Next-Generation Simulations for XFEL-Plasma Interactions with Solid Density Targets with PIConGPU

Towards Predictive 3D Modeling

A. Huebl[1,2], R. Widera[1], R. Pausch[1,2], M. Garten[1,2], H. Burau[1,2], A. Matthes[1,2], B. Worpitz[4], F. Koller[1], T. Kluge[1], J. Vorberger[1], A. Debus[1], T. Cowan[1,2], U. Schramm[1,2], H.-K. Chung[3] and M. Bussmann[1]

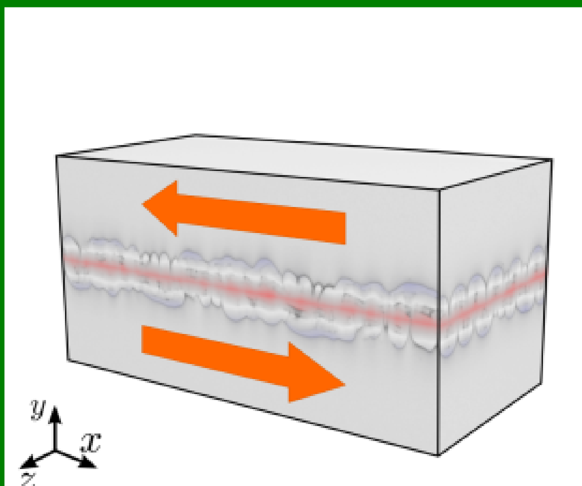
[1] Helmholtz-Zentrum Dresden - Rossendorf
[2] Technische Universität Dresden
[3] International Atomic Energy Agency

3rd European Advanced Accelerator Concepts Workshop

Elba, September *27th 2017*

Plasma Instabilities

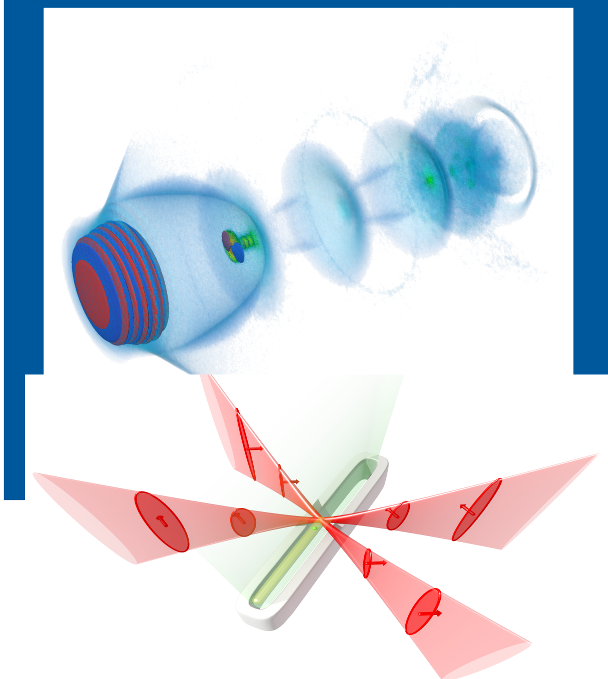
- Astrophysics
- Beam-Plasmas



0.75 x 10^{11} particles

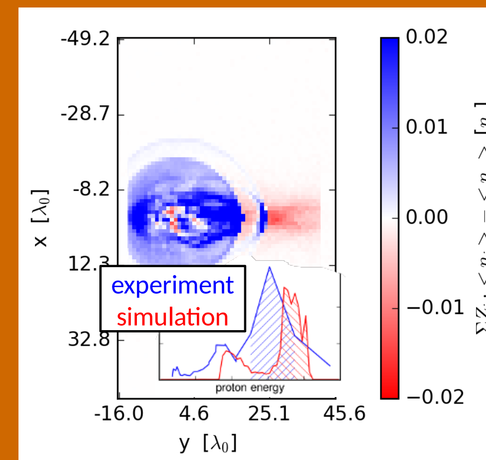
Electron Acceleration with Lasers

- Compact X-Ray sources
- Push the Energy Frontier



Ion Acceleration with Lasers

- Hadron Therapy
- HED



~1 PB / run

P. Hilz, T.M. Ostermayr, A. Huebl et al., in review (2017)
L. Obst et al., **Sci Rep. 7**:10248 (2017), DOI:10.1038/s41598-017-10589-3
J. Couperius et al., **Nat Commun. 8**:487 (2017), DOI:10.1038/s41467-017-00592-7 | A. Debus et al., in review (2017)
R. Pausch et al., **Physical Review E** (2017), DOI:10.1103/PhysRevE.96.013316

- **Modern Hardware**
- **Exascale?**

  common misunderstandings

  opportunities for HEDP & laser-plasmas
- **Data Challenge for Simulations**
- **Community & Sustainability**

