Simulations of Laser Plasma Interaction

Michael Bussmann

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Theoretical Prerequisites

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \vec{\nabla} f + \vec{F} \cdot \frac{df}{d\vec{p}} = 0$$

$$\frac{df_{i(s,z)}}{dt} = \frac{\partial f_{i(s,z)}}{\partial t} + \frac{\vec{p}_{i(s,z)}}{m_{i(s,z)}} \cdot \vec{\nabla} f_{i(s,z)} + \vec{F} \cdot \frac{df_{i(s,z)}}{d\vec{p}_{i(s,z)}} = 0$$

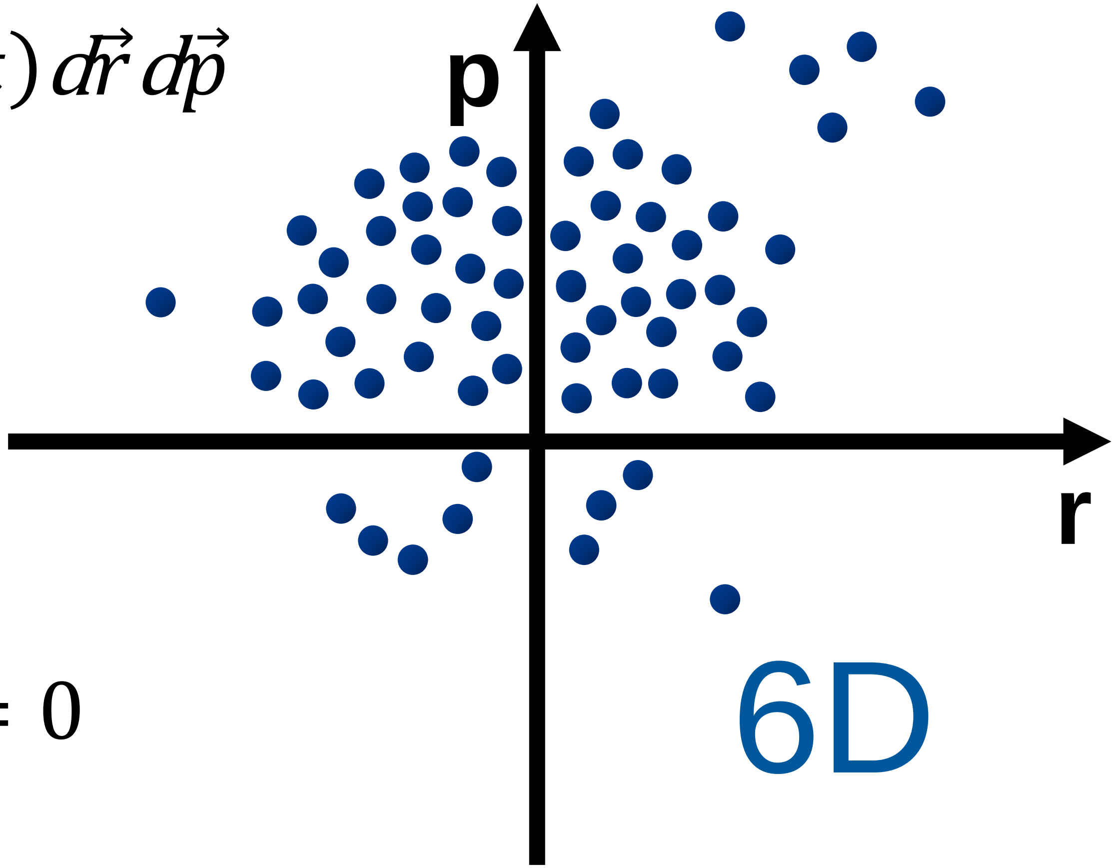
$$= \frac{\partial f_e}{\partial t} + \frac{\vec{p}_e}{m_e} \cdot \vec{\nabla} f_e + \vec{F} \cdot \frac{df_e}{d\vec{p}_e} = 0$$

Collisionless Boltzmann Equation

$$dN = f(\vec{r}(t), \vec{p}(t), t)\, d\vec{r}\, d\vec{p}$$

f is the phase space density at time t

$$\frac{df}{dt} = \left.\frac{\partial f}{\partial t}\right|_{collisions} = 0$$

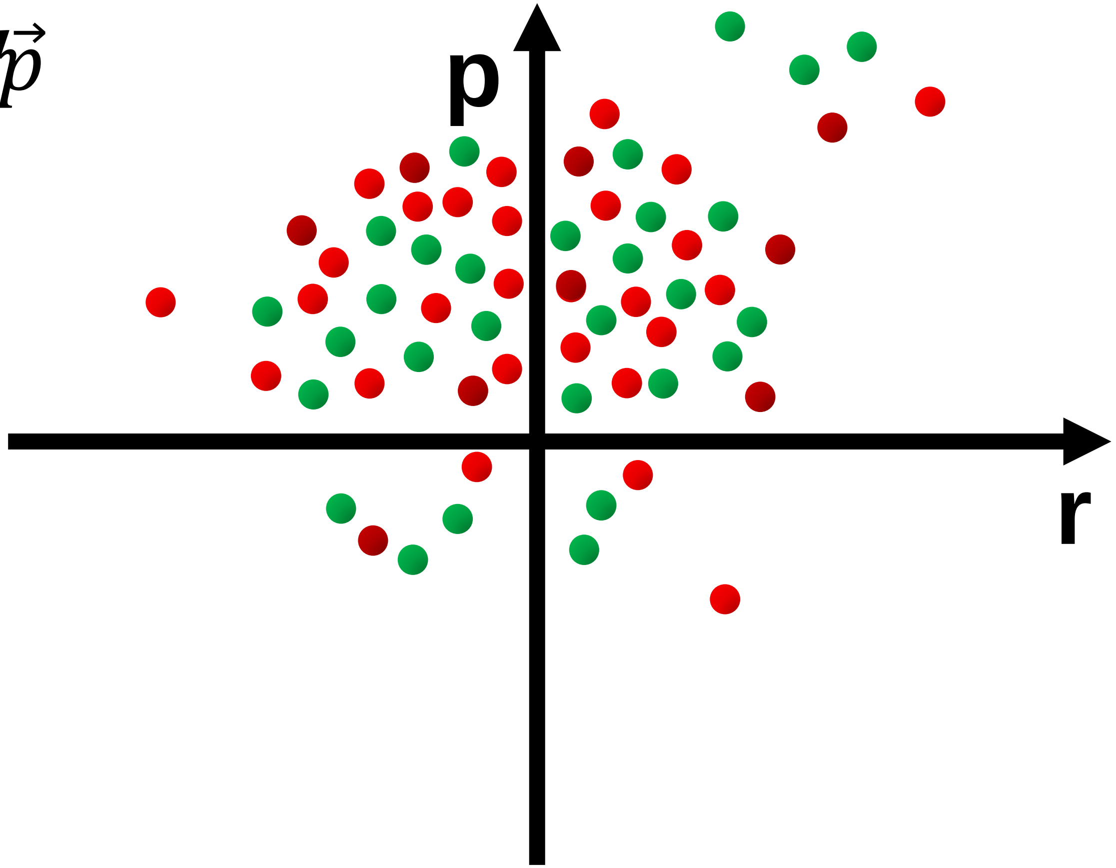


Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The Vlasov Equations for a collisionless multi-species plasma

$$dN_{i(s,z)} = f_{i(s,z)}\, d\vec{r}\, d\vec{p}$$
$$dN_e = f_e\, d\vec{r}\, d\vec{p}$$

$$\frac{df_{i(s,z)}}{dt} = 0\ \forall i(s,z)$$
$$\frac{df_e}{dt} = 0$$



$$\rho(\vec{r},t) = \sum_s \sum_z \int e\left(Z_{s,z} f_{i(s,z)} - f_e\right) d\vec{p}$$

The Vlasov-Maxwell Equations – What are the forces?

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla} f + \vec{F} \cdot \frac{df}{d\vec{p}} = 0$$

$$\frac{df_{i(s,z)}}{dt} = \frac{\partial f_{i(s,z)}}{\partial t} + \vec{v}_{i(s,z)} \cdot \vec{\nabla} f_{i(s,z)} + \vec{F} \cdot \frac{df_{i(s,z)}}{d\vec{p}_{i(s,z)}} = 0$$

$$\frac{df_e}{dt} = \frac{\partial f_e}{\partial t} + \vec{v}_e \cdot \vec{\nabla} f_e + \vec{F} \cdot \frac{df_e}{d\vec{p}_e} = 0$$

DRESDEN concept

HZDR

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The Vlasov-Maxwell Equations – The Lorentz force

$$\vec{F}_{i(s,z)} = Z_{i(s,z)} e \left(\vec{E} + \frac{\vec{v}_{i(s,z)}}{c} \times \vec{B} \right)$$

$$\vec{F}_{e} = - e \left(\vec{E} + \frac{\vec{v}_{e}}{c} \times \vec{B} \right)$$

$$\vec{v}_x = \frac{\vec{p}_x}{\gamma_x m_x} = \frac{\vec{p}_x}{\sqrt{m_x^2 + \left(\frac{\vec{p}_x}{c}\right)^2}}, x \in \{i(s,z), e\}$$

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The Vlasov-Maxwell Equations – Fields mediate interactions

$$\vec{F}_x = Z_x e\left(\vec{E} + \frac{\vec{v}_x}{c} \times \vec{B}\right)$$

$$\vec{\nabla} \times \vec{B} = \frac{1}{c}\left(4\pi\vec{j} + \frac{\partial \vec{E}}{\partial t}\right)$$ Ampere's Law

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$$ Faraday's Law

$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho$$ Gauss's Law

$$\vec{\nabla} \cdot \vec{B} = 0$$ Gauss's Law

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The Vlasov-Maxwell Equations – Currents created by plasma

$$\vec{F}_x = Z_x e \left(\vec{E} + \frac{\vec{v}_x}{c} \times \vec{B} \right)$$

$$\vec{\nabla} \times \vec{B} = \frac{1}{c} \left(4\pi \vec{j} + \frac{\partial \vec{E}}{\partial t} \right)$$ Ampere's Law

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t}$$ Faraday's Law

$$\vec{j}(\vec{r}, t) = \sum_s \sum_z \int e\left(Z_{s,z} f_{i(s,z)} \vec{v}_{i(s,z)} - f_e \vec{v}_e \right) d\vec{p}$$

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The Vlasov-Maxwell Equations Cheat Sheet

$$\frac{df_{i(s,z)}}{dt} = \frac{\partial f_{i(s,z)}}{\partial t} + \vec{v}_{i(s,z)} \cdot \vec{\nabla} f_{i(s,z)} + \vec{F}_{i(s,z)} \cdot \frac{df_{i(s,z)}}{d\vec{p}_{i(s,z)}} = 0 \qquad \vec{F}_{i(s,z)} = Z_{i(s,z)} e\left(\vec{E} + \frac{\vec{v}_{i(s,z)}}{c} \times \vec{B}\right)$$

$$\frac{df_e}{dt} = \frac{\partial f_e}{\partial t} + \vec{v}_e \cdot \vec{\nabla} f_e + \vec{F}_e \cdot \frac{df_e}{d\vec{p}_e} = 0 \qquad \vec{F}_e = -e\left(\vec{E} + \frac{\vec{v}_e}{c} \times \vec{B}\right)$$

$$\vec{\nabla} \times \vec{B} = \frac{1}{c}\left(4\pi\vec{j} + \frac{\partial \vec{E}}{\partial t}\right) \quad \text{Ampere's Law}$$

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t} \quad \text{Faraday's Law}$$

$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho \quad \text{Gauss's Law}$$

$$\vec{\nabla} \cdot \vec{B} = 0 \quad \text{Gauss's Law}$$

$$\vec{v}_x = \frac{\vec{p}_x}{\gamma_x m_x} = \frac{\vec{p}_x}{\sqrt{m_x^2 + \left(\frac{\vec{p}_x}{c}\right)^2}}, x \in \{i(s,z), e\}$$

$$\vec{j}(\vec{r},t) = \sum_s \sum_z \int e\left(Z_{s,z} f_{i(s,z)} \vec{v}_{i(s,z)} - f_e \vec{v}_e\right) d\vec{p}$$

$$\rho(\vec{r},t) = \sum_s \sum_z \int e\left(Z_{s,z} f_{i(s,z)} - f_e\right) d\vec{p}$$

$$dN_{i(s,z)} = f_{i(s,z)}\, d\vec{r}\, d\vec{p}$$

$$dN_e = f_e\, d\vec{r}\, d\vec{p}$$

DRESDEN concept HZDR

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The Vlasov-Maxwell Equations

- Phase space density is coserved for every species
- Electric and magnetic fields mediate interaction
- Close-range interactions neglected
- Current densities and charge densities change fields

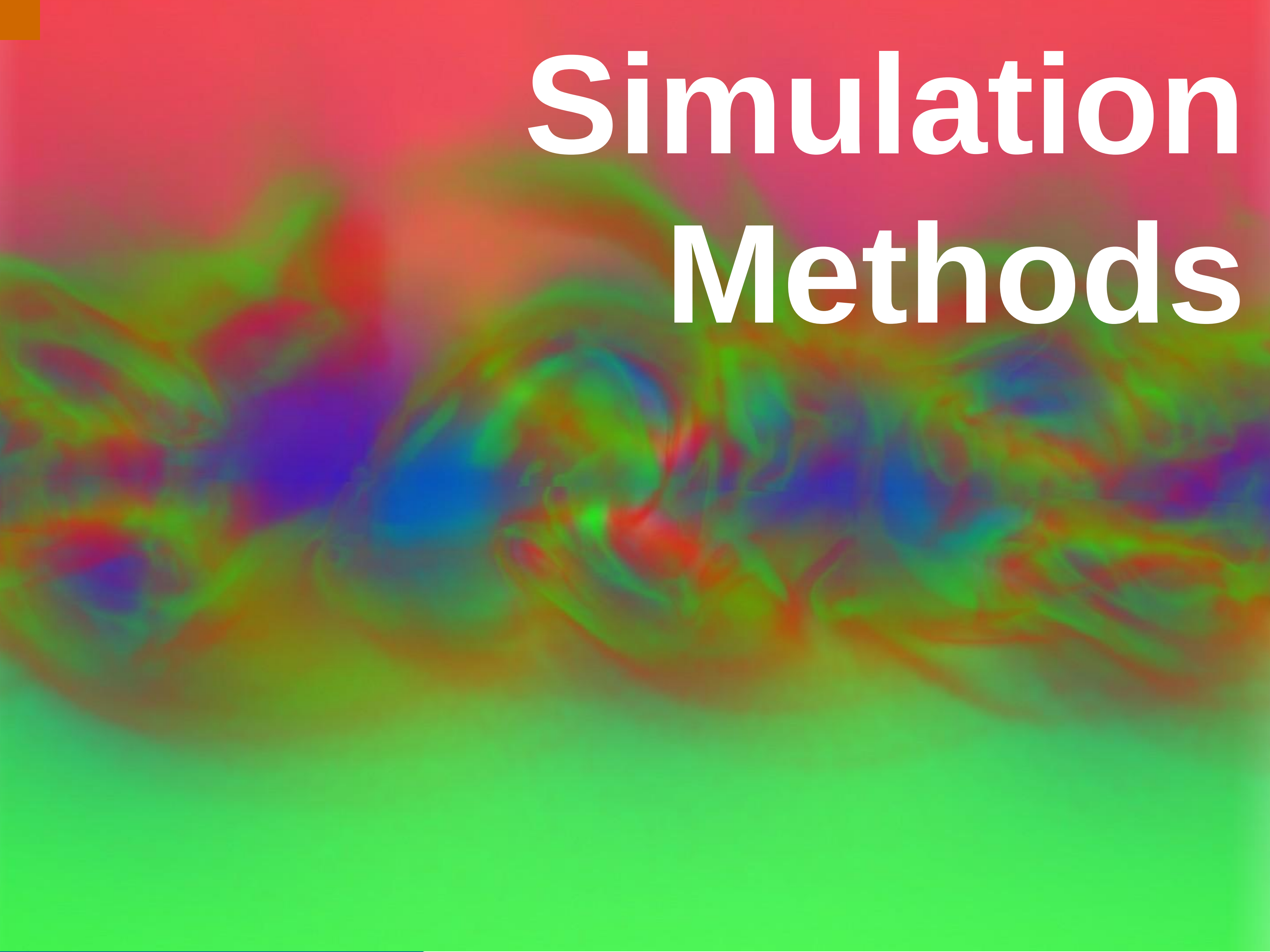
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The Vlasov-Maxwell Equations

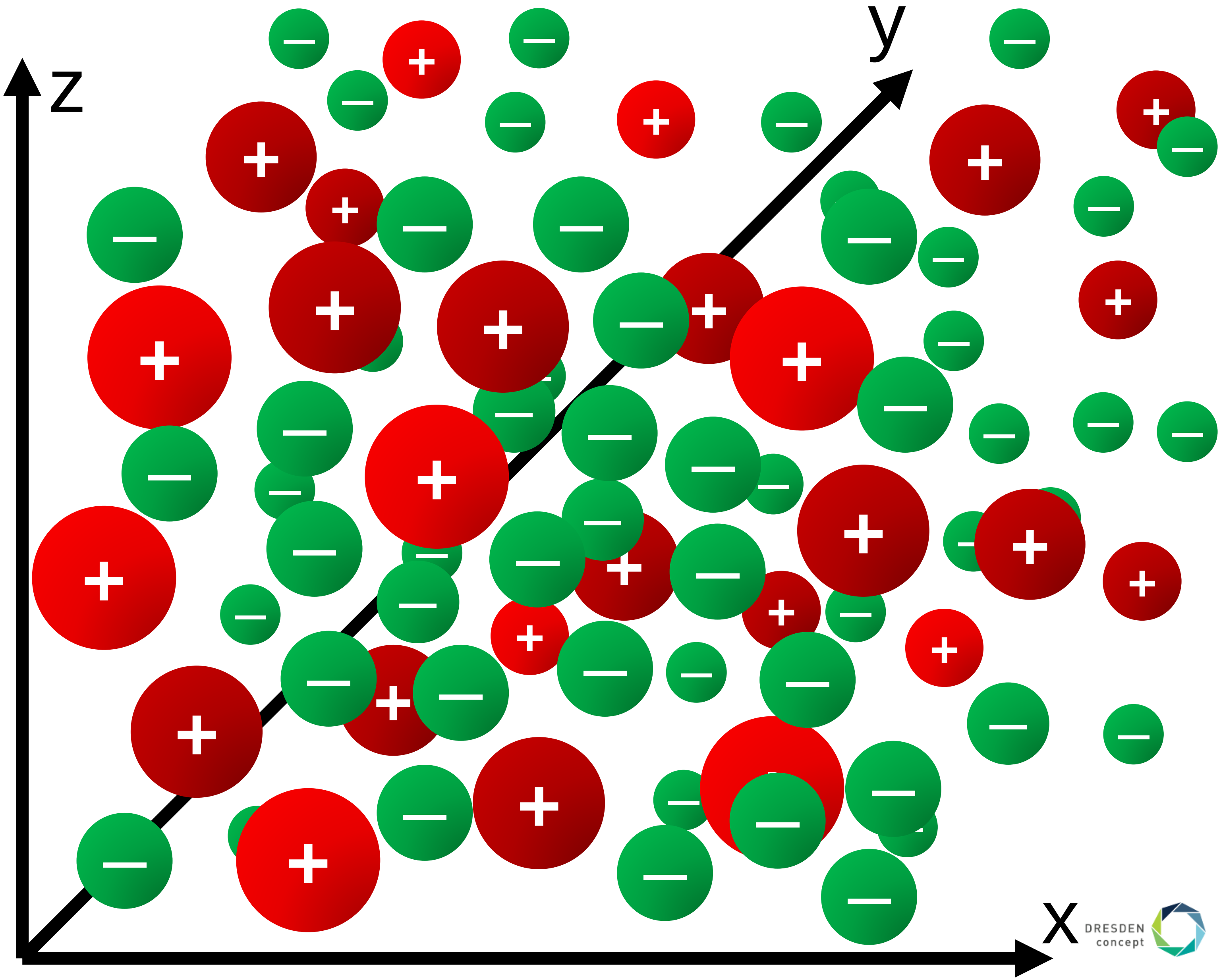
Method	Resource
„Vlasov-Maxwell Equations“	A. A. Vlasov, *The Vibrational Properties of an Electron Gas*, **Soviet Physics Uspekhi. 10(6), 721**, 1968

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

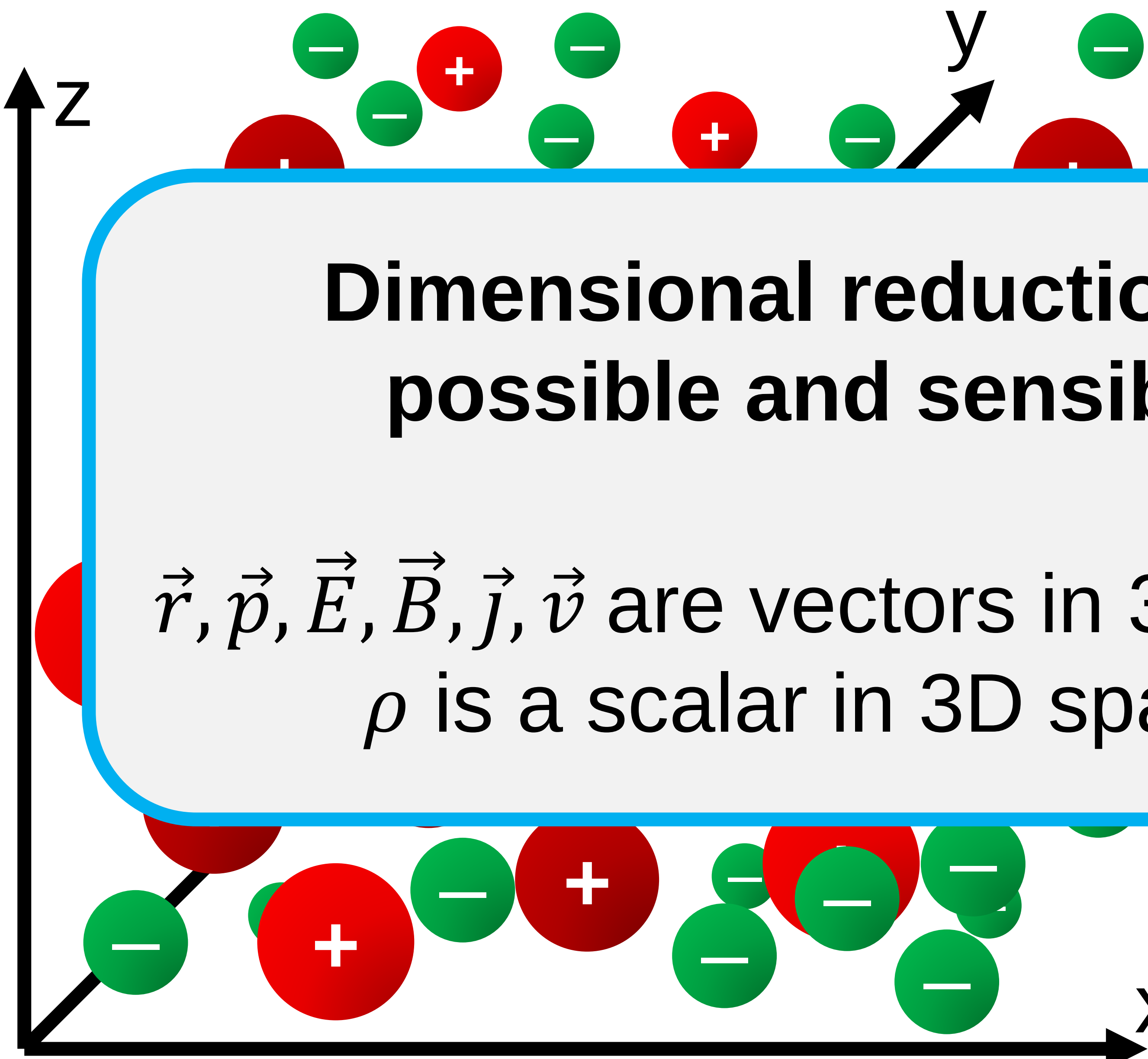
Simulation Methods



Methods to „probe“ the Vlasov-Maxwell Equations – Going „3D“



Methods to „probe“ the Vlasov-Maxwell Equations – Going „3D“



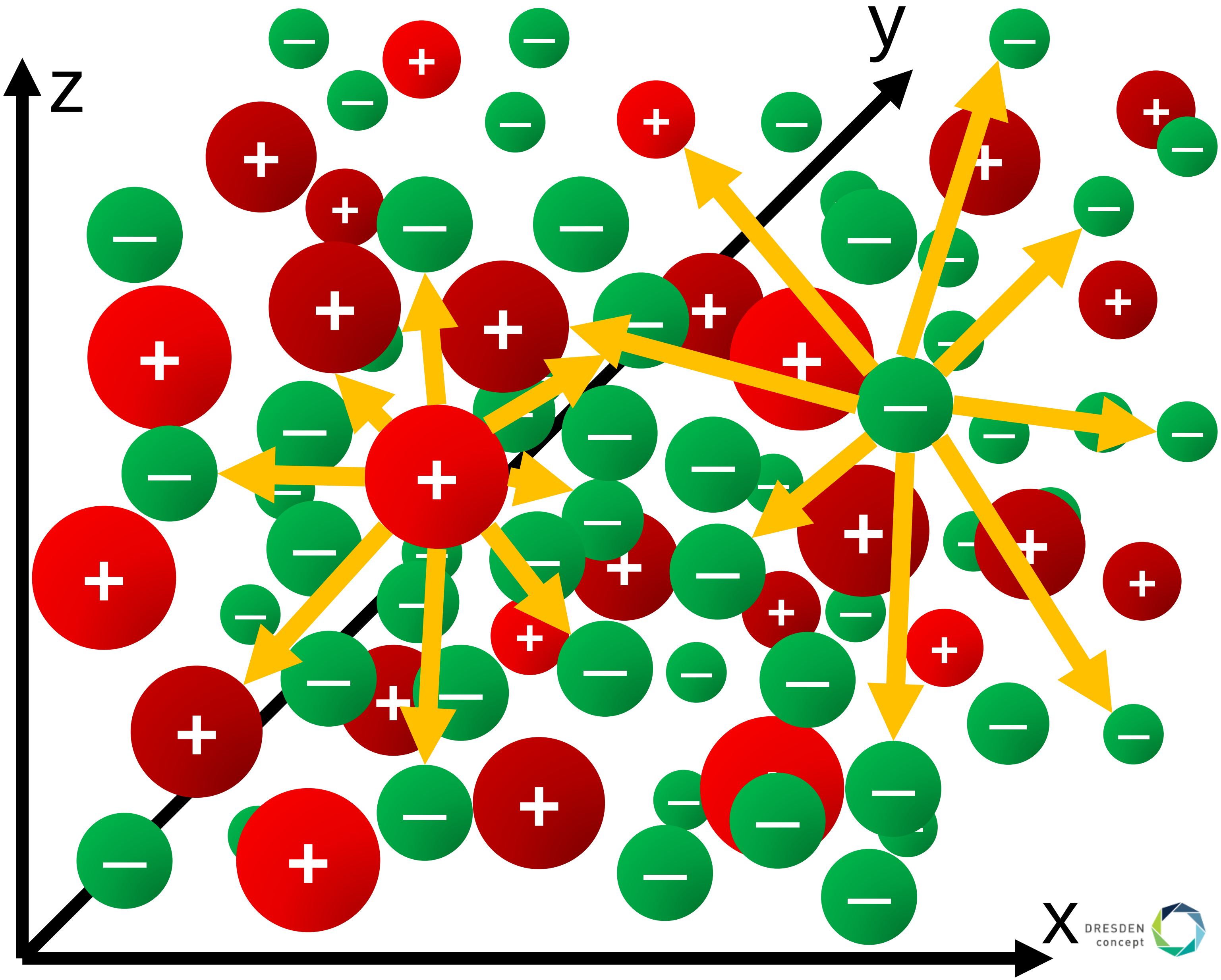
Dimensional reduction is possible and sensible

$\vec{r}, \vec{p}, \vec{E}, \vec{B}, \vec{j}, \vec{v}$ are vectors in 3D space

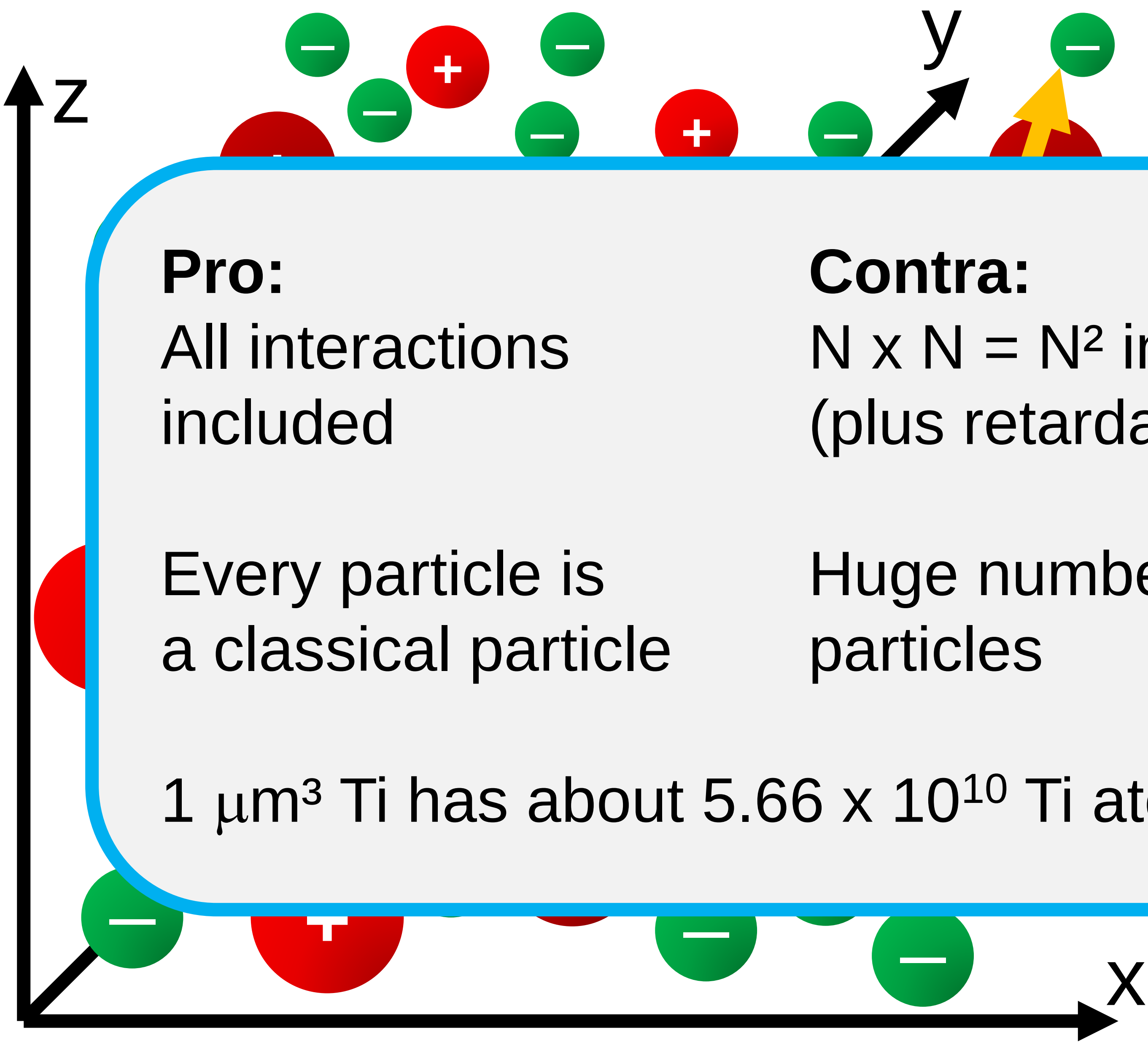
ρ is a scalar in 3D space

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Molecular Dynamics for probing the Vlasov-Maxwell-Equations



