

Exascale Laser Plasma Physics - From Computational Speed to Predictions



A. Huebl^{1,2}

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K. Bastrakova,¹ A. Debus,¹ S. Ehrig,¹ M. Werner,^{1,2} B. Worpitz,³ A. Matthes,^{1,2}
S. Rudat,^{1,2} S. Starke,¹ T. Kluge,¹ T.E. Cowan,^{1,2} U. Schramm,^{1,2} and M. Bussmann¹

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³ LogMeln, Inc.

Invited Talk I4.203

46th European Physical Society Conference on Plasma Physics (EPS 2019)

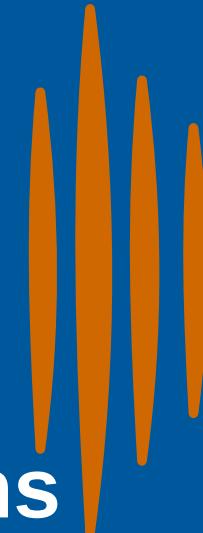
Milano (Italy), July 11th 2019



Outline

- Contemporary PIC Simulations
 - *PIConGPU as a scientific instrument*
 - *selected challenges in Exascale computing*
- Predictive Capabilities for Experimental Campaigns
 - *systematic understanding under uncertain conditions*
 - *a new look on multi-species effects*

PICon GPU

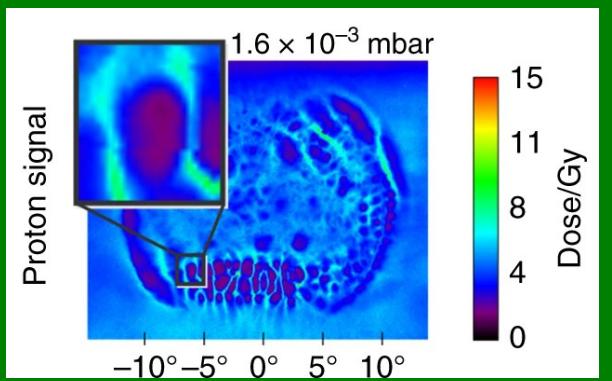


Particle-in-Cell Simulations for the Exascale Era

Research Topics

Plasma Instabilities

- Astrophysics
- Control of Laser-Plasmas

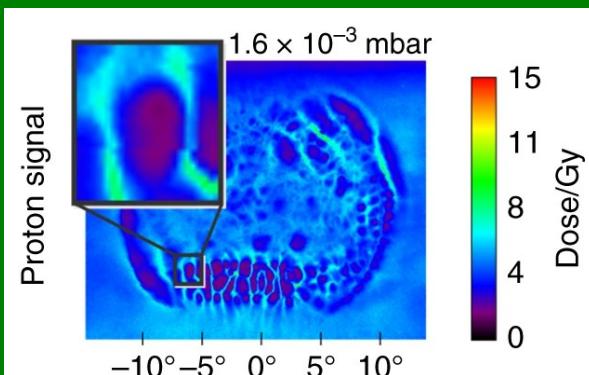


L. Obst-Huebl et al., Nat. Comm. 9, 5292 (2018)

Research Topics

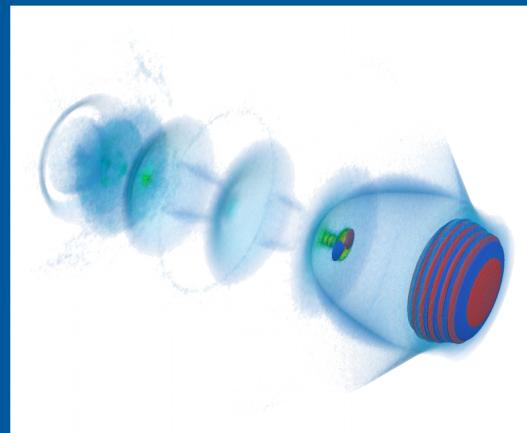
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Laser-Electron Acceleration

- Compact X-Ray sources
- Push the Energy Frontier

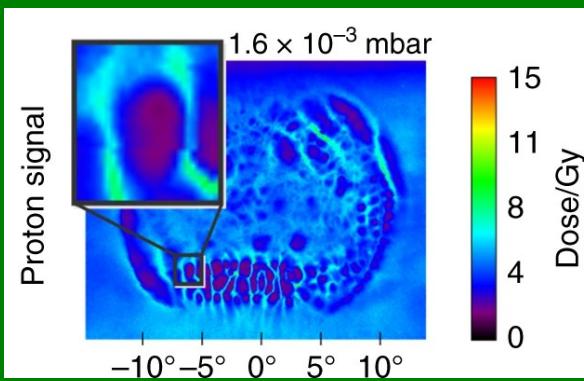


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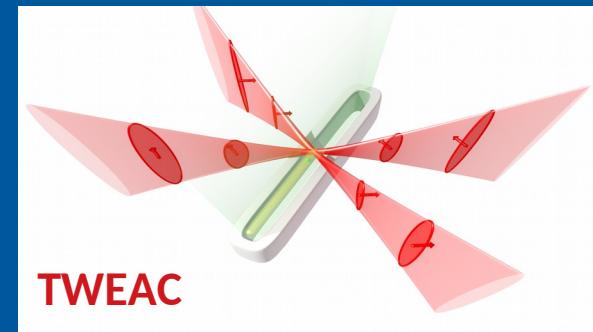
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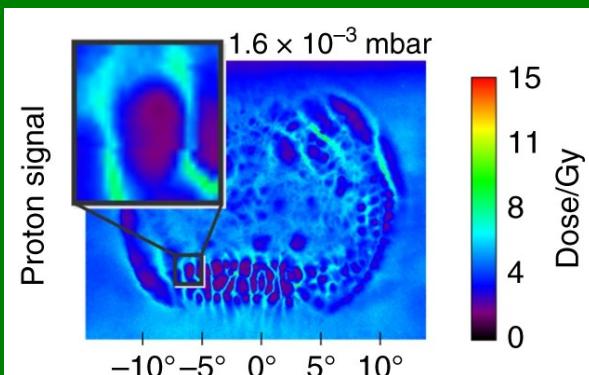


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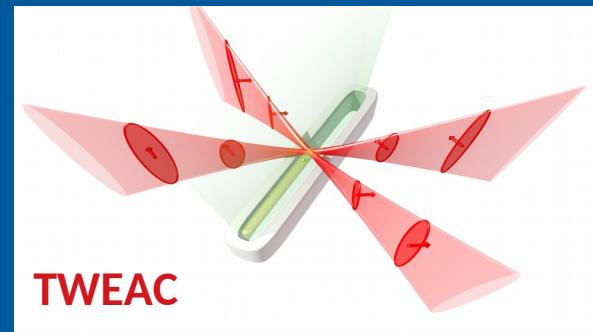
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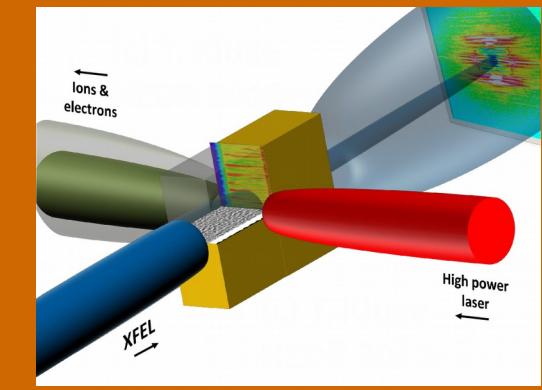
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Laser-Ion Acceleration

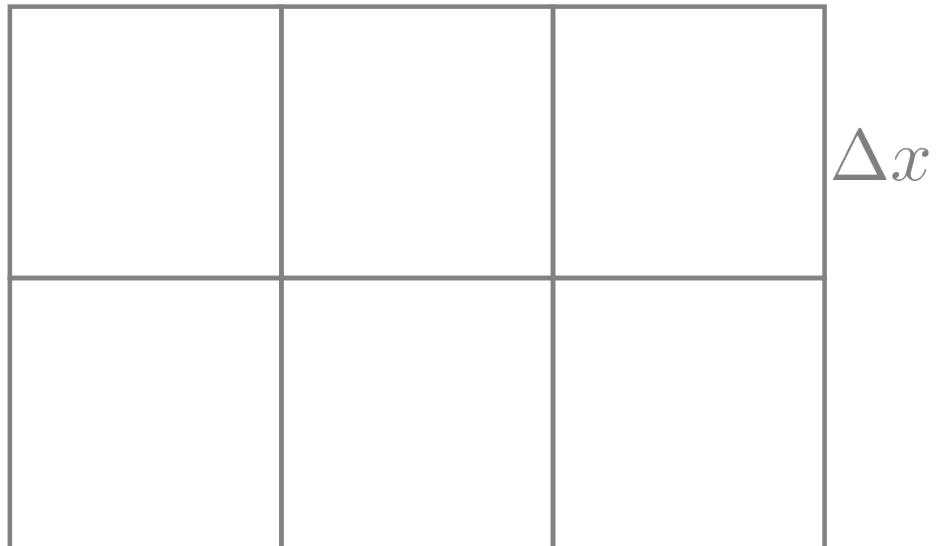
- Compact Ion Sources
- HED Physics



L. Obst-Huebl et al., Nat. Comm. **9**, 5292 (2018); J. Couperius et al., Nat. Comm. **8**, 487 (2017); A. Debus et al., under review (2019); P. Hilz et al., Nat. Comm. **9**, 423 (2018); T. Kluge et al., PRX **8**, 031068 (2018)

Particle-in-Cell

Basic Principle

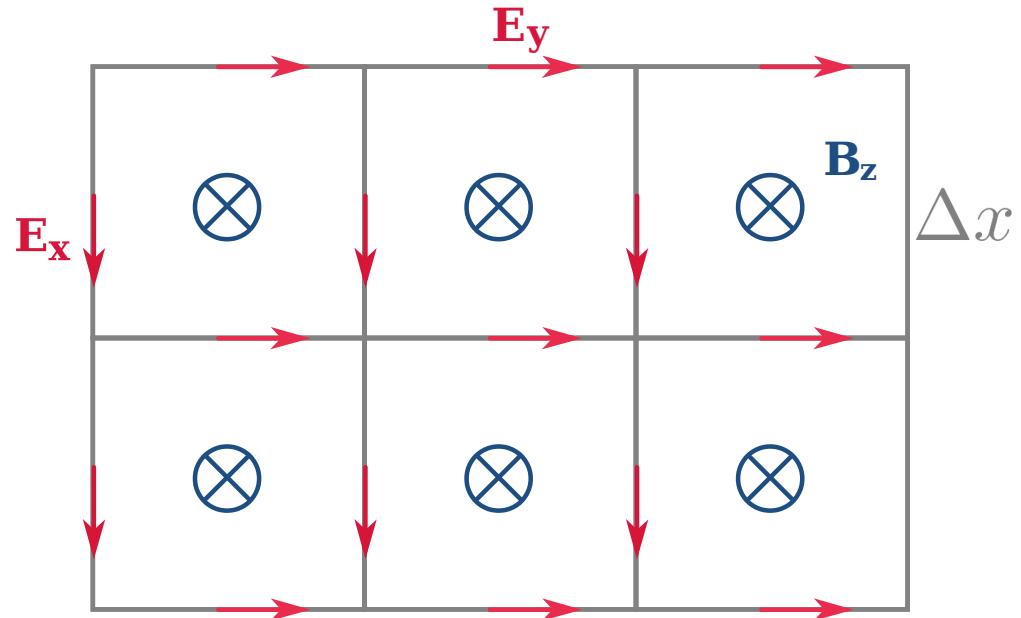


- Eulerian



Particle-in-Cell

Basic Principle



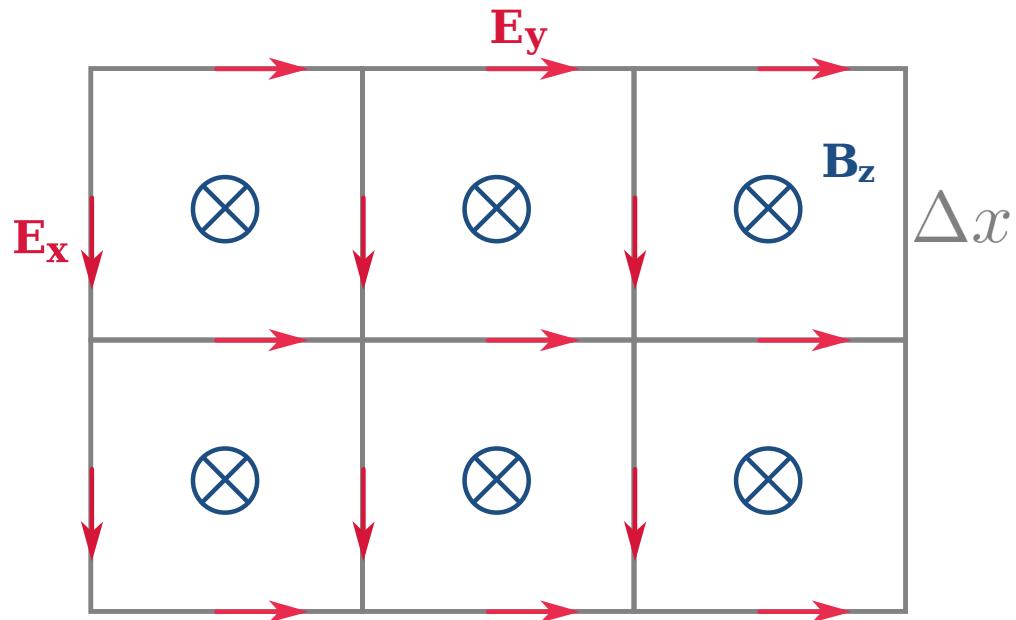
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

- Eulerian: electro-magnetic fields

PIConGPU

Particle-in-Cell

Basic Principle



self-consistent,
linearized
time step:

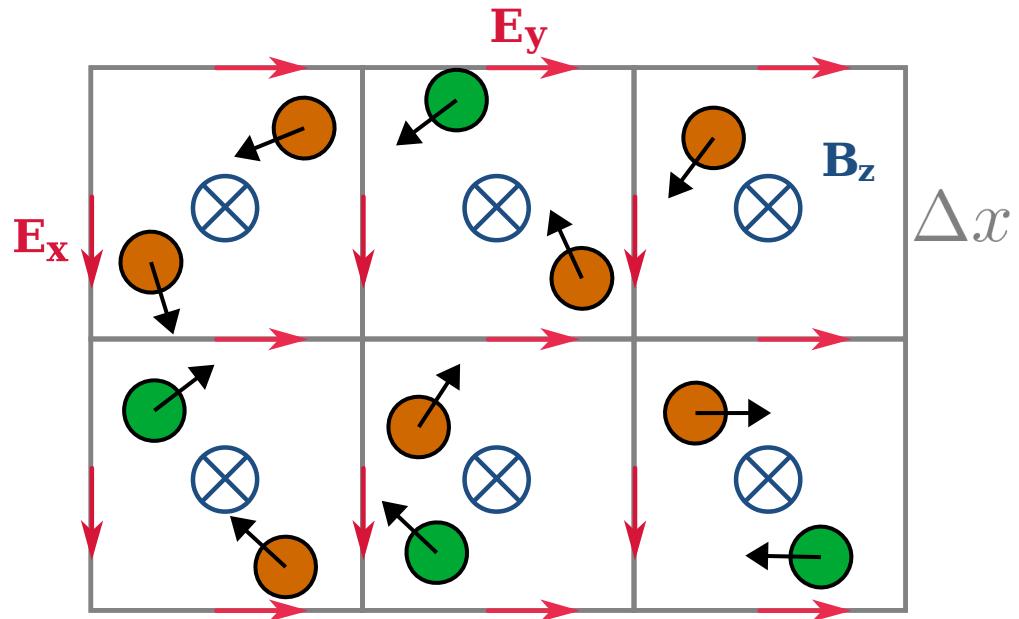
$$\frac{\partial \mathbf{A}}{\partial t} \rightarrow \frac{\Delta \mathbf{A}}{\Delta t}$$
$$c\Delta t \lesssim \Delta x$$

$$\nabla \times \mathbf{E} = - \frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{B} = + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

