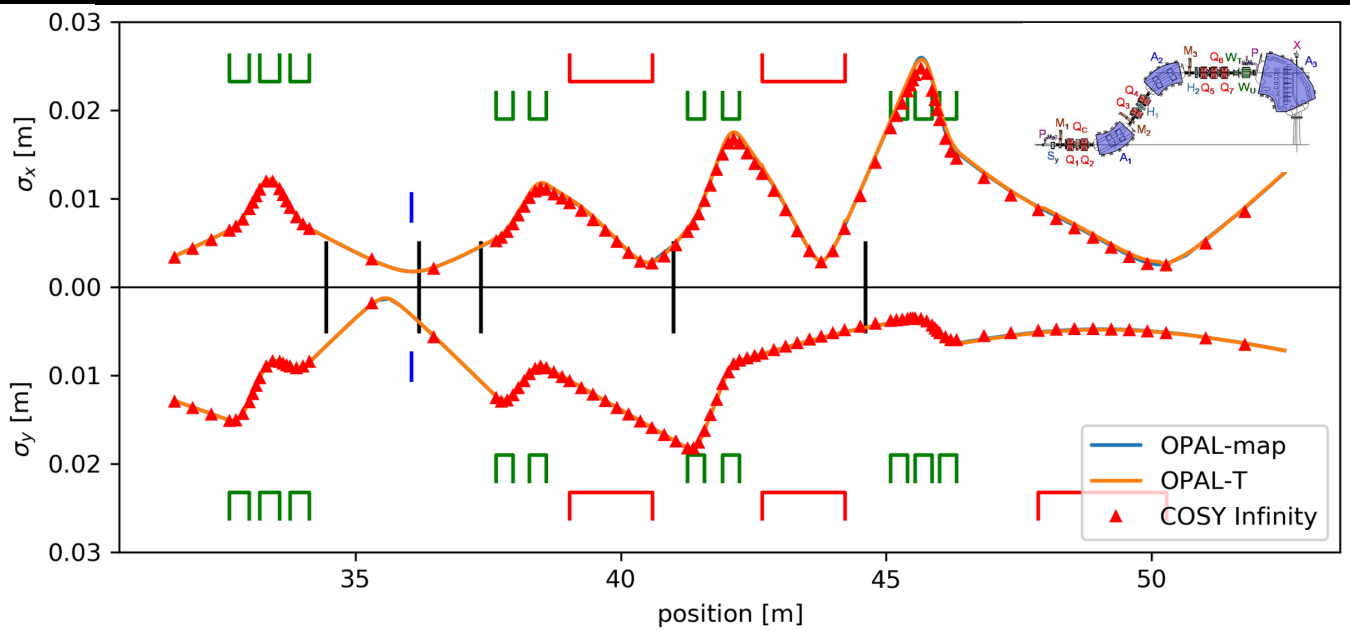
- OPAL paper
- OPAL-Map
- Computing Hardware Independence
- OPAL and Radiation (MSc project Arnau Albà)

OPAL-map (work in progress)

s is the independent variable $\mathscr{M}(s), v \in \mathfrak{R}^6, \mathscr{M} \in Sp(2d)$







- Elements (D,Q,S) up to any order are implemented
- No space charge yet: $\mathscr{M}(s) = M_{\text{ext}}(s/2) \otimes M_{\text{sc}}(s) \otimes M_{\text{ext}}(s/2) + \mathcal{O}(s^3)$

Computing Hardware Independence

- The finite difference SAAMG-PCG solver is based on first generation Trilinos
- FFT-solver and particle matter interaction can use the GPU one 1 node via. DKS