Molecular Dynamics for probing the Vlasov-Maxwell-Equations



Pro:
All interactions included

Every particle is a classical particle

Contra:
N x N = N² interactions (plus retardation)

Huge number N of particles

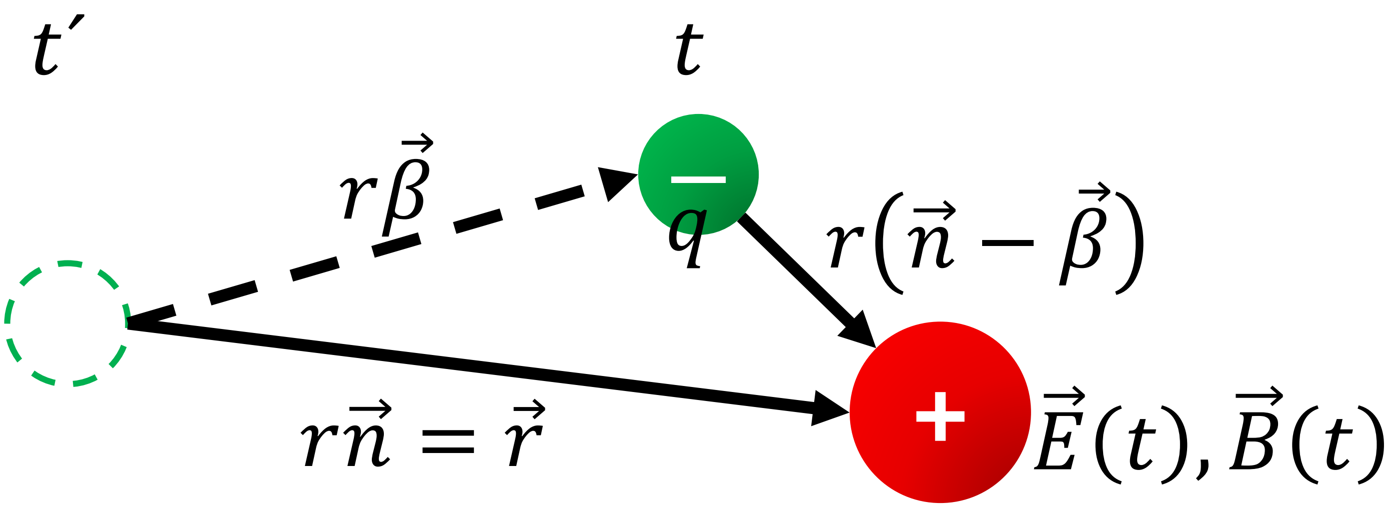
1 μm³ Ti has about 5.66 x 10^{10} Ti atoms

Efficient Molecular Dynamics on High Performance Computers (HPC)

Method	Resource
„Barnes-Hut"-like Tree Code	J. Barnes, P. Hut, *A hierarchical O(N log N) force-calculation algorithm*, **Nature, 324(4), 446,** 1986
Fast Multipole Methods	N. Engheta, et al., *The Fast Multipole Method for Electromagnetic Scattering Computation*, **IEEE Transactions on Antennas and Propagation 40, 634**, 1992

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The problem of retardation in Molecular Dynamics — Bookkeeping

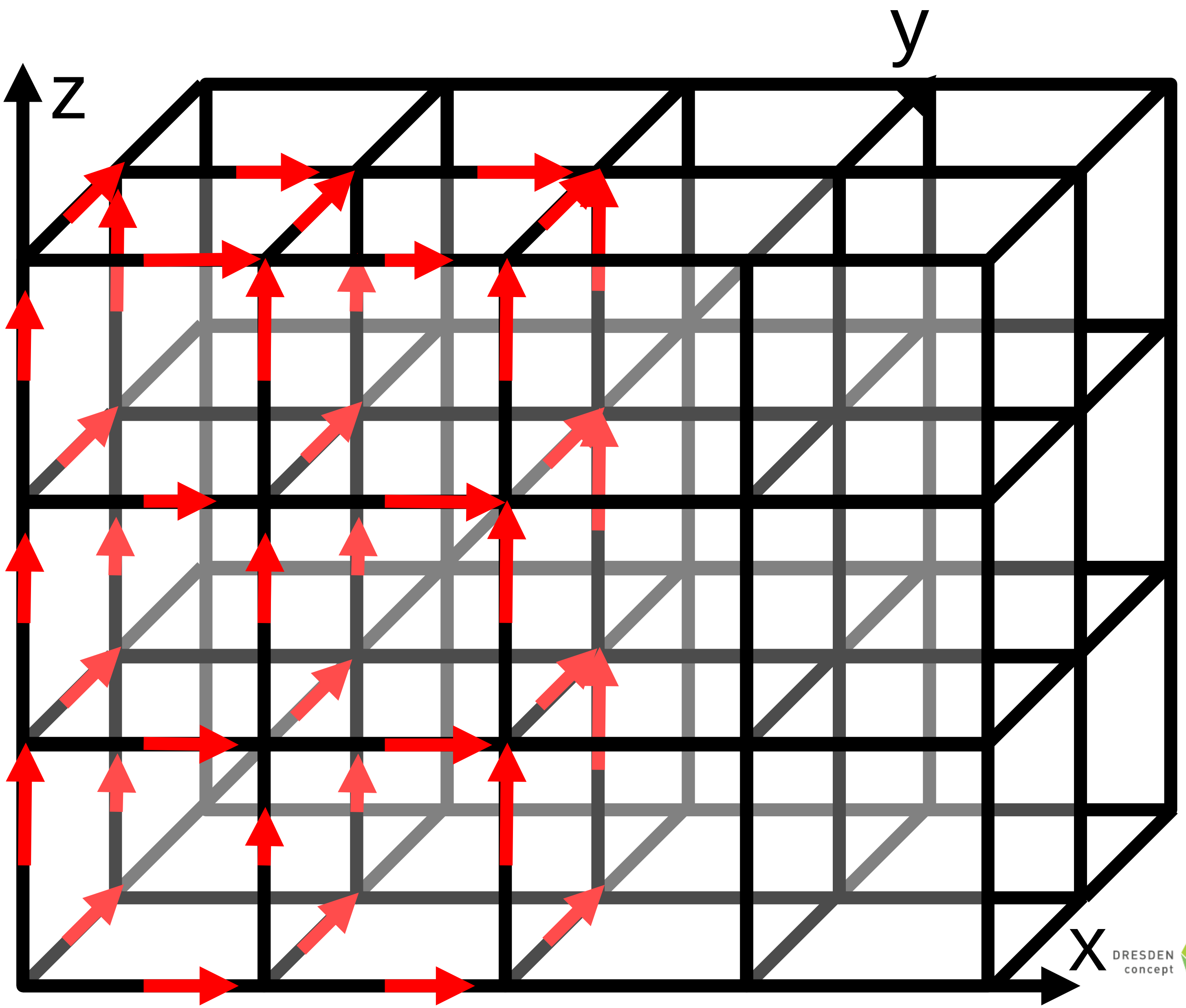


$$\vec{E}(t) = \frac{q}{4\pi\varepsilon_0} \frac{(1-\beta^2)(\vec{n}-\vec{\beta})}{r^2(1-\vec{n}\cdot\vec{\beta})^3} + \frac{\vec{n}\times\left((\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}\right)}{cr(1-\vec{n}\cdot\vec{\beta})^3}\Bigg|_{t'}$$

$$\vec{B}(t) = \frac{\vec{n}\times\vec{E}(t)}{c}\Bigg|_{t'}$$

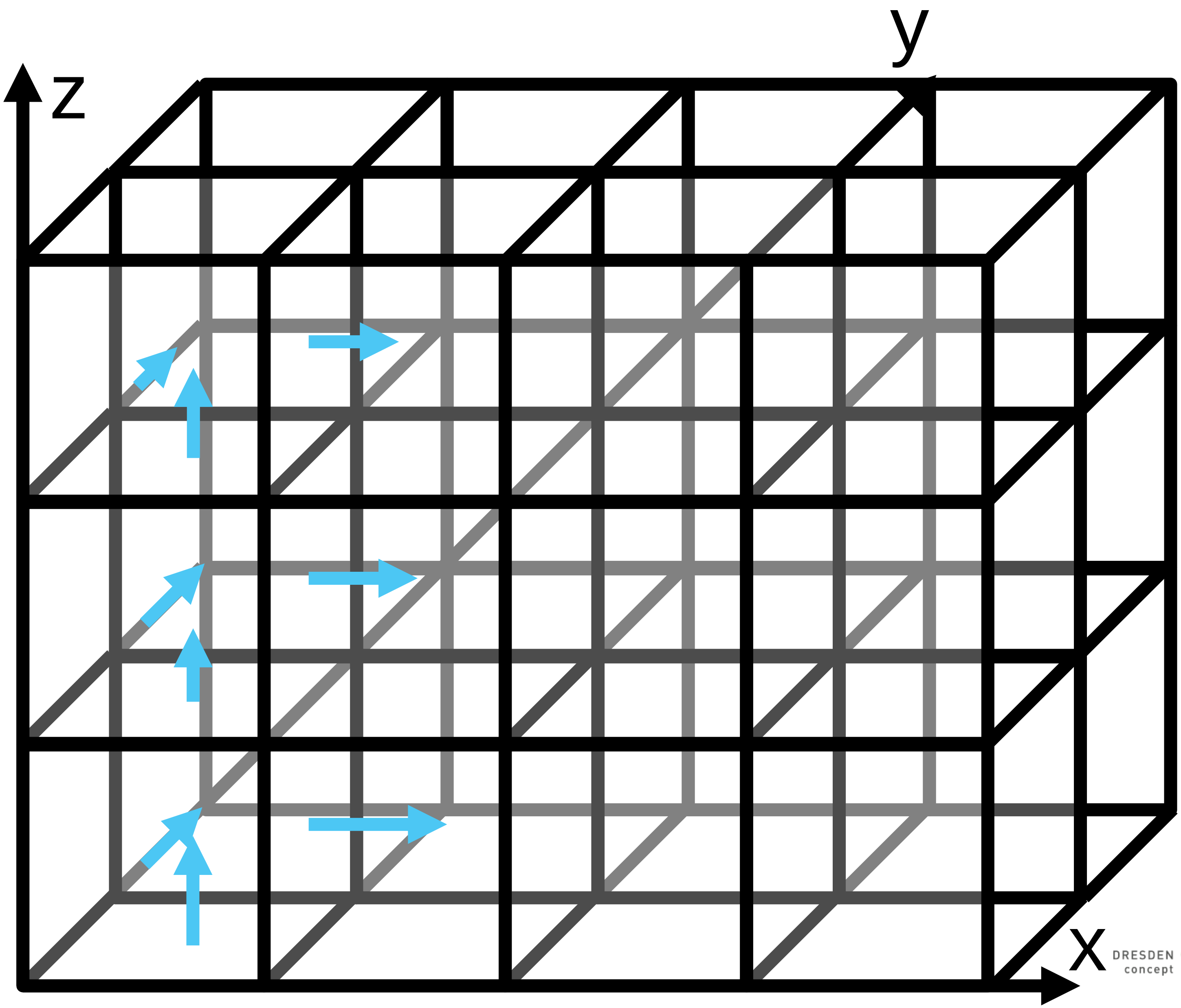
Liénard-Wiechert Fields

Long-range interactions via **electric** fields…

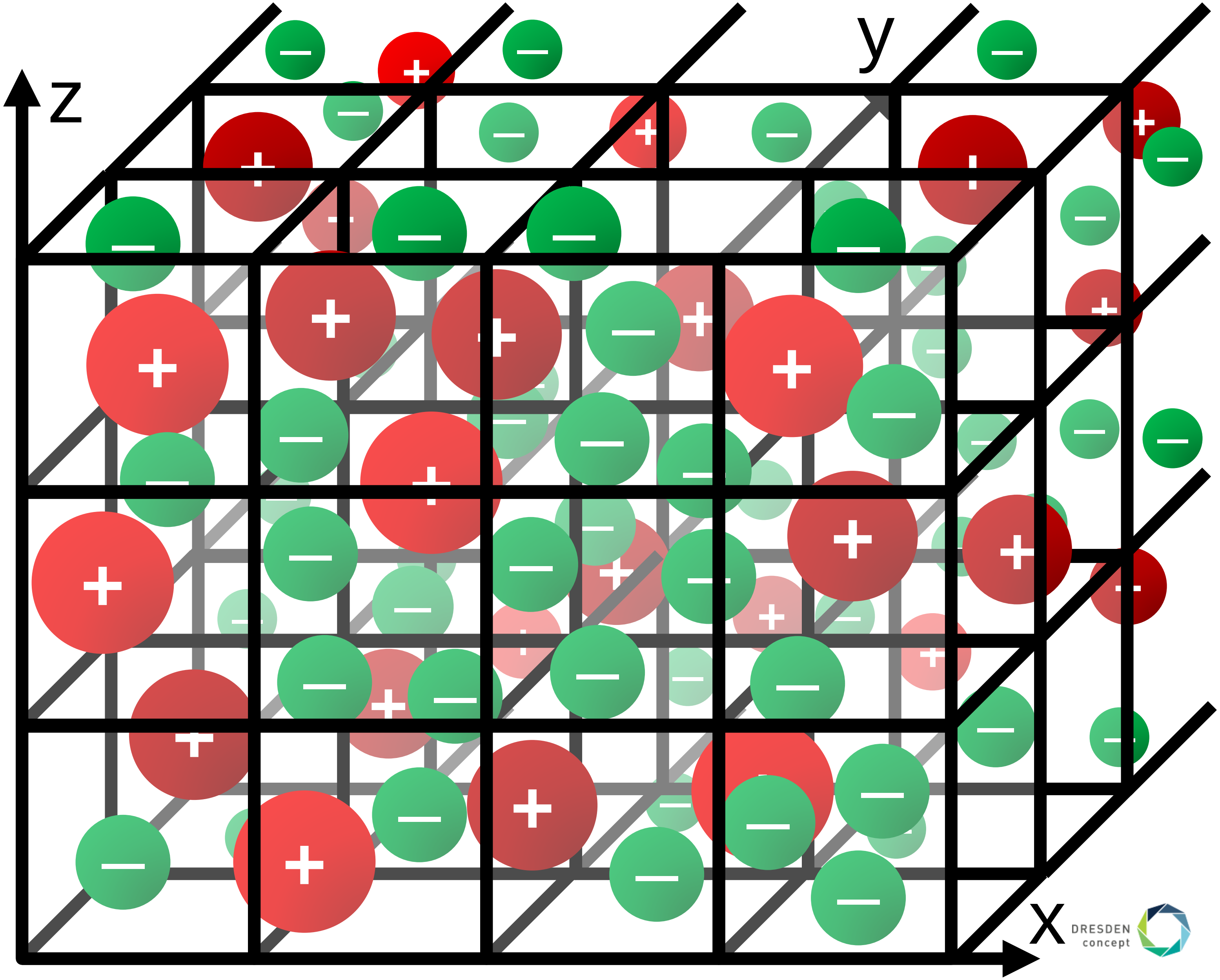


Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

… and **magnetic** fields (displaced by ½ grid cell)

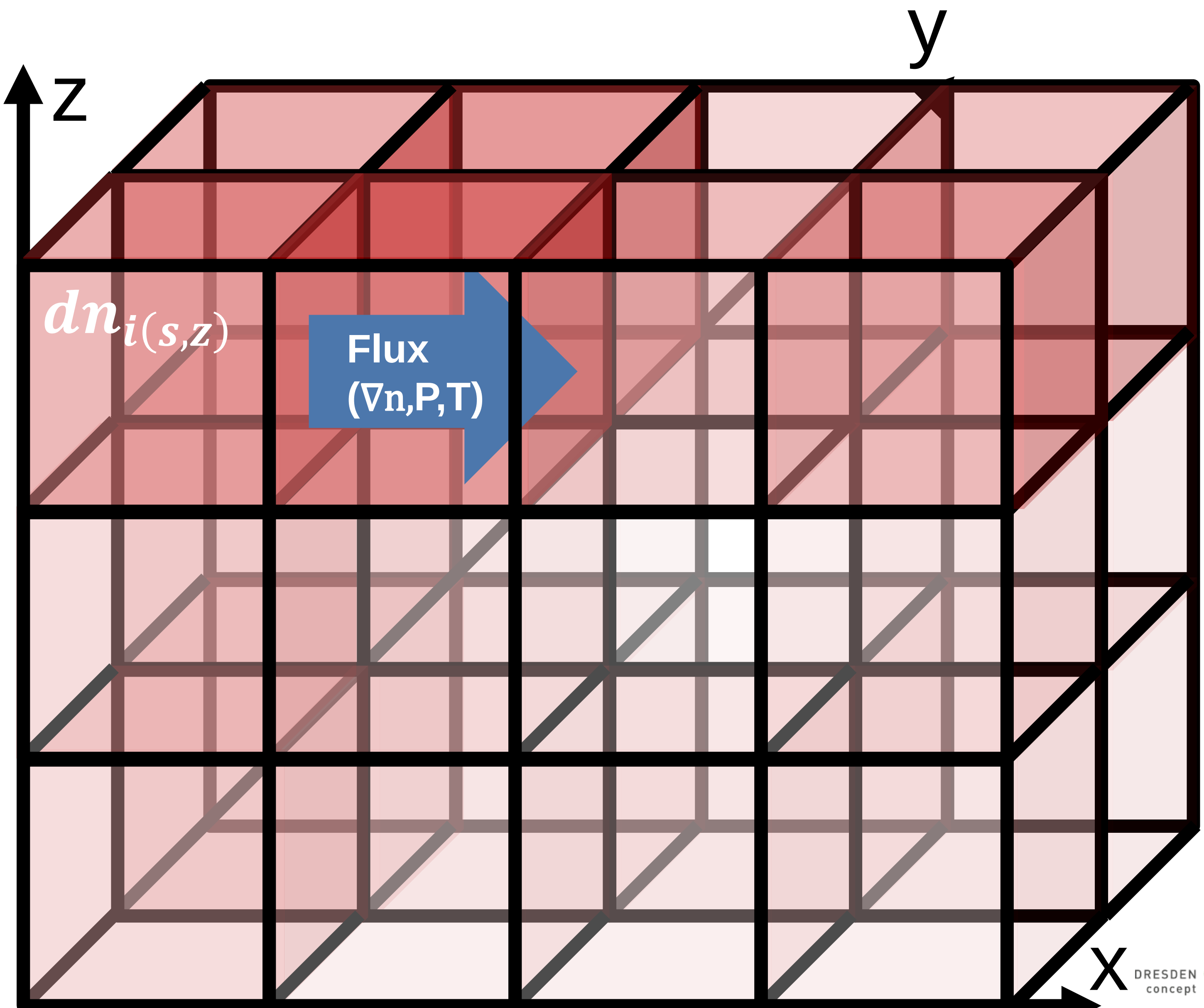


Average the particle densities n over a grid



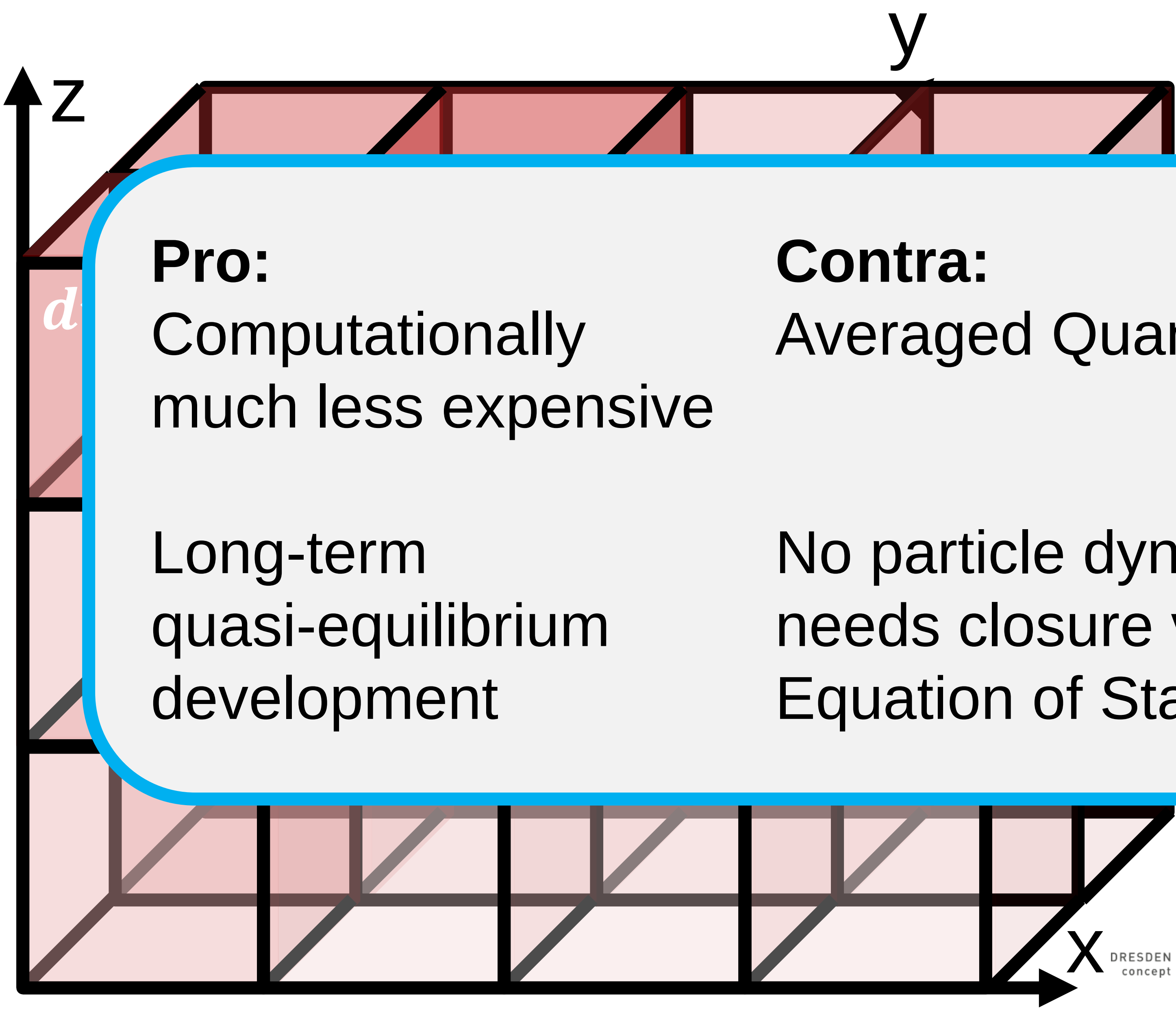
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Fluid Methods for probing the Vlasov-Maxwell-Equations



Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Fluid Methods for probing the Vlasov-Maxwell-Equations



Pro:

Computationally much less expensive

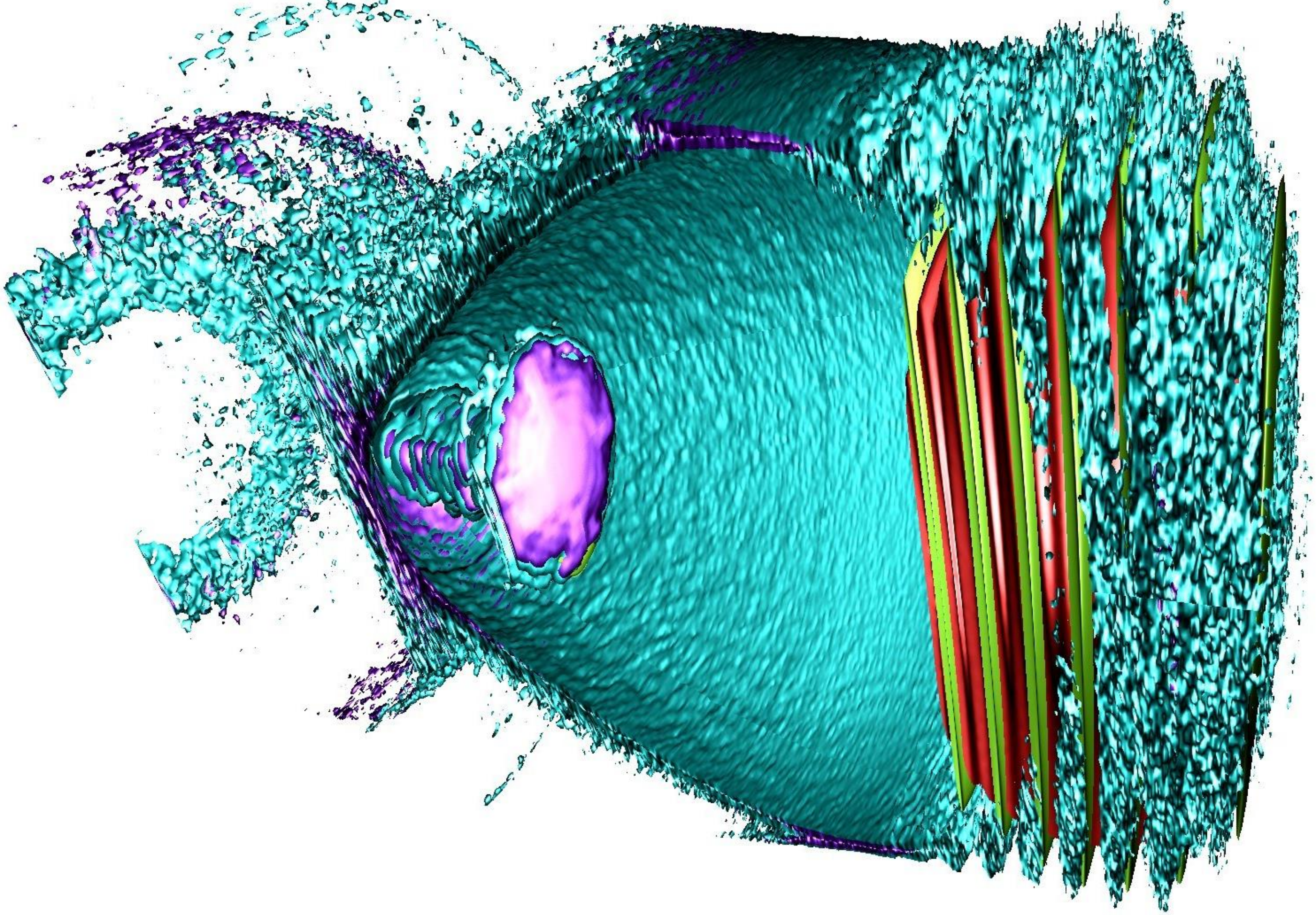
Long-term quasi-equilibrium development

Contra:

Averaged Quantities

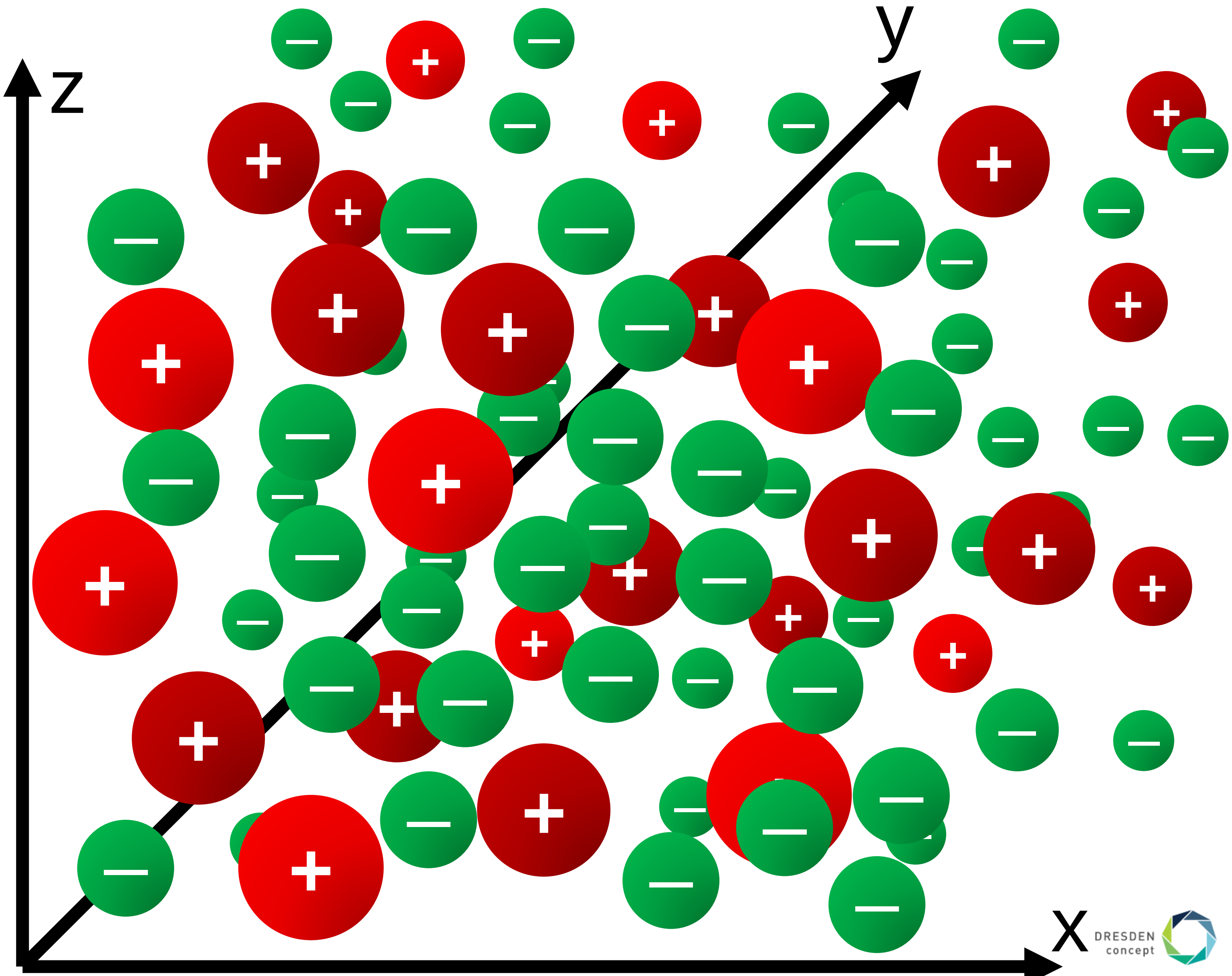
No particle dynamics, needs closure via Equation of State