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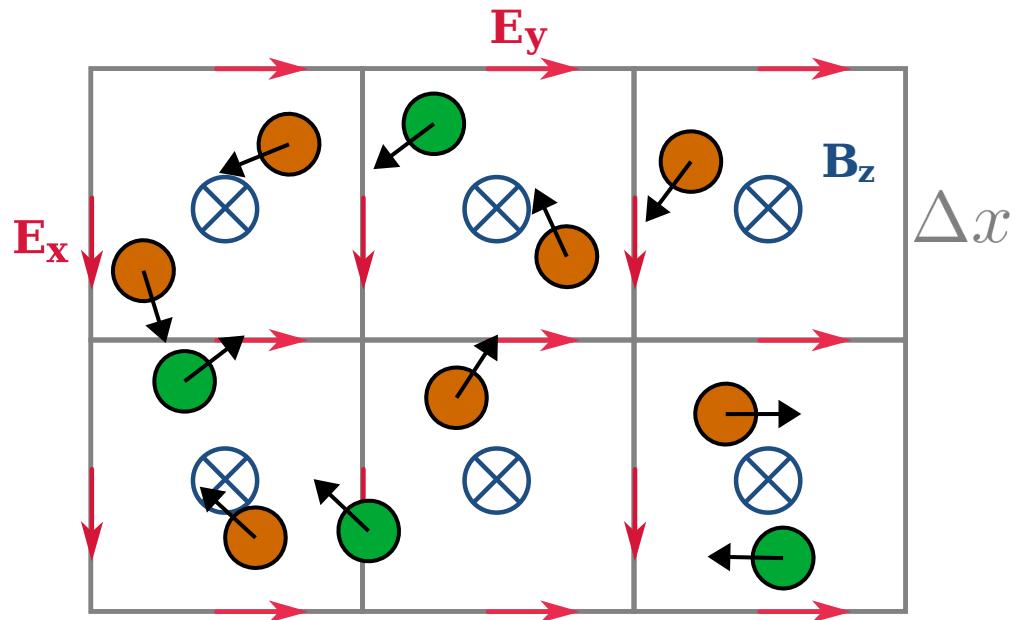
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- Lagrangian: particles in Vlasov-equation



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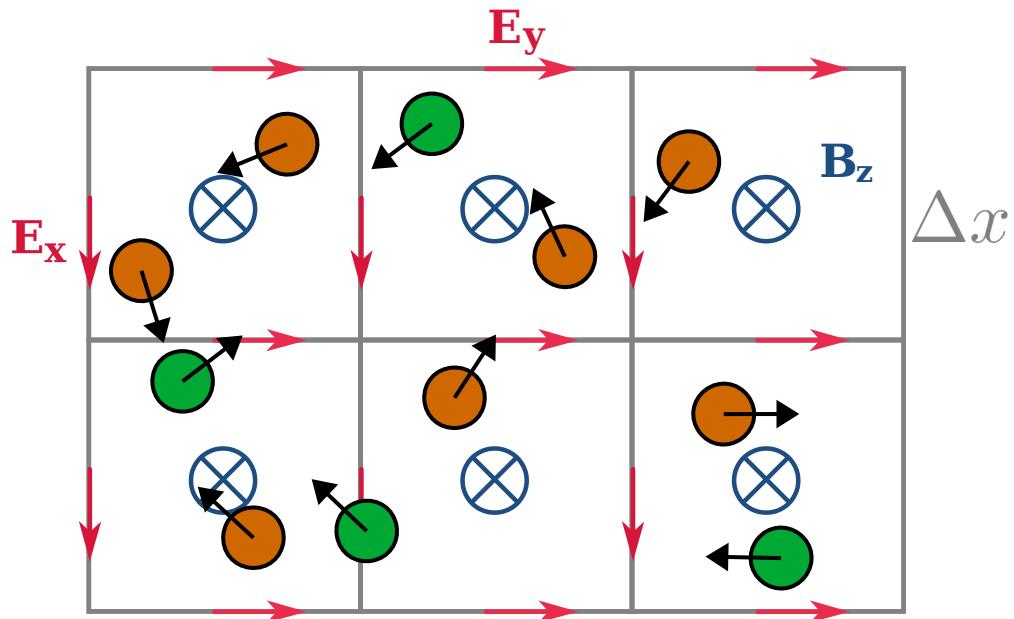
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

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Particle-in-Cell Basic Principle



initial & boundary
conditions:

$$\nabla \cdot \mathbf{E} = \frac{1}{\varepsilon_0} \sum_s \rho_s$$
$$\nabla \cdot \mathbf{B} = 0$$

self-consistent,
linearized
time step:

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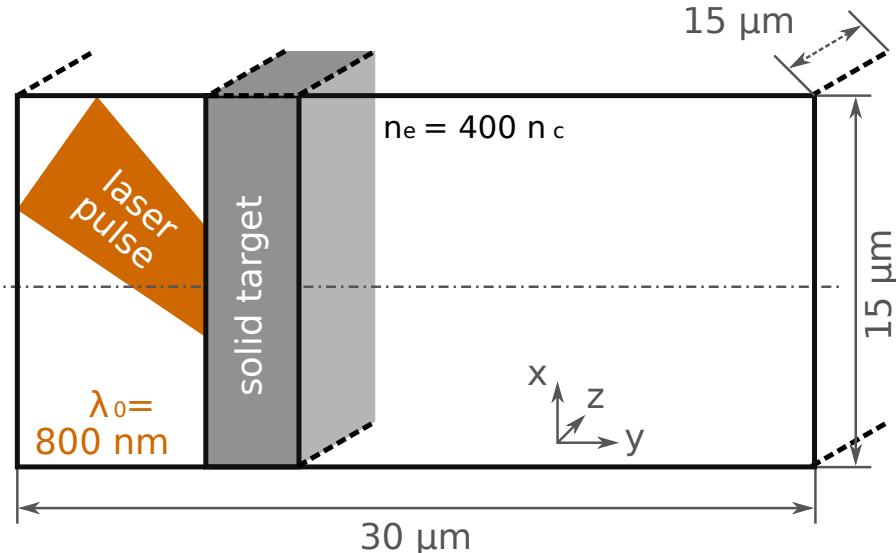
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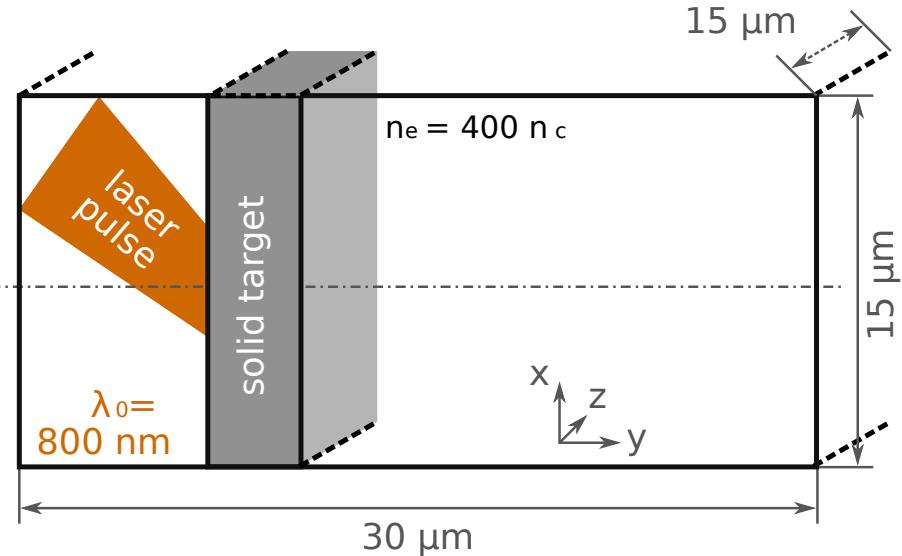
Simulation Requirements

A moderate, 3D Laser-Ion Acceleration Setup



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A moderate, 3D Laser-Ion Acceleration Setup



$$\Delta t \cdot \omega_{p,e} \leq 0.1$$

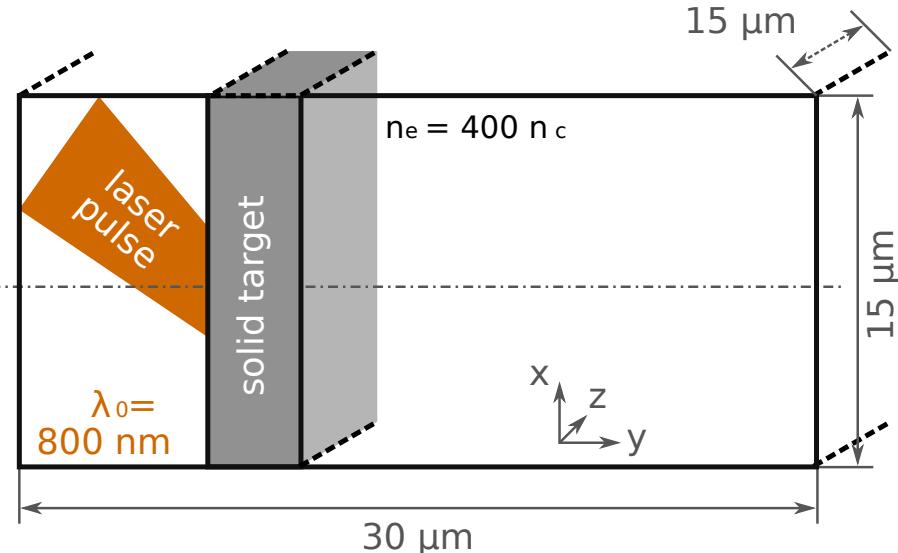
$$\Delta t = 2.1 \text{ as}$$

$$\Delta x, \Delta y, \Delta z = 1.1 \text{ nm}$$

$$N_{x,y,z} = 13\,600 \times 13\,600 \times 27\,000$$
$$= 5 \cdot 10^{12}$$

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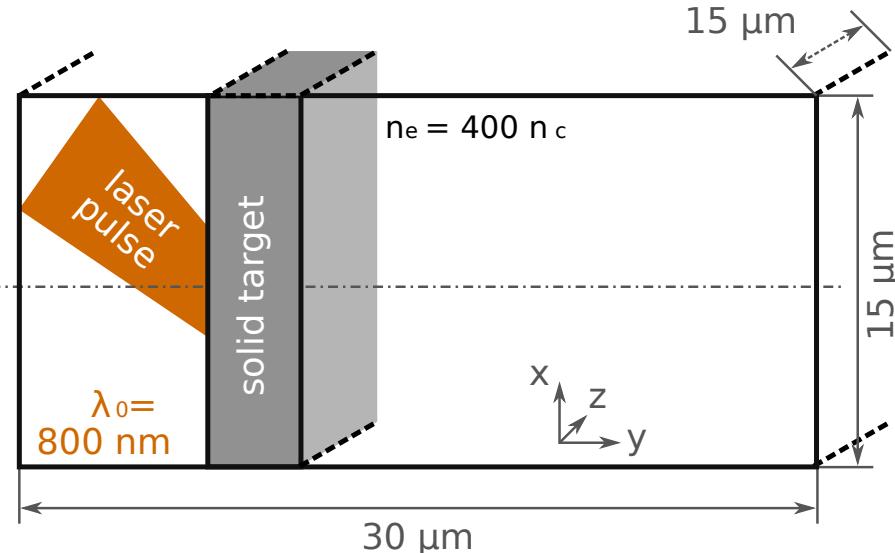
+ 10^{12} particles

each $\mathcal{O}(1\,000)$ Operations

$\times 100\,000$ steps

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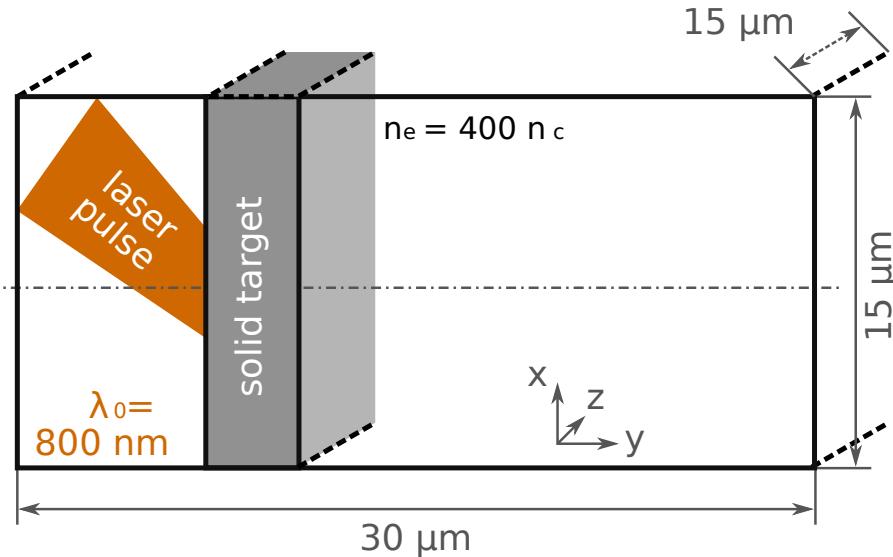
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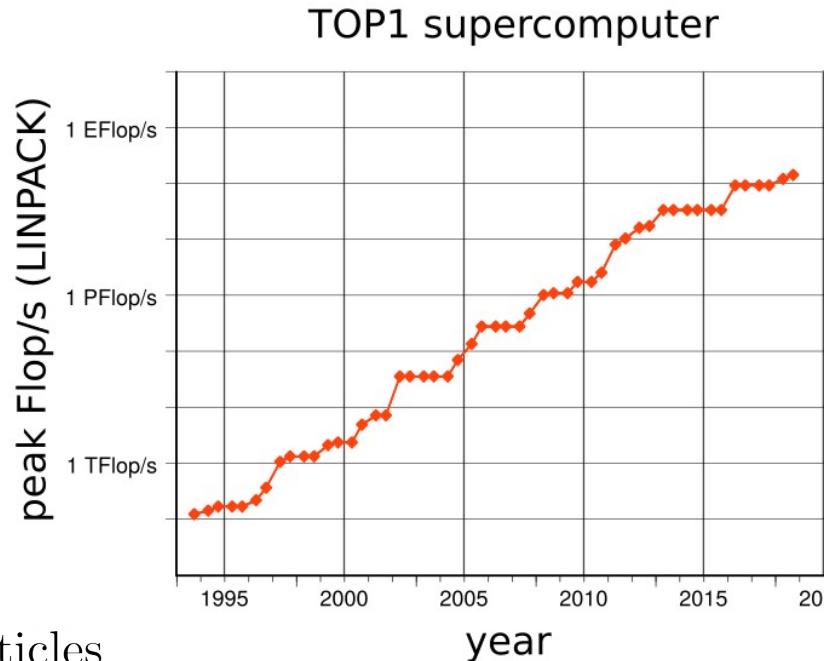
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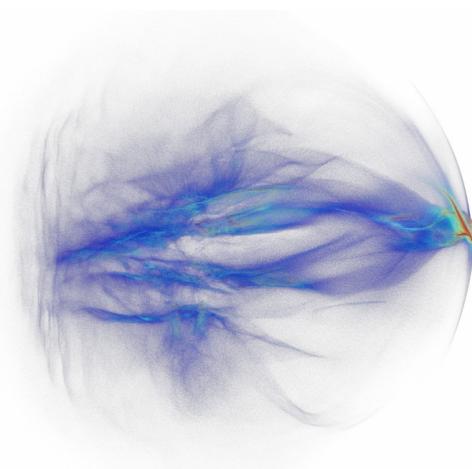
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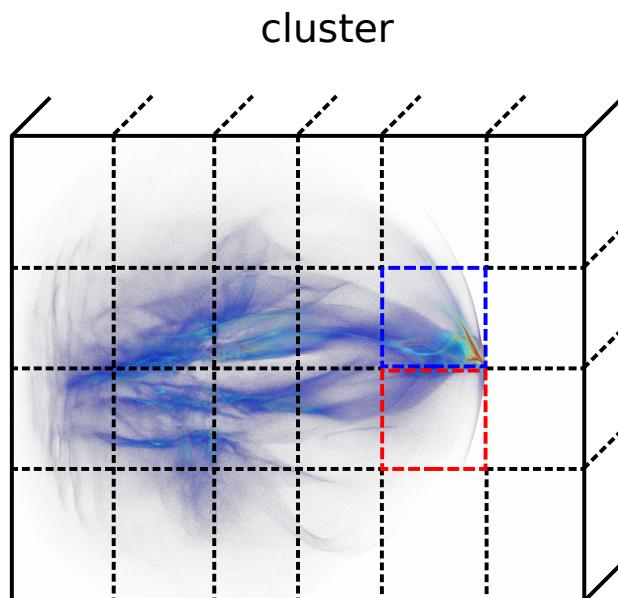
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B. Worpitz, Master's Thesis (2015)
E. Zenker, A. Huebl et al., IPDPSW (2016)