Two Problems for the future

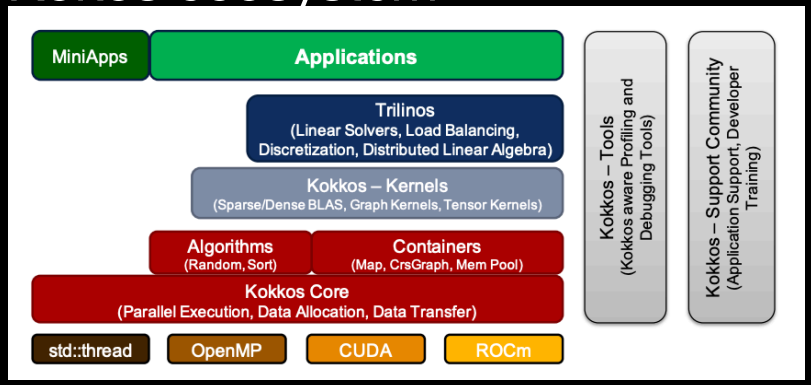
- Computing HW topologies changing toward ML (data science)
- One of the striking features of OPAL is the seemingly integration with HPC

We made a first attempt towards a future based on Kokos

M. Frey, U. Locans, A. Adelmann
On Architecture and Performance of Adaptive Mesh Refinement in an Electrostatics Particle-In-Cell Code
CPC Vol 247 (2020)
https://doi.org/10.1016/j.cpc.2019.106912

- [x] use only second generation Trilinos
- [ ] IPPL & Kokos integration

Kokos ecosystem



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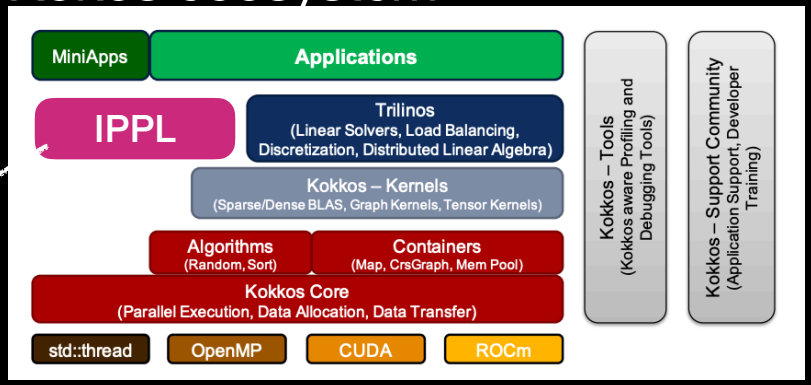
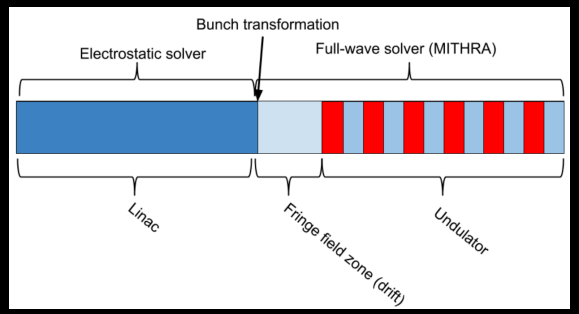


OPAL and Radiation (MSc project Arnau Albà)



MITHRA 1.0: A full-wave simulation tool for free electron lasers
A Fallahi et al, CPC Vol 228 (2018) 10.1016/j.cpc.2018.03.011