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de



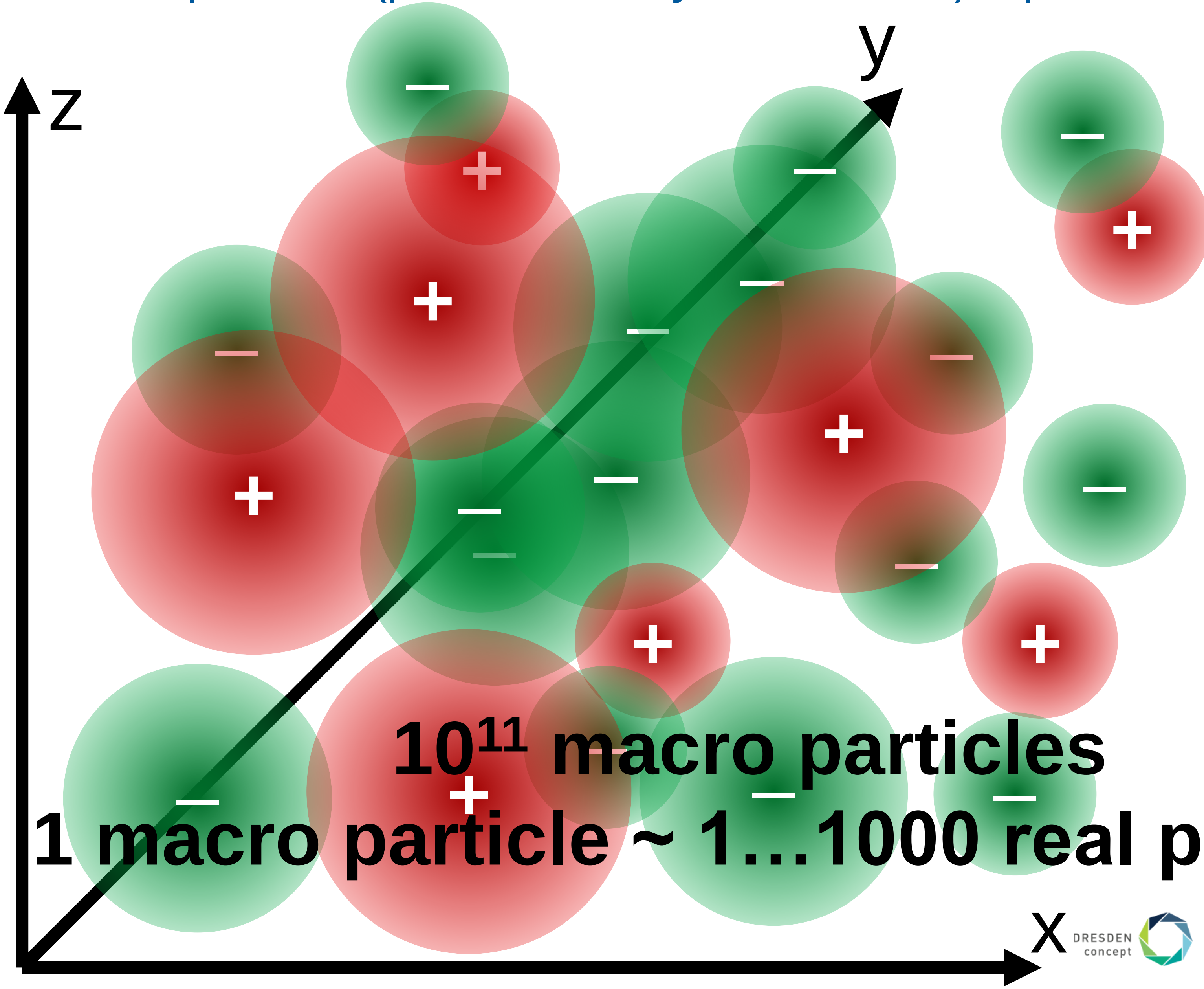
Particle-in-Cell

The PIC Method for probing the Vlasov-Maxwell-Equations



Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Macro particles (particle density distributions) replace real particles



10^{11} macro particles

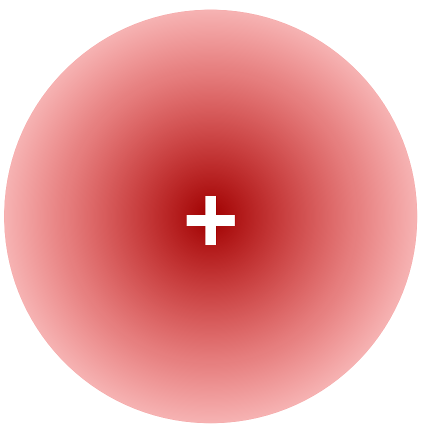
1 macro particle ~ 1…1000 real particles

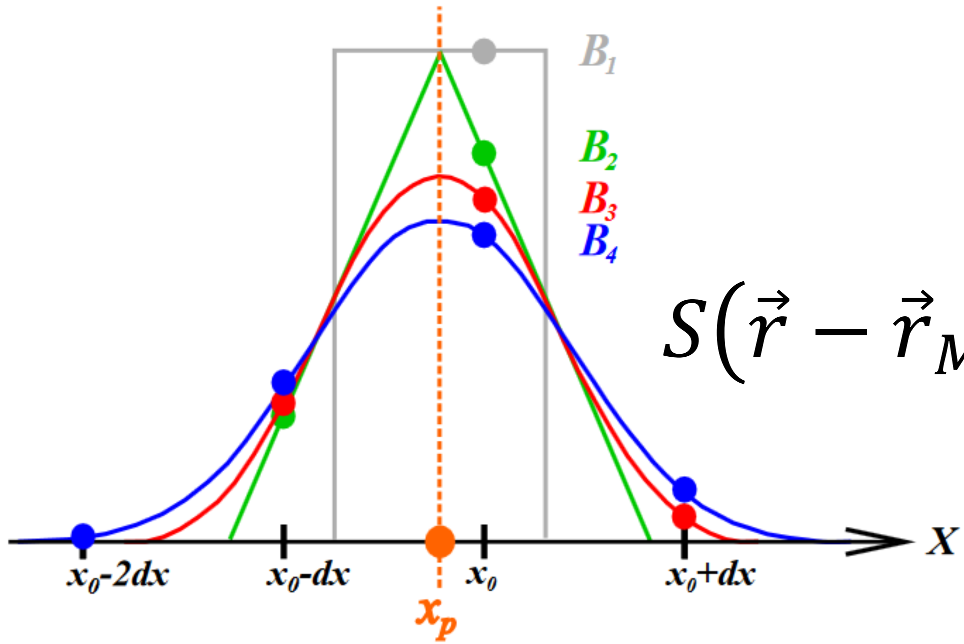
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Macroparticles (particle density distributions) replace real particles

$$f_{MP(x)}(\vec{r},\vec{p}) = w_x \delta\left(\vec{p}-\vec{p}_{MP(x)}\right) S\left(\vec{r}-\vec{r}_{MP(x)}\right)$$

$$\int\int f_{MP(x)}(\vec{r},\vec{p},t)\ d\vec{r}d\vec{p} = \int\int f_x(\vec{r},\vec{p},t)\ d\vec{r}d\vec{p}$$



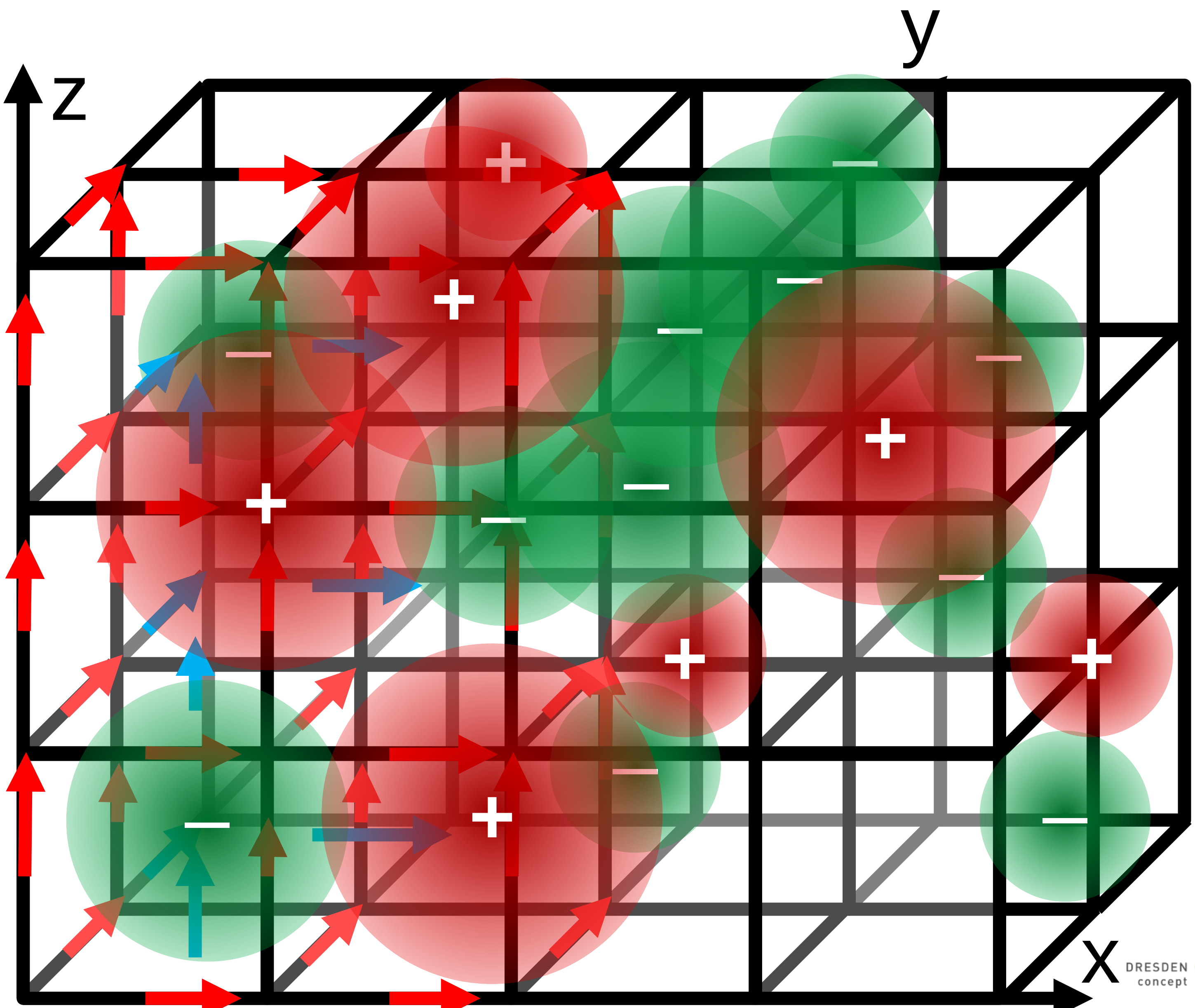


$$S\left(\vec{r}-\vec{r}_{MP(x)}\right)$$

T. Haugbølle, J.T. Frederiksen, Å. Nordlund,
Photon-plasma: A modern high-order particle-in-cell code,
Phys. Plasmas 20, 062904, 2013

DRESDEN concept HZDR

Fields are discretized on a (regular rectilinear) grid



$$l_{cell} \approx \lambda_{min}$$

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

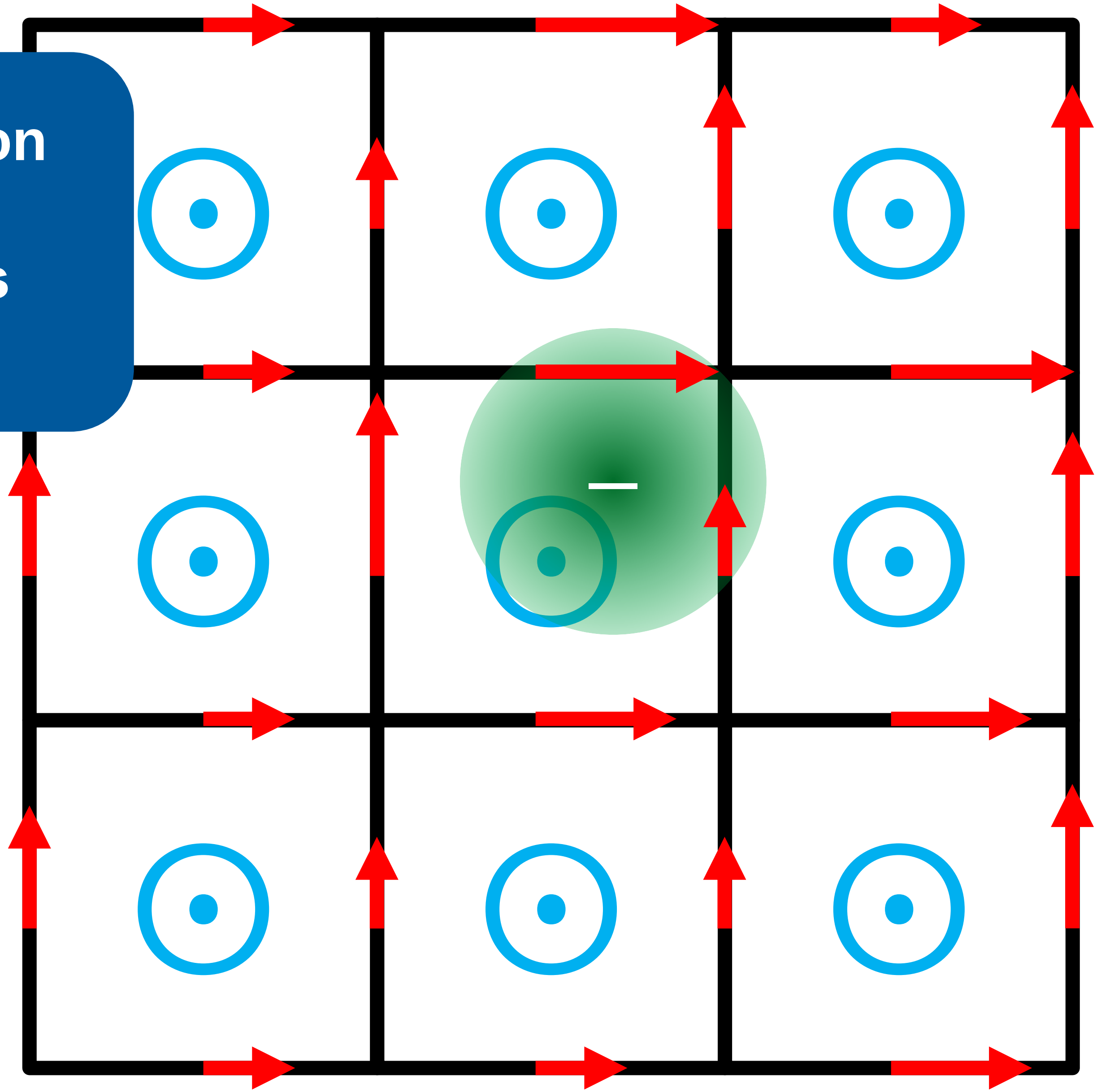
Field discretization on a rectilinear grid – The Yee Lattice

Method	**Resource**
„Yee-Lattice“	K.S. Yee, *Numerical solution of initial boundary value problems involving Maxwell’s equations in isotropic media*, **IEEE Transactions on Antennas and Propagation. 14, 302**, 1966

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Performing the particle-in-cell algorithm

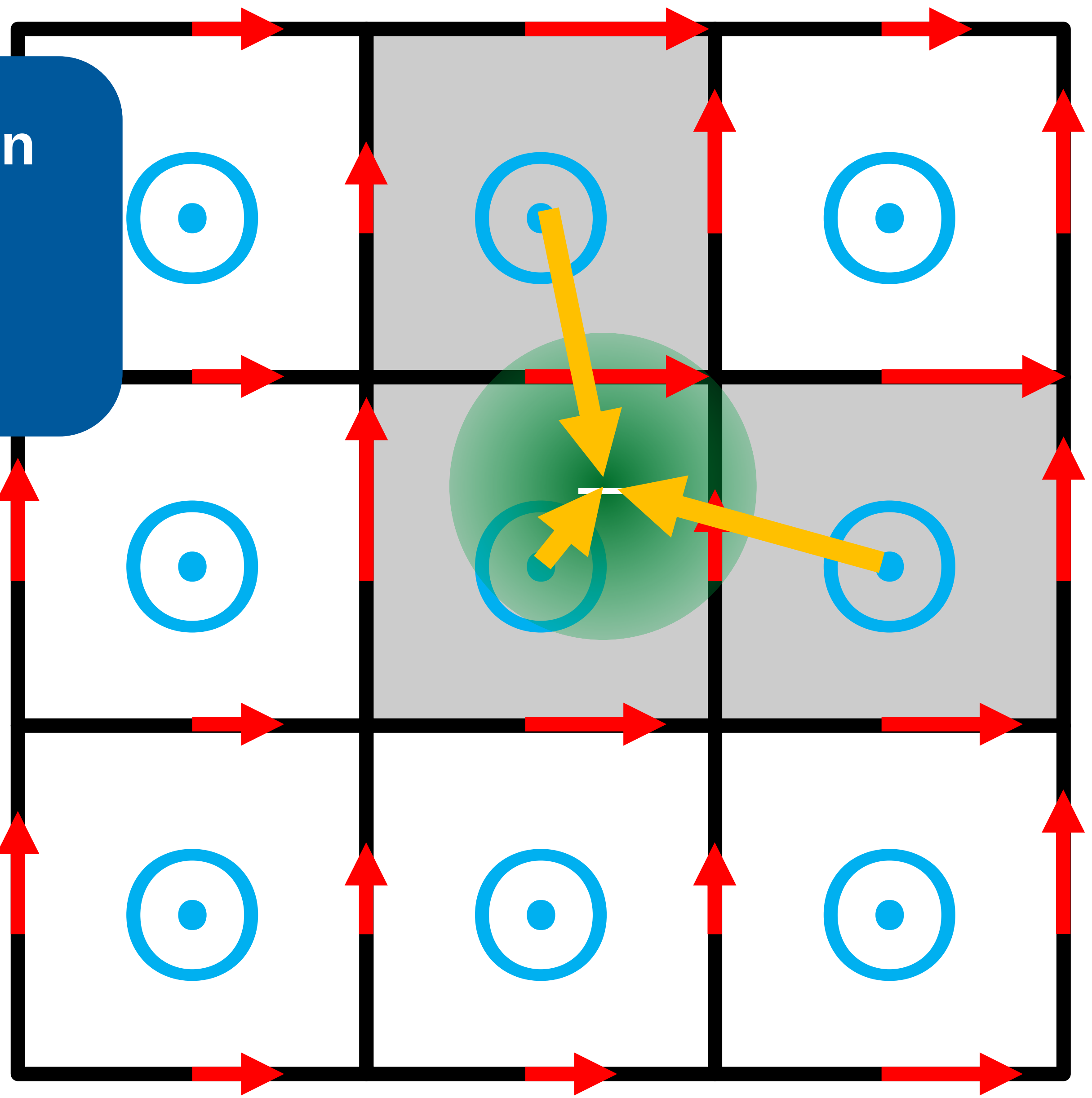
Field interpolation on the macroparticle's position



Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Fields interpolation (1 cell)

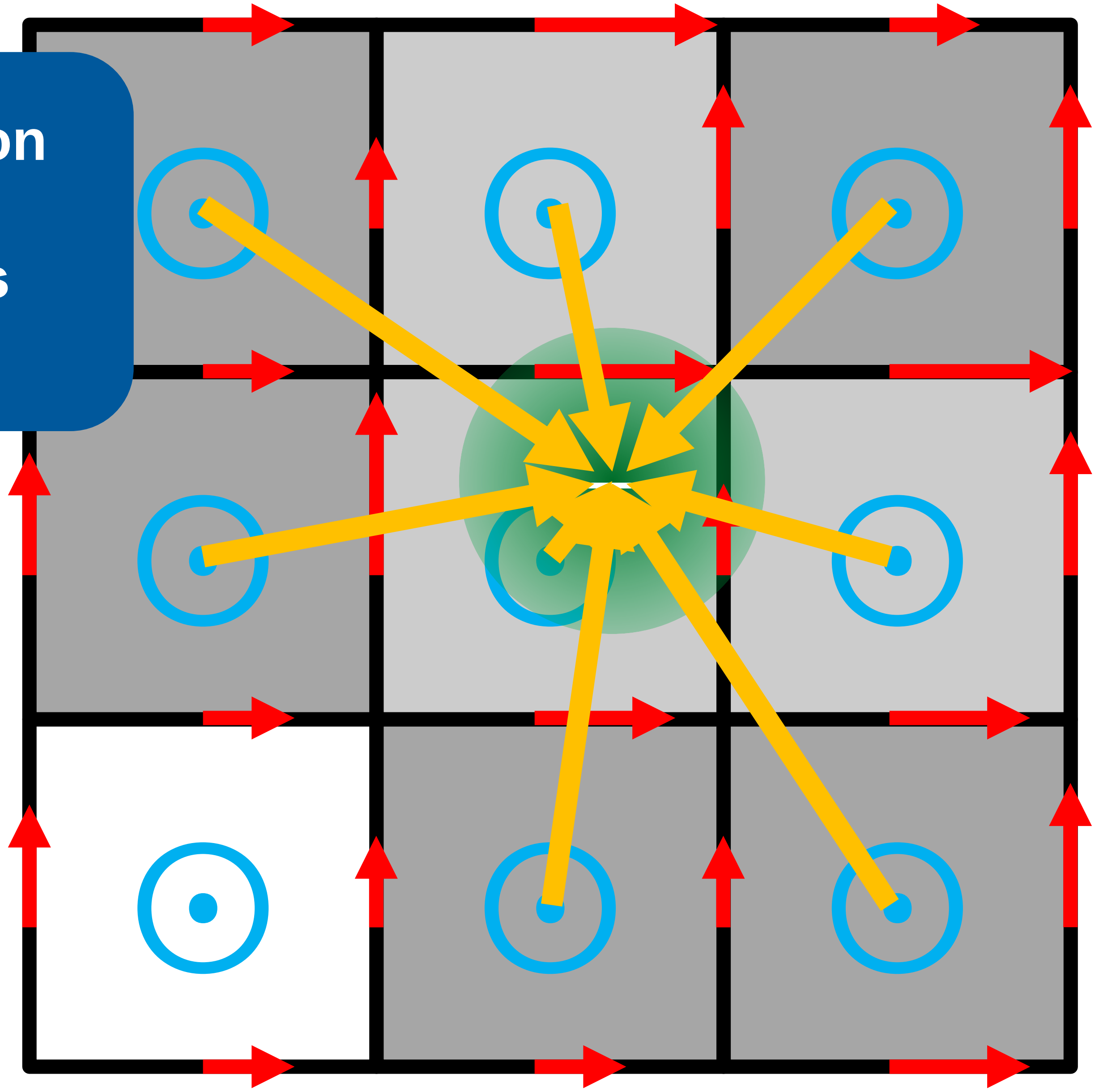
Field interpolation on the macroparticle‘s position



Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Fields interpolation (2 cells)

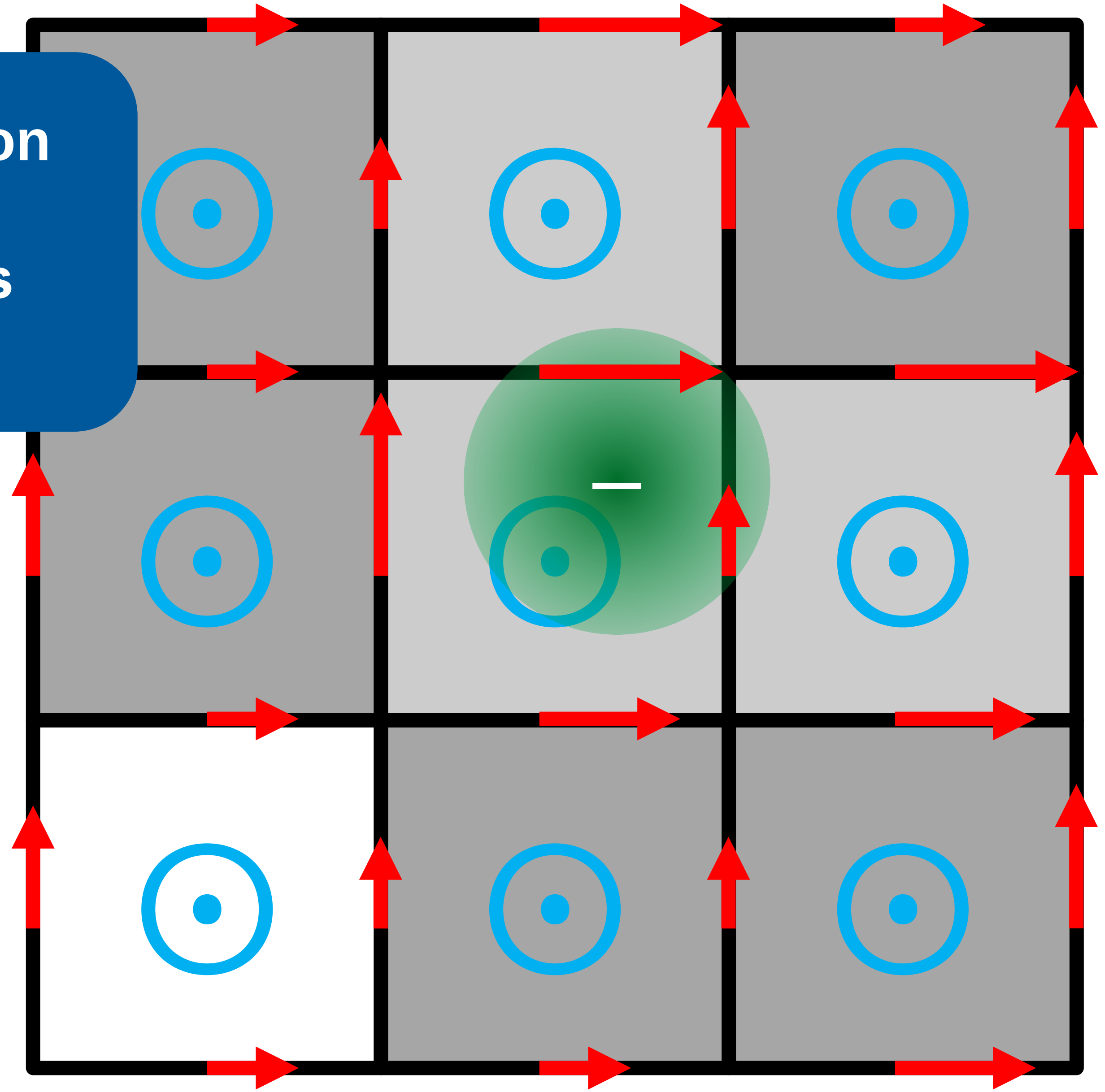
Field interpolation on the macroparticle‘s position



Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Fields interpolation — We need a lot of cells around each MP

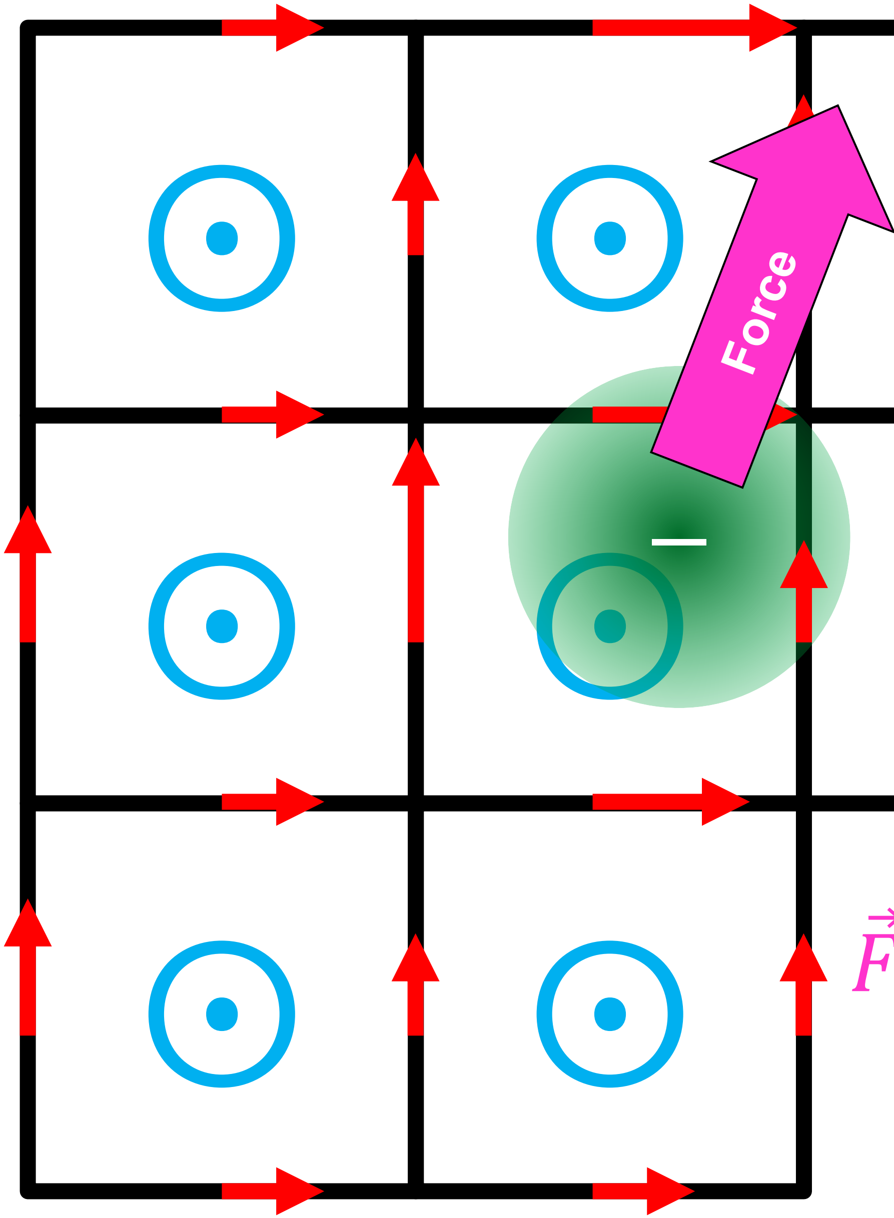
Field interpolation on the macroparticle's position



- **Use several cells around each MP for higher accuracy**
- **Act on the macro particle according to the shape function *S***

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

„Particle pusher“ (Integration of Equation of Motion)