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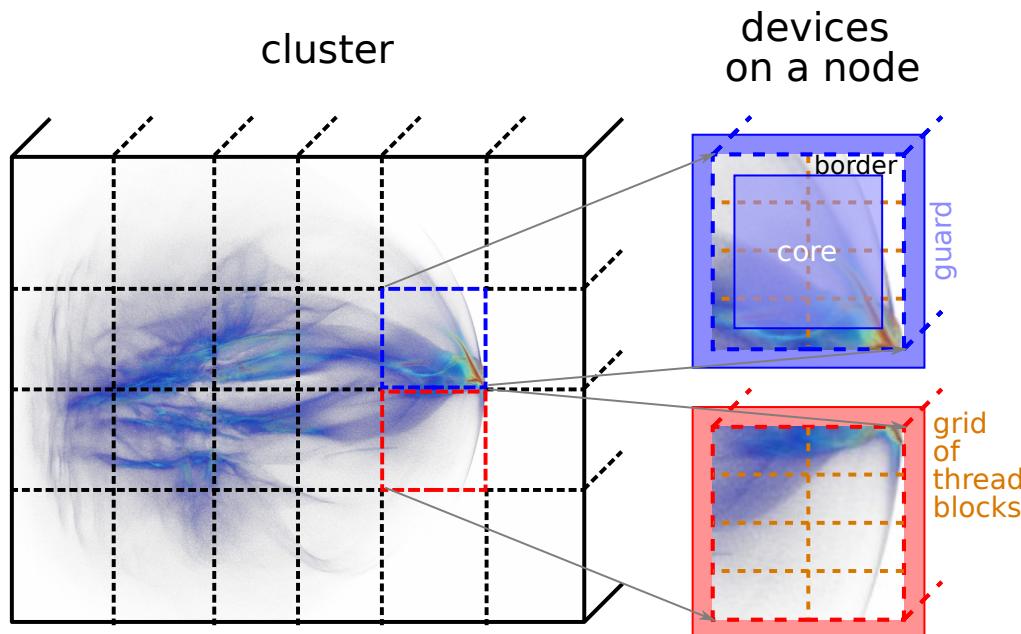
Deeply nested, 3D, Domain Decomposition



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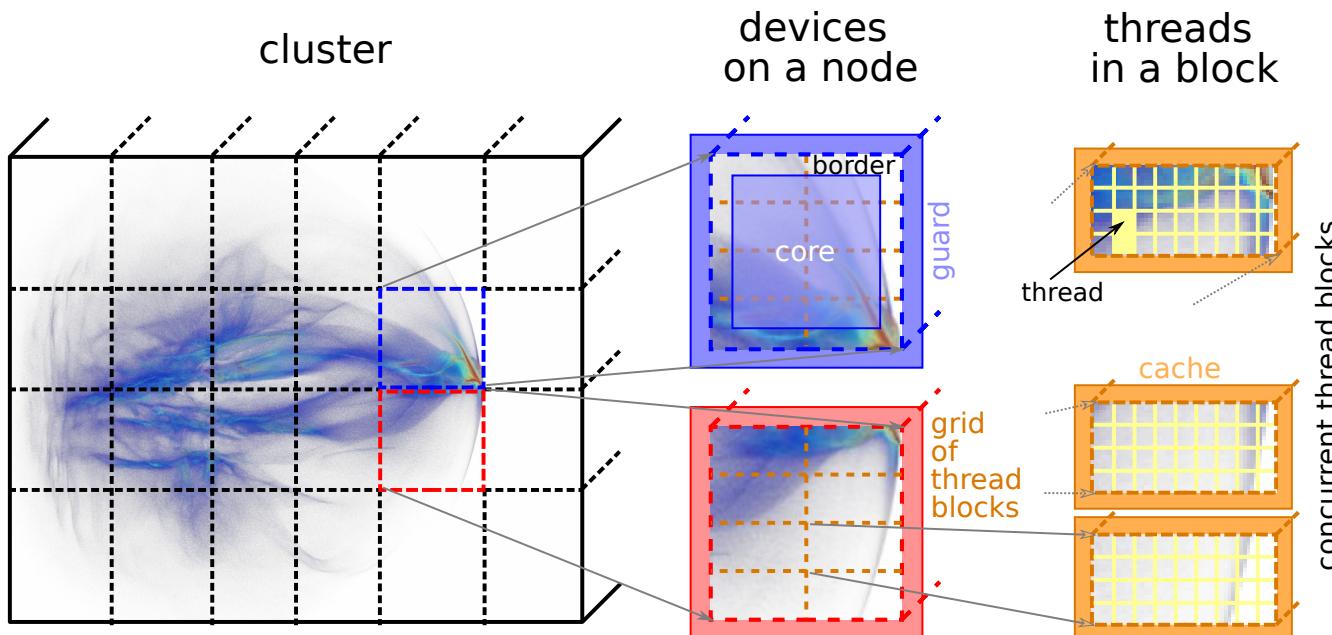
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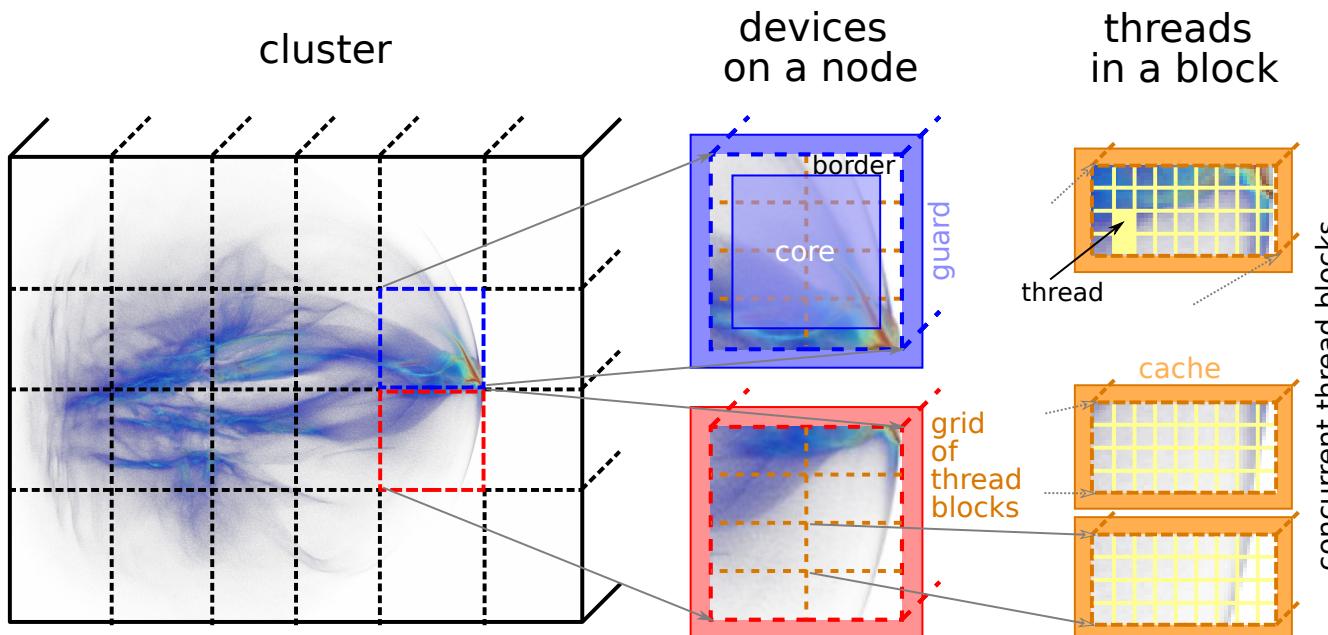
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Deeply nested, 3D, Domain Decomposition



*typical time
to solution:*

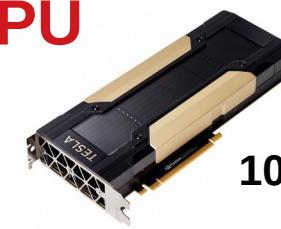
CPU



72 cores
288 threads

1 week

GPU



5120 cores
100'000 threads

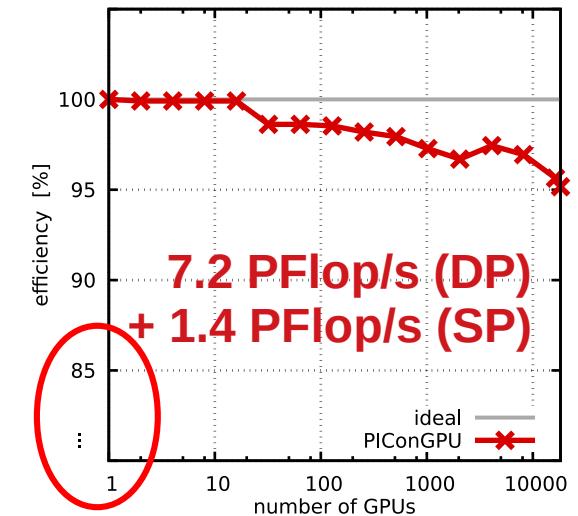
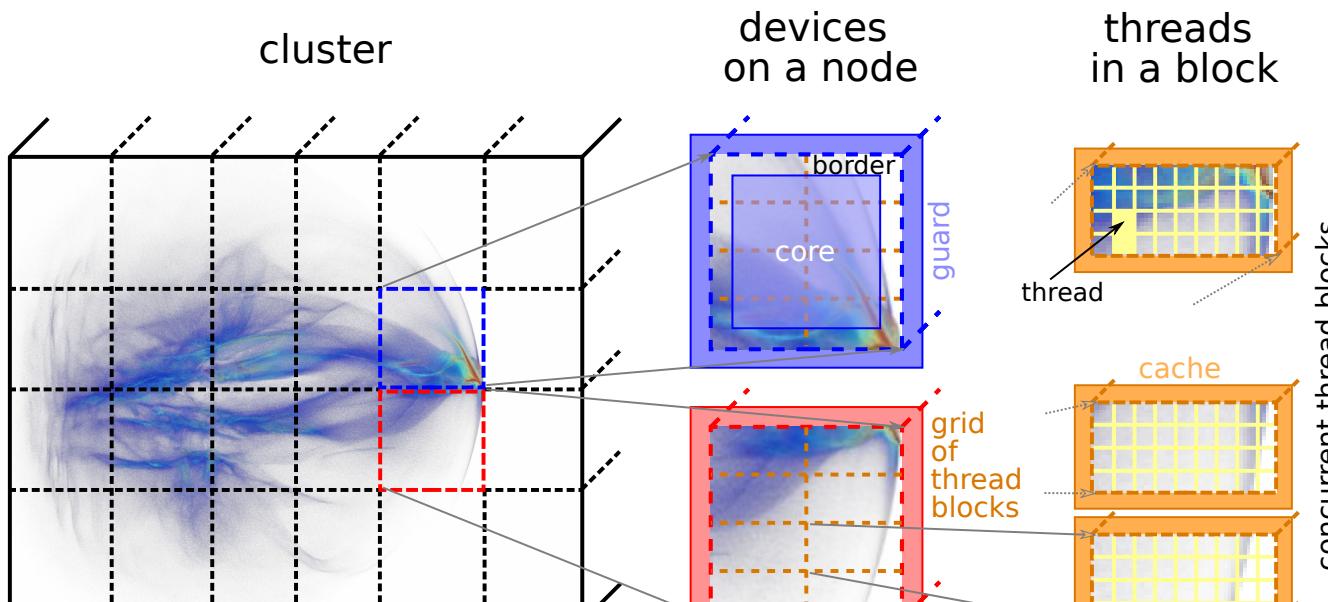
8 hours

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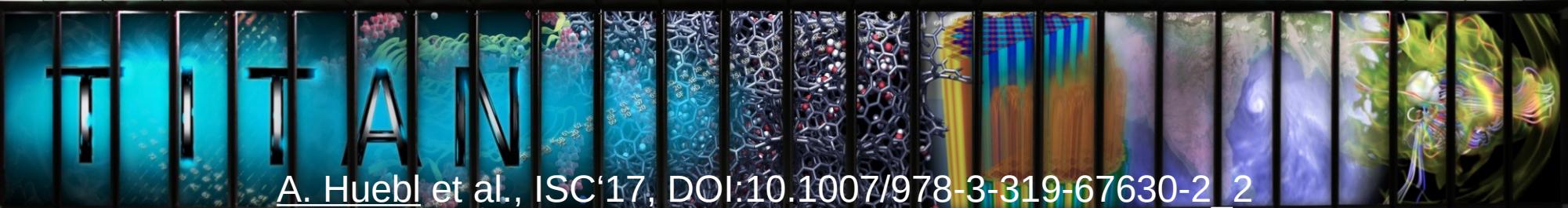
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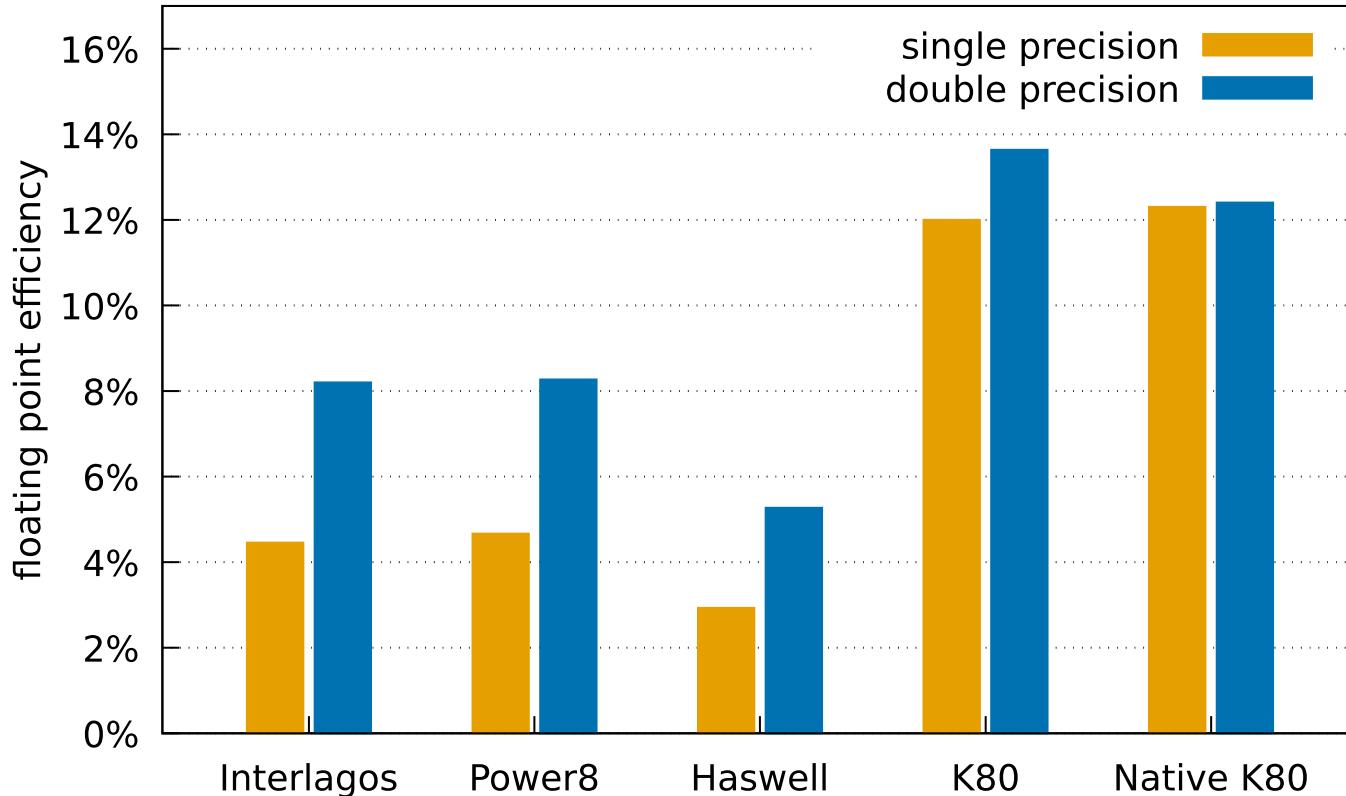


M. Bussmann, A. Huebl et al., SC'13, DOI:10.1145/2503210.2504564



PIConGPU on alaka

Performance after only 3 (!) weeks



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Maintainability
PIConGPU +
PMacc code lines

Before: 80k LOC
(20k in kernels)
After: 50k LOC
(1 year)

Parallelization

Managing Expectations & Predictive Capabilities

PetaFlop/s (2008): 10^{15} floating point operations / second

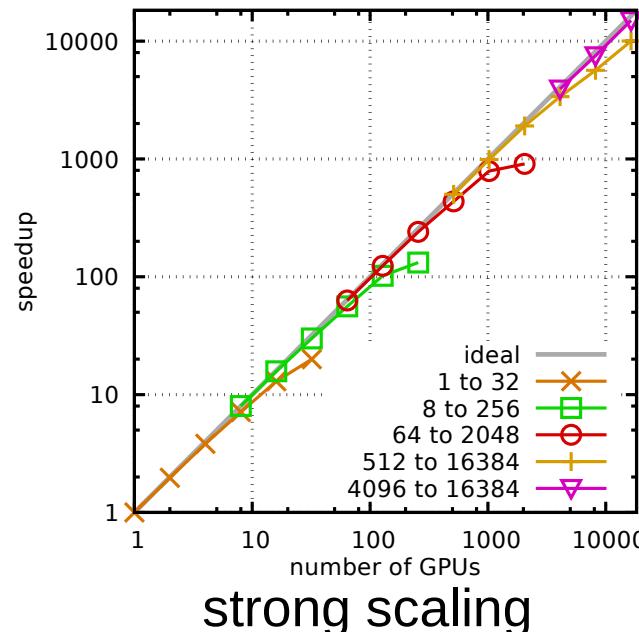
ExaFlop/s (2021)

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ExaFlop/s (2021) will **not** deliver simulation results $10^3 \times$ faster, but enables simulations of

- larger problems (size, resolution)
- more complex problems*
- more problems**

within the same time to solution!