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   MESHRESOLUTION = { 40e-6, 40e-6, 2e-6},
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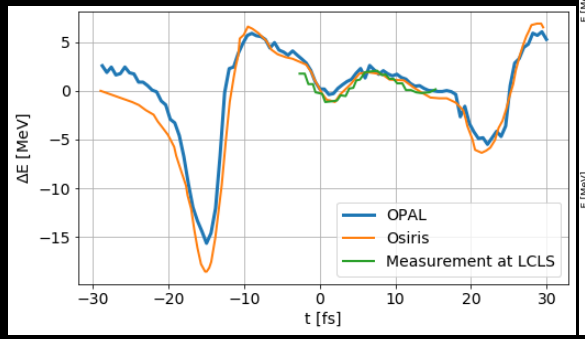
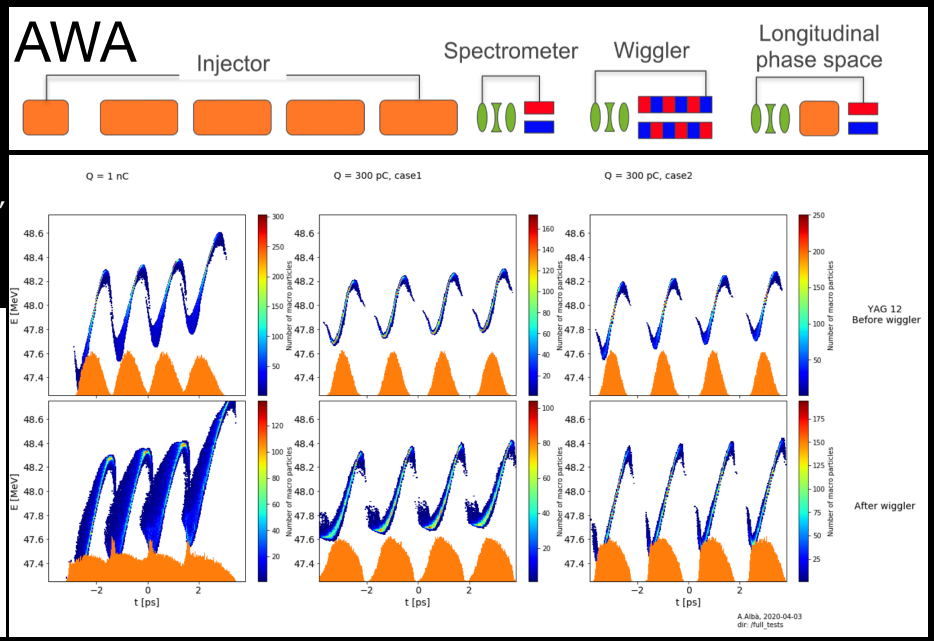


Phase-Stable Self-Modulation of an Electron Beam in a Magnetic Wiggler James P. MacArthur et al.,
PRL Vol 123 (2019)

https://doi.org/10.1103/PhysRevLett.123.214801

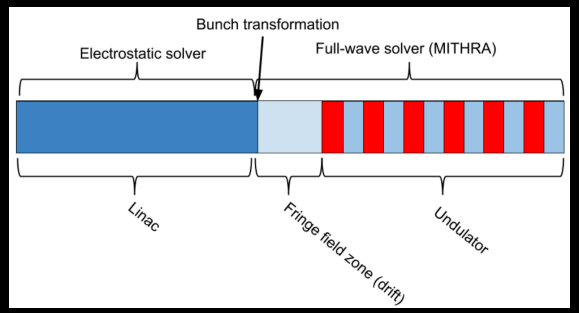


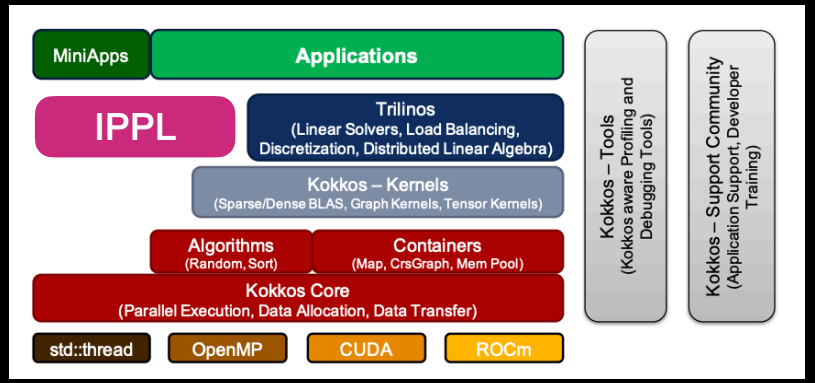
★full-wave solver (3D) attached to the undulator element (OPAL-t)
➡ ok for now ➡ this enables 3D S2E simulations of compact FELs

★full-wave solver should be a FIELDSOLVER (➡ radiation in dipoles etc.)

How to proceed

- ☑ need to keep the quality of code and examples as high as necessary
- ★ attract new developer / maintainer
- ★ respond to “sw technology challenges”
- ★ respond to physics challenges





- ★ pyOPAL will attract a lot of users