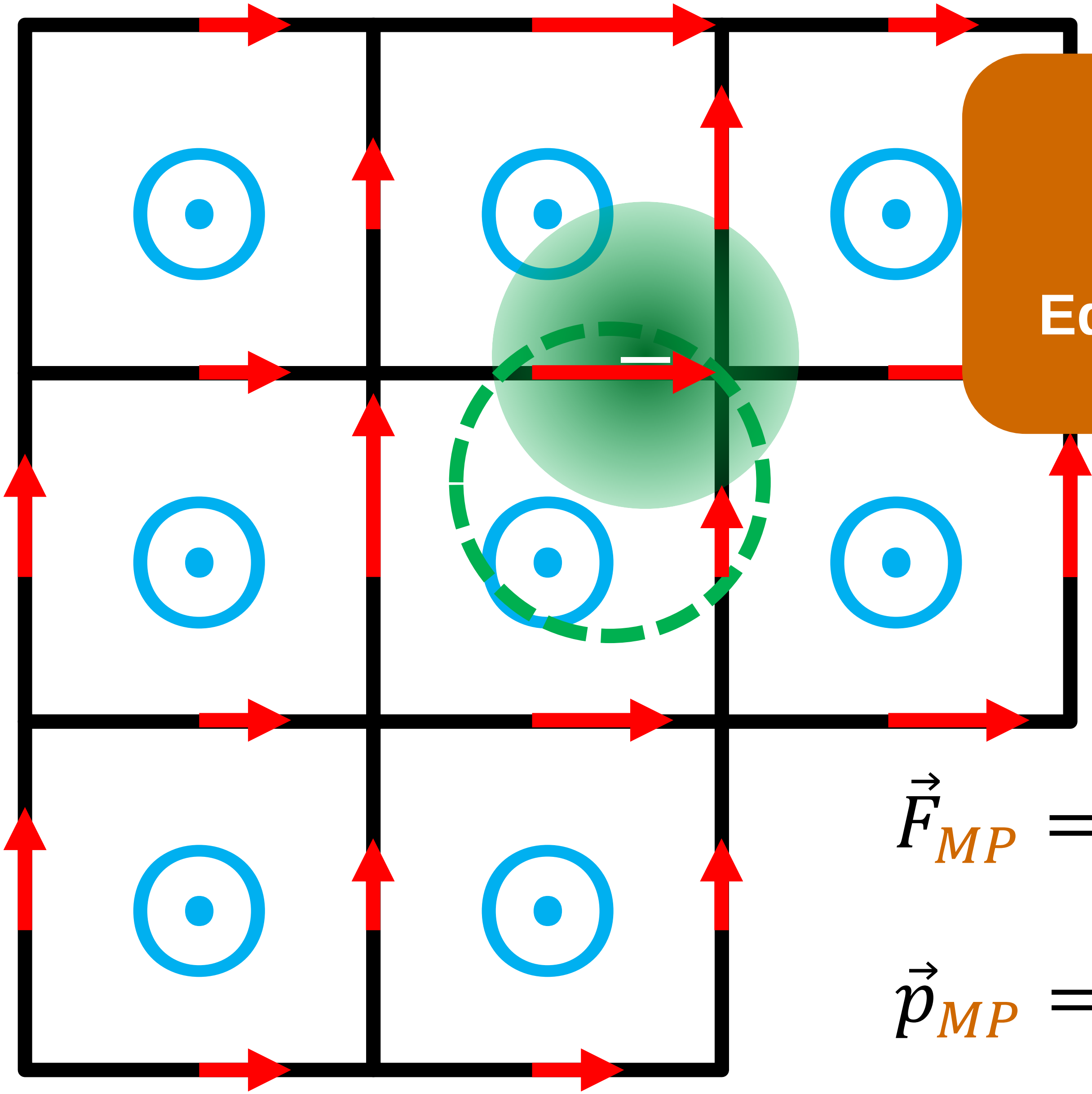


Particle Pusher Integration of Equation of Motion

$$\vec{F}_{MP} = Q_{MP}\, e \left(\vec{E} + \frac{\vec{v}_{MP}}{c} \times \vec{B} \right)$$

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

„Particle pusher“ (Integration of Equation of Motion)

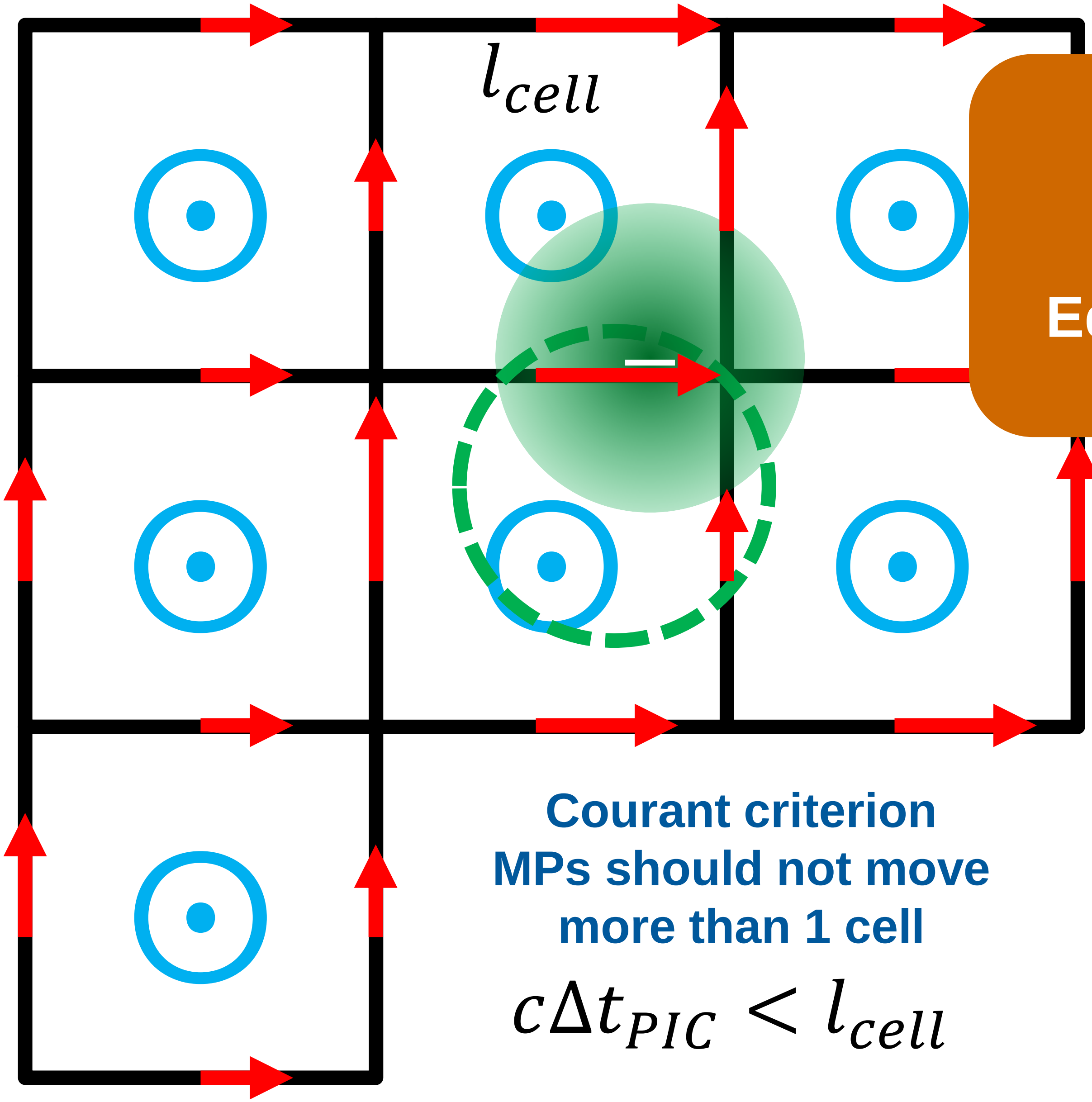


Particle Pusher Integration of Equation of Motion

$$\vec{F}_{MP} = \frac{d\vec{p}_{MP}}{dt}$$

$$\vec{p}_{MP} = \gamma_{MP} m_{MP} \frac{d}{dt}\vec{r}_{MP}$$

„Particle pusher“ (Integration of Equation of Motion)



Particle Pusher Integration of Equation of Motion

- **Energy and momentum conservation?**
- **Sub-stepping in time (leapfrog)**

Courant criterion
MPs should not move more than 1 cell

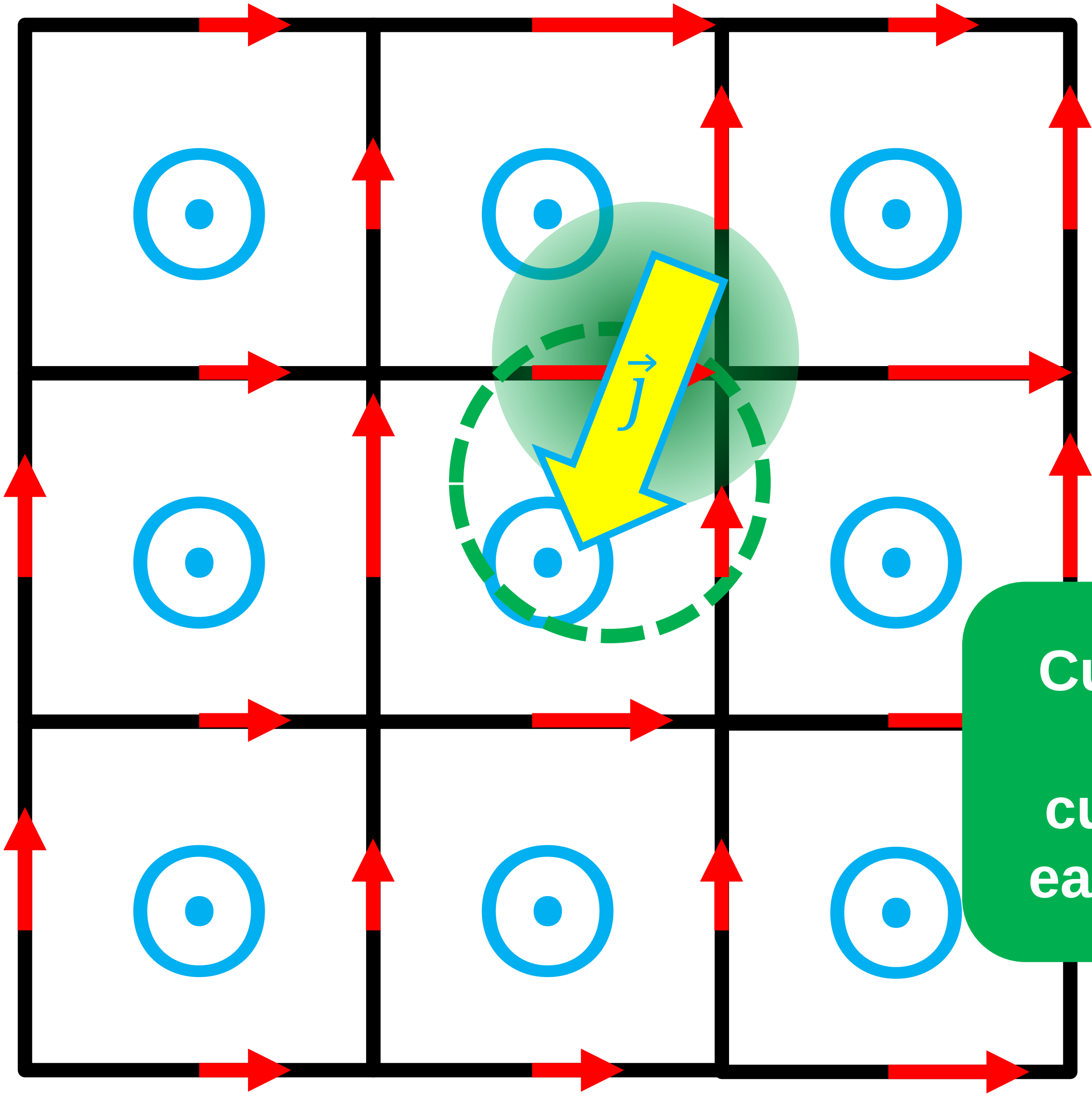
$$c\Delta t_{PIC} < l_{cell}$$

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

„Particle pusher“ (Integration of Equation of Motion)

Method	Resource
„Boris-Pusher“	J.P. Boris, *Relativistic plasma simulation-optimization of a hybrid code,* **Proceedings of the 4th Conference onNumerical Simulation of Plasmas, Naval Res. Lab., Washington, D.C.**, **3**, 1970
„Vay-Pusher“	J.-L. Vay, D.P. Grote, R.H. Cohen, A. Friedman, *Novel methods in the Particle-In-Cell accelerator Code-Framework Warp,* **Computational Science & Discovery 5(1), 014019**, 2012

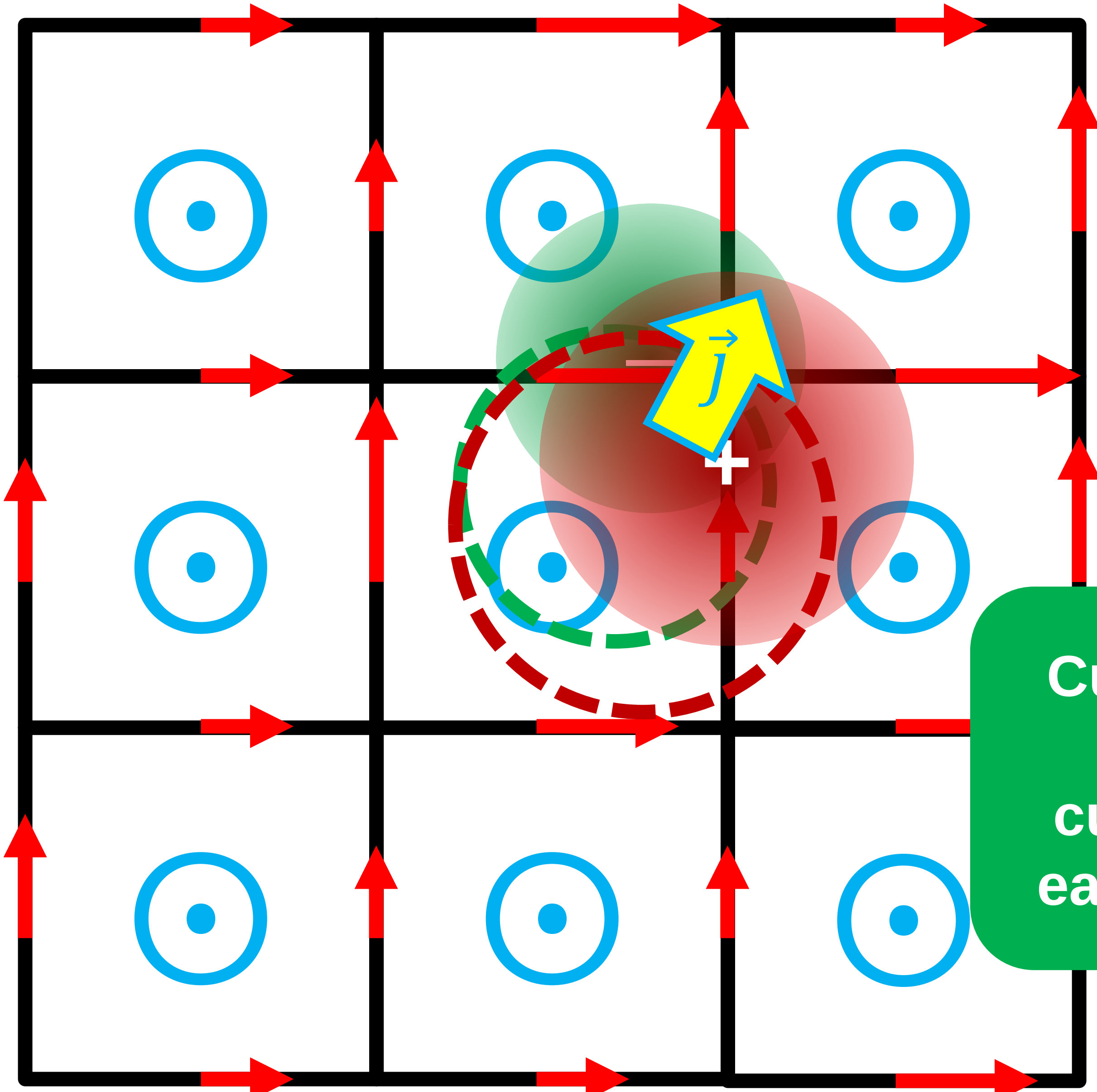
„Current Deposition“ – Computing the current density



Current Deposition Computing the current density for each macro particle

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The only relevant measure is the total current of all MP

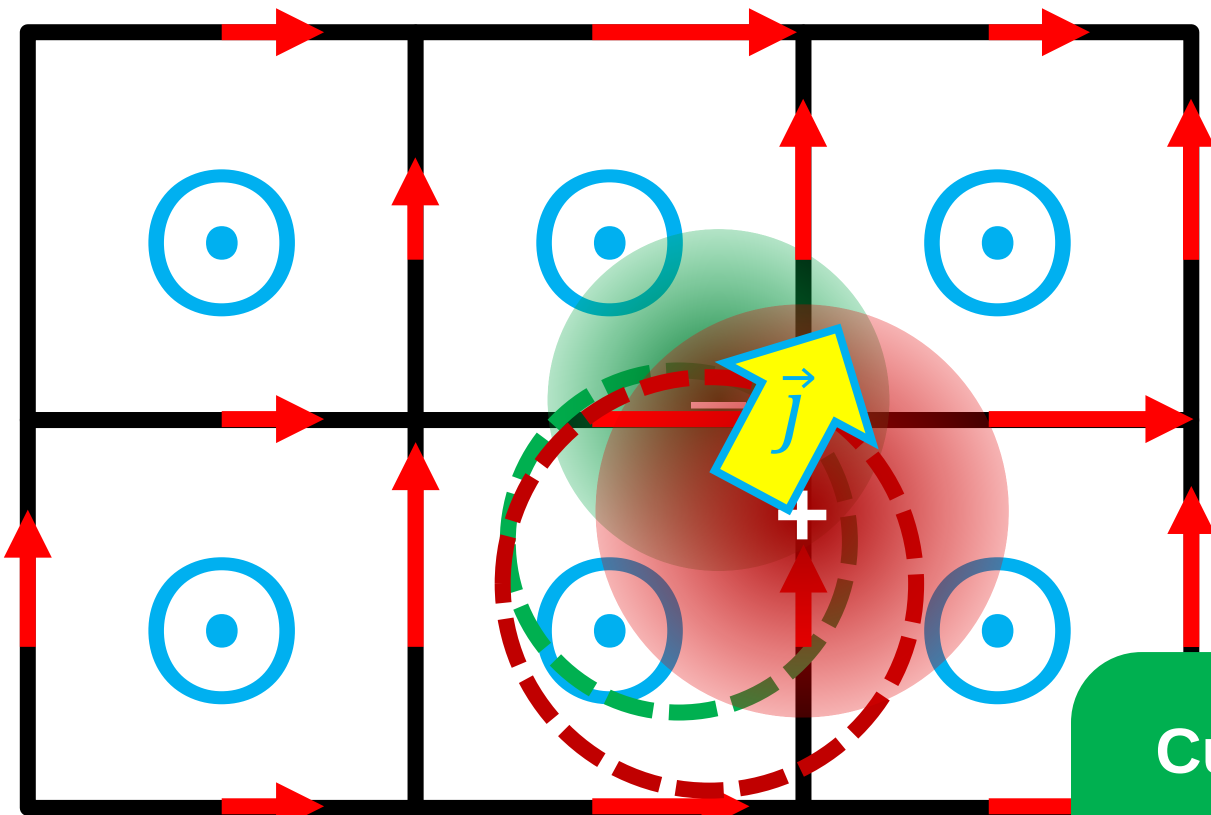


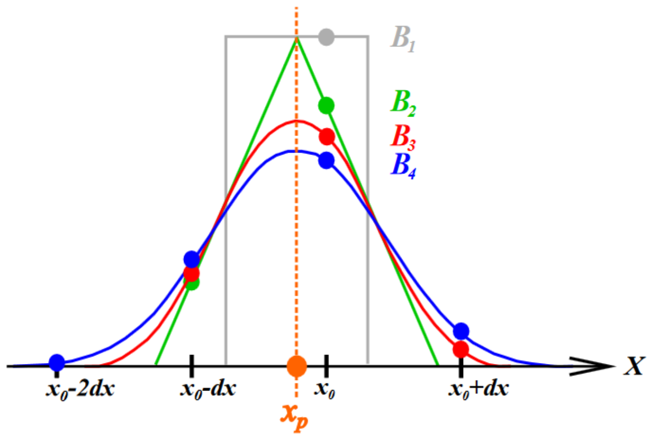
$$\vec{j} = \sum_{i}^{MP} \vec{j}_i$$

Current Deposition Computing the current density for each macro particle

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The only relevant measure is the total current of all MP



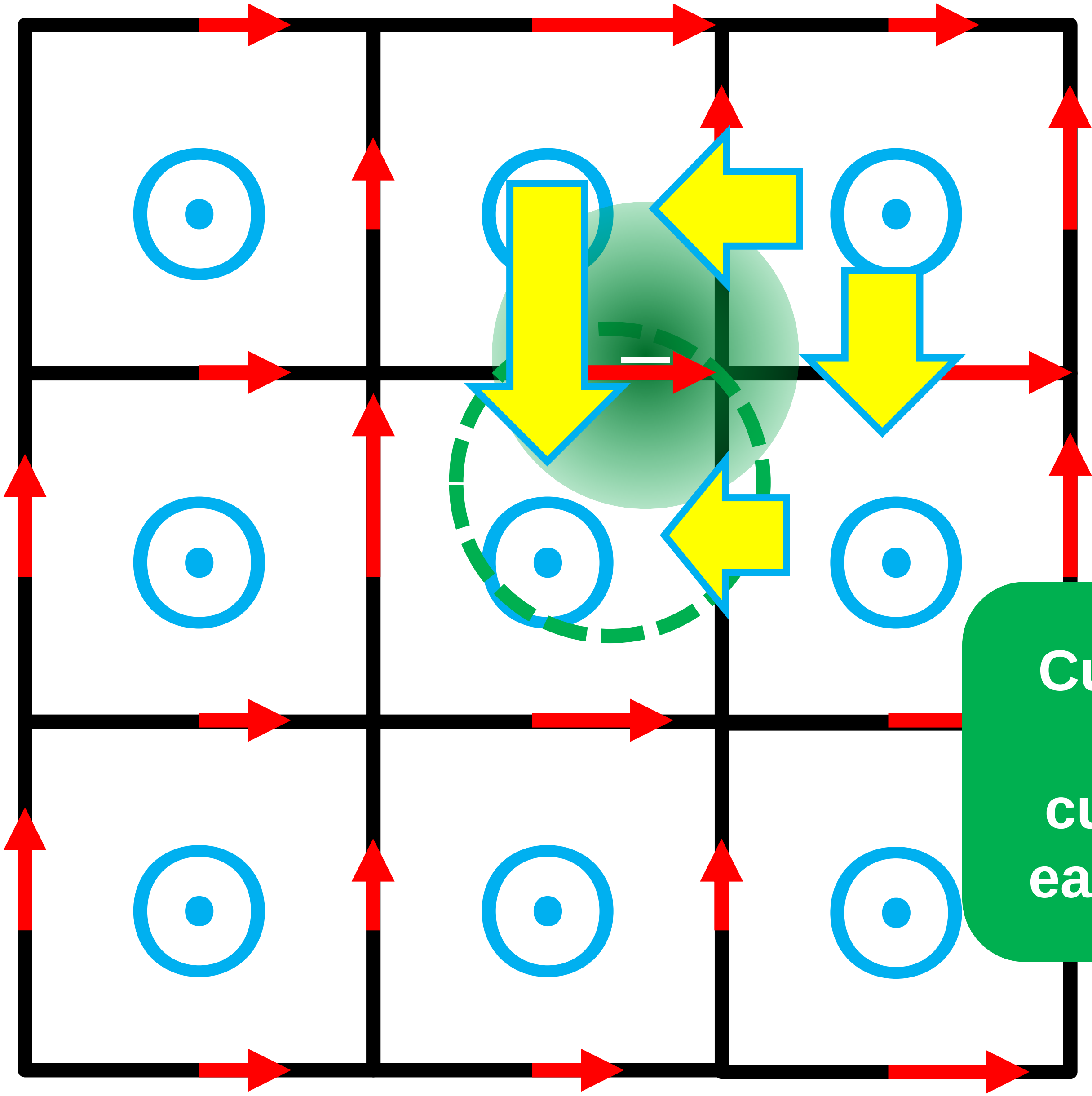


Discrete MPs create noise in current

Current Deposition Computing the current density for each macro particle

$$\vec{j} = \sum_{i}^{MP} Q_{MP} \int f_{MP} \, d\vec{l}_{cell}$$

Current splitting schemes – Achieving conservation of charge



$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho$$

Current Deposition
Computing the current density for each macro particle

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

„Current Deposition“ – Computing the total current density

Method	Resource
„Villasenor-Buneman“	J. Villasenor, O. Buneman, *Rigorous charge conservation for local electromagnetic field solvers*, **Computer Physics Communications 69(2-3), 306**, 1992
„Esirkepov“	T. Zh. Esirkepov, *Exact charge conservation scheme for Particle-in-Cell simulation with an arbitrary form-factor*, **Computer Physics Communications 135(2), 144**, 2001
„Umeda“/“Zig-zag“	T Umeda, et al., *A new charge conservation method in electromagnetic particle-in-cell simulations*, **Computer Physics Communications 156(1), 73,** 2003

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

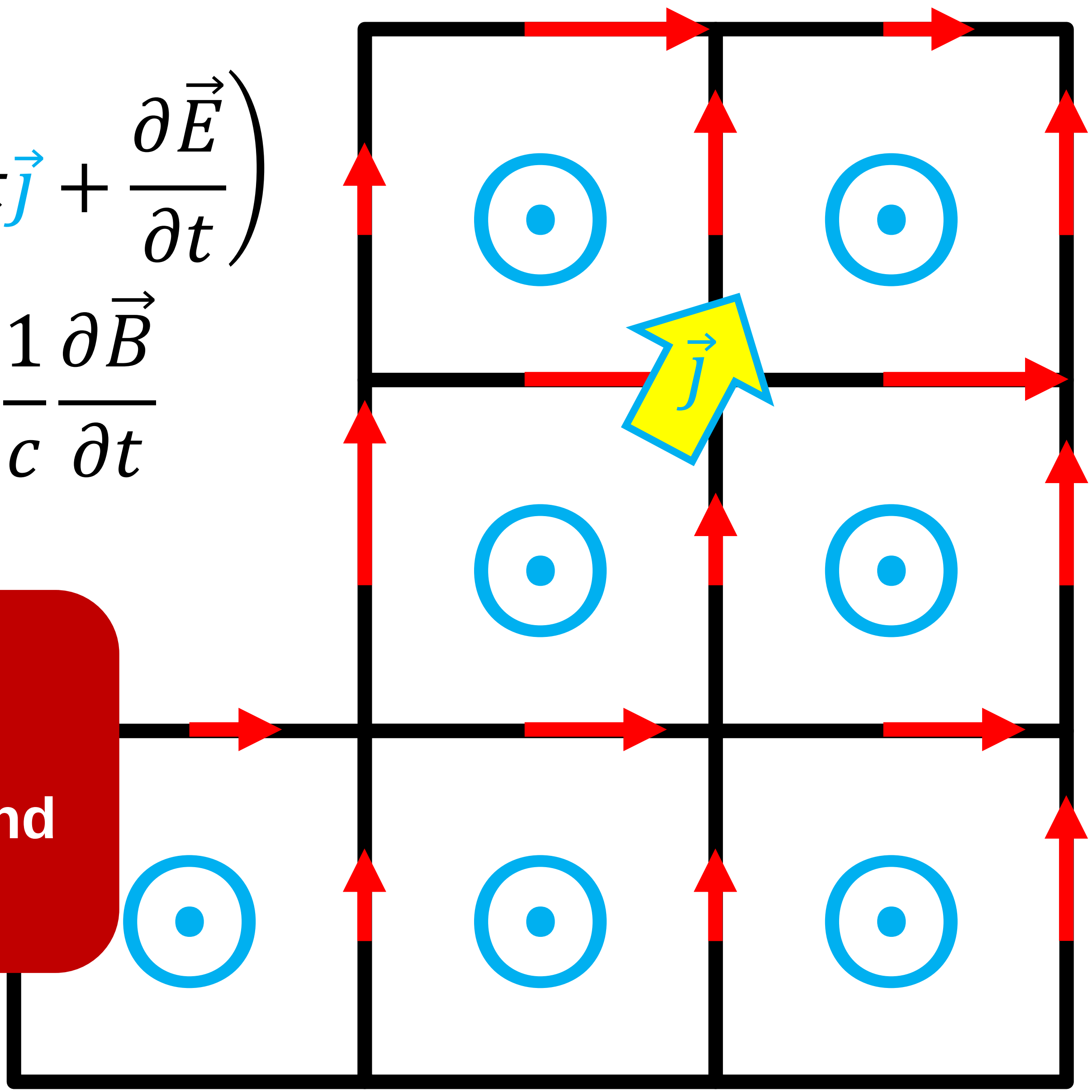
„Maxwell Solver“ – Solving 50% of Maxwell‘s Equations

$$\vec{\nabla} \times \vec{B} = \frac{1}{c}\left(4\pi\vec{j} + \frac{\partial \vec{E}}{\partial t}\right)$$

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$$

Maxwell Solver

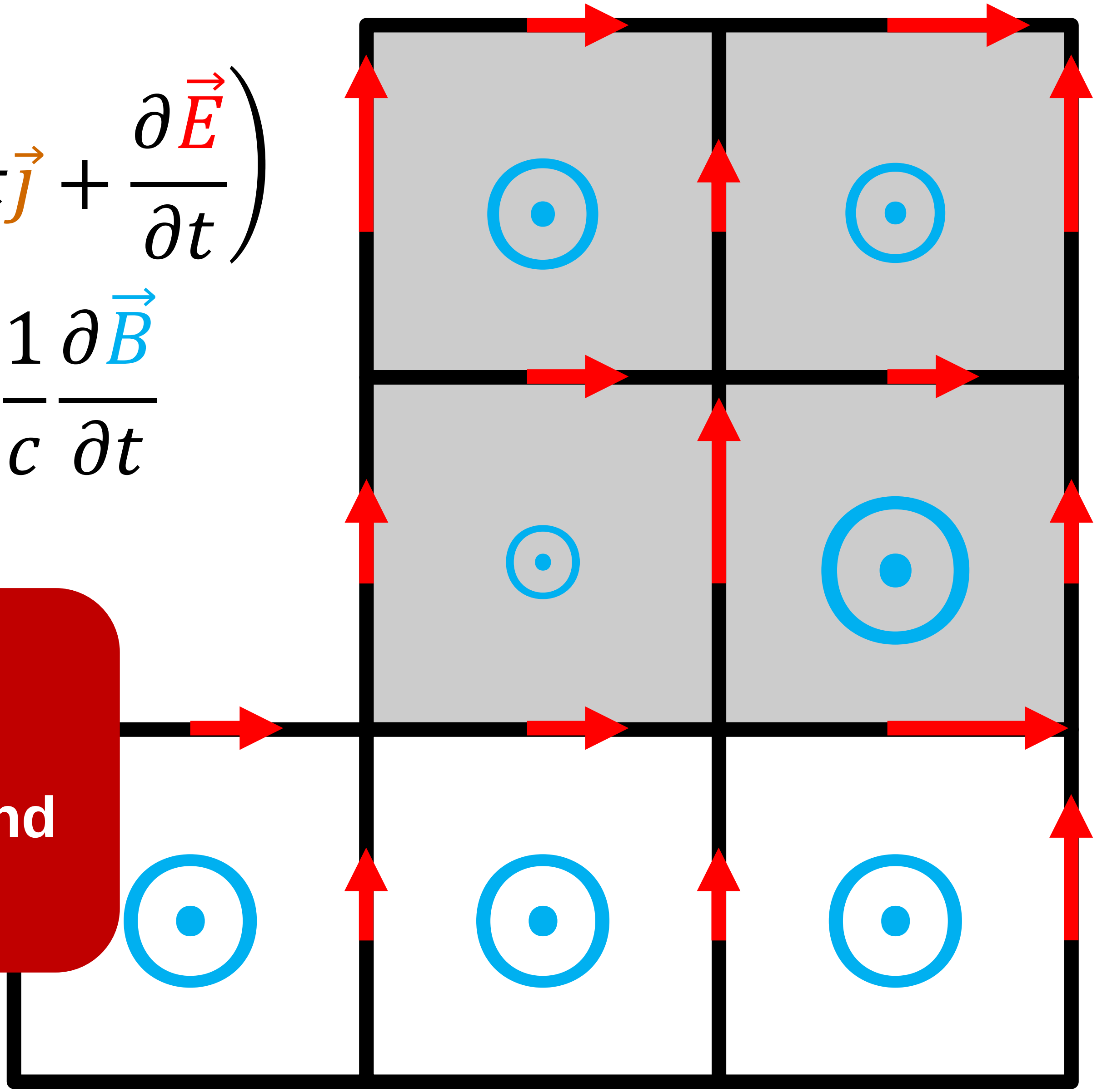
Solve Ampére‘s and Faraday‘s Law



„Maxwell Solver“ – Solving 50% of Maxwell‘s Equations

$$\vec{\nabla} \times \vec{B} = \frac{1}{c}\left(4\pi \vec{j} + \frac{\partial \vec{E}}{\partial t}\right)$$