Parallelization

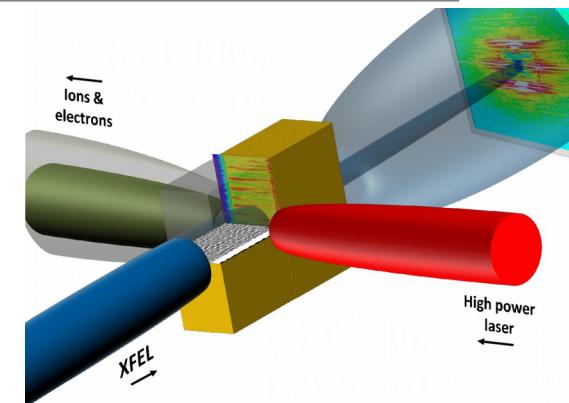
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* extend modeled micro-physics

- X-Ray scattering
- non-LTE atomic physics
- advanced collisions
- QED processes
- etc.

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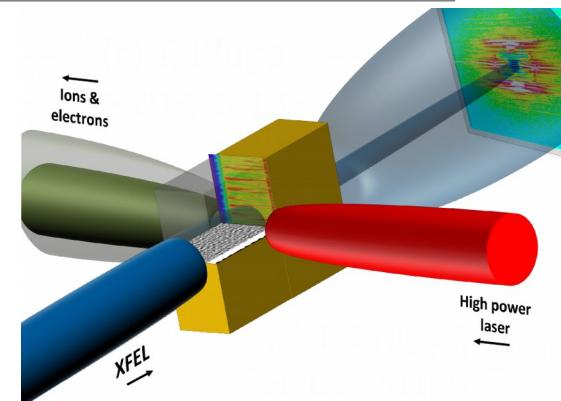
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** investigate systematical & statistical errors

- *input uncertainties*
- *numerical schemes*

* extend modeled micro-physics

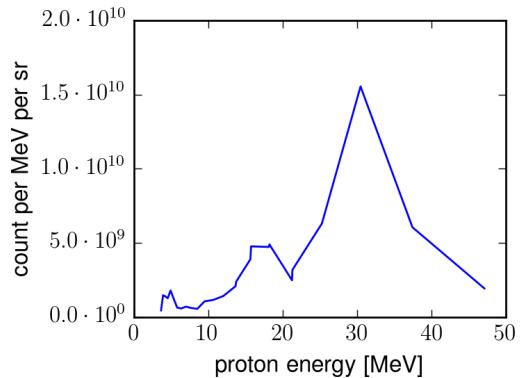
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Scientific Data Workflows

The actual Exascale / PByte Challenge

- every ~7 years:
8x compute power but only **2.5x** I/O bandwidth

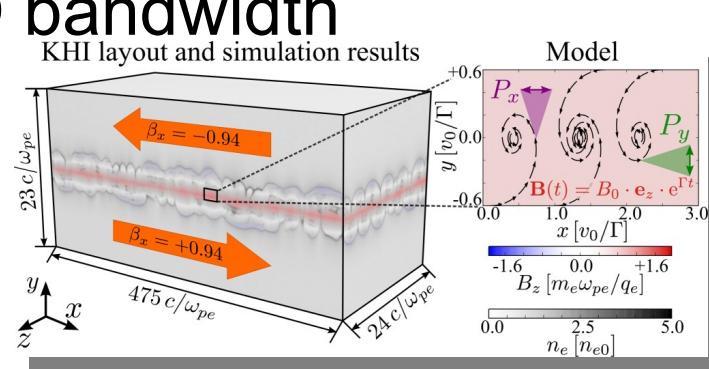
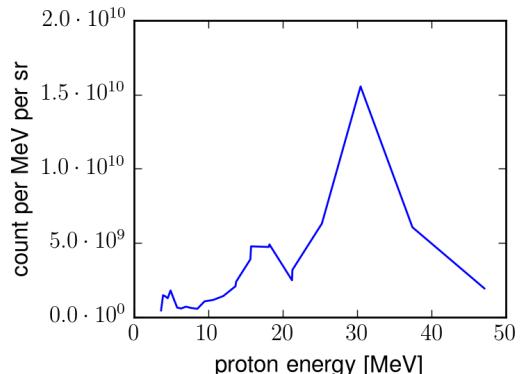


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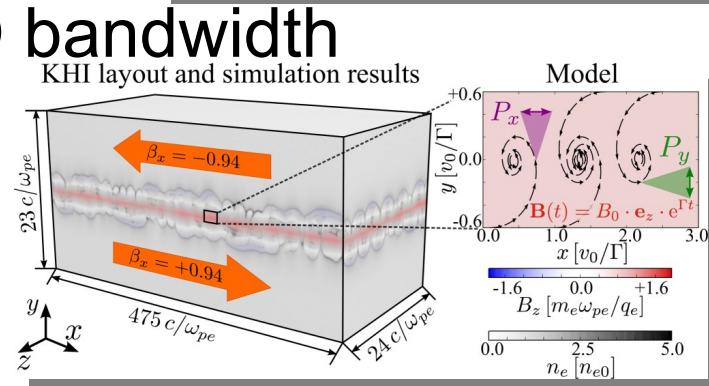
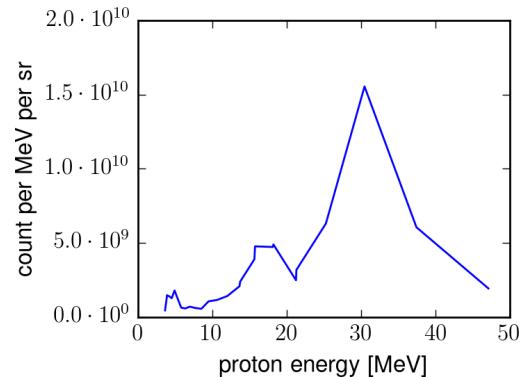


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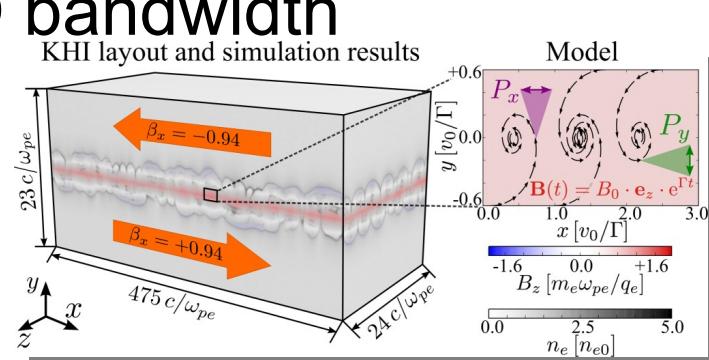
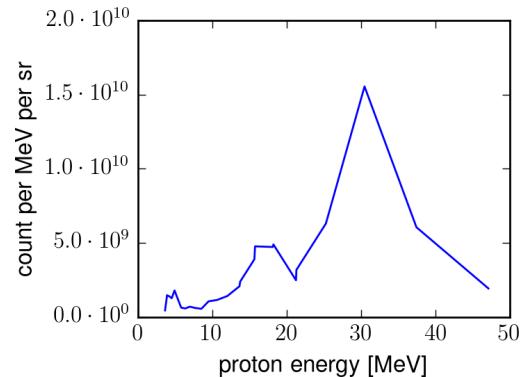
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- exchange:  standard & API, streaming

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 The HDF Group

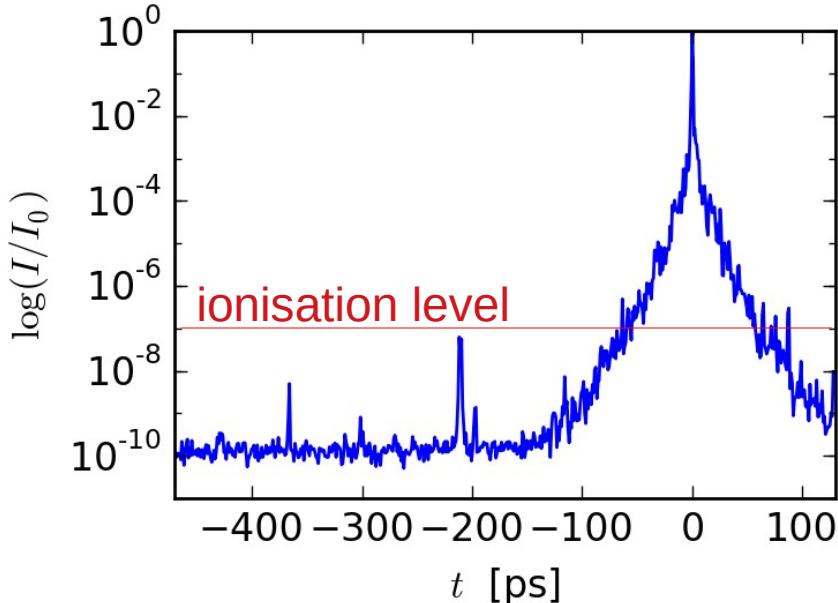


Predictive Capabilities for Experimental Campaigns

Predictive 3D Simulations

Volumetric Ion Acceleration with Micron-Scale Spheres

Sensitive Initial Conditions



$\varnothing=1\mu\text{m}$
 $n_e=400n_c$

autocorrelator measurement

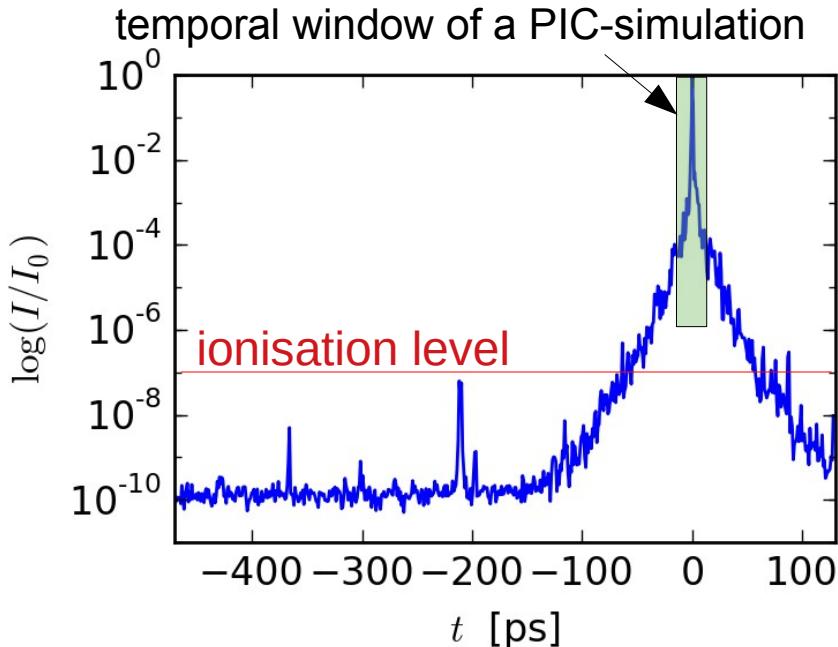
PHELIX laser: $\tau_0=500$ fs, $a_0=17$, $\lambda_0=1.054$ μm

P. Hilz, T. Ostermayr, A. Huebl et al., Nat. Comm. 9, 423 (2018); Talk this morning by P. Hilz

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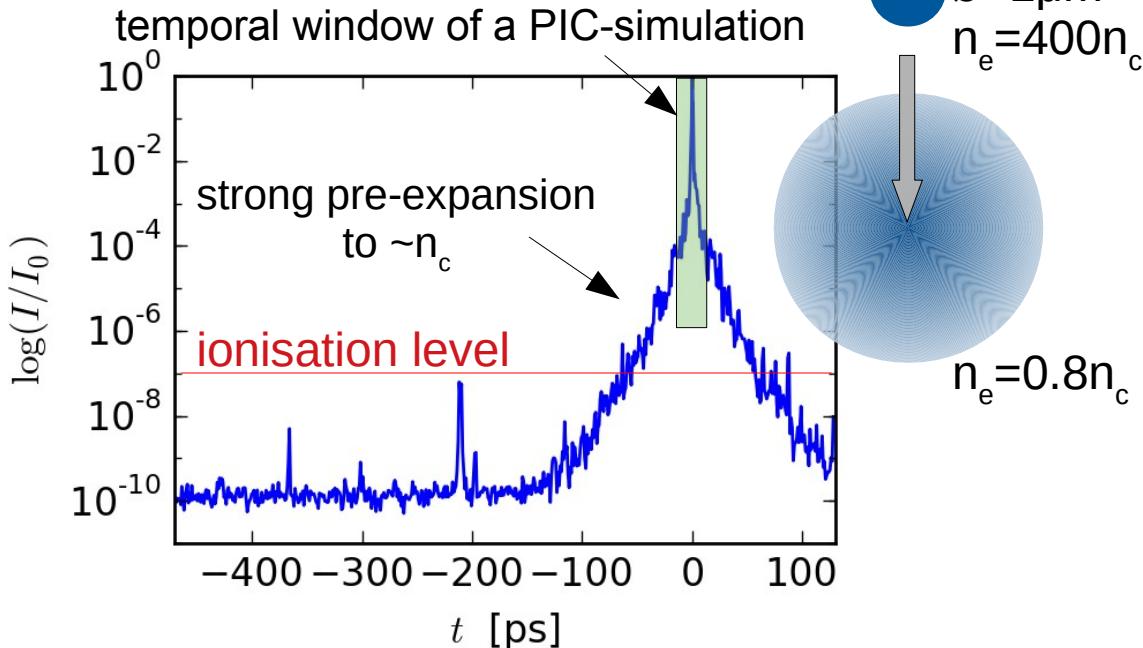
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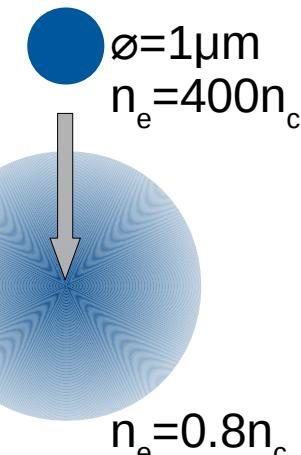
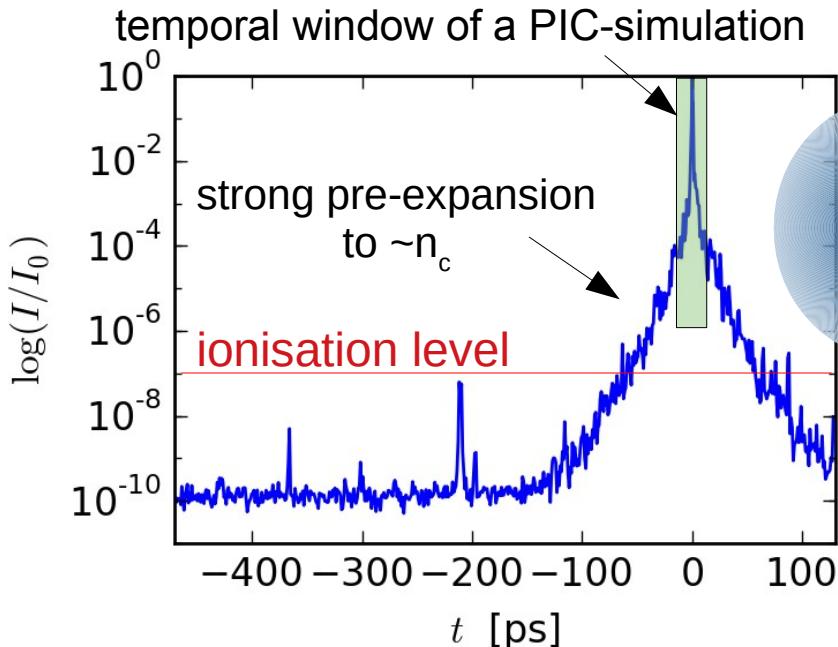
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P. Hilz, T. Ostermayr, A. Huebl et al., Nat. Comm. 9, 423 (2018); Talk this morning by P. Hilz