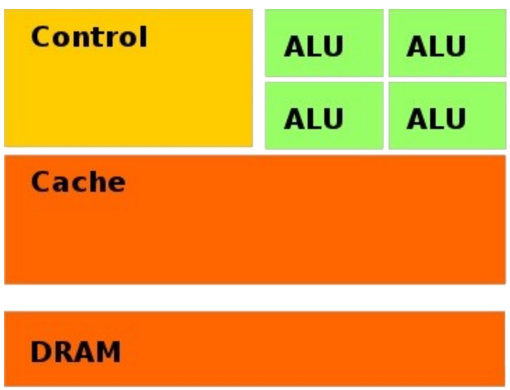
Axel Huebl | HZDR - Research Group Computer Assisted Radiation Physics | picongpu.hzdr.de

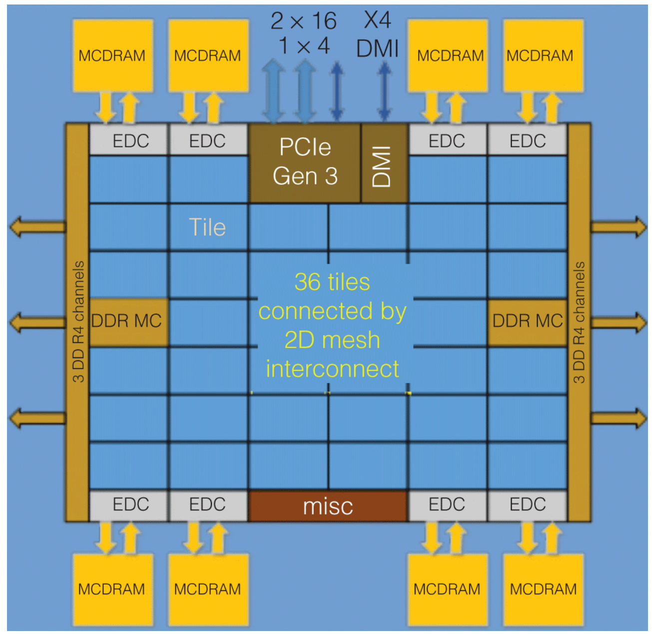
Modern Hardware

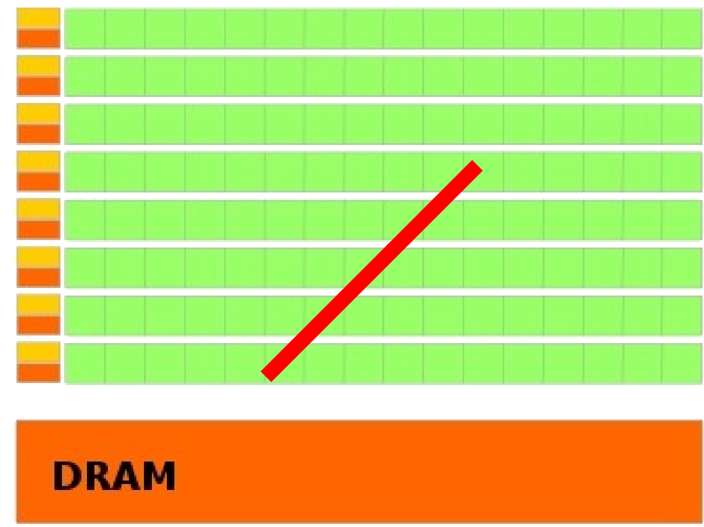
Architectures (simplified)