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$$



Maxwell Solver

Solve Ampére‘s and Faraday‘s Law

The particle-in-cell Cycle

Field interpolation on the macroparticle‘s position

→

Particle Pusher
Integration of Equation of Motion

↓

Current Deposition
Computing the current density for each macro particle

←

Maxwell Solver

Solve Ampére‘s and Faraday‘s Law

↑ (back to Field interpolation)

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Books on Particle-in-Cell Techniques

Method	**Resource**
„Particle-Mesh“ Basics	R.W. Hockney, J.W. Eastwood *Computer Simulation Using Particles*
„Particle-in-Cell“ for Plasmas	C.K. Birdsall, A.B. Langdon *Plasma Physics via Computer Simulation*
„Particle-in-Cell“ Theory	Yu.N. Grigoryev *Numerical "Particle-in-cell" Methods: Theory and Applications*

It‘s all wrong!!!
Issues with PIC

Issues for the Particle-in-Cell Technique – An incomplete list

Problem	Resource
Energy Conservation	S. Markidis, G. Lapenta, *The energy conserving particle-in-cell method*, **Journal of Computational Physics 230(18), 7037**, 2011
Momentum Conservation	G.B. Jacobs, J.S. Hesthaven, *Implicit–explicit time integration of a high-order particle-in-cell method with hyperbolic divergence cleaning*, **Computer Physics Communications 180(10), 1760**, 2009
Charge Conservation	„Villasenor-Buneman“, „Esirkepov“, „Umeda“/“Zig-Zag“, etc.
„Numerical Heating“	E. Cormier-Michel, et al., *Unphysical kinetic effects in particle-in-cell modeling of laser wakefield accelerators*, **Phys. Rev. E 78, 016404**, 2008
„Close Collisions“	Y. Sentoku, A.J. Kemp, *Numerical methods for particle simulations at extreme densities and temperatures: Weighted particles, relativistic collisions and reduced currents*, **Journal of Computational Physics 227(14), 6846**, 2008

DRESDEN concept HZDR

Issues for the Particle-in-Cell Technique – An incomplete list

Problem	Resource
Field Ionization	R. Nuter et al., *Field ionization model implemented in Particle In Cell code and applied to laser-accelerated carbon ions*, **Phys. Plasmas 18, 033107**, 2011
Collisional Ionization	A.J. Kemp, et al., *Modeling ultrafast laser-driven ionization dynamics with Monte Carlo collisional particle-in-cell simulations*, **Phys. Plasmas 11, 5648,** 2004
Energy Transport in overdense Plasmas	R. Mishra, et. al., *Collisional particle-in-cell modeling for energy transport accompanied by atomic processes in dense plasmas*, **Phys. Plasmas 20, 072704**, 2013
„Numerical Dispersion“	R. Lehe, et al., *Elimination of Numerical Cherenkov Instability in flowing-plasma Particle-In-Cell simulations by using Galilean coordinates*, **arXiv:1608.00227 [physics.plasm-ph]**, 2016
Phase space sampling	M. Vranic, et al., *Particle merging algorithm for PIC codes*, Computer Physics Communications 191, 65, 2015
…	…

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Issues for the Particle-in-Cell Technique

- Not all methods are implemented in every PIC code

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Issues for the Particle-in-Cell Technique

- Not all methods are implemented in every PIC code
- Some methods cannot be implemented together

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Issues for the Particle-in-Cell Technique

- Not all methods are implemented in every PIC code
- Some methods cannot be implemented together
- Some methods interact spuriously with others

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Issues for the Particle-in-Cell Technique

- Not all methods are implemented in every PIC code
- Some methods cannot be implemented together
- Some methods interact spuriously with others
- Some methods have limited applicability

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Issues for the Particle-in-Cell Technique

- Not all methods are implemented in every PIC code
- Some methods cannot be implemented together
- Some methods interact spuriously with others
- Some methods have limited applicability
- Some methods are approximate

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Issues for the Particle-in-Cell Technique

- Not all methods are implemented in every PIC code
- Some methods cannot be implemented together
- Some methods interact spuriously with others
- Some methods have limited applicability
- Some methods are approximate
- Some methods are hard to parallelize

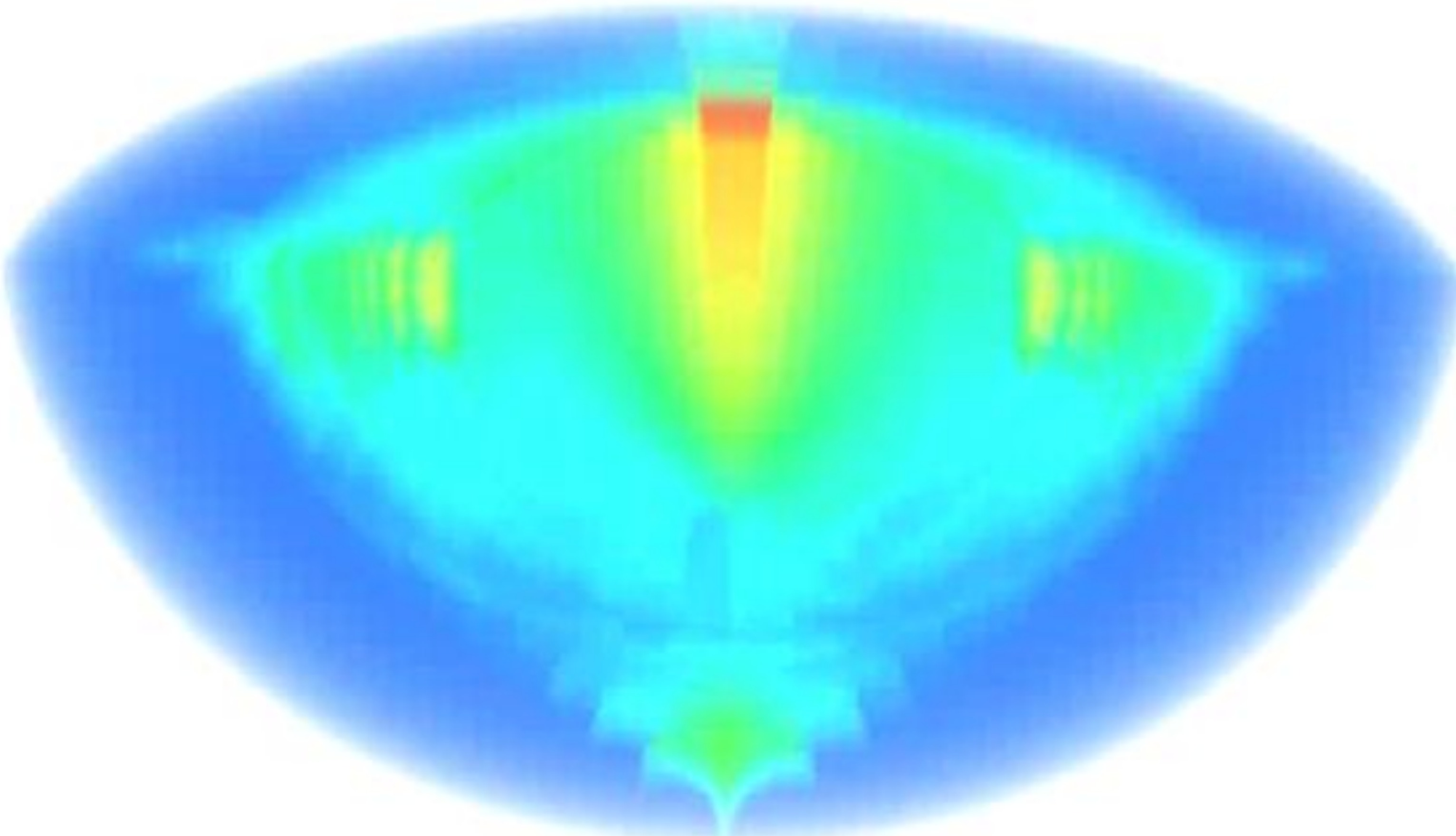
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Issues for the Particle-in-Cell Technique

- Not all methods are implemented ... PIC code
- Some methods cannot ... ether
- Some method ... with others
- Som ... ed applicability
- S ... are approximate
- Som ... methods are hard to parallelize

PIC is a SAMPLING TECHNIQUE!

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de



Why we need Exascale

How can I predict what I will measure?

- As discussed: Methods have their faults

DRESDEN concept HZDR

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

How can I predict what I will measure?

- As discussed: Methods have their faults
- PIC-sampling requires reruns with varying sampling

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

How can I predict what I will measure?

- As discussed: Methods have their faults
- PIC-sampling requires reruns with varying sampling
- Monte-Carlo sampling (Ionization, etc.), too

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

How can I predict what I will measure?

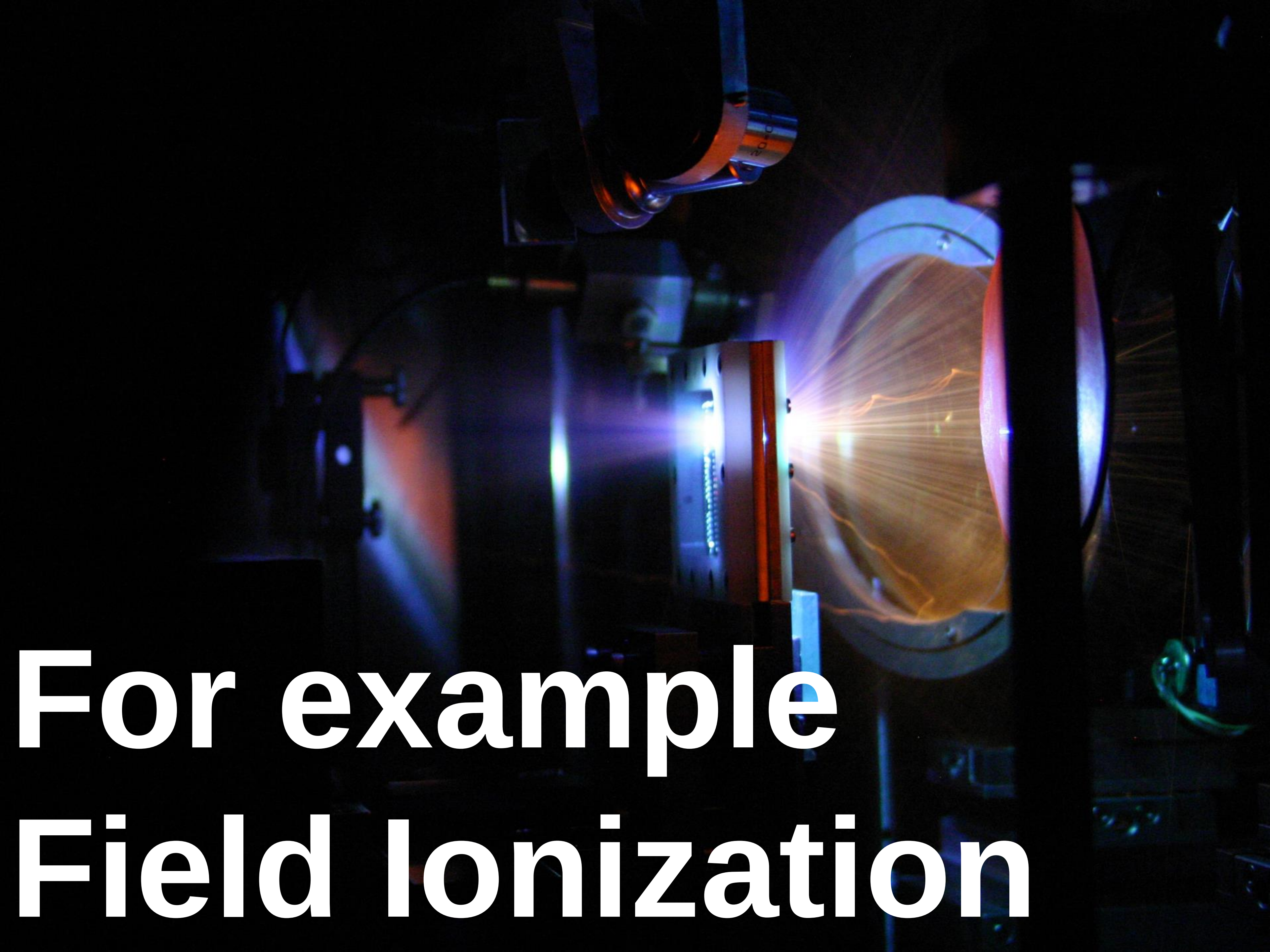
- As discussed: Methods have their faults
- PIC-sampling requires reruns with varying sampling
- Monte-Carlo sampling (Ionization, etc.), too
- Initial parameters not well known from Experiment

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

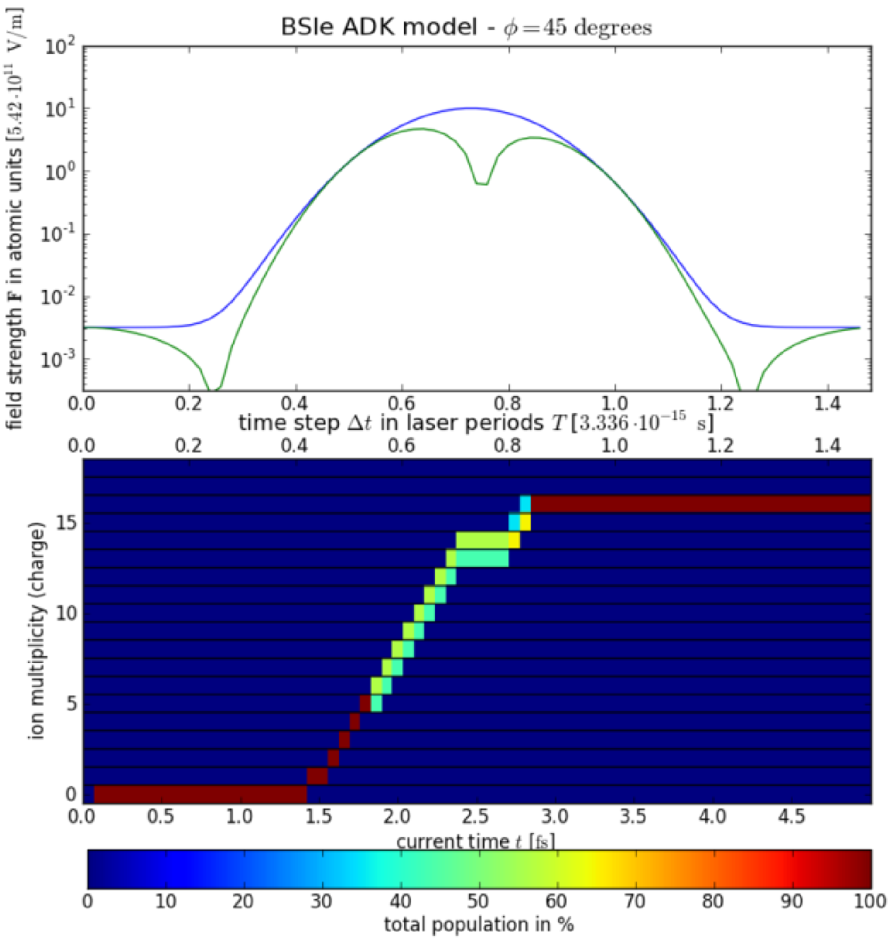
How can I predict what I will measure?

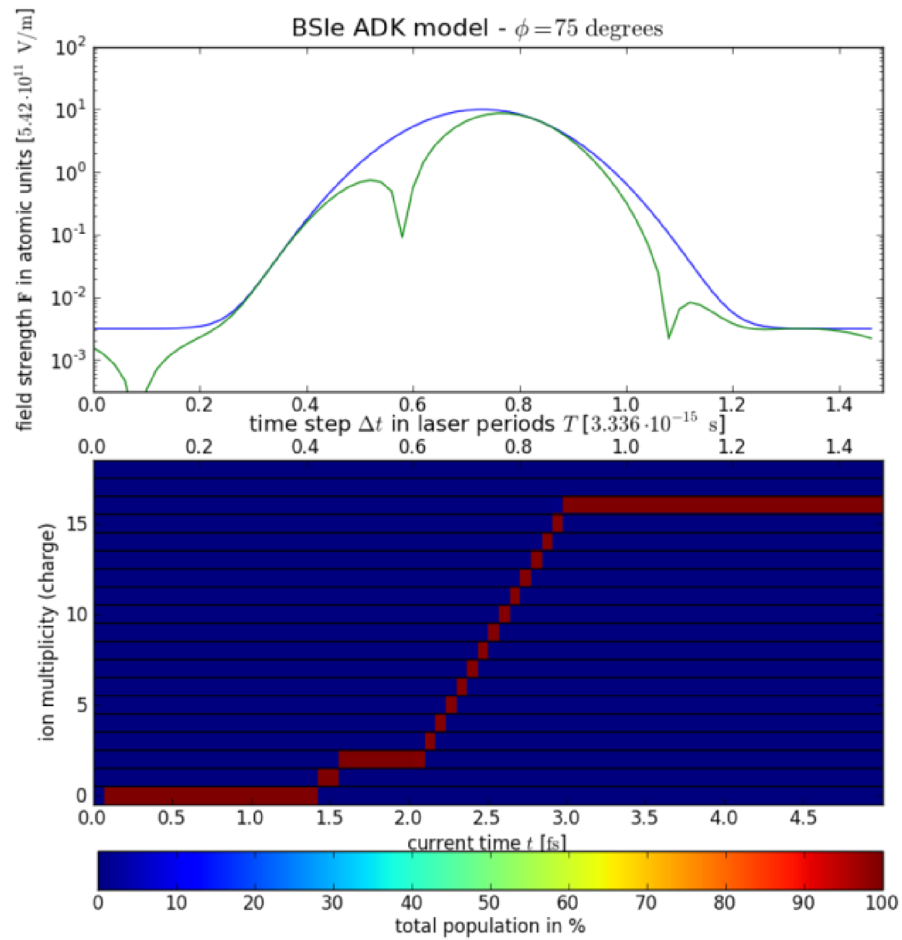
- As discussed: Methods have their faults
- PIC-sampling requires reruns with varying sampling
- Monte-Carlo sampling (Ionization, etc.), too
- Initial parameters not well known from Experiment
- Simulate what is measured!

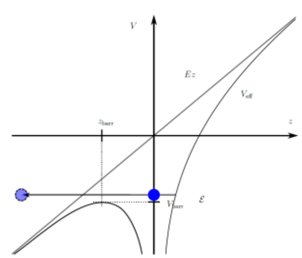
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de


For example
Field Ionization

Carrier-envelope Phase influences Femtosecond Field Ionization

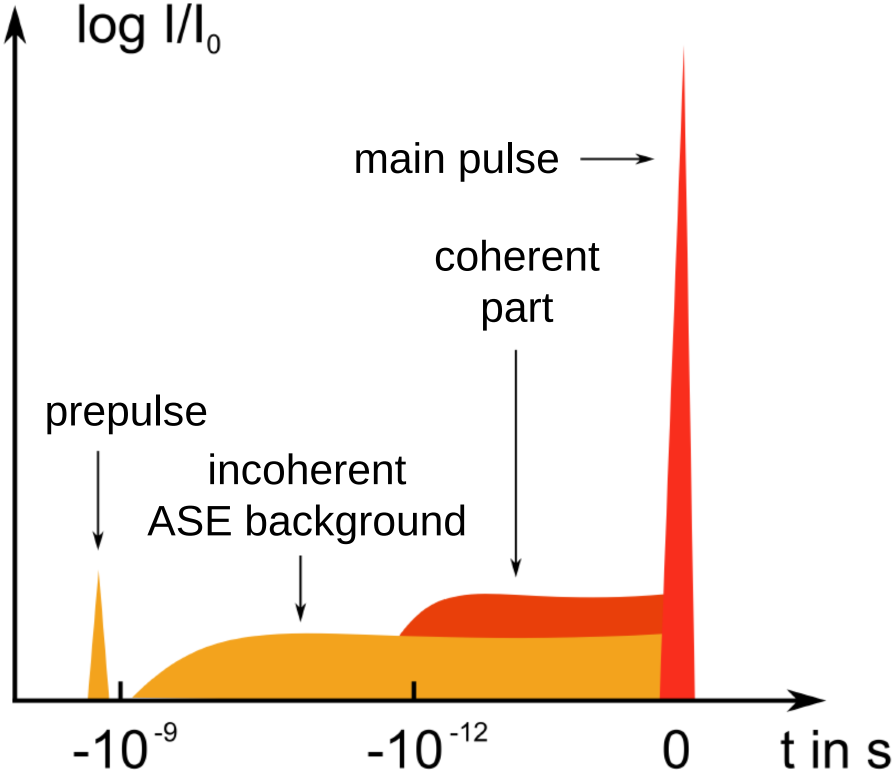


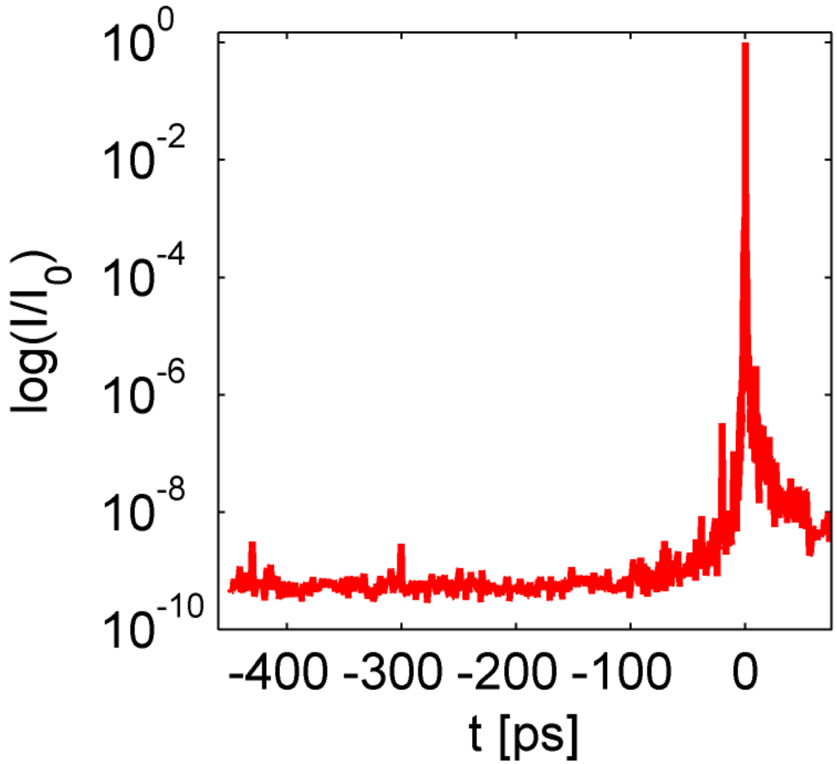




Argon ions, λ = 1 μm, Ammosov, Delone, Krainov Barrier Suppression Ionization
Marco Garten

At best we know the Laser Contrast at one position in the beam

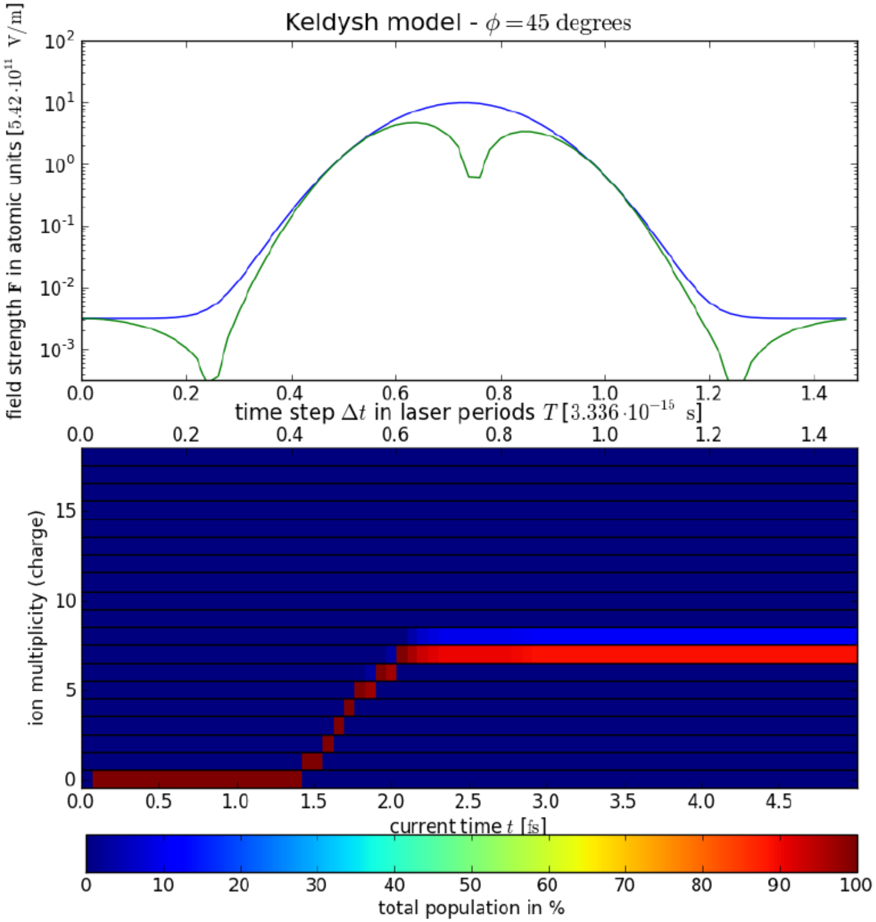


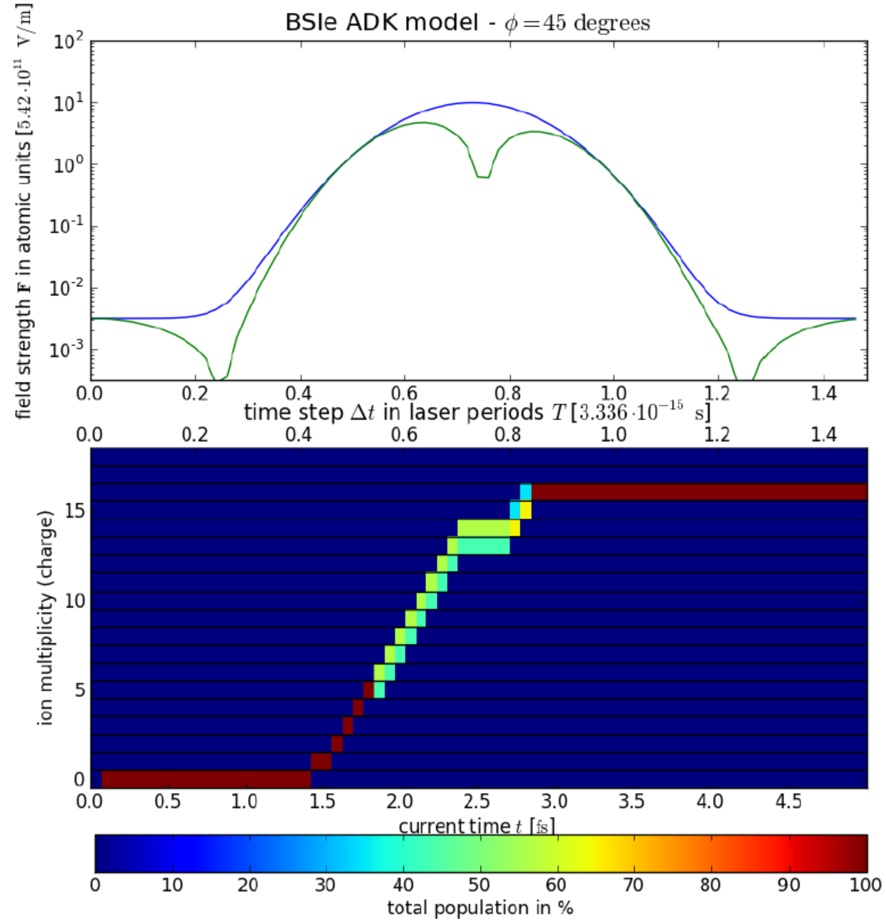


Josefine Metzkes

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Choice of Field Ionization Model determines Charge State



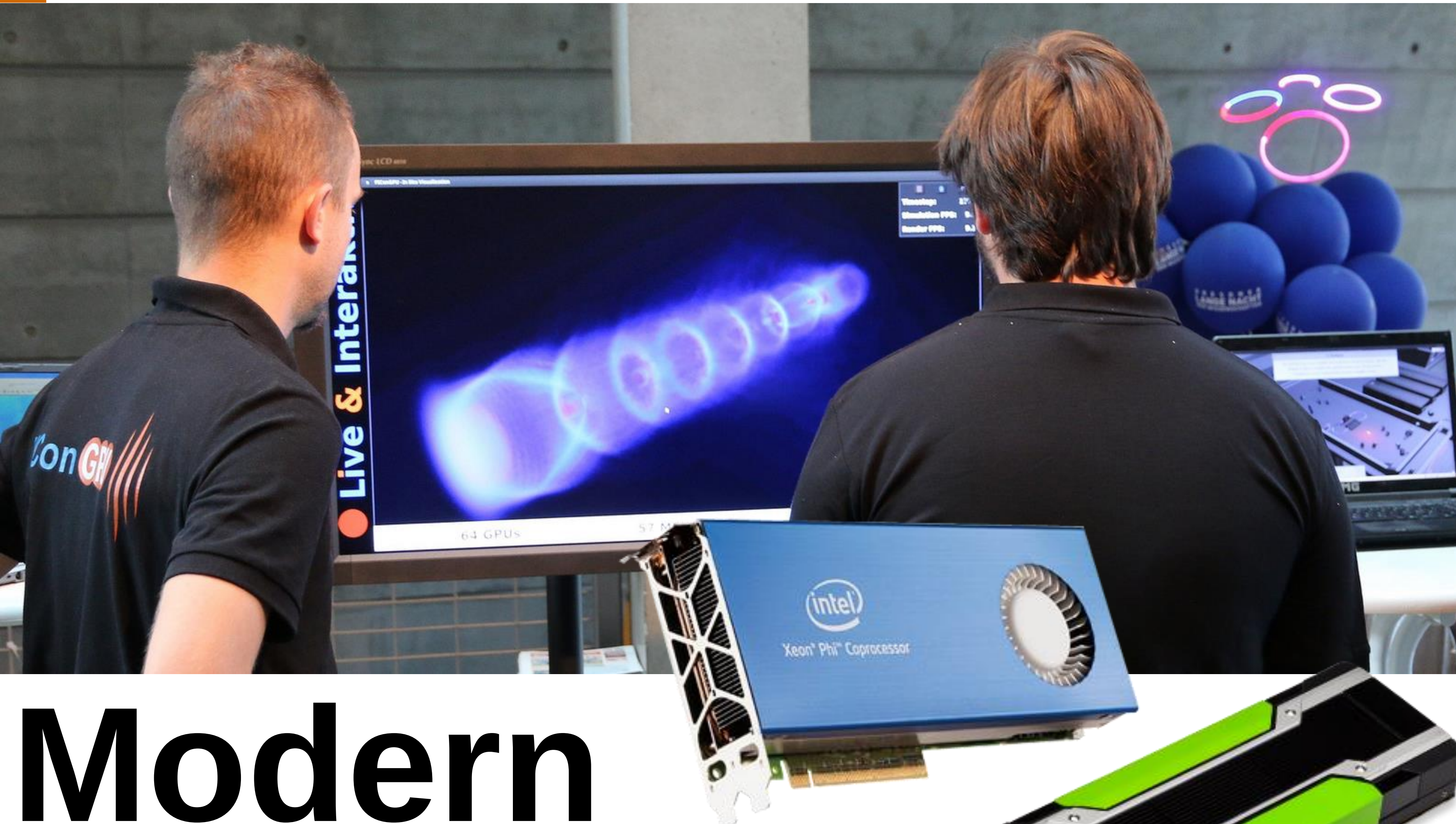


Argon ions, λ = 1 μm, Keldysh vs. ADK, Marco Garten

Solution: High performance computing

- **Repeat simulations for…**
- … computing stochastic errors from sampling
- … computing systematic errors from models
- … parameter scans in range of initial conditions
- Integrate simulated (synthetic) diagnostics

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de



Modern Hardware

Modern HPC Systems

TOP 10 Sites for June 2016

For more information about the sites and systems in the list, click on the links or view the complete list.