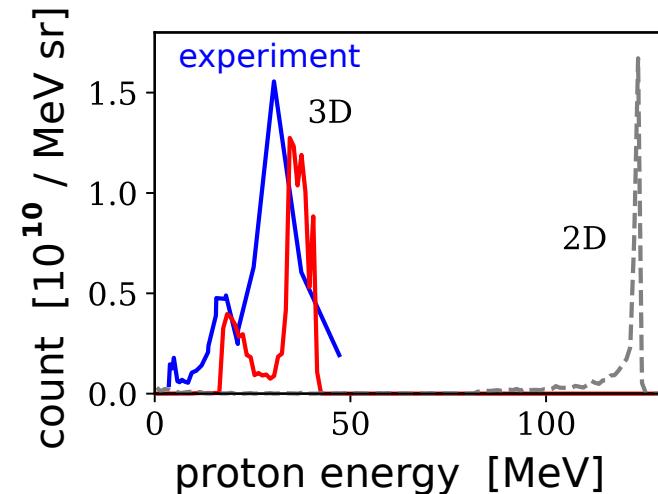
Predictive 3D Simulations

Volumetric Ion Acceleration with Micron-Scale Spheres

Sensitive Initial Conditions



Proper, 3D Geometry



autocorrelator measurement

PHELIX laser: $\tau_0=500$ fs, $a_0=17$, $\lambda_0=1.054$ μm

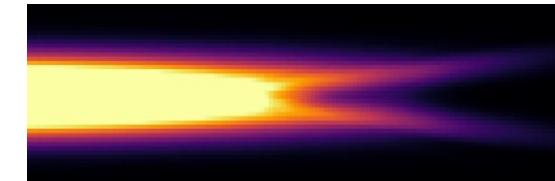
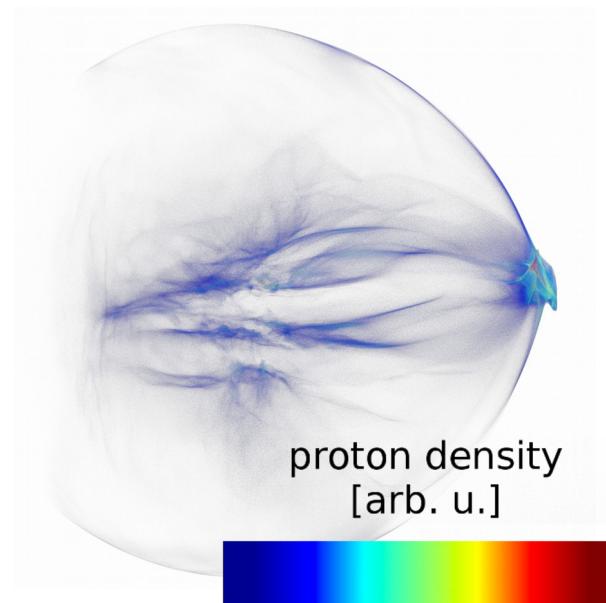
**10 MCPUh & 1 PByte data
on 8'000 GPUs in 16h**

P. Hilz, T. Ostermayr, A. Huebl et al., Nat. Comm. 9, 423 (2018); Talk this morning by P. Hilz

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Volumetric Ion Acceleration of μm -Spheres

- Electrons
 - *volumetric interaction after expansion*
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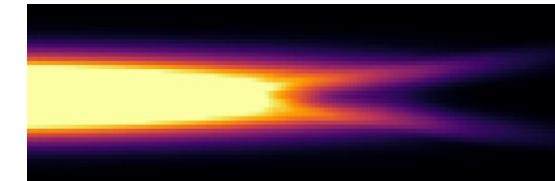


P. Hilz, T. Ostermayr, A. Huebl et al., Nat. Comm. **9**, 423 (2018); Talk this morning by P. Hilz

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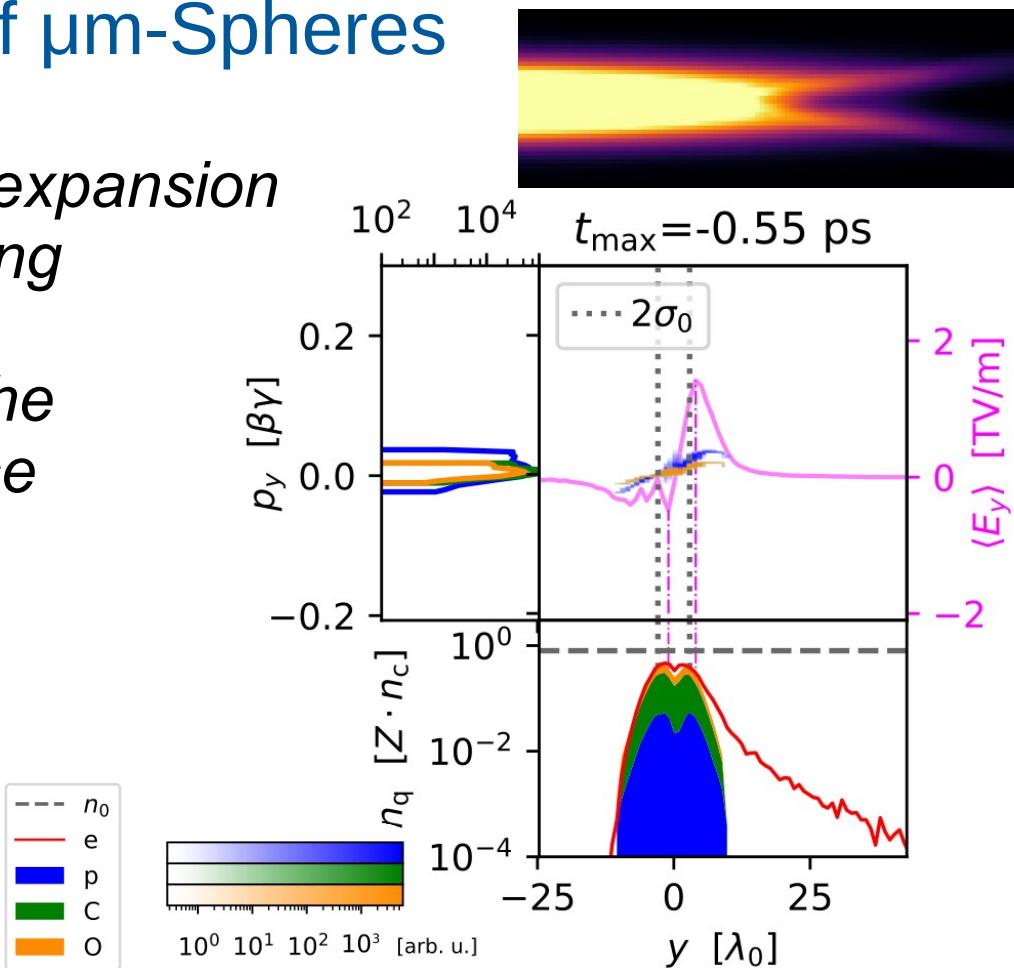


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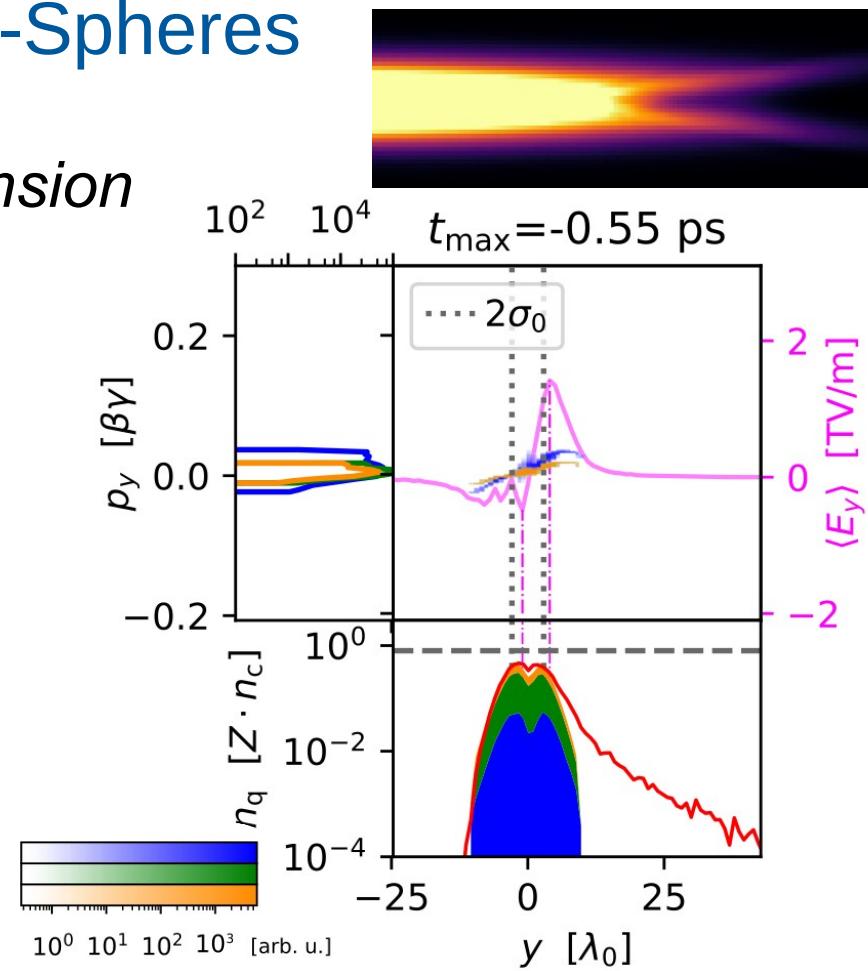
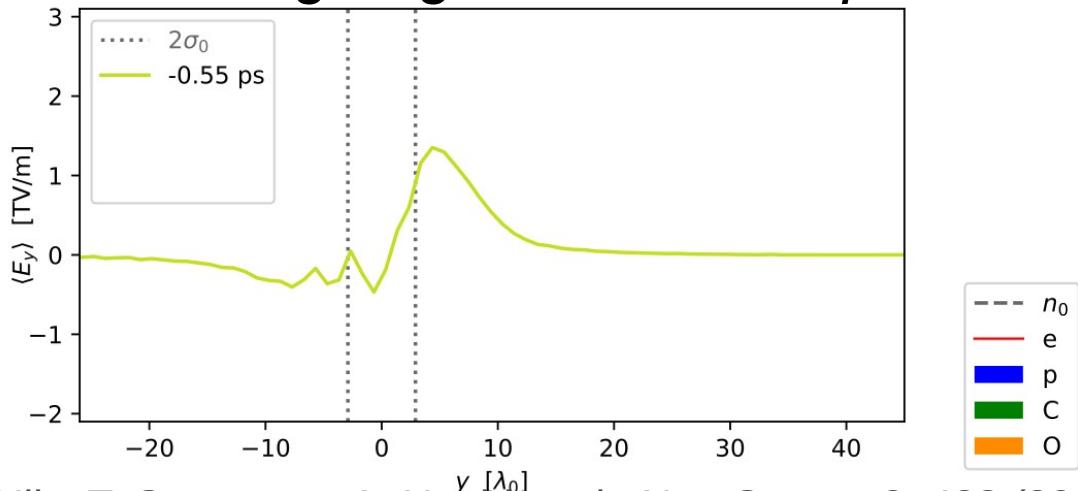


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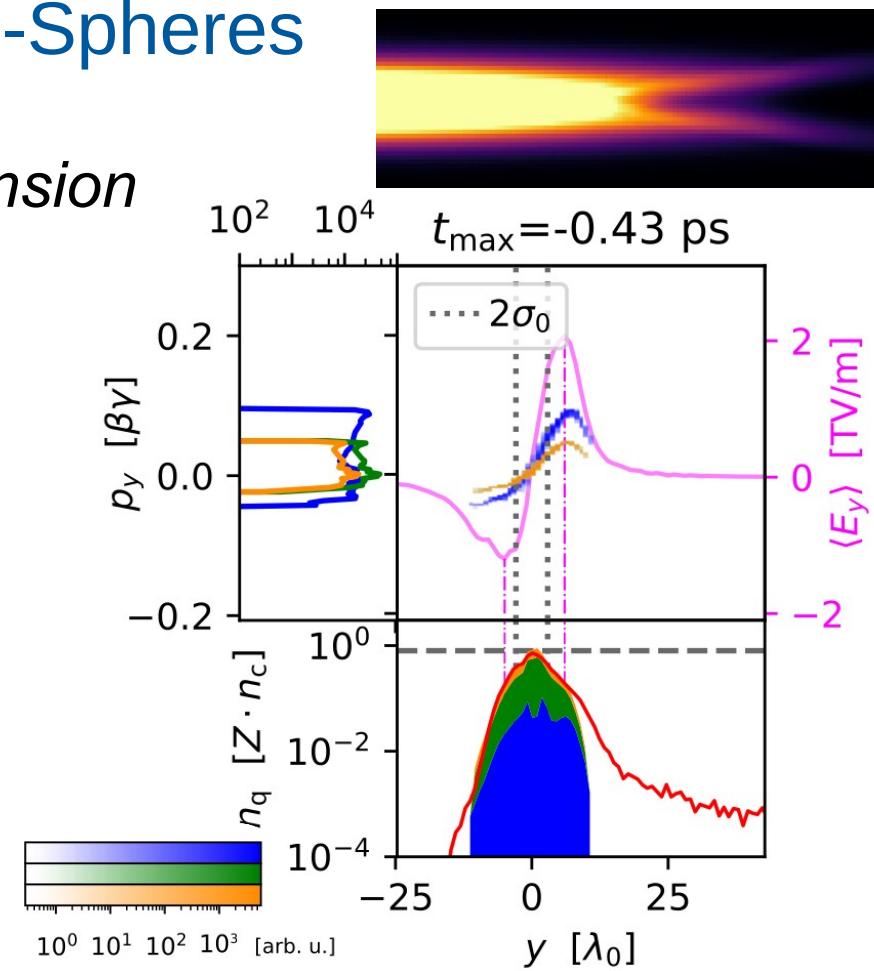
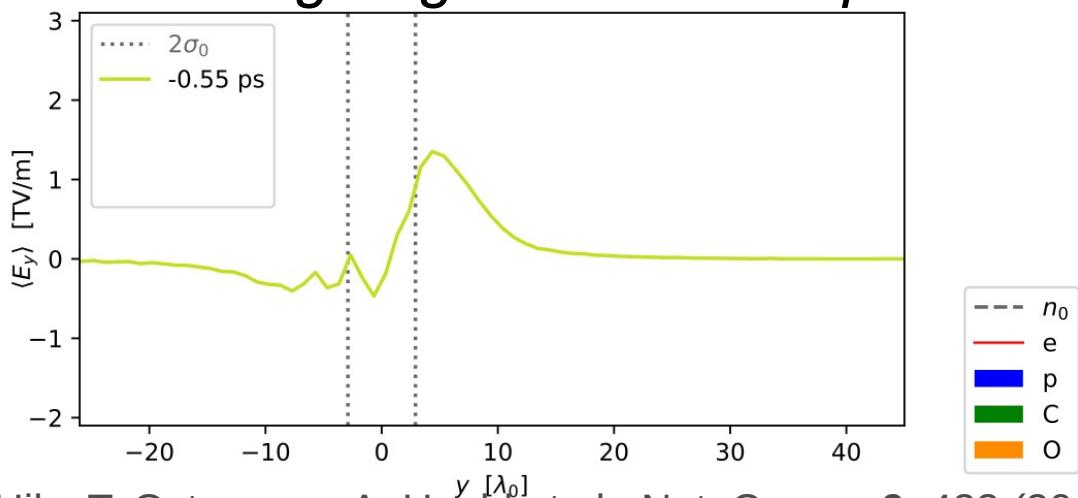