More Parallelism, End of Sequential Speedup

CPU → **GPGPU**







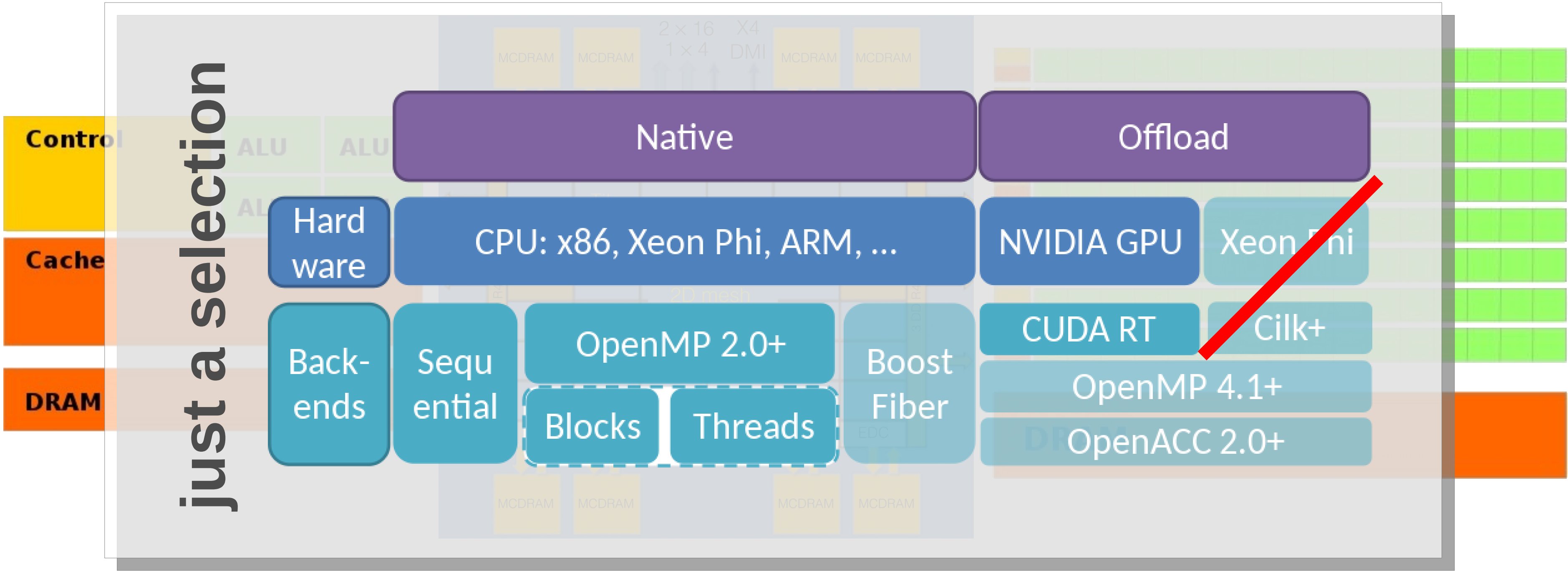
multi-core → many-core

Image sources: CUDA reference guide (Nvidia); Intel

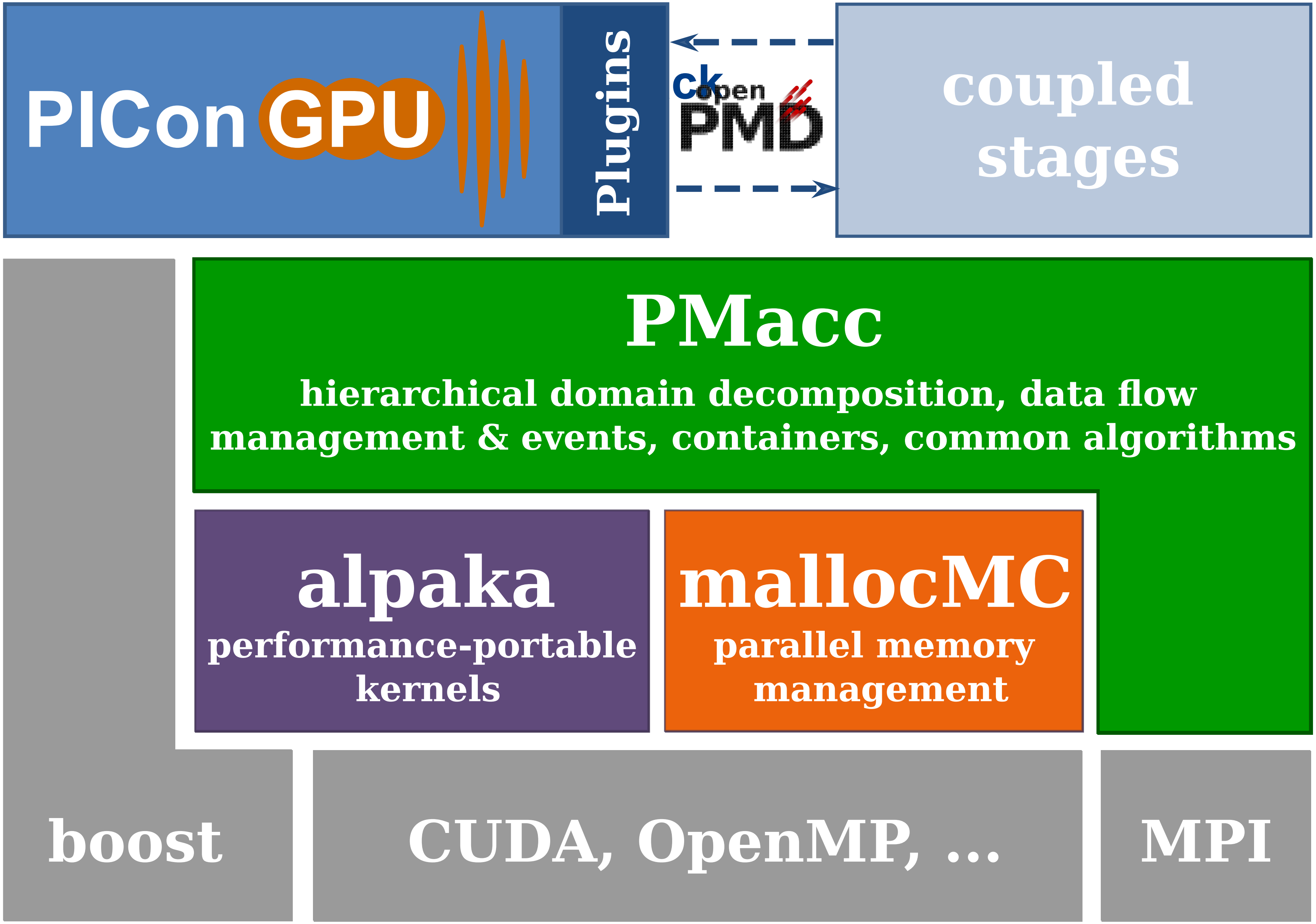
Architectures (simplified)