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)	Architecture	Best Practice Programming
1	National Supercomputing Center in Wuxi China	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371	SW26010	OpenAcc
2	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808	Intel Xeon Phi	TBB, OpenMP
3	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209	Nvidia Tesla	CUDA
4	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890	IBM PowerPC	OpenMP
5	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660	Sparc 64	OpenMP
6	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945		
7	DOE/NNSA/LANL/SNL United States	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	301,056	8,100.9	11,078.9		Intel x86	TBB, OpenMP

DRESDEN concept HZDR

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Modern HPC Systems

TOP 10 Sites for June 2016

For more information about the sites and systems in the list, click on the links or view the complete list.

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)	Architecture	Best Practice Programming
1	National Supercomputing Center in Wuxi Ch	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C	10,649,600	93,014.6	125,435.9	15,371	SW26010	OpenAcc
2	Na Gu Ch						Intel Xeon Phi	TBB, OpenMP
3	DO La Un	Cray Inc.					Nvidia Tesla	CUDA
4	DO Un						IBM PowerPC	OpenMP
5	RI Co Ja						Sparc 64	OpenMP
6	DO La Un							
7	DOE/NNSA/LANL/SNL United States	Trinity - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	301,056	8,100.9	11,078.9		Intel x86	TBB, OpenMP

Almost all systems in the TOP 10 HPC list have a different architecture

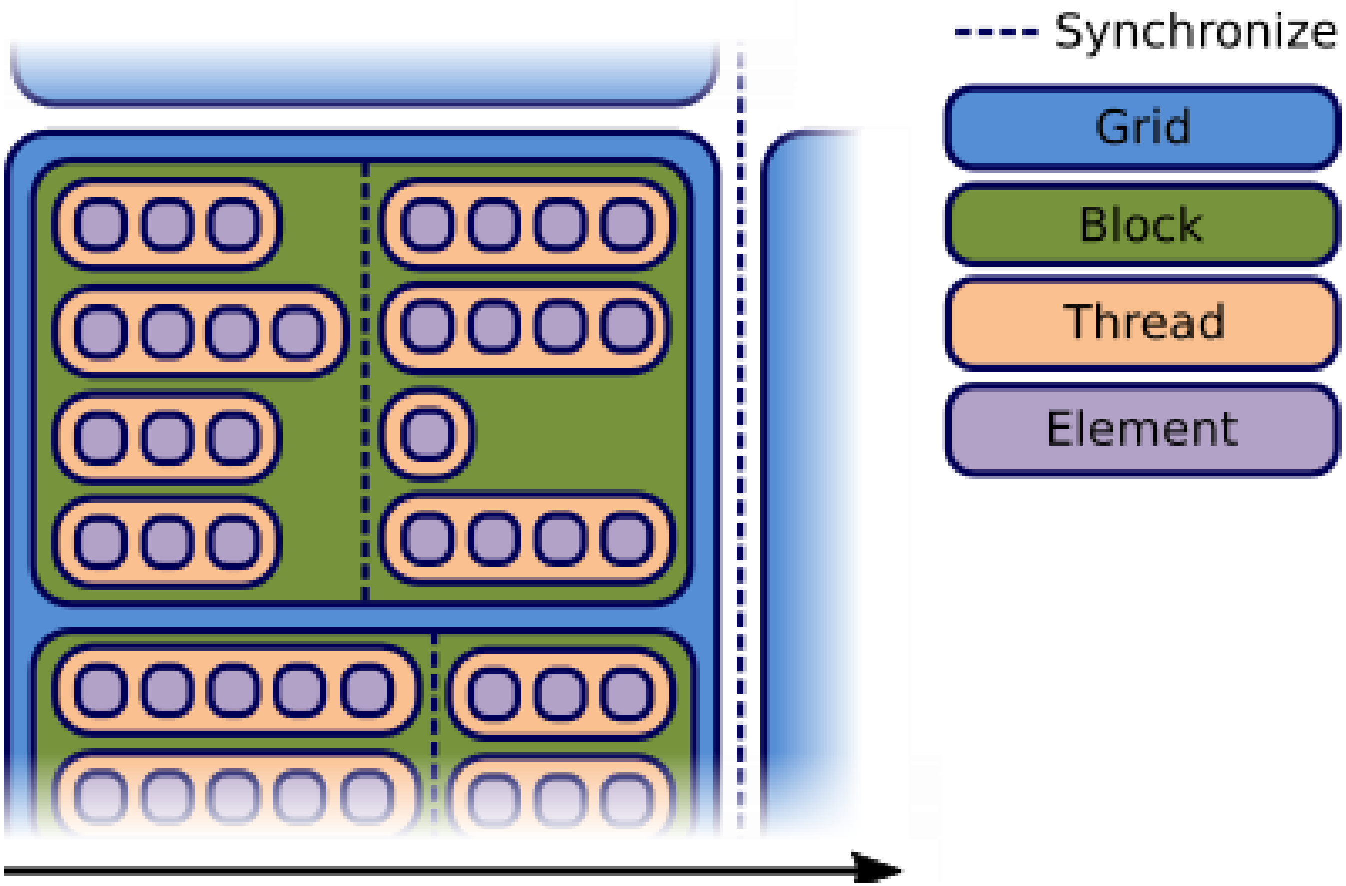
There is not a single programming model that provides you performance on all architectures (forget about OpenCL)

DRESDEN concept

HZDR

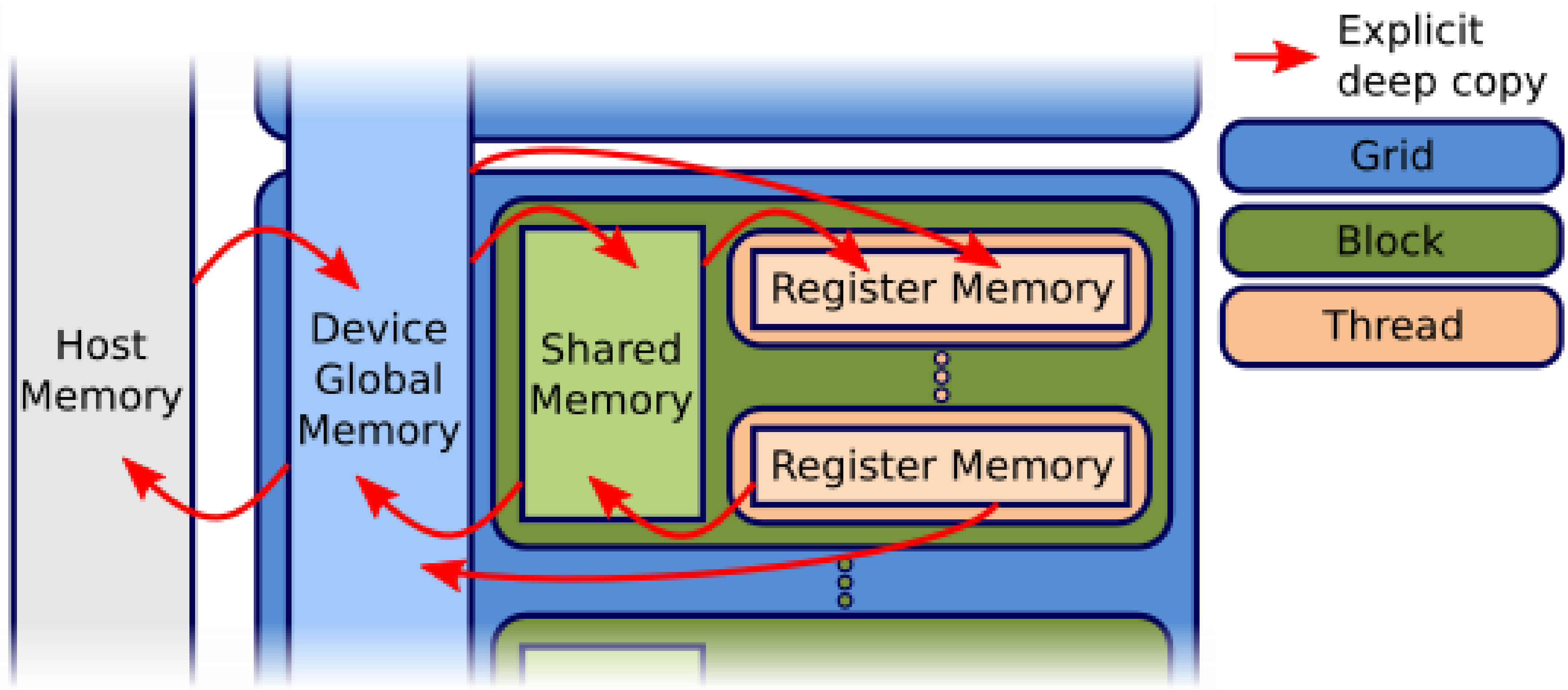
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Modern Hardware – Levels of Parallelism

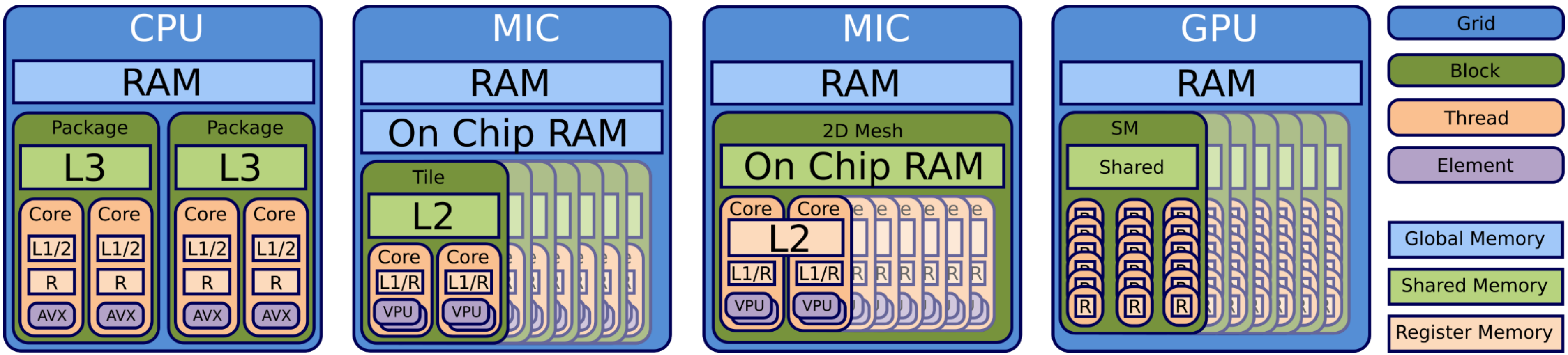


Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Modern Hardware – Memory Hierarchy



Modern Hardware – Mapping of Hierarchies to Hardware



90 % of code is management, 10% Physics

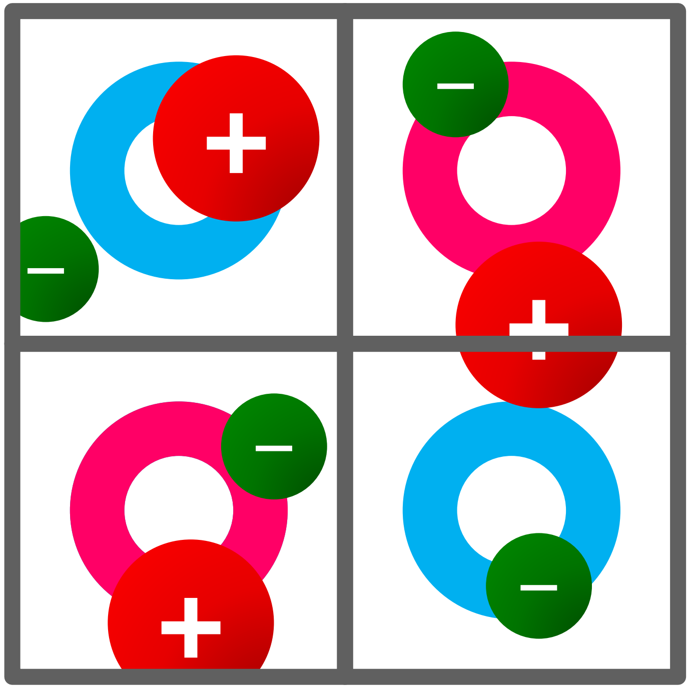
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

How do you get fast?

- Put everything you need in the fastest memory (data parallelism)
- Do independent parts of the algorithm in parallel (task parallelism)

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

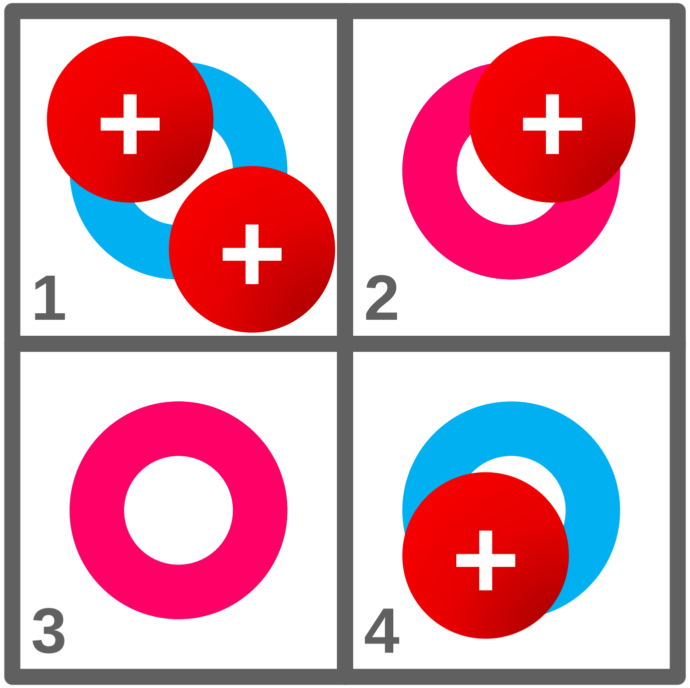
Domain Decomposition – Field and Particle Domain

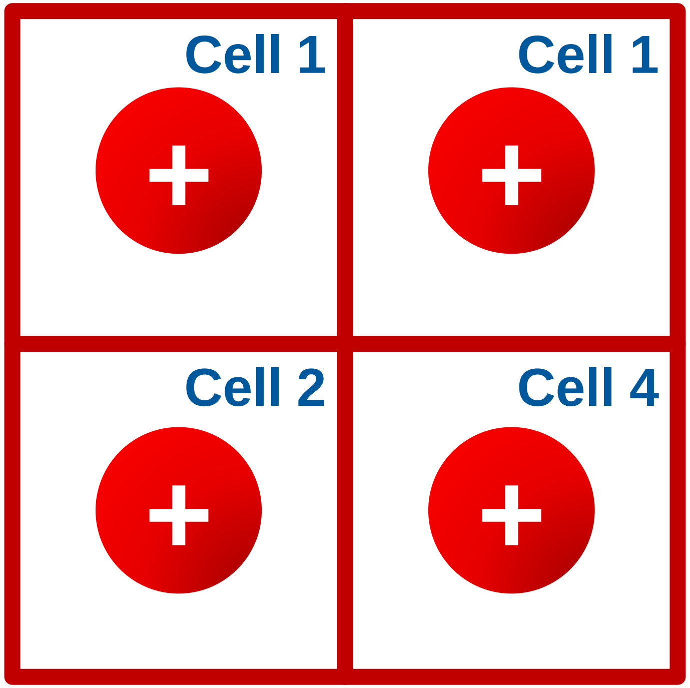


Field Domain **Particle Domain**

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Use Vectorized, Sorted Data Structures

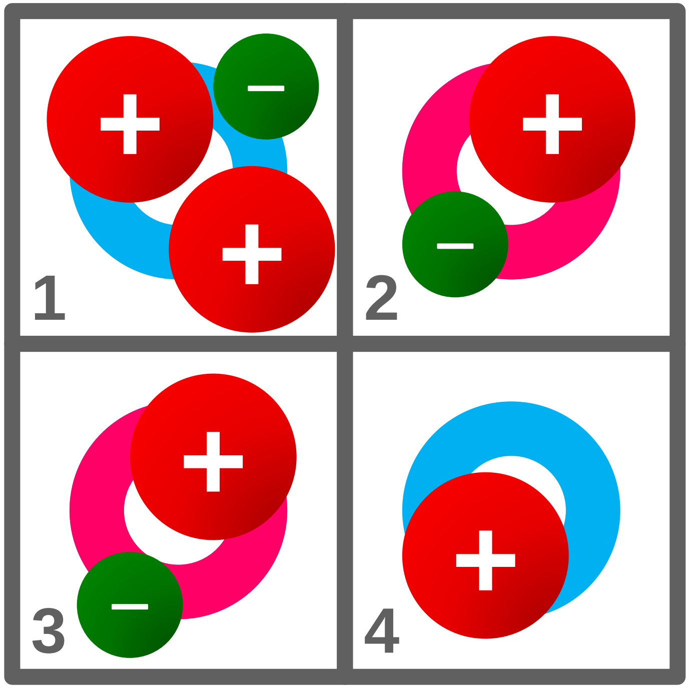


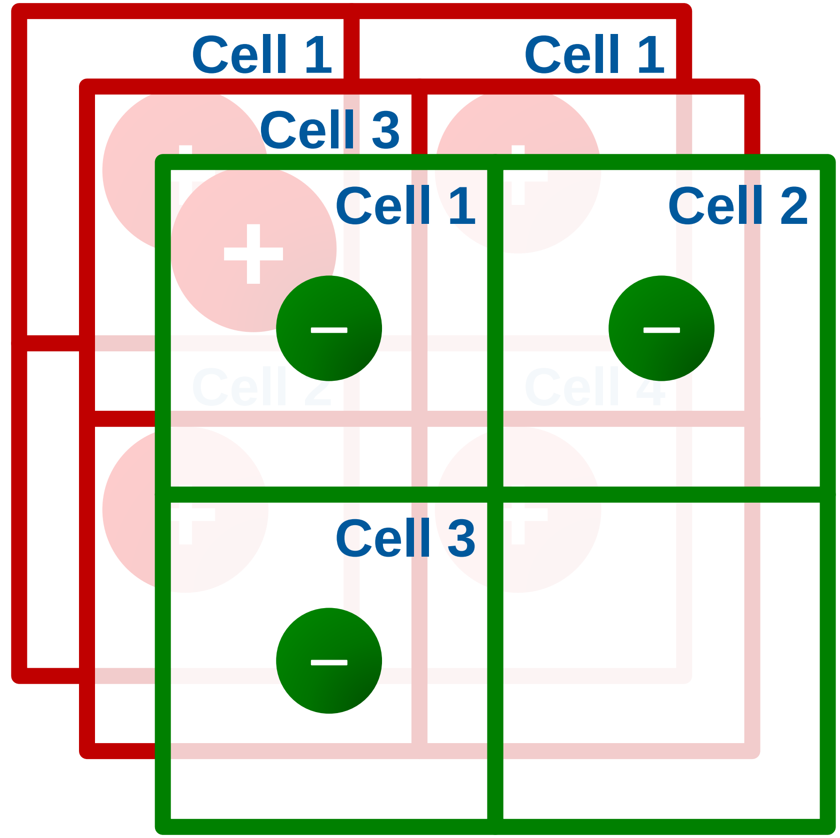


Field Domain **Particle Domain**

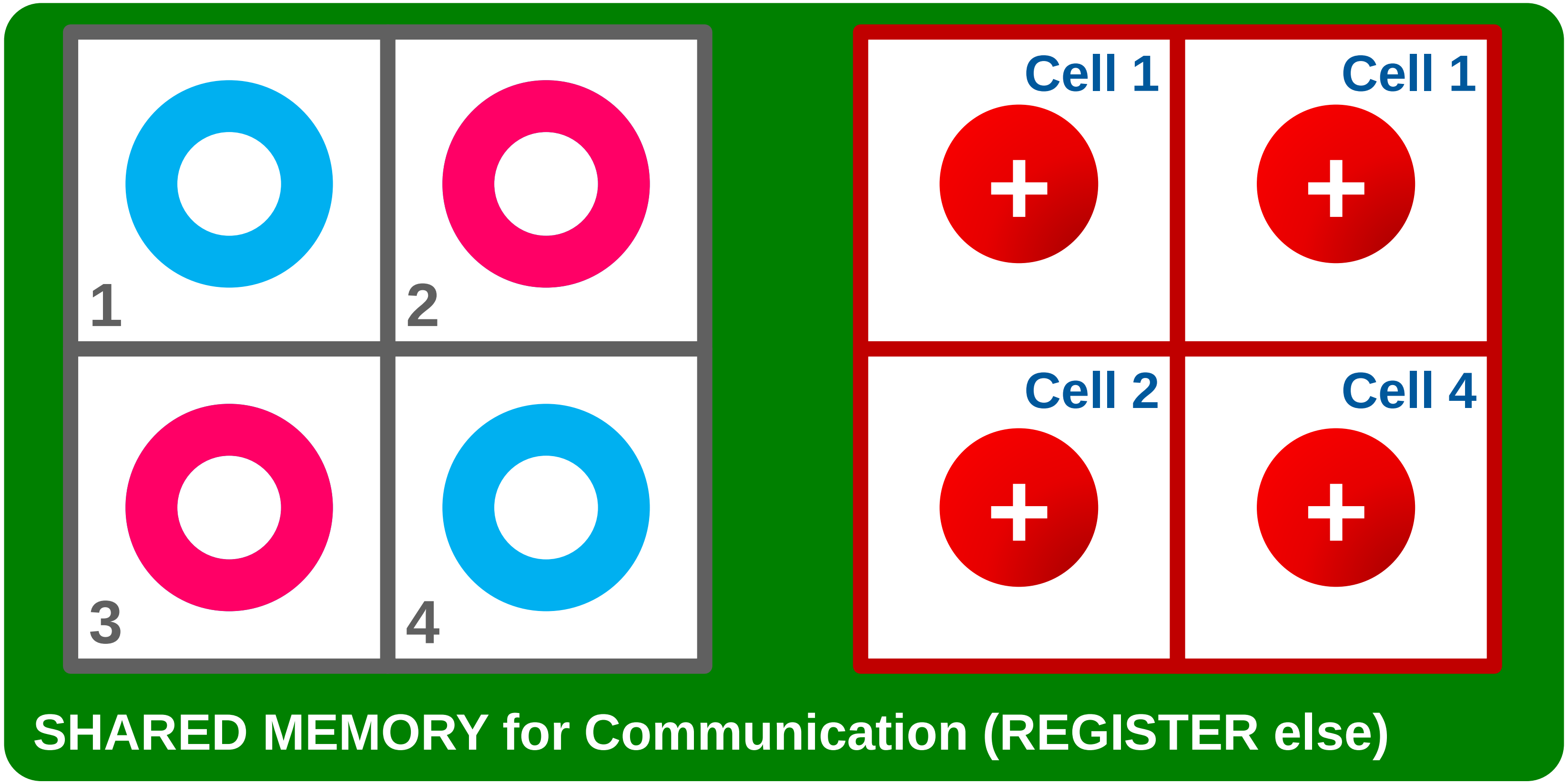
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Add Particles