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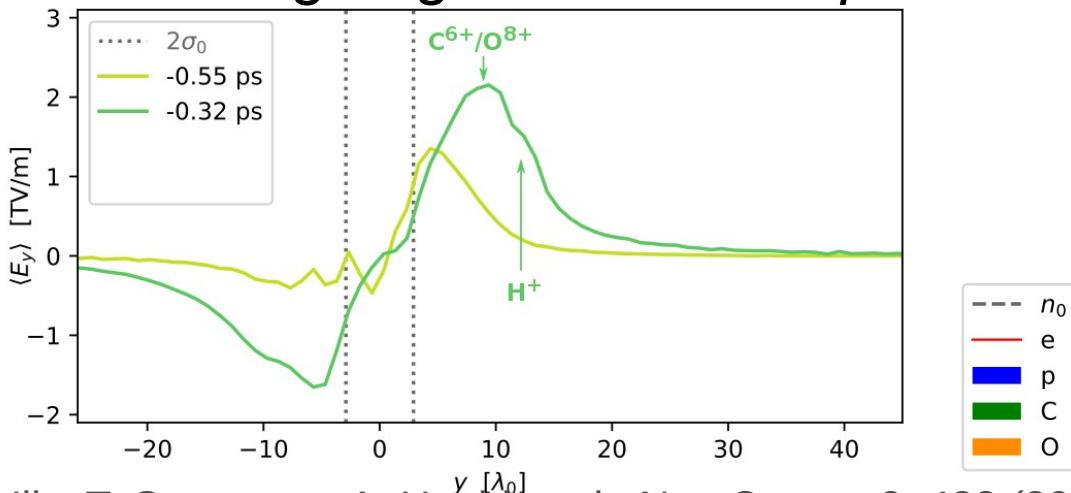


P. Hilz, T. Ostermayr, A. Huebl et al., Nat. Comm. 9, 423 (2018); Talk this morning by P. Hilz

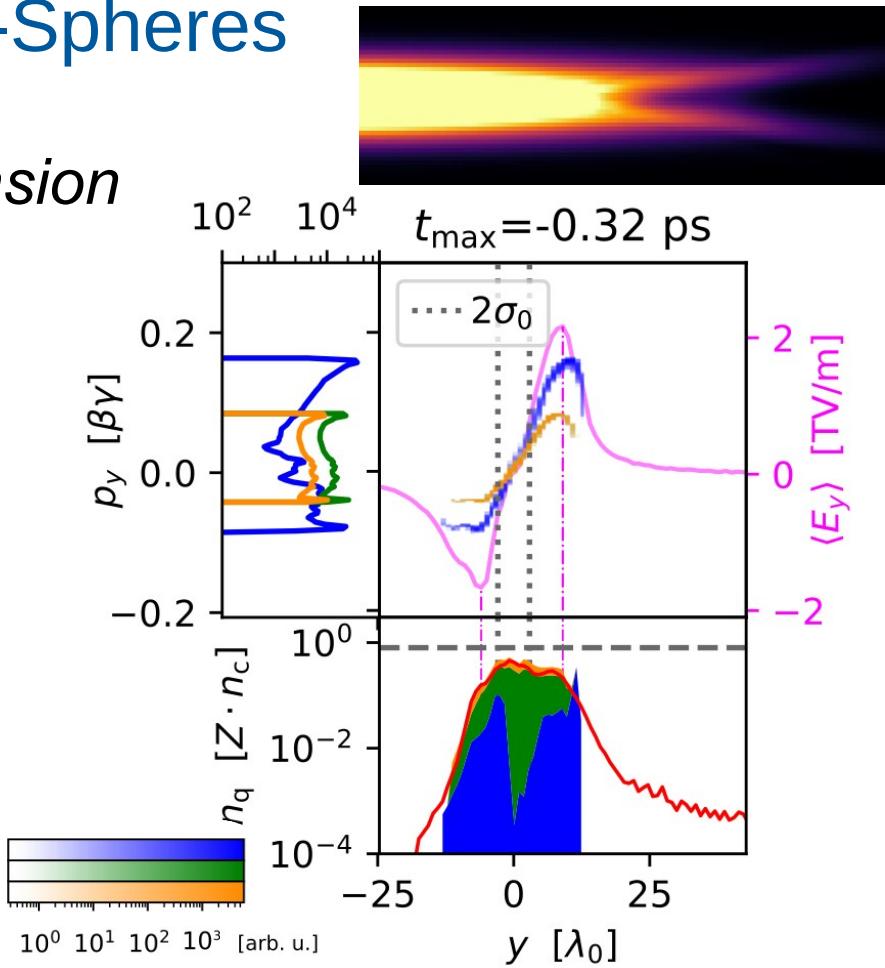
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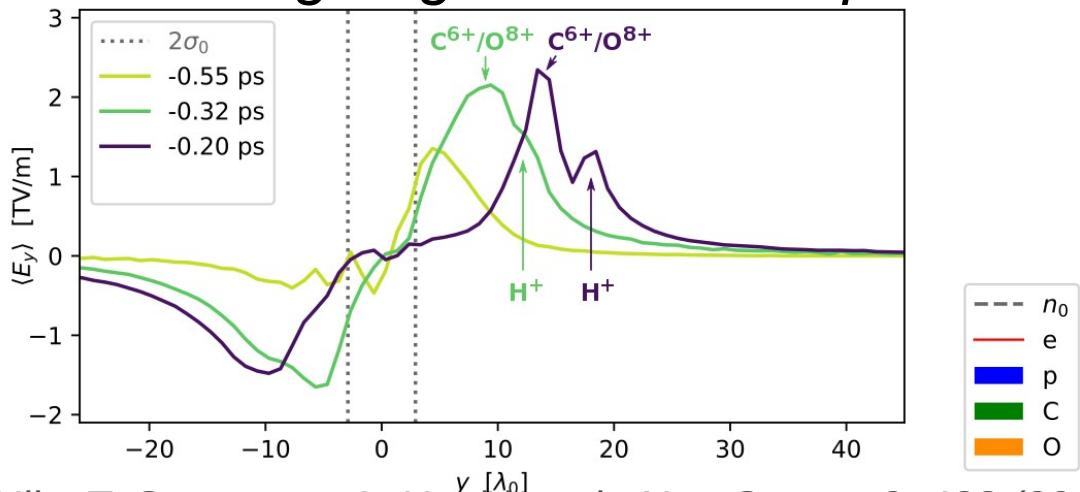
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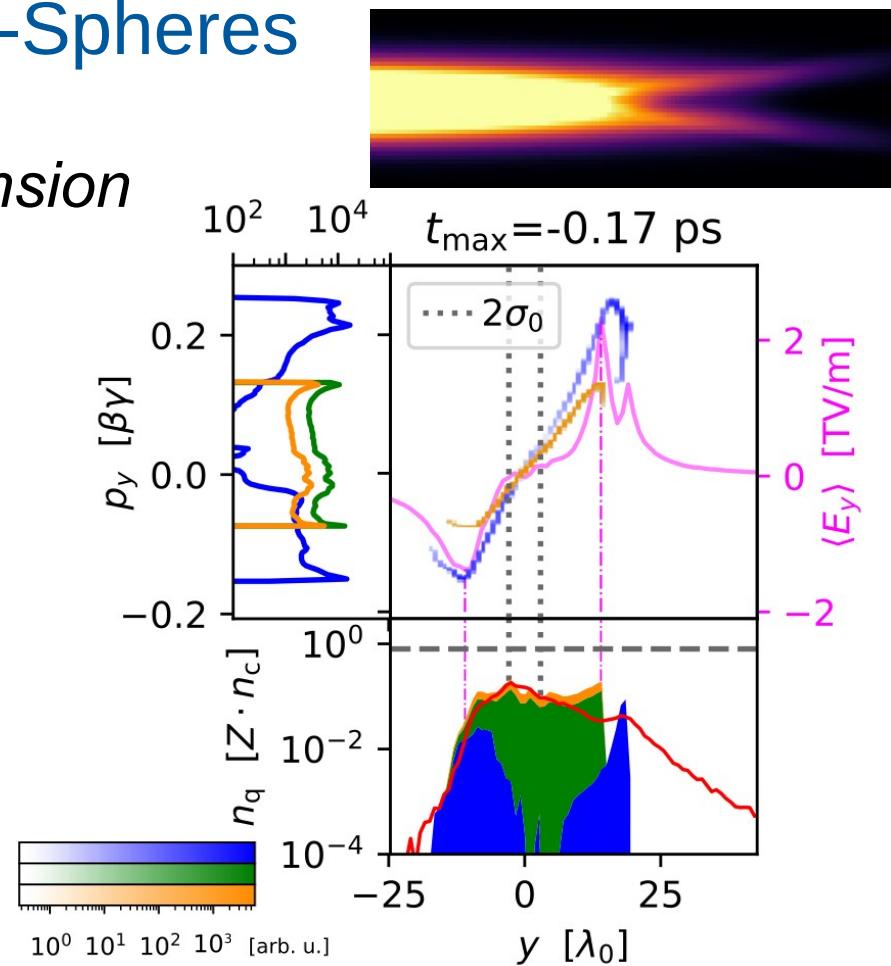
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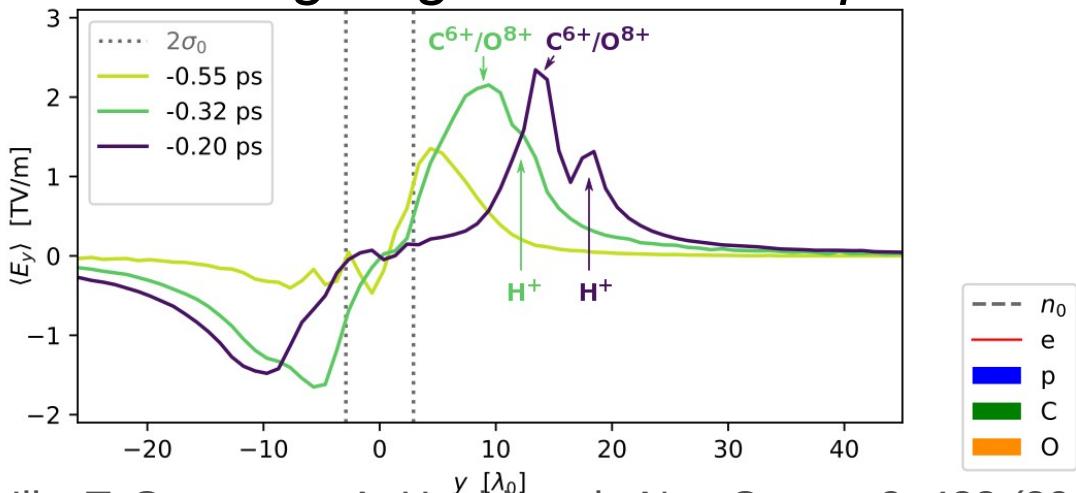
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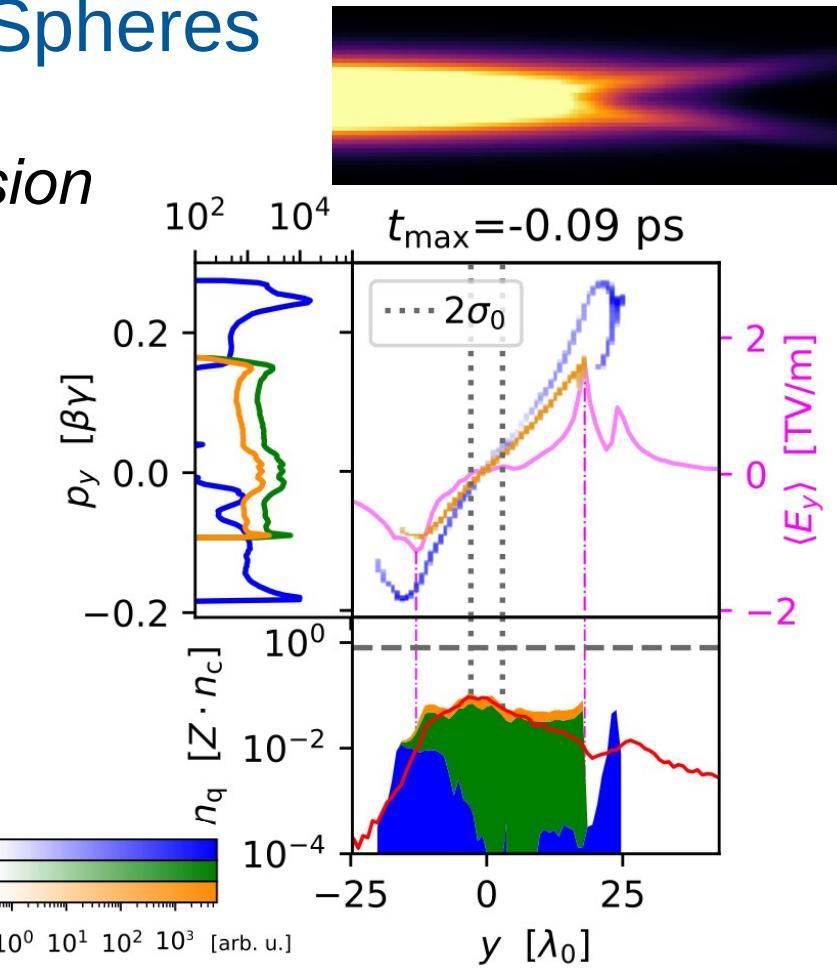
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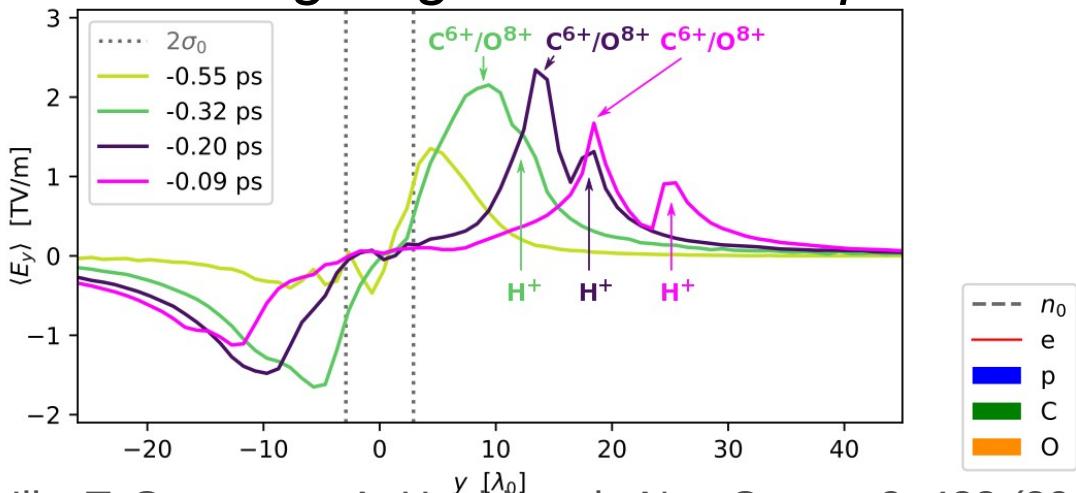
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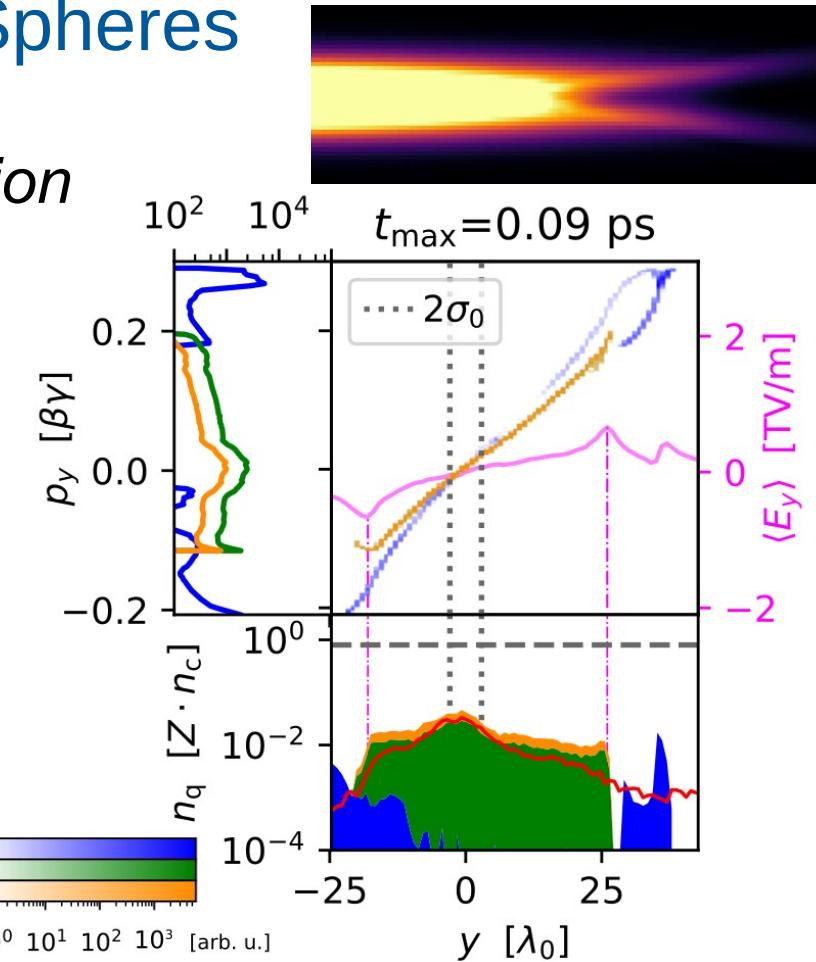
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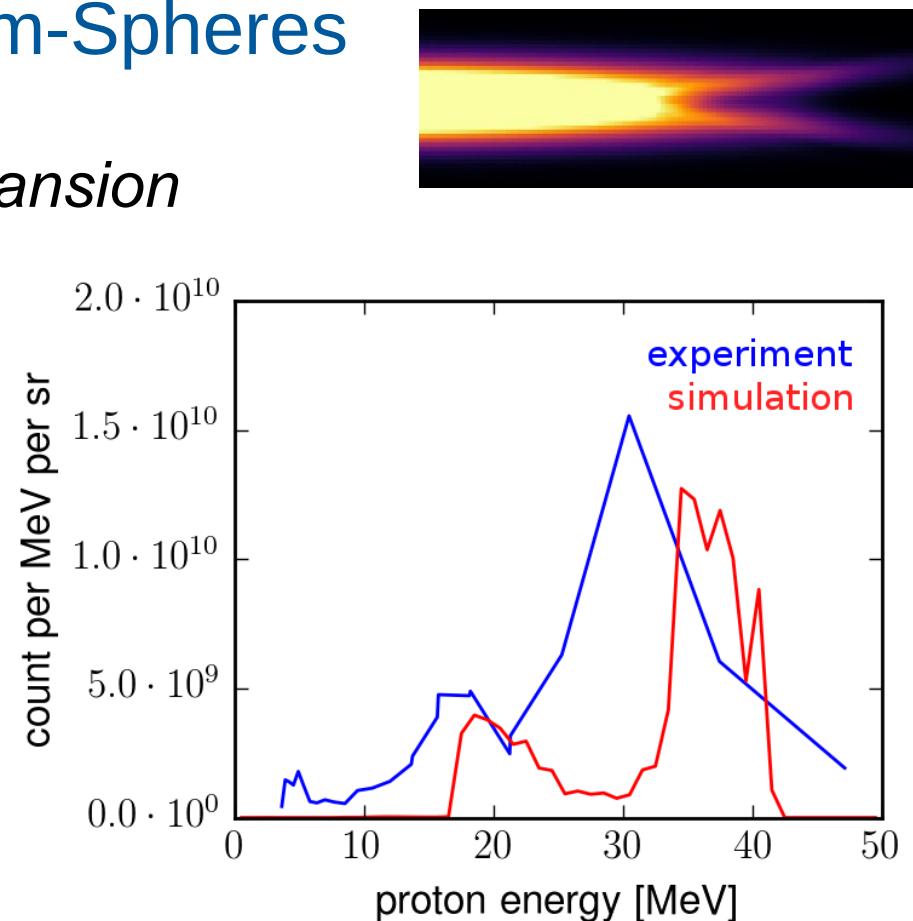
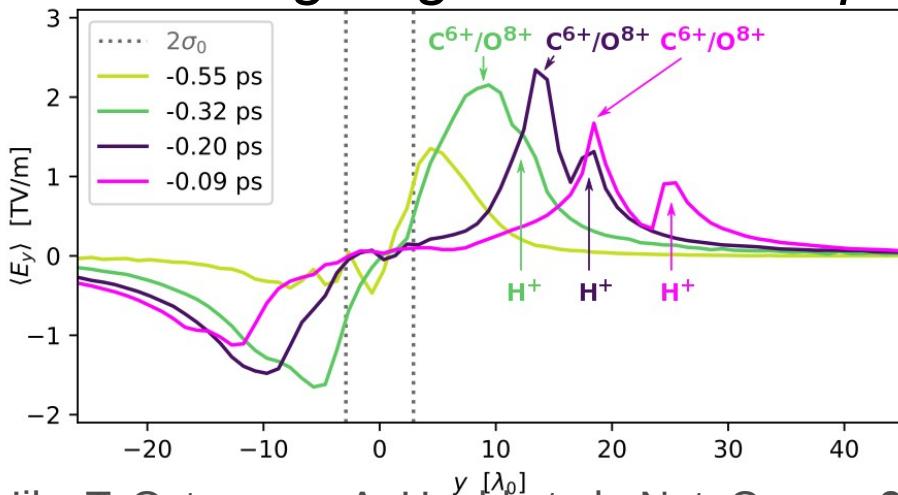
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Revisiting Multi-Species Effects in TNSA