More Parallelism, End of Sequential Speedup

CPU → **GPGPU**



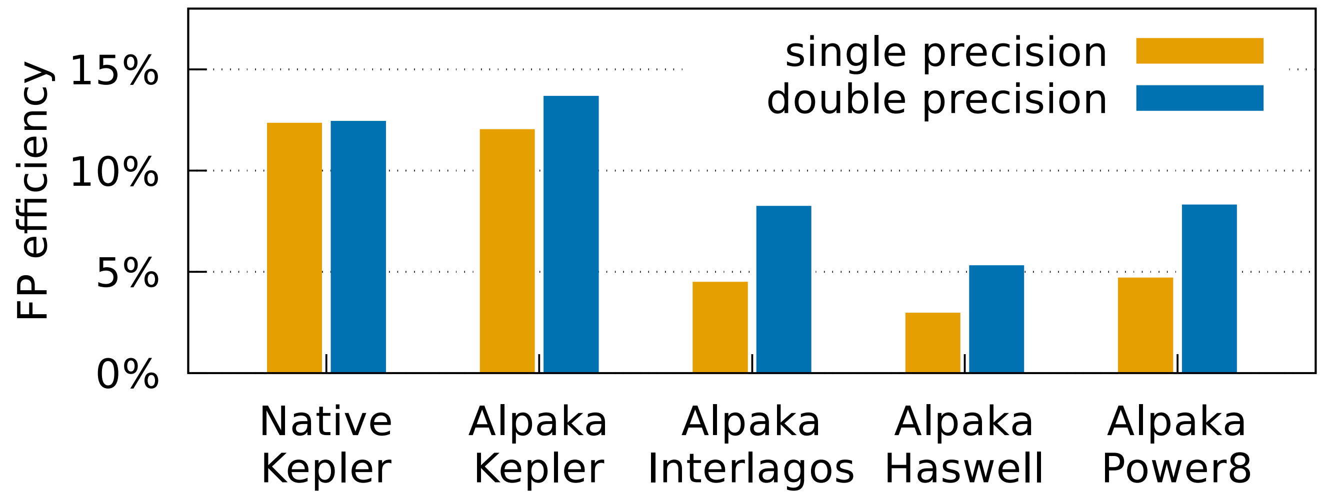
multi-core → many-core



E. Zenker et al., IPDPS (2016), DOI:10.1109/IPDPSW.2016.50
A. Matthes et al., P3MA - ISC'17 (2017), *in-press*

Alpaka: Single-Source, Performance Portable Kernels

PICon*GPU*? … on CPU ...KNL …ARM ...OpenPOWER!



weeks. Through this abstraction, the ported PIConGPU implementation is executable on AMD, IBM, Intel, and NVIDIA architectures. The code was not just ported, but has been moved to a generic *single-source* multi-platform programming model. Thus, PIConGPU never needs to be ported again.

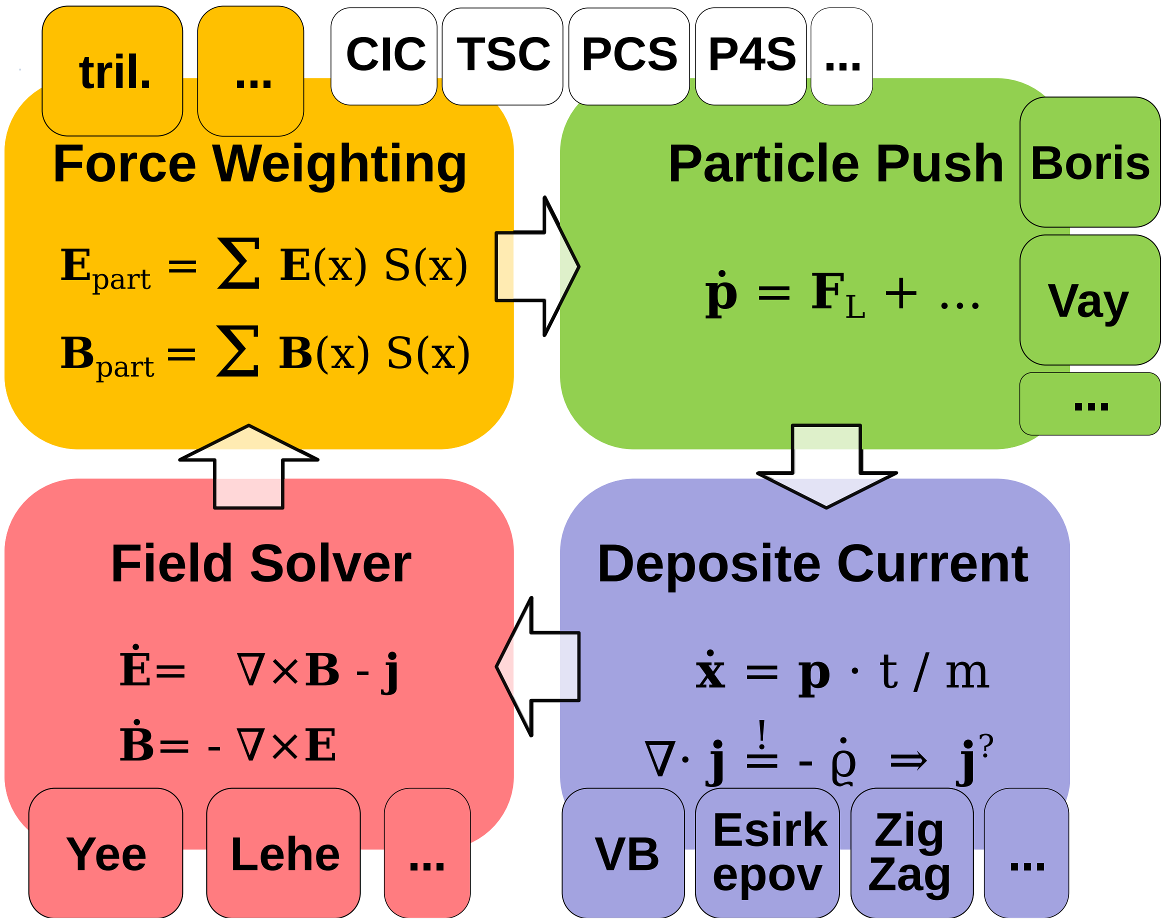
No GPU? No Problem! pic-build **-b cuda** / **-b omp2b:knl**

Installation: spack install picongpu

E. Zenker et al., ISC (2016), DOI:10.1007/978-3-319-46079-6_21
A. Matthes et al., ISC (2017), in-press, arXiv:1706.10086

Algorithmic Agility: ALL work with & on ALL

Single-Source, Performance Portable C++, 27k LOC



+ field ionization

+ synchrotron & bremsstrahlung

+ radiation reaction

+ merging

+ in-situ diagnostics

+ scalable I/O

+ ...

A. Gonoskov et al. (2015), DOI:10.1103/PhysRevE.92.023305, P.T. Luu et al. (2016), DOI:10.1016/j.cpc.2016.01.009 (DA: **H. Burau**); D. Bauer, P. Mulser (1999). DOI:10.1103/PhysRevA.59.569, L. V. Keldysh (1965) (MA: **M. Garten**); M. Vranic et al. (2015), DOI:10.1016/j.cpc.2016.04.002 (**R. Pausch**); A. Huebl et al. (2017), *in-press*, arXiv:1706.00522

Exascale?
misunderstandings vs. opportunities

Computational Speed → Predictive Capability

PetaFlop/s: 10^{15} floating point operations / second

ExaFlop/s won't solve *today's* problems *10^3x faster, but*

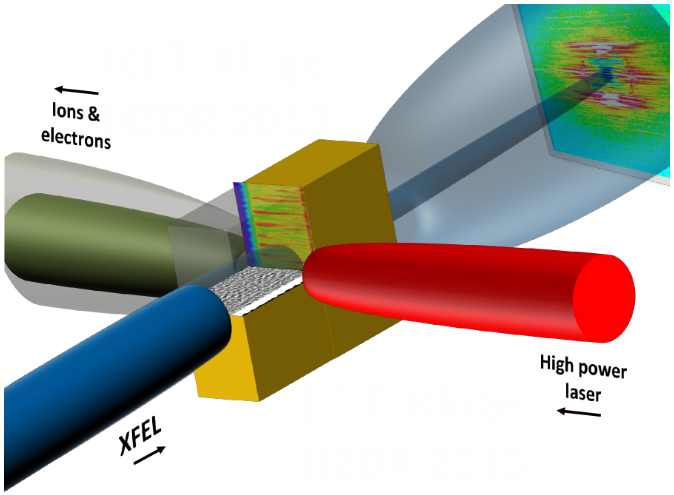
- **larger problems**
- **more problems***
- **more complex problems***

in the same <u>time to solution</u>!

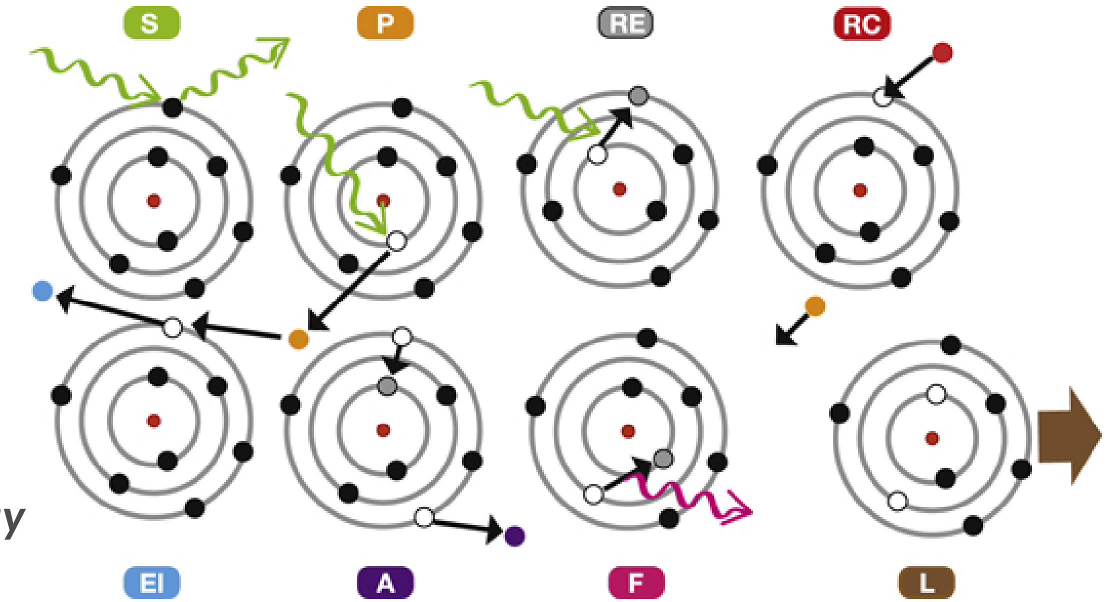
*** investigate systematical & statistical errors!**

upcoming

HiBEF Helmholtz International Beamline for Extreme Fields at the European XFEL



See talk of M. Garten earlier today



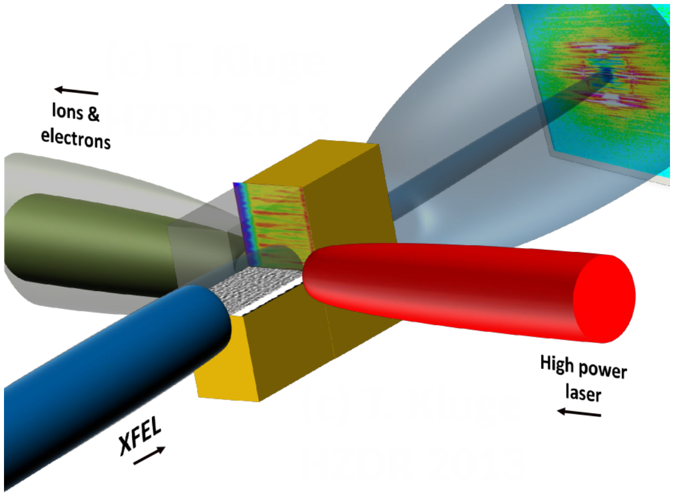
List of non-LTE atomic processes:

- photo ionization & rad. recombination
- resonant absorption & spontaneous decay
- collisional excitation & deexcitation
- collisional ionization & 3-body recombination
- autoionization & dielectr. recombination

Image: P.J. Ho, C. Knight
J. Phys. B: At., Mol. Opt. Phys. (CC-BY 2017)

HiBEF Helmholtz International Beamline for Extreme Fields at the European XFEL

upcoming



"structural"
atomic data

Model 1	Model 2
K^2L^7	Model 1+
$K^2L^6 + n$	$K^1L^6M^1 + n$
$K^2L^5M^1 + n$	
$K^1L^7 + n$	
$K^2L^8M^4$	Model 1 +
$K^2L^8M^3 + n_1$	$K^2L^7M^4 + n_1$
$K^2L^8M^2N^1 + n_2$	$K^2L^7M^3N^1 + n_2$
$K^2L^7M^4 + n_1$	$K^2L^6M^5 + n_1$
$K^1L^8M^4 + n_1$	$K^2L^6M^4N^1 + n_2$
	$K^1L^8M^3N^1 + n_2$
	$K^1L^7M^5 + n_1$
	$K^1L^7M^4N^1 + n_2$

H.-K. Chung et al. High Energy Density Physics 1 (2005) 3-12
H.-K. Chung et al. High Energy Density Physics 3 (2007) 57-64

FLYCHK / SCFLY

- 0D collisional-radiative model
- screened-hydrogenic levels

self-consistent coupling

PIConGPU

- ab initio, electro-magnetic plasmas

Multi-Physics: Non-LTE Atomic Physics

removed from summary

PIConGPU

FLYlite

$$\frac{\mathrm{d}\tilde{\mathrm{n}}}{\mathrm{d}t} = \underline{\mathbf{R}} \cdot \tilde{\mathrm{n}}$$