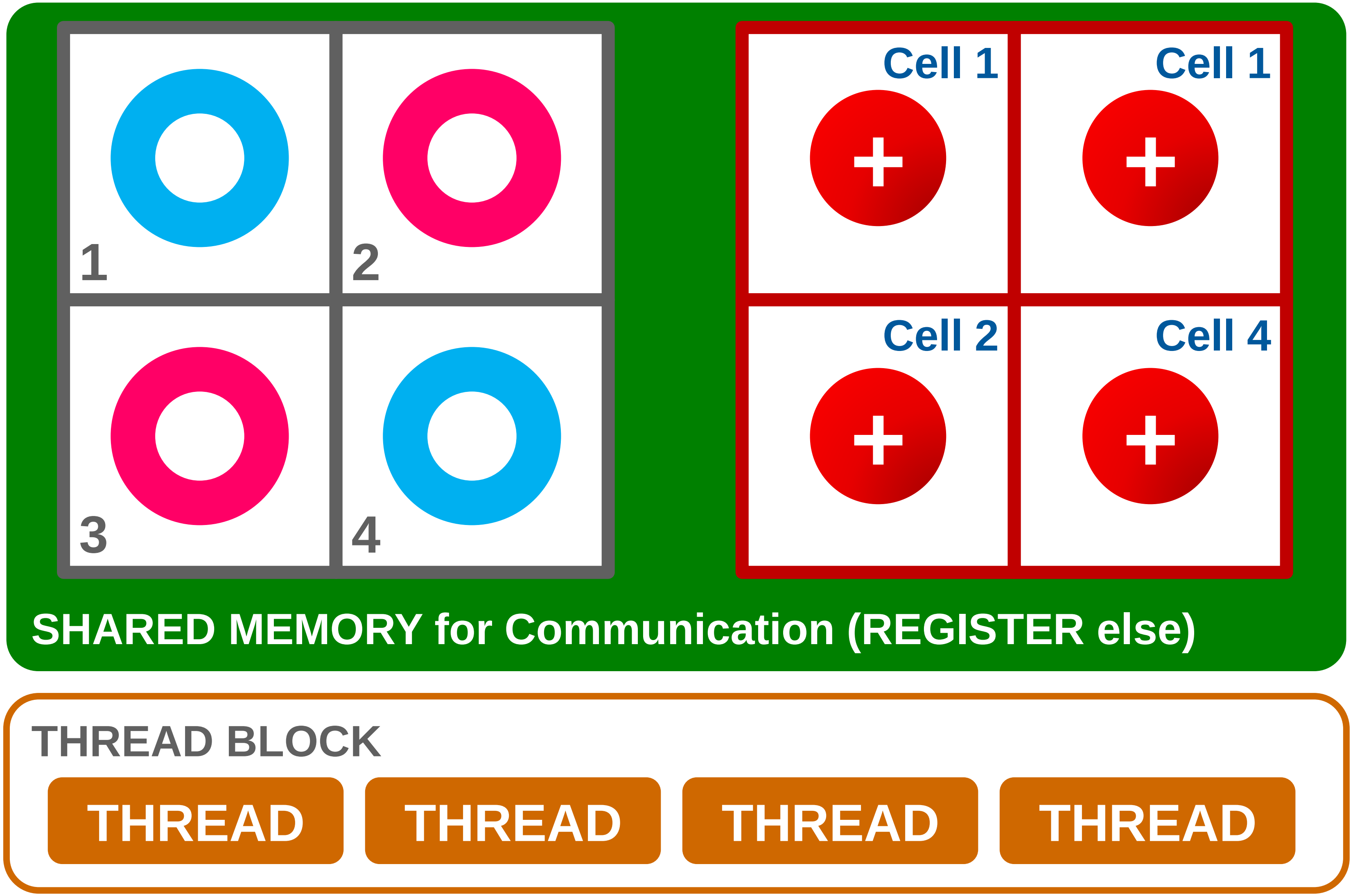


Put Data in Fast Memory

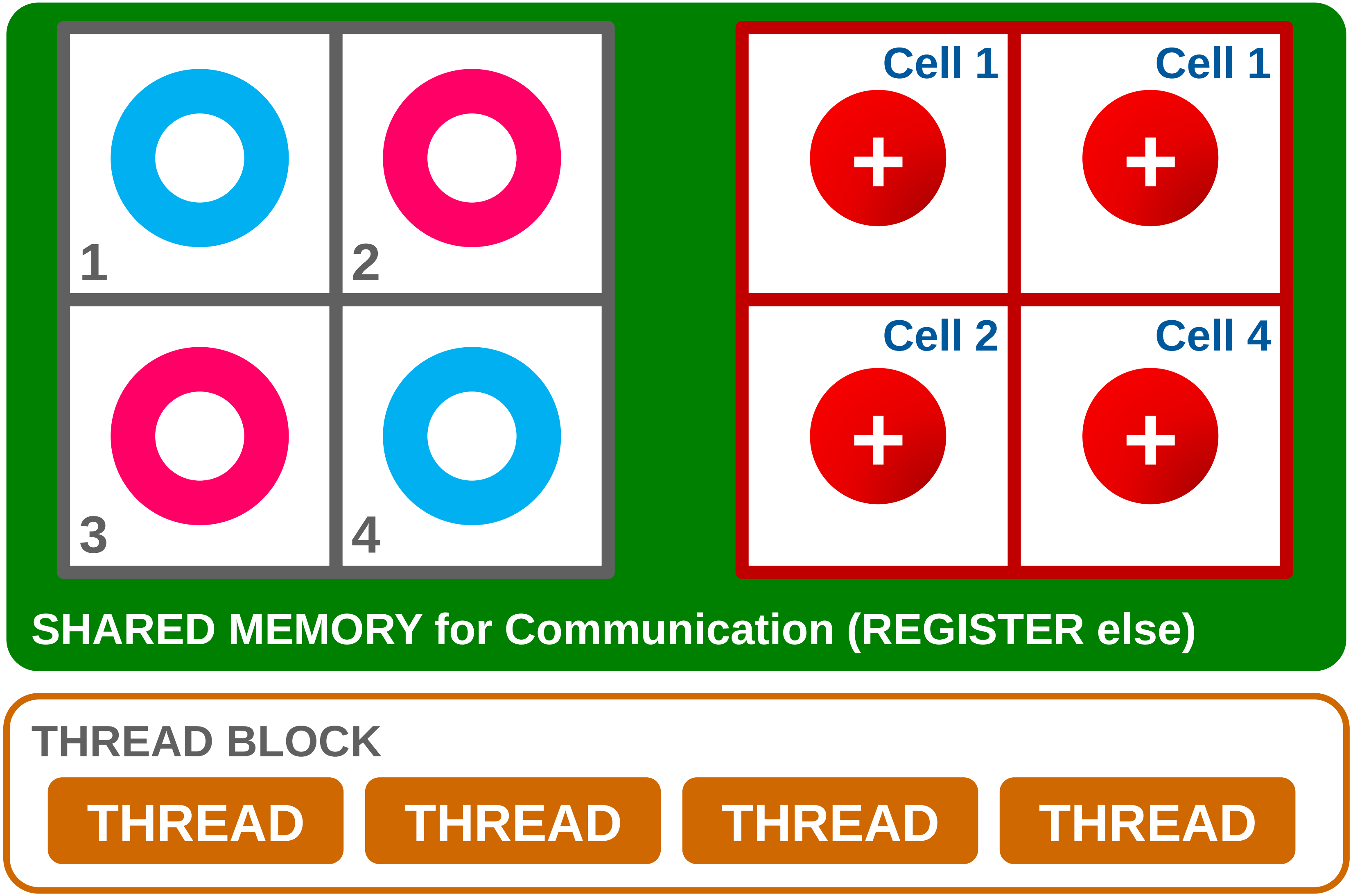


Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Cell-wise Threading

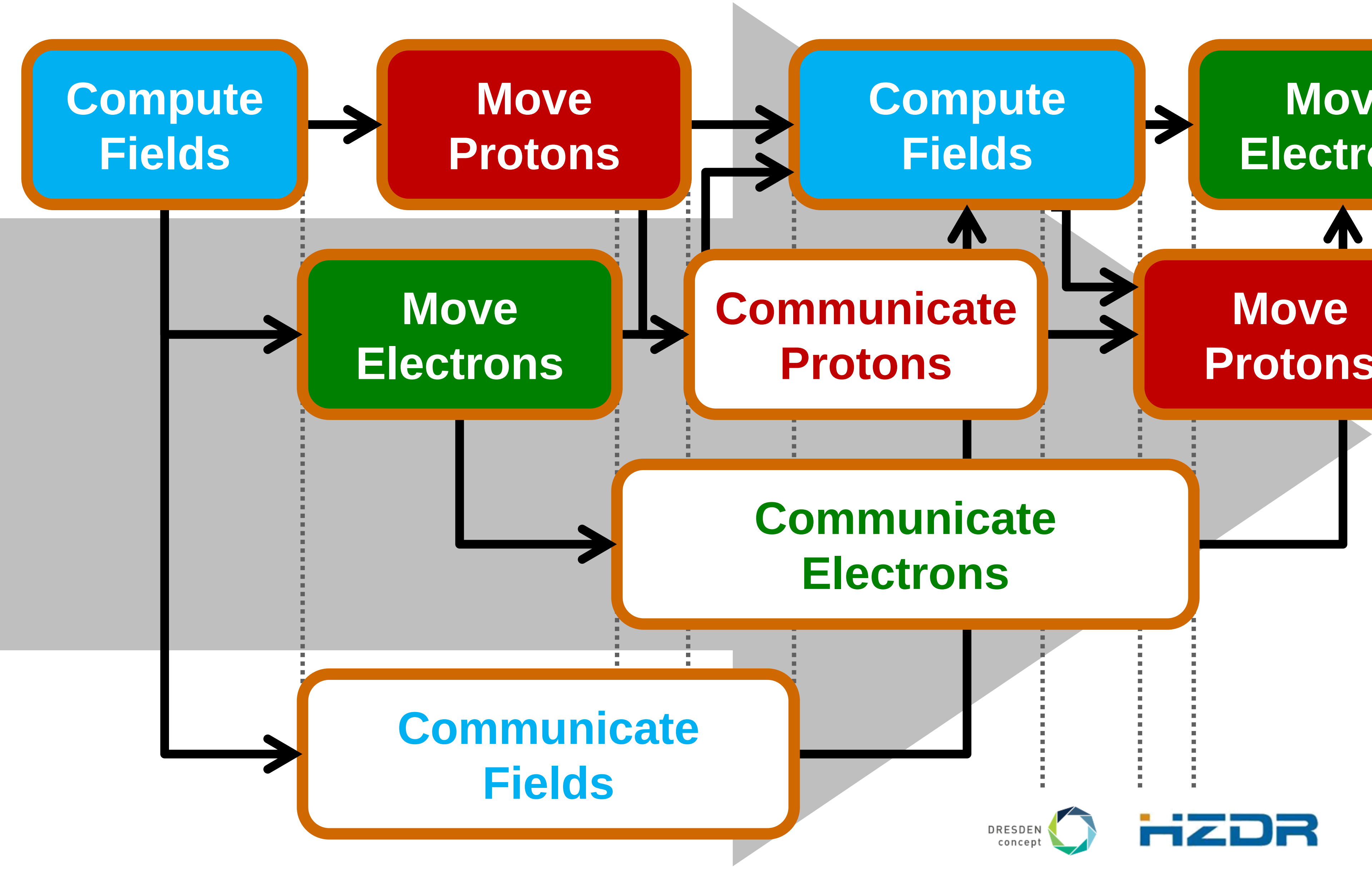


Particle-wise Threading



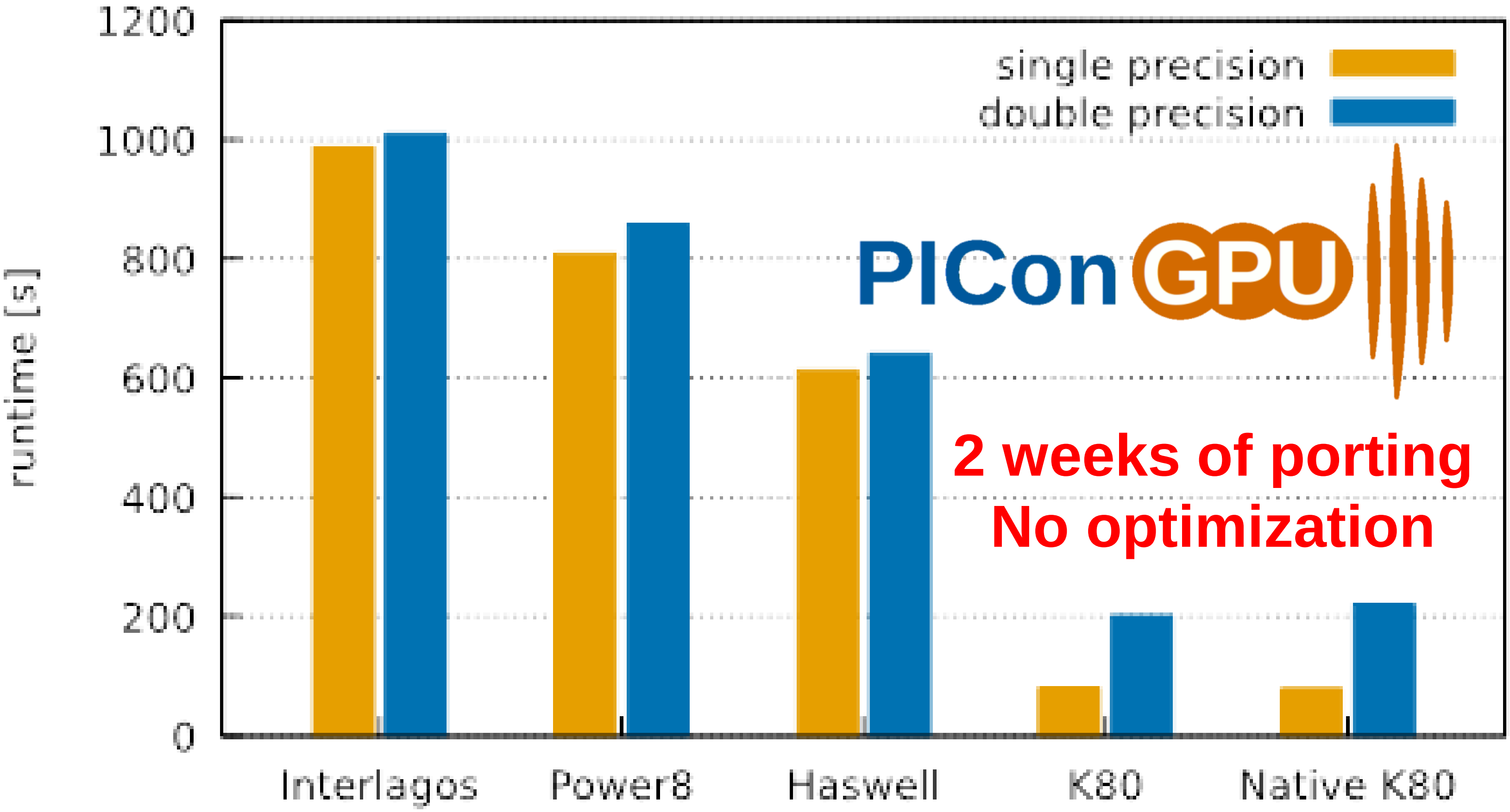
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Tasks — Concurrent Kernels, Asynchronous Communication



Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

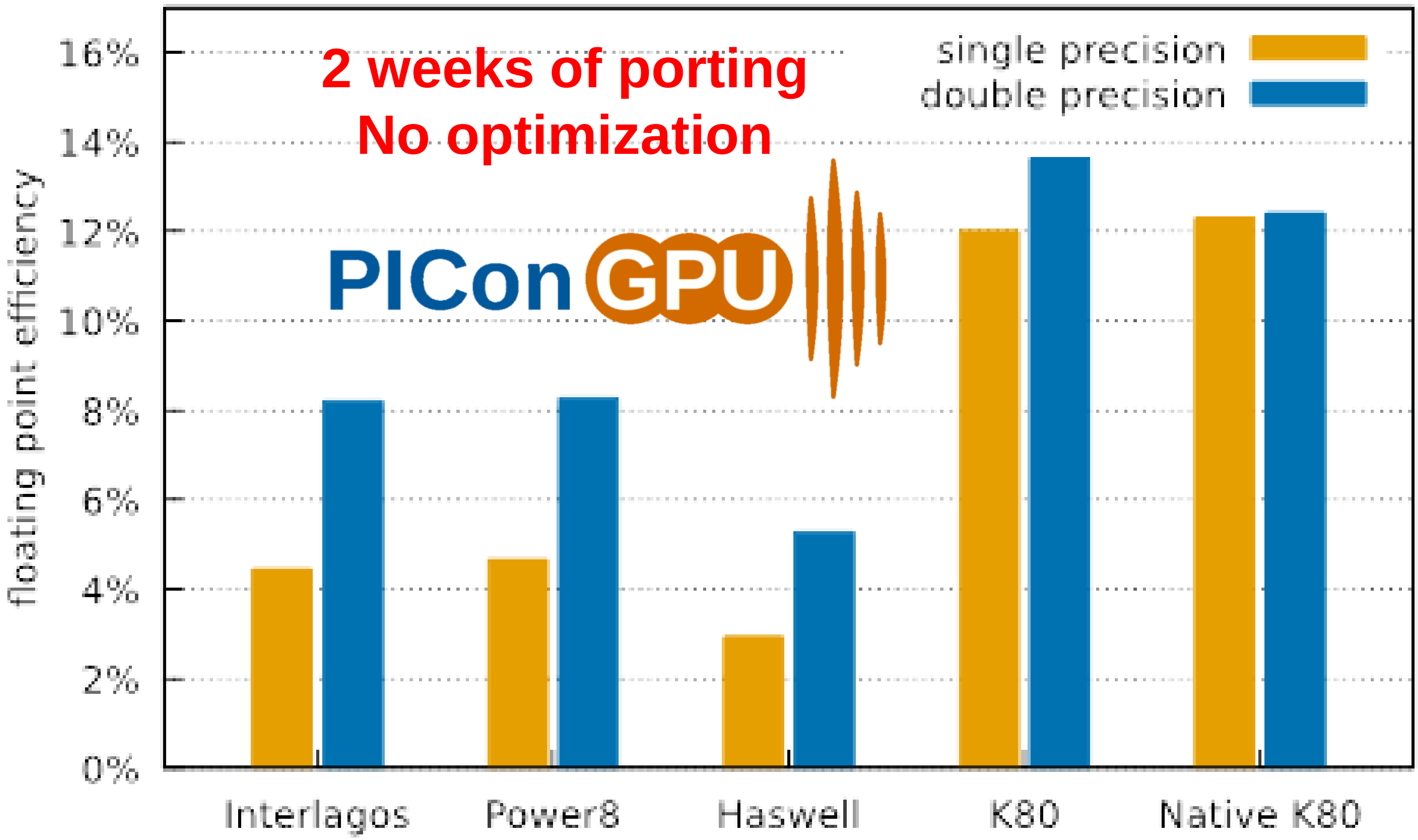
PIC on EVERY hardware with a single source



DRESDEN concept

HZDR

PIC is memory bound (you do not need or can use FLOPs)

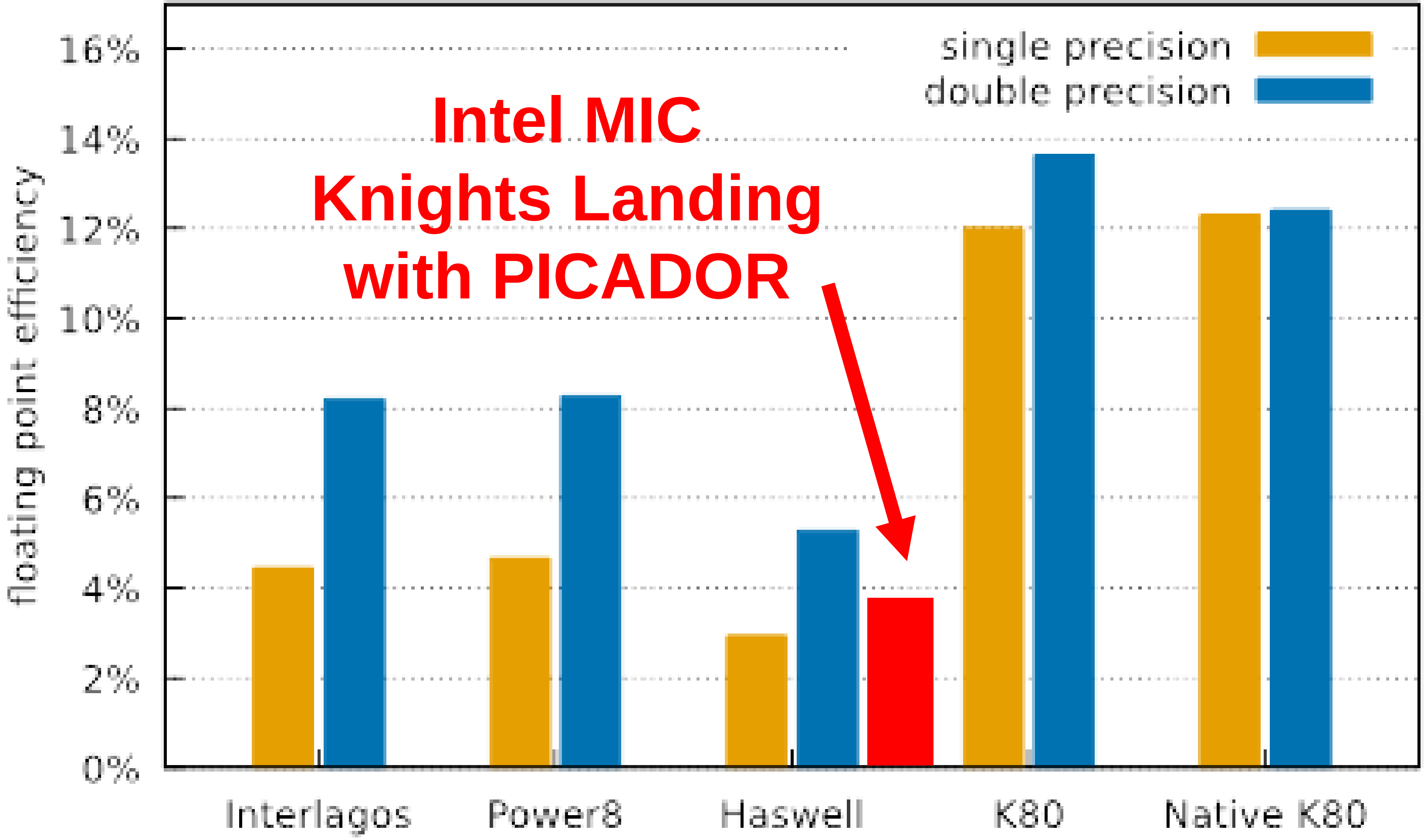


DRESDEN concept

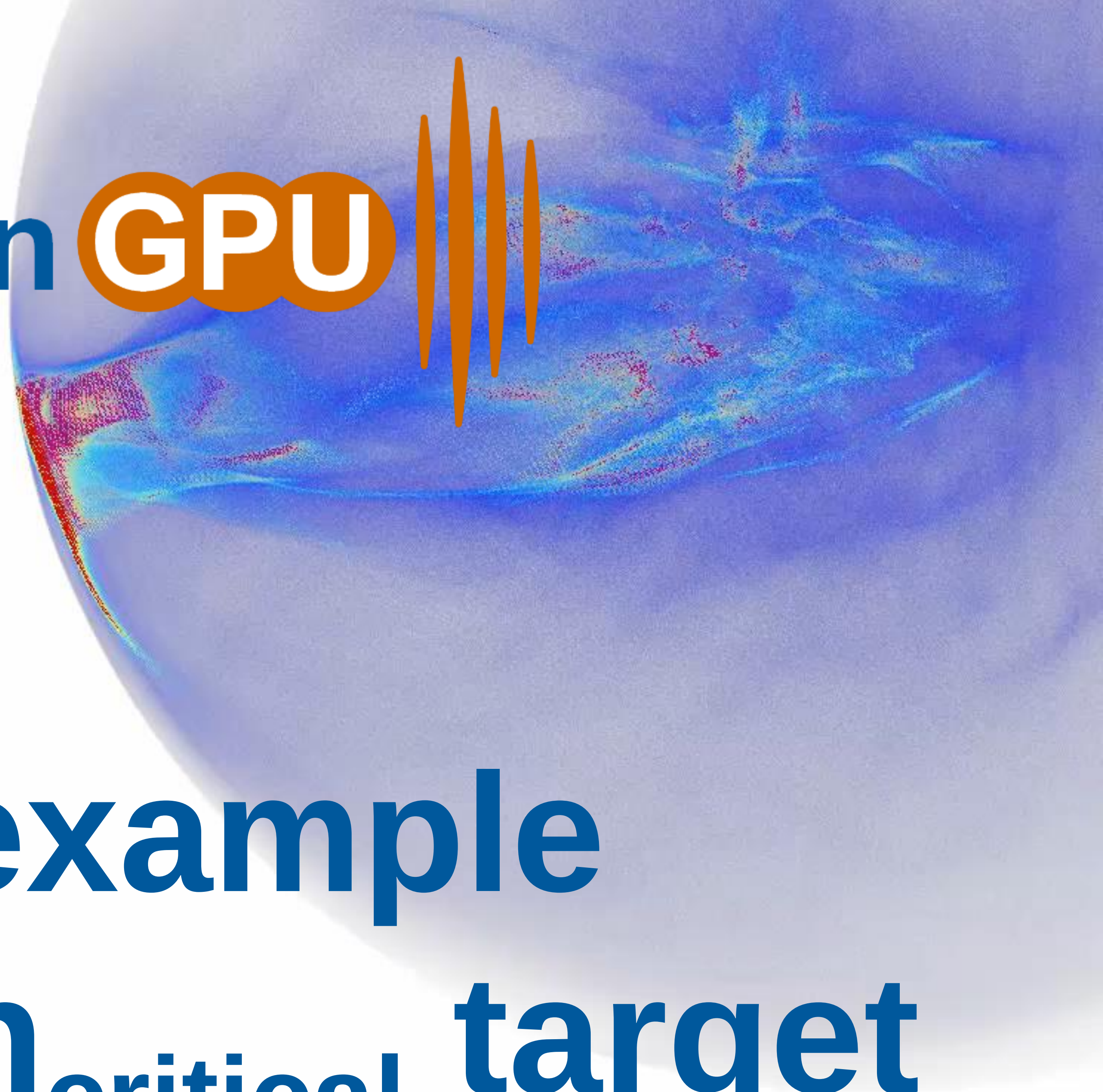
HZDR

Maybe we are just not smart enough?

I. Surmin, et al., *Co-design of a particle-in-cell plasma simulation code for Intel Xeon Phi: a first look at Knights Landing*, **arXiv:1608.01009 [cs.DC]**



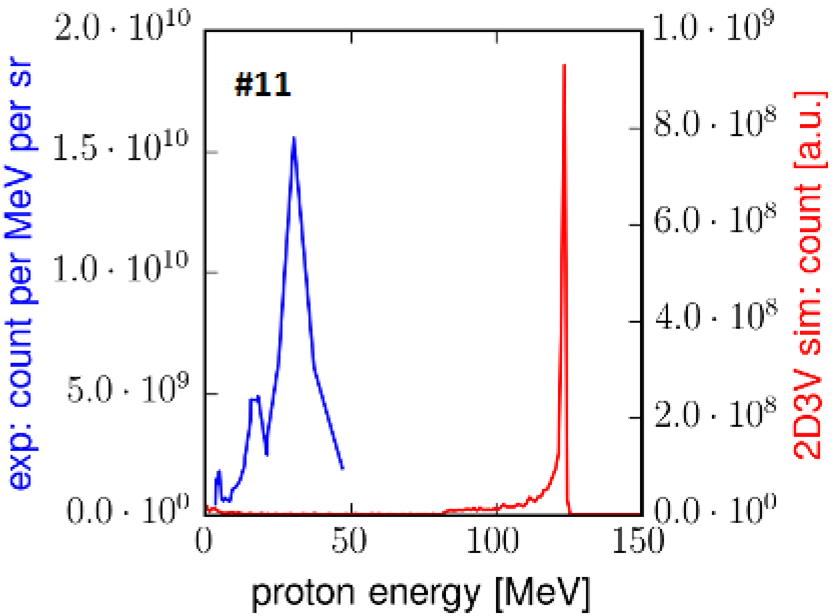
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

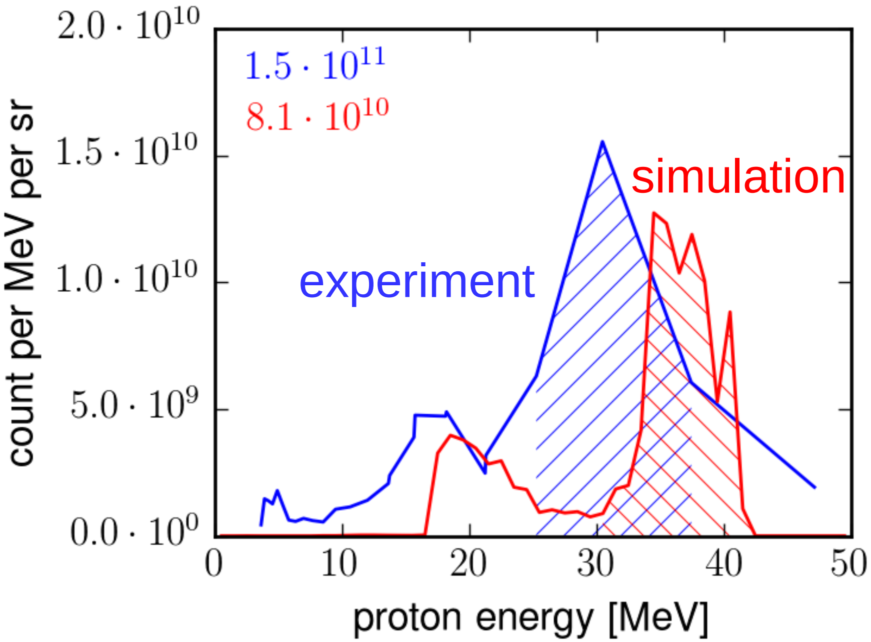


PIConGPU

For example
400 $n_{critical}$ target

The difference between 2D and 3D for a spherical Target





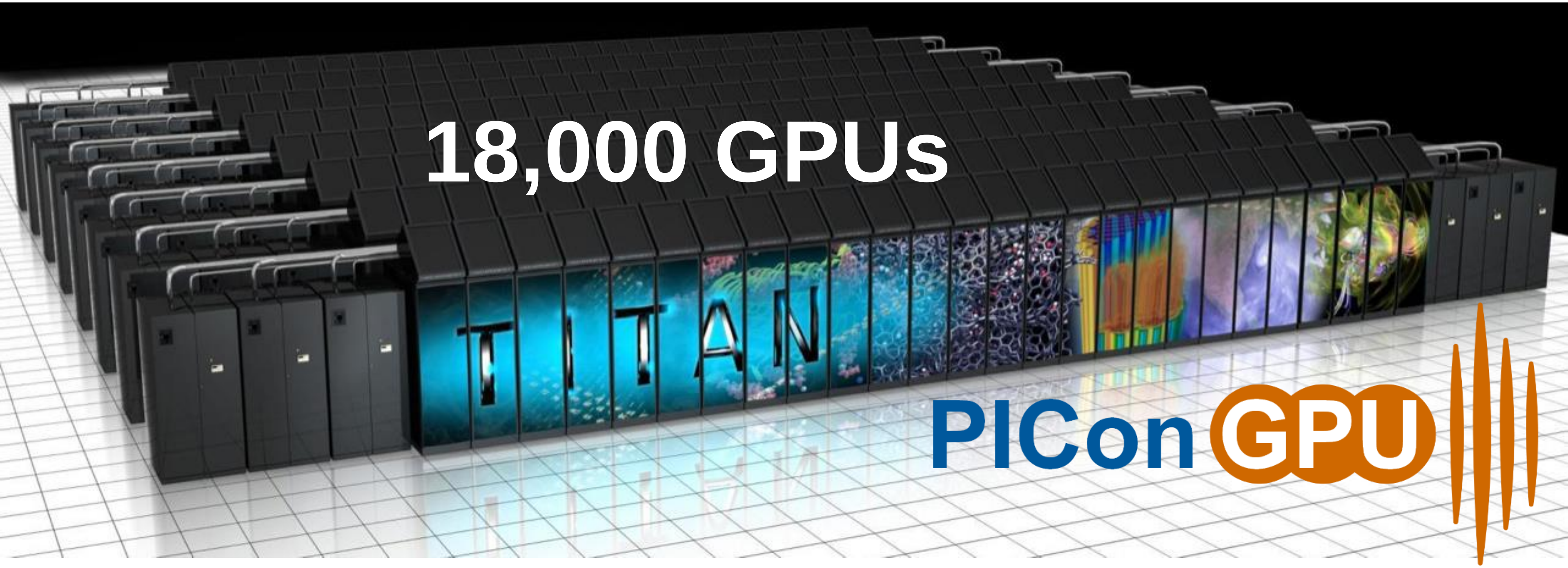
2D3V **3D3V**

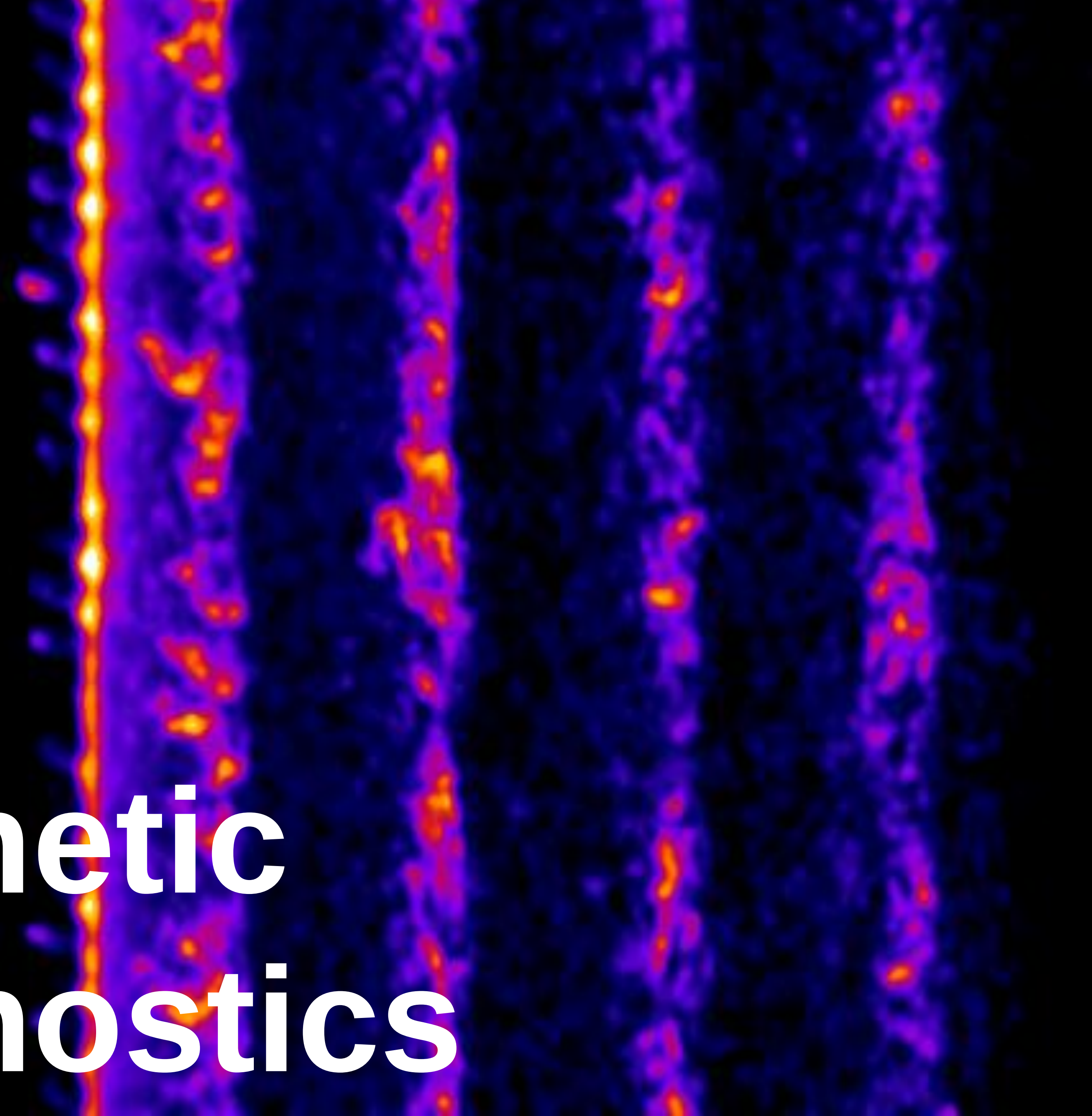
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