Spectral Signatures as Macroscopic Observable

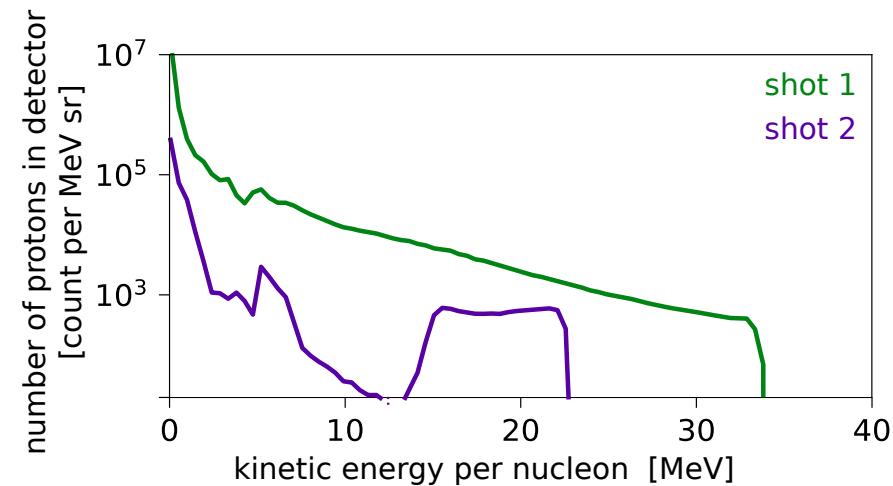
- omnipresent in laser-ion acceleration as distribution $f(Z)$
 - exception: pure $Z=1$ (e.g. Hydrogen) targets
- mechanism is well-known

C. Joshi et al., APL **34** (1979); F. Begay et al., Physics of Fluids **25** (1982); M. Allen et al., PoP **10** (2003);
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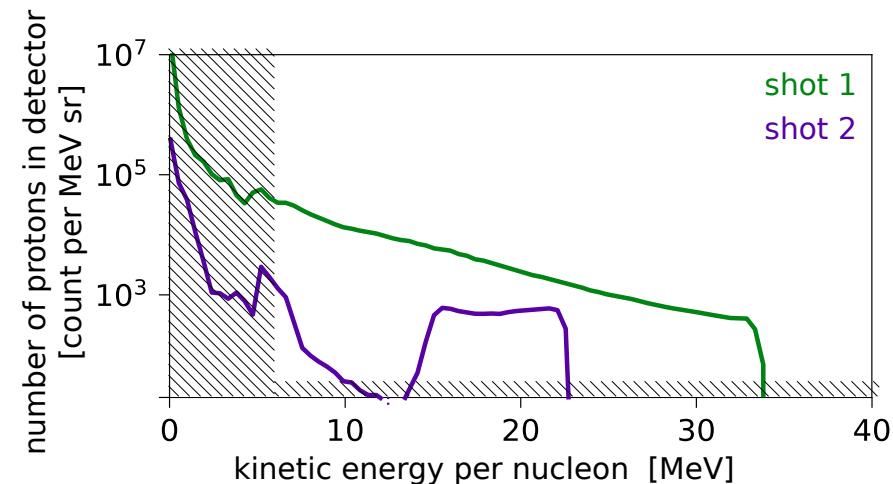


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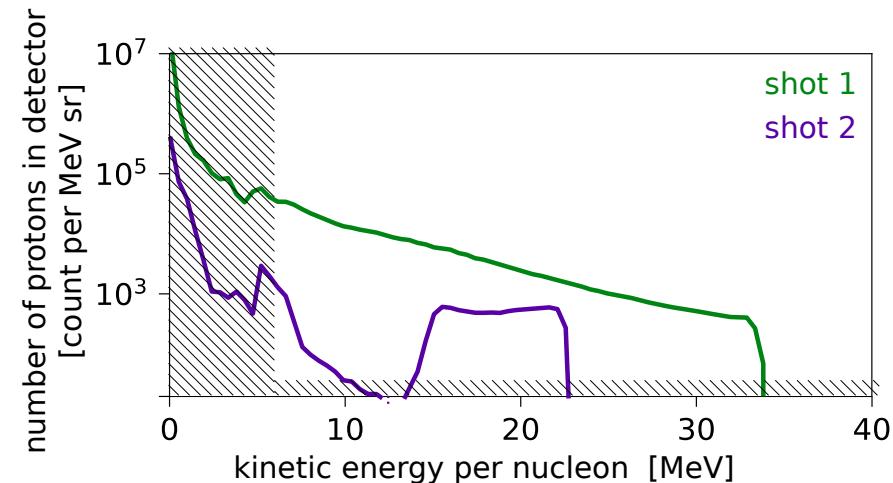


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 - spectral signatures can mimic alternative acceleration mechanism
- analytical models *only for limits of mixtures*



C. Joshi et al., APL **34** (1979); F. Begay et al., Physics of Fluids **25** (1982); M. Allen et al., PoP **10** (2003);
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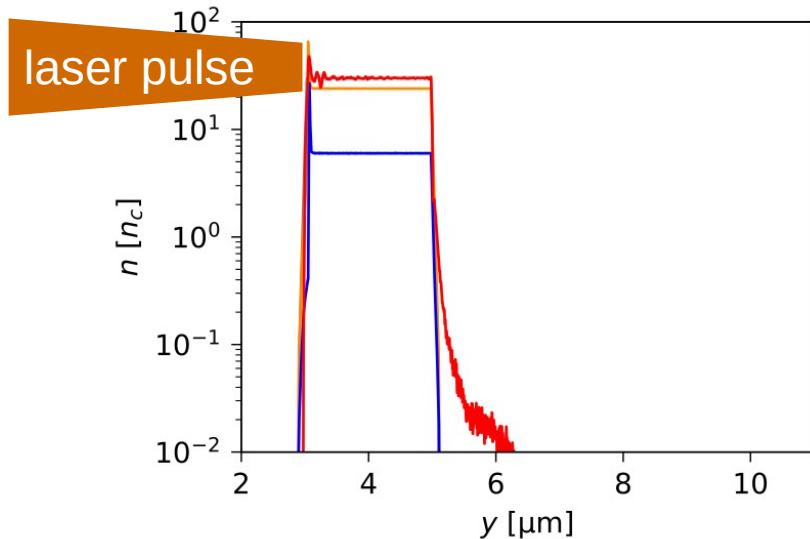
Multi-Species Effects

Flat 2 μm Deuterium-Hydrogen Target, $n_e = 30n_c$

$a_0 = 16, \tau_0 = 30\text{fs}$

- ^1_1H ^2_1H d=80%

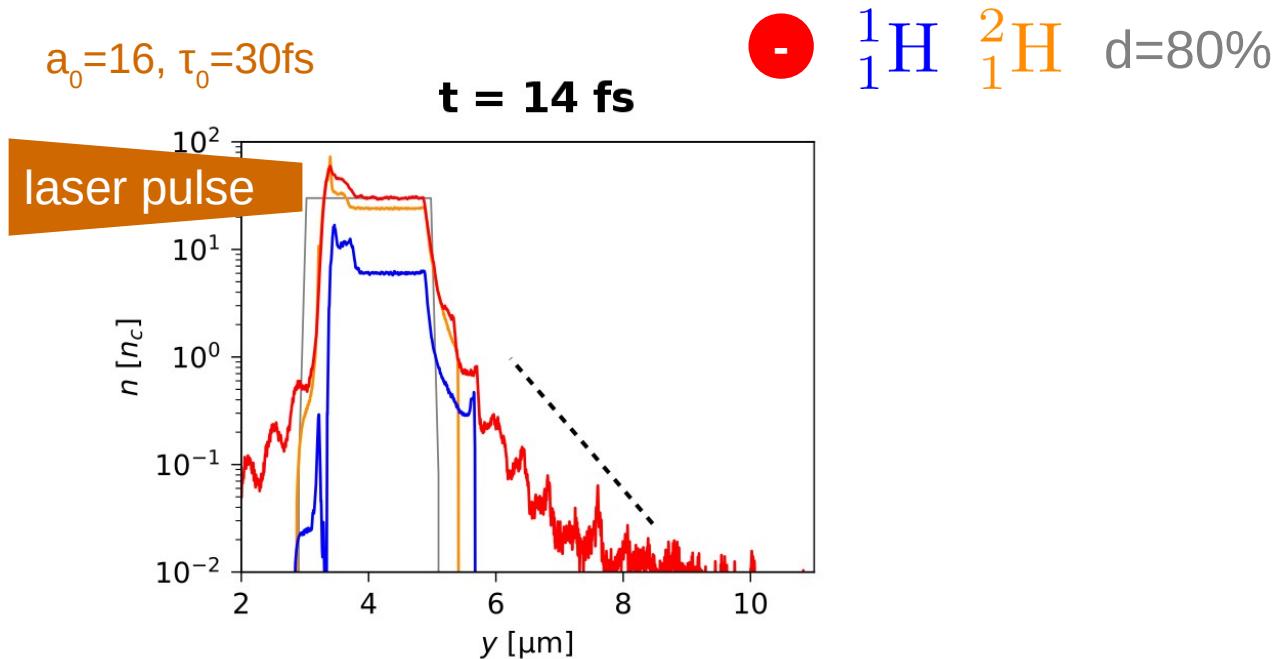
$t = -25\text{ fs}$



P. Mora, PRL 90, 18 (2003); A. Huebl et al., arXiv:1903.06428, submitted (2019)

Multi-Species Effects

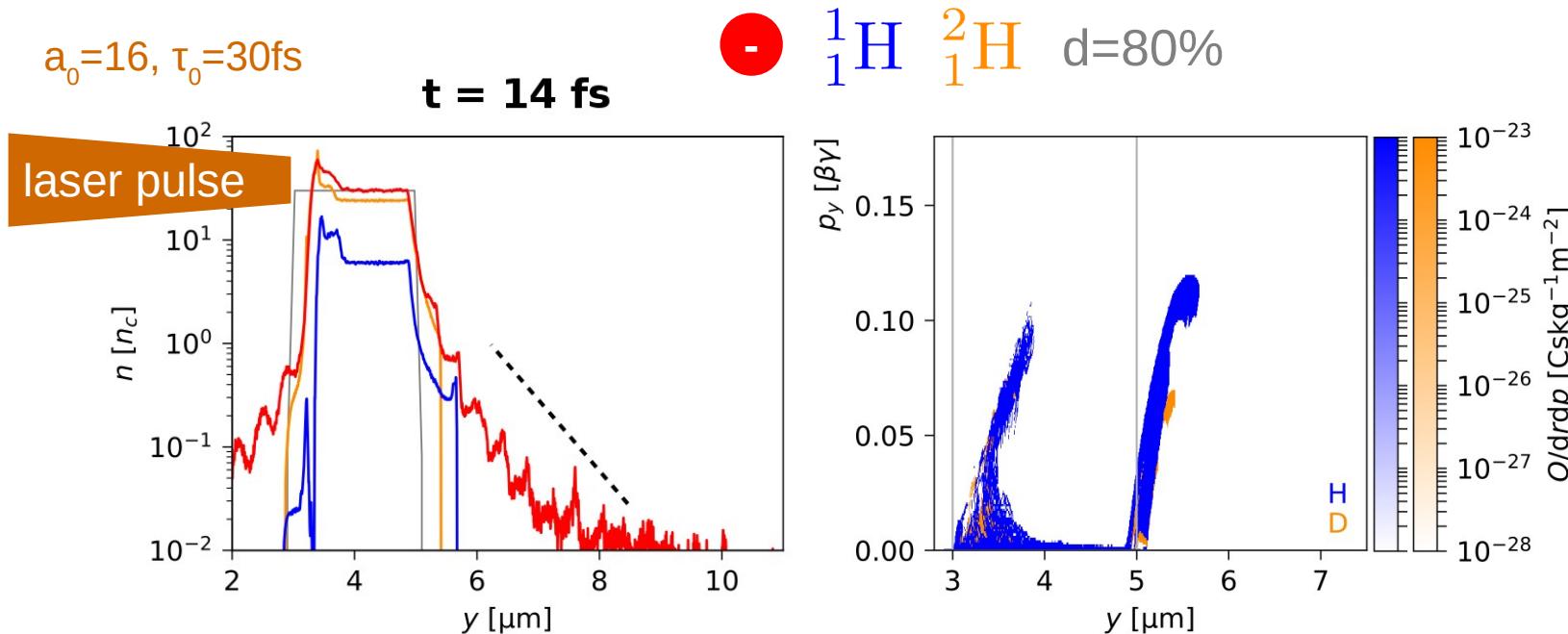
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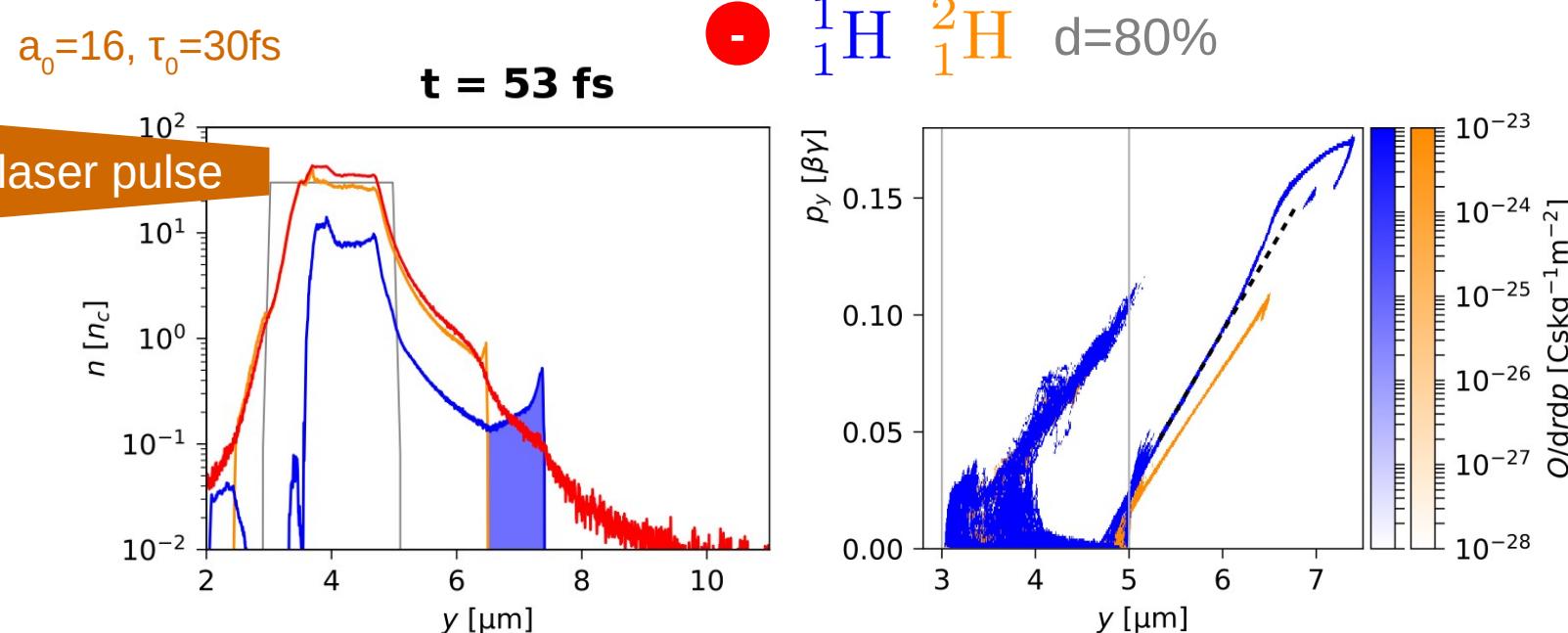
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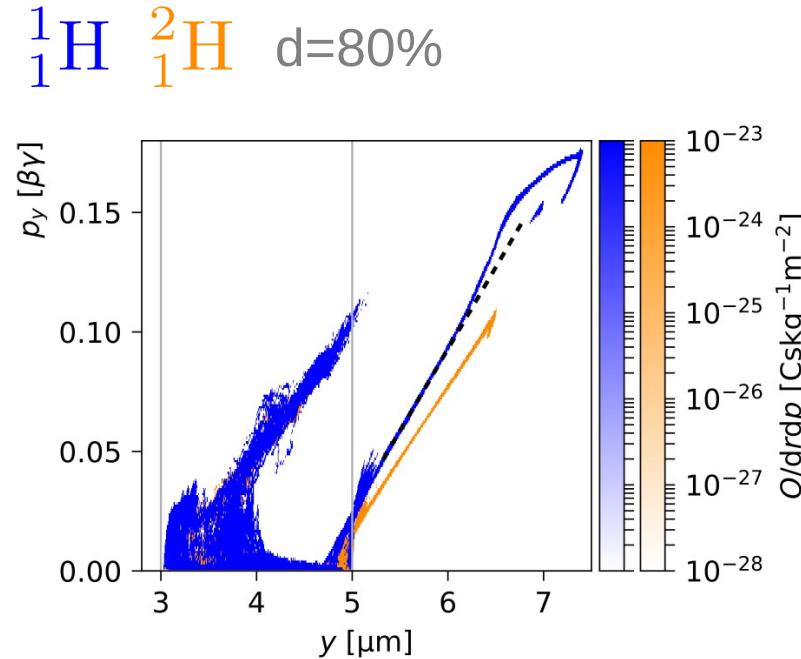
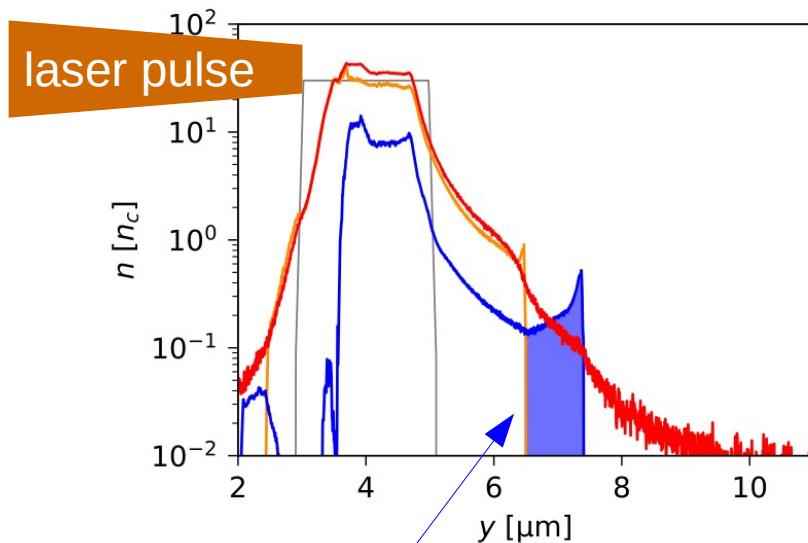
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- ^1_1H ^2_1H $d = 80\%$

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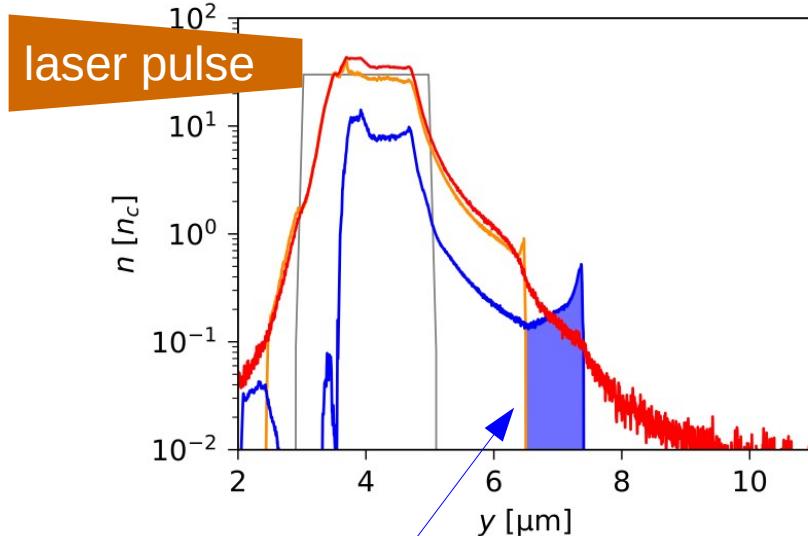
$$\Delta E_D^{\text{ctf}} = \frac{Z_H q_e}{\varepsilon_0} \int_{y_D^{\text{ctf}}}^{y_H^{\text{ctf}}} n_H \cdot dy$$

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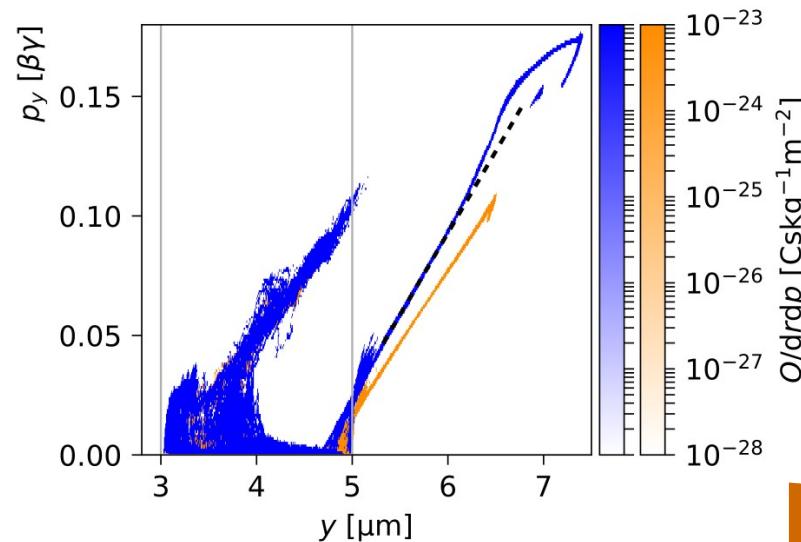
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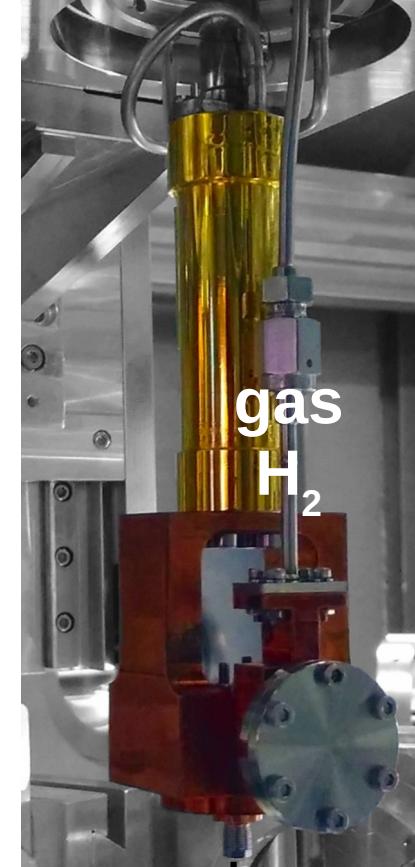
$a_0=16$, $\tau_0=30\text{fs}$ $t = 53 \text{ fs}$ - ${}^1_1\text{H}$ ${}^2_1\text{H}$ $d=80\%$



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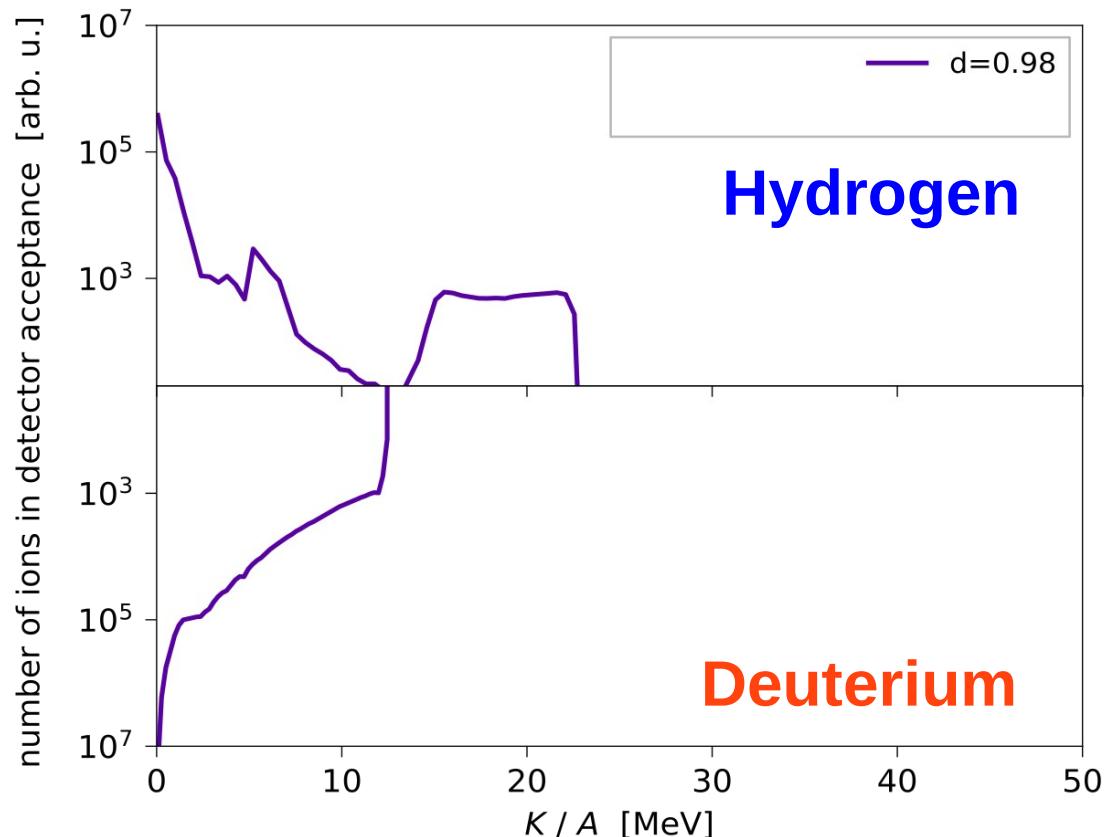
Approach: systematic mixing
laser pulse
solid H_2



P. Mora, PRL **90**, 18 (2003); A. Huebl et al., arXiv:[1903.06428](https://arxiv.org/abs/1903.06428), submitted (2019)
S. Göde et al., PRL **118**, 19 (2017); L. Obst et al., Scientific Reports **7**, 10248 (2017)

Analytical Model: Point of Modulation

Connection to Microscopic Electron Ensemble Properties