removed from summary

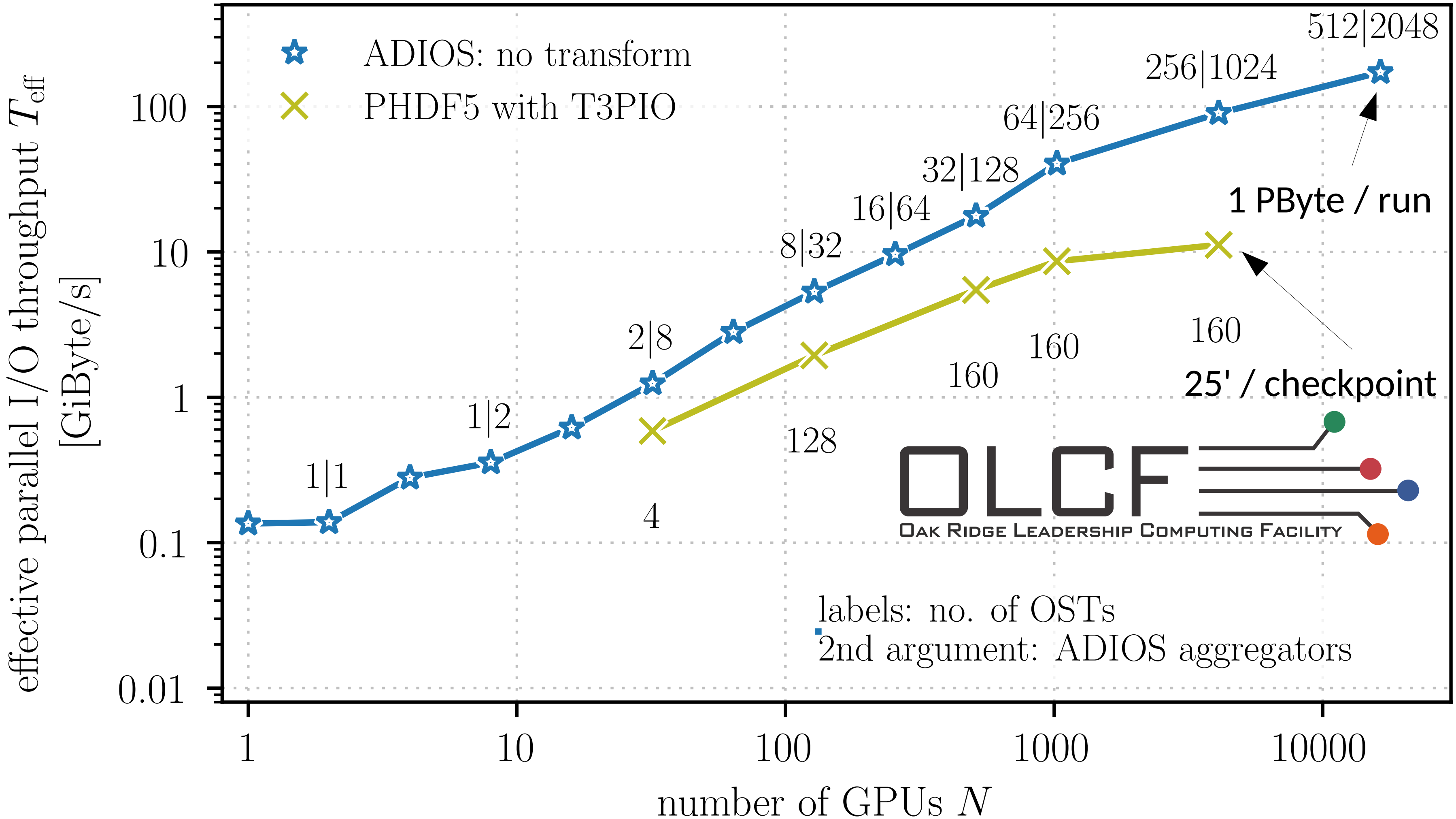
References for SCFLY/FLYlite models: [ColEx] H.-K. Chung et al. (2007), Mewe (1972), [ColIon] A. Burgess, M.C. Chidichimo (1983), [RadEx] Screended Oscillators, e.g. R.M. More (1981/91), [RadIon] J. H. Scofield (1983), H. A. Kramers (1923), [Auto] Rates, [IPD] J.C. Stewart, K.D. Pyatt (1966)

Data Challenge for Simulations

Data Reduction Challenge

Titan I/O Weak Scaling

$$T_{\text{eff}} \equiv \frac{N \times S}{t_{\text{I/O}}}$$



A. Huebl et al., DRBSD-1 - ISC'17 (2017), *in-press*, arXiv:1706.00522

Data Reduction Challenge

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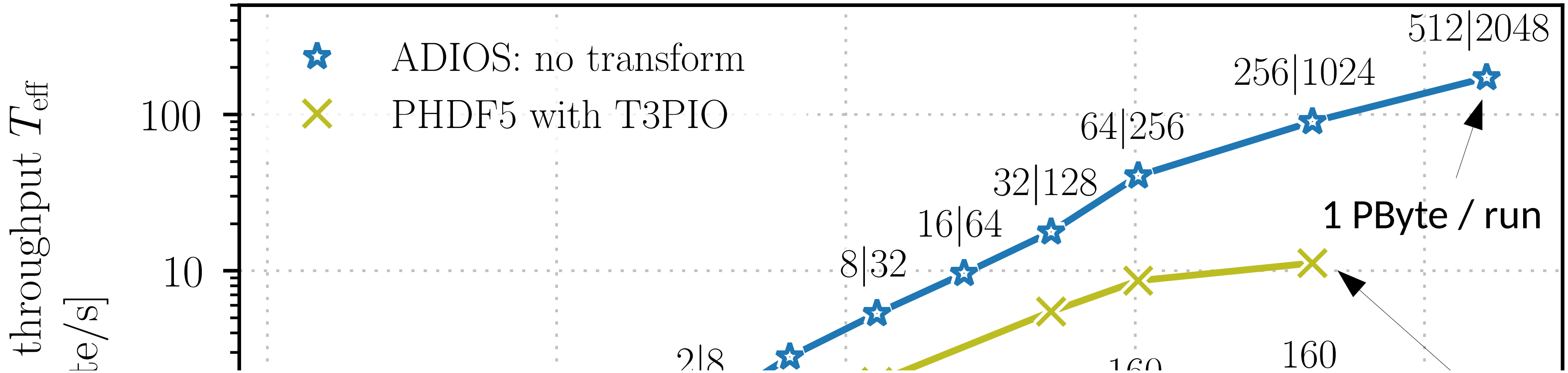
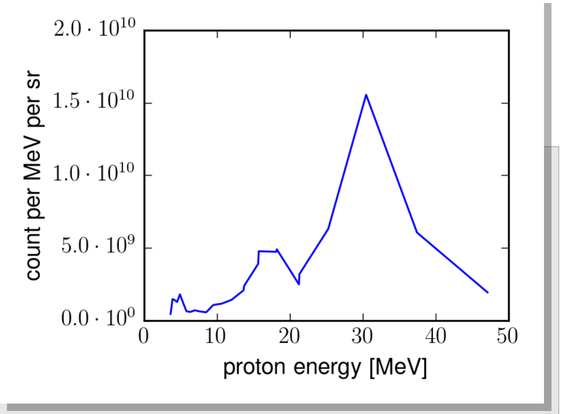


FEATURE	TITAN	SUMMIT
Application Performance	Baseline	5-10x Titan
Number of Nodes	18,688	~4,600
Node performance	1.4 TF	> 40 TF
File System	32 PB, 1 TB/s, Lustre©	250 PB, 2.5 TB/s, GPFS™
Peak power consumption	9 MW	15 MW

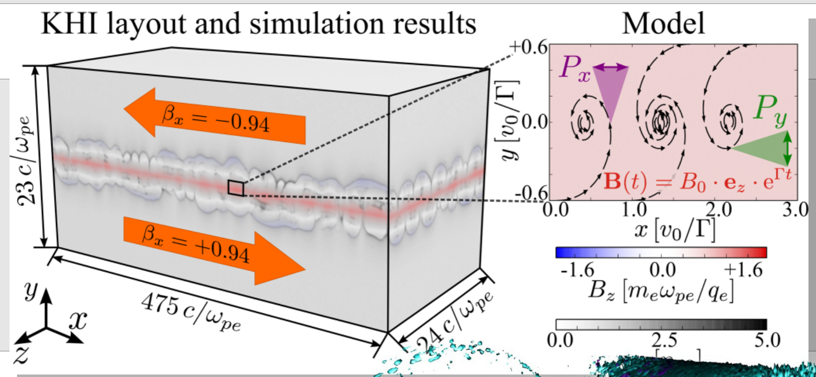
www.olcf.ornl.gov/summit

A. Huebl et al., DRBSD-1 - ISC'17 (2017), *in-press*, arXiv:1706.00522

Data Reduction: In Situ (Plugins)

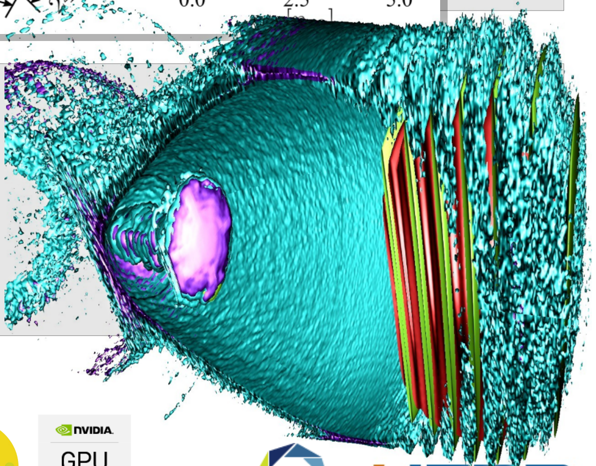


Binning of a spectrogram
Creation of a phase space image



In situ radiation diagnostics
(see talk of R. Pausch)

Ray-cast or photo-realistic ray-trace
Aggressive (lossy) data reduction



A. Huebl et al. (2014), DOI:10.1109/TPS.2014.2327392
R. Pausch et al. (2017), DOI:10.1103/PhysRevE.96.013316
A. Matthes, A. Huebl et al., ISC'16 (2016), DOI:10.14529/jsfi160403
A. Huebl et al., ISC'17 (2017), *in-press*, arXiv:1706.00522

Community & Sustainability

Open Science Approach

github.com/
ComputationalRadiationPhysics

source: open, contributable, docs

review: open issues & changelogs

methodology: documented workflows

education: resources & integrations

data: standardized, versioned

reproducibility

quality

sustainability

exchange

after-user

A. Huebl et al., openPMD 1.0.0 (2015), DOI:10.5281/zenodo.33624

PIConGPU

Thank you for your attention!

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EUCALL | NVIDIA GPU CENTER OF EXCELLENCE | DRESDEN concept | HZDR