The difference between 2D and 3D in resources

- 1 x 2D3V: ~300 GB, 130 GPUhrs
- 1 x 3D3V: ~250 TB, 500.000 GPUhrs

5 ps

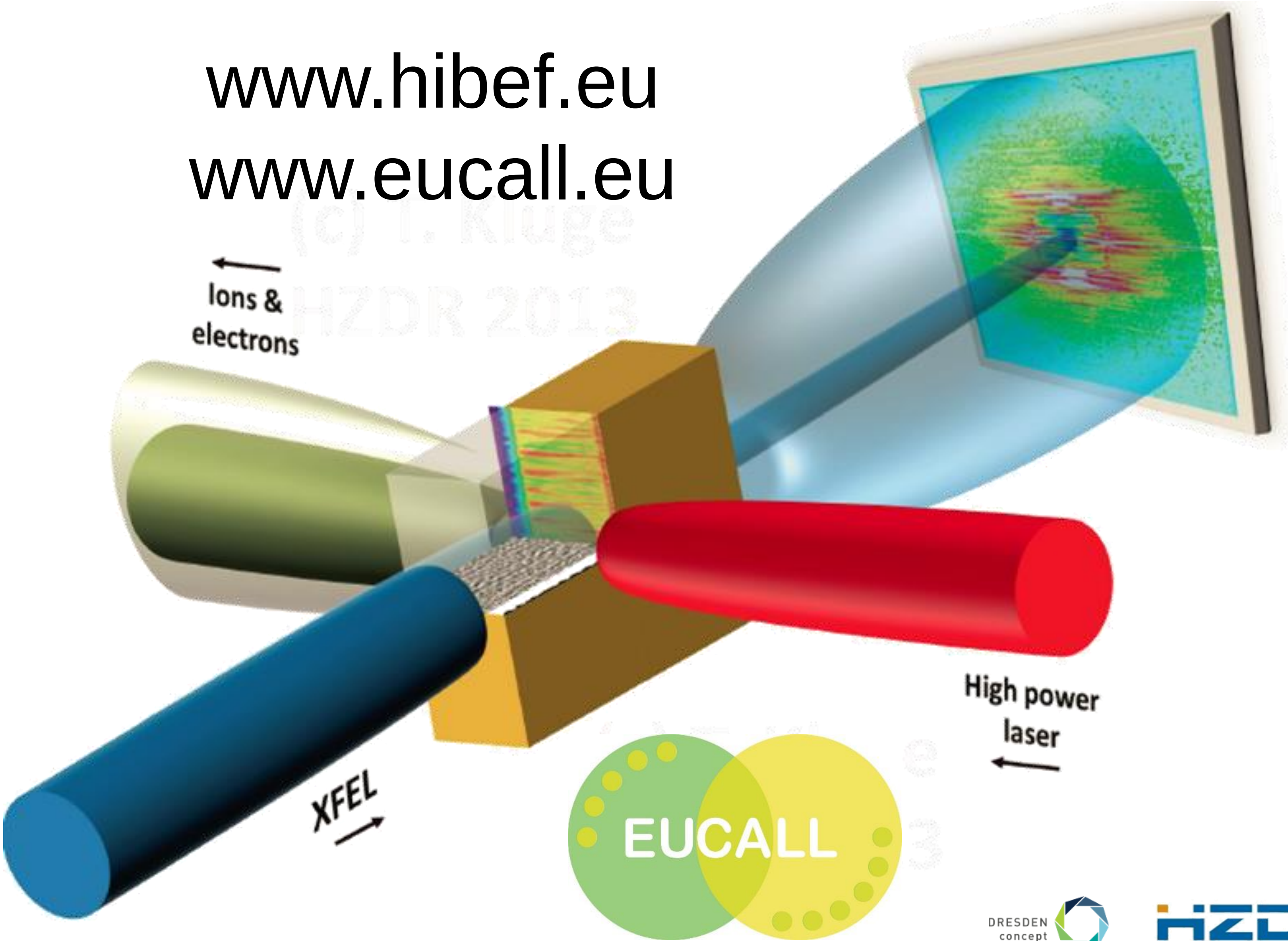




Synthetic Diagnostics

A look inside the tool box – X-Ray free electron lasers for probing

www.hibef.eu
www.eucall.eu

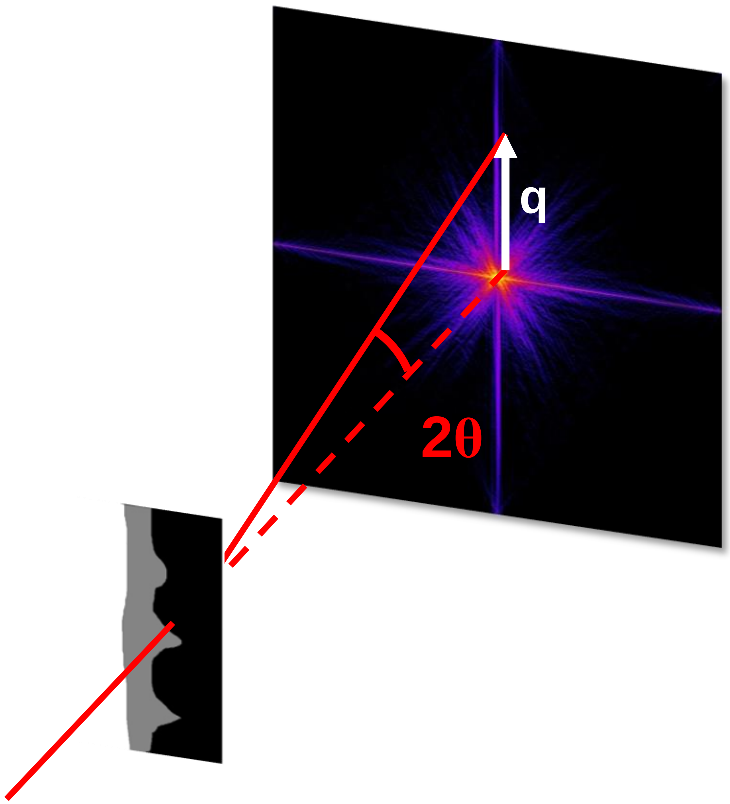


Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Small **A**ngle **X**-Ray **S**cattering (SAXS) in a nutshell

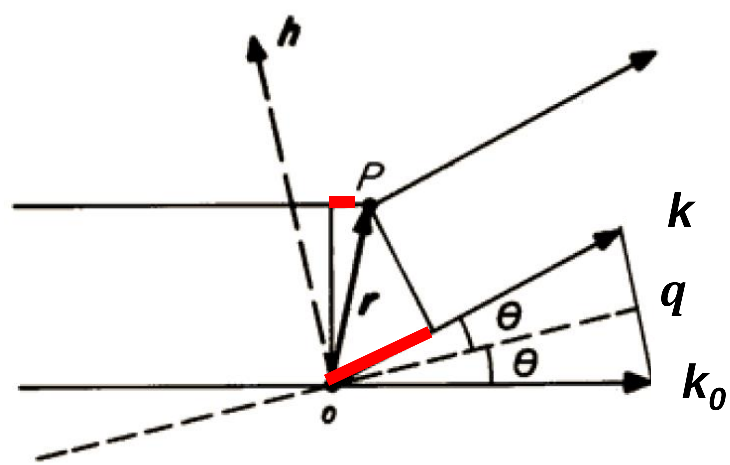
$$\Phi = \Phi_0 \cdot \Delta\Omega \cdot T \cdot \epsilon \cdot \left| r_0 \cdot \int n_e(\vec{r}) \cdot e^{i\vec{q}\vec{r}} d\vec{r} \right|^2$$

Flux	Solid angle	Trans-mission	Detection efficiency	Thomson scattering cross section	Fourier transform of e⁻ density



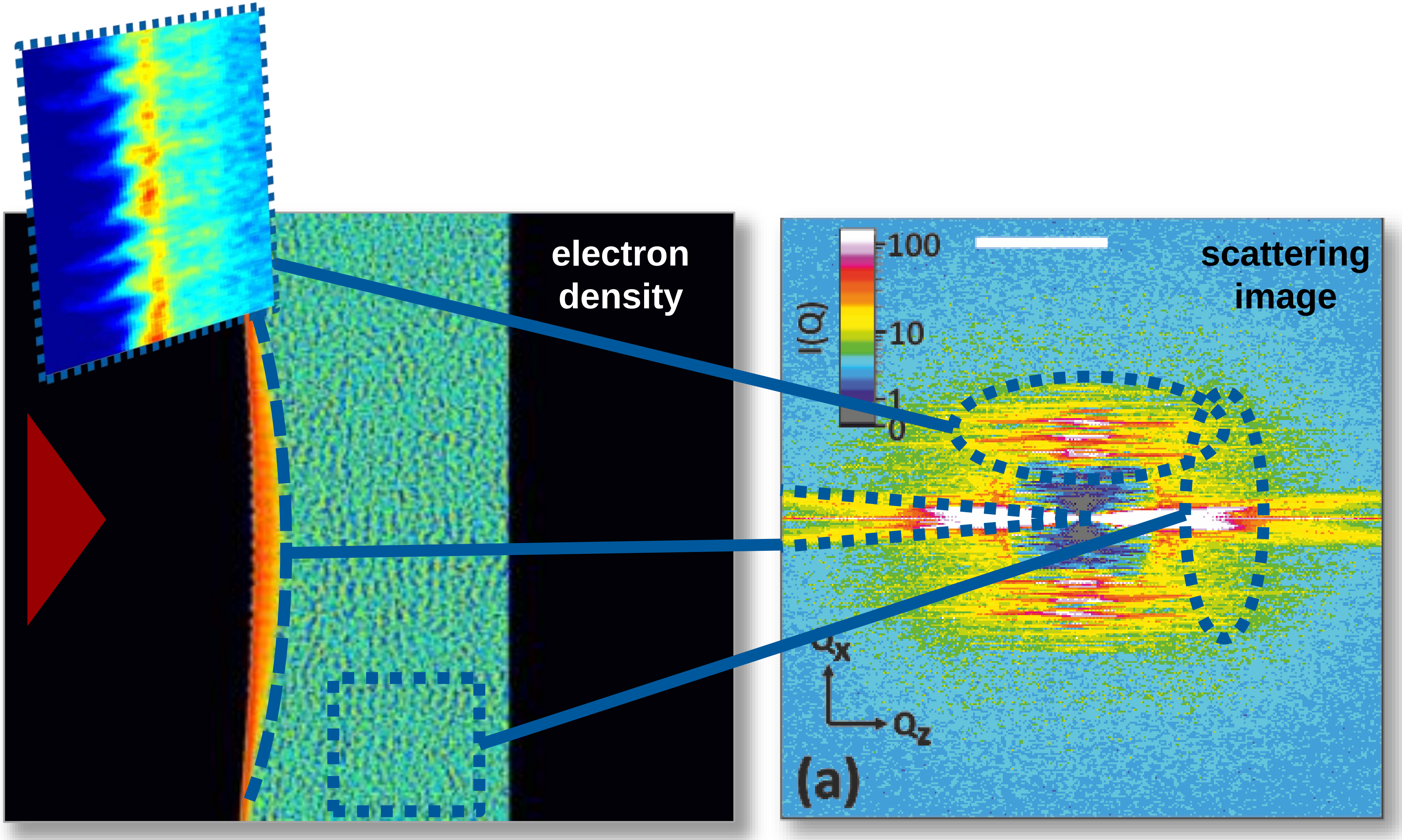
$$q = |\boldsymbol{k} - \boldsymbol{k_0}| = \frac{4\pi}{\lambda} \sin\Theta$$

$$\Delta\phi = -\boldsymbol{r}(\boldsymbol{k} - \boldsymbol{k_0}) = -\boldsymbol{r}\boldsymbol{q}$$

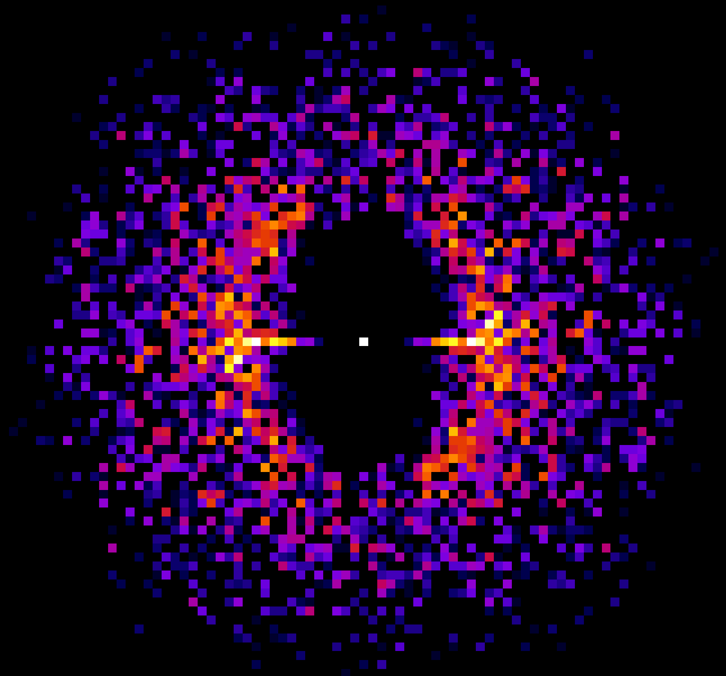


Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

What would we see if we probed the instabilities by SAXS?

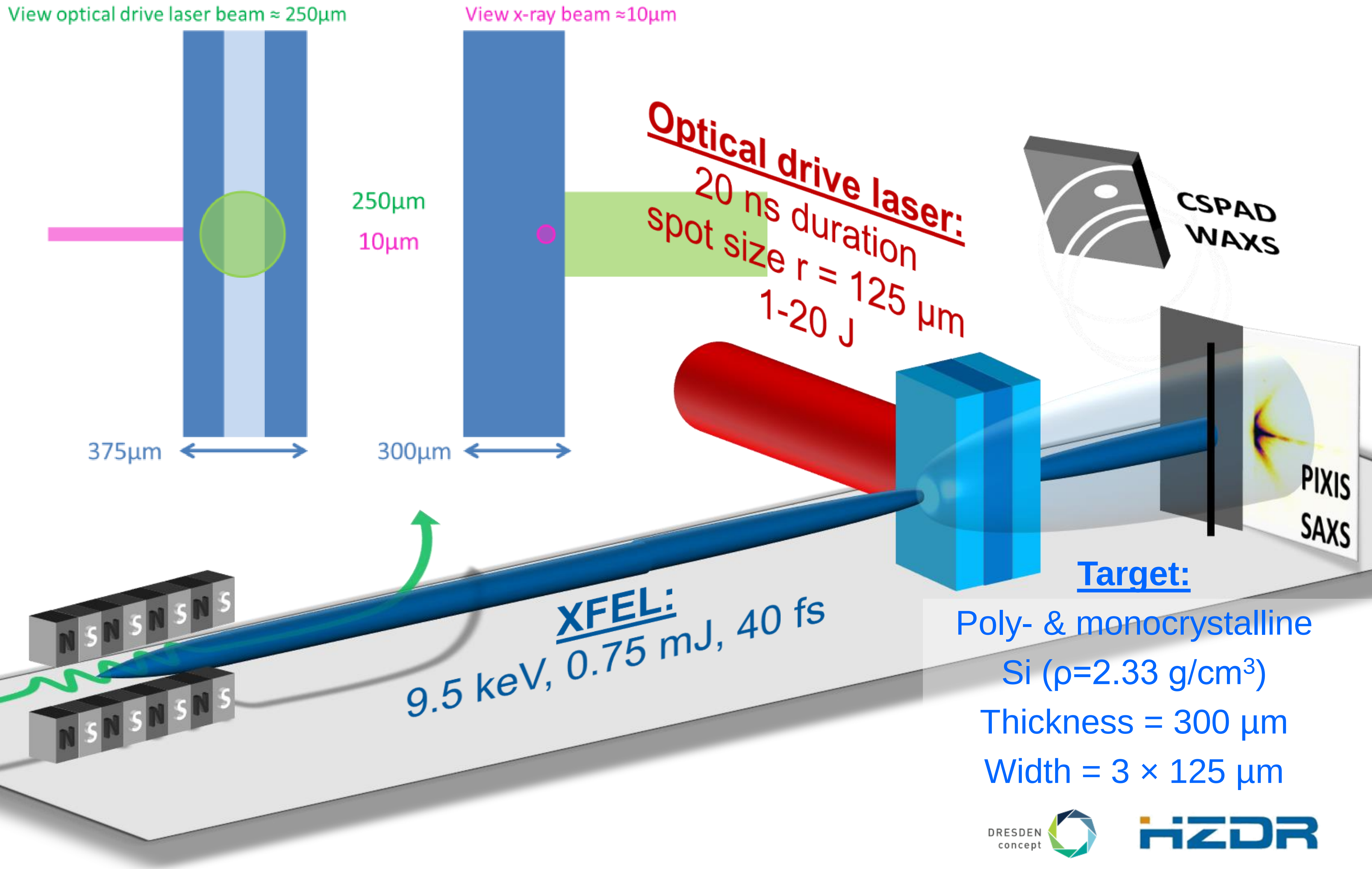


Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de



Compare to Experiment

LH88 beam time at LCSL (E. McBride, A. Pelka, M. Roedel, et al.)



Target:

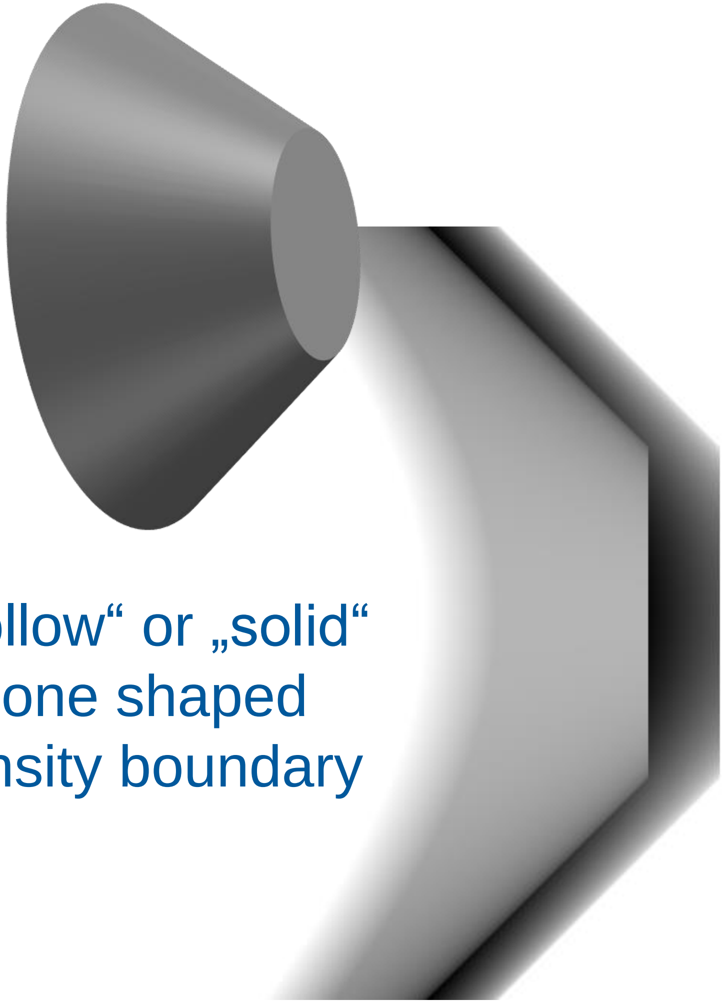
Poly- & monocrystalline

Si (ρ=2.33 g/cm^3)

Thickness = 300 µm

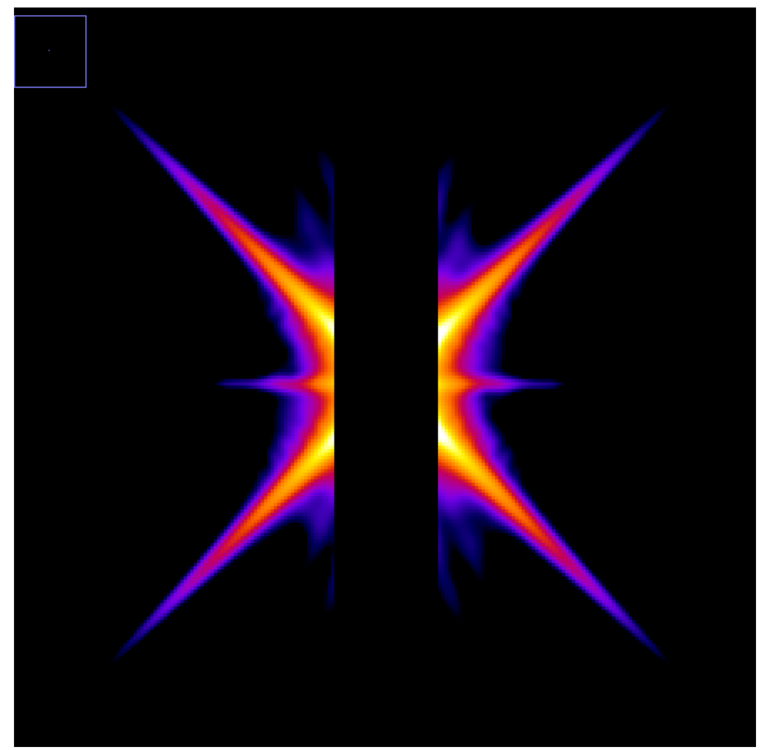
Width = 3 × 125 µm

SAXS is great for electron density jumps, so what do we see?



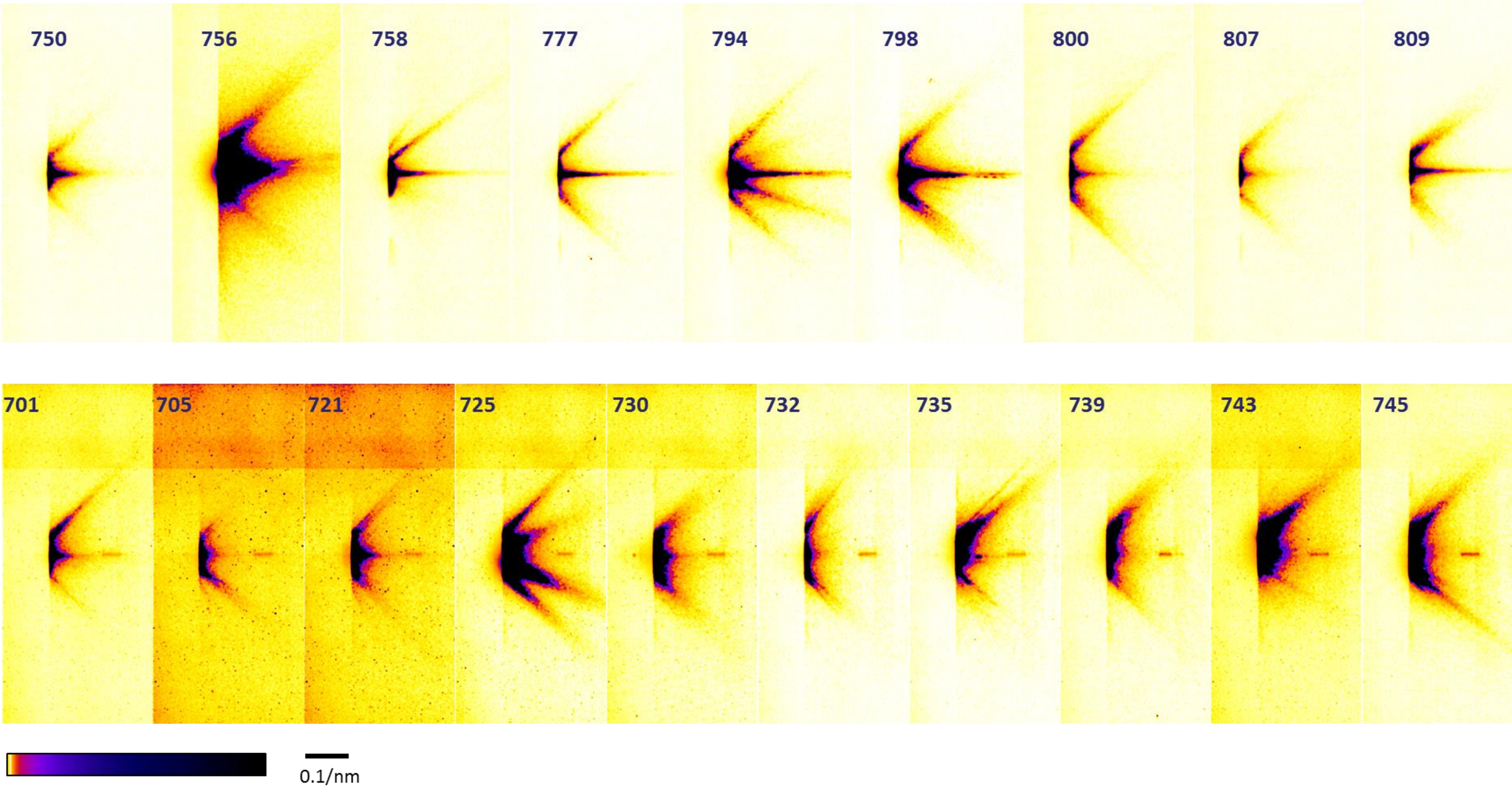
„Hollow“ or „solid“ cone shaped density boundary

$|FT|^2$



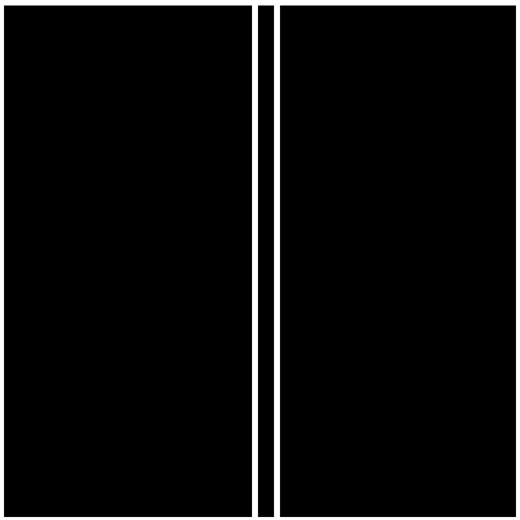
Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

SAXS is great for electron density jumps, so what do we see?

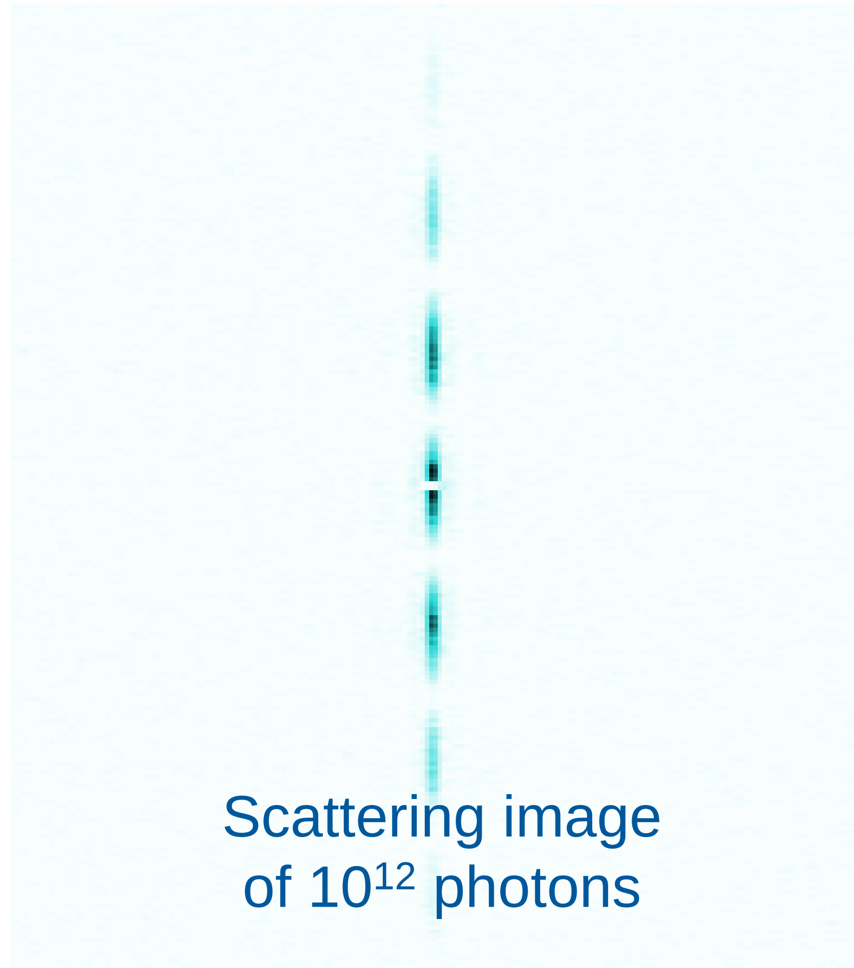


Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

10^{12} X-ray photons scattered on double slit in simulation



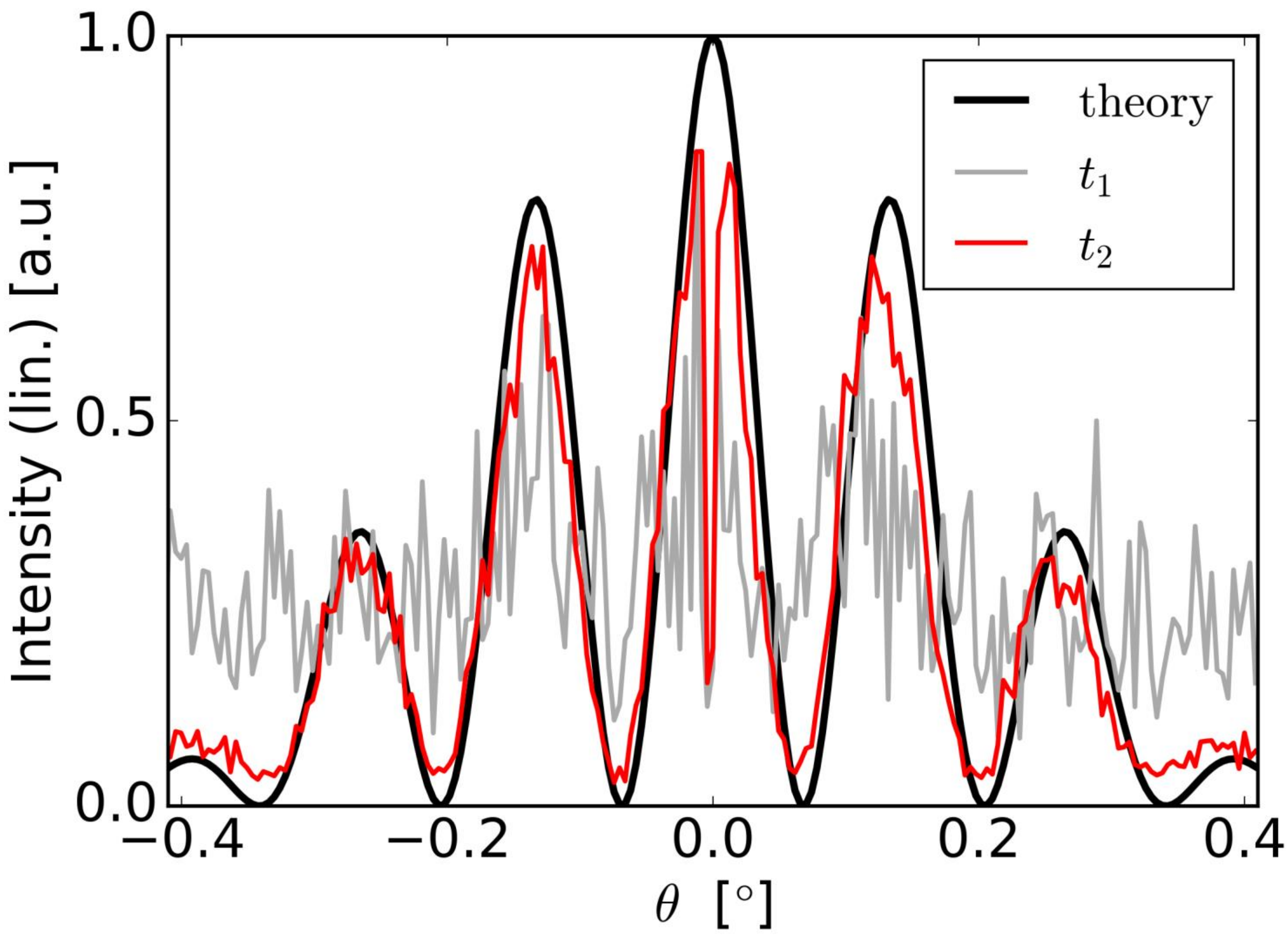
Double slit
3D density



Scattering image
of 10^{12} photons

Michael Bussmann · Computational Radiation Physics · www.hzdr.de/crp
m.bussmann@hzdr.de

Next: In-situ X-ray scattering / radiation transport / atomic physics




Thank you!
www.hzdr.de/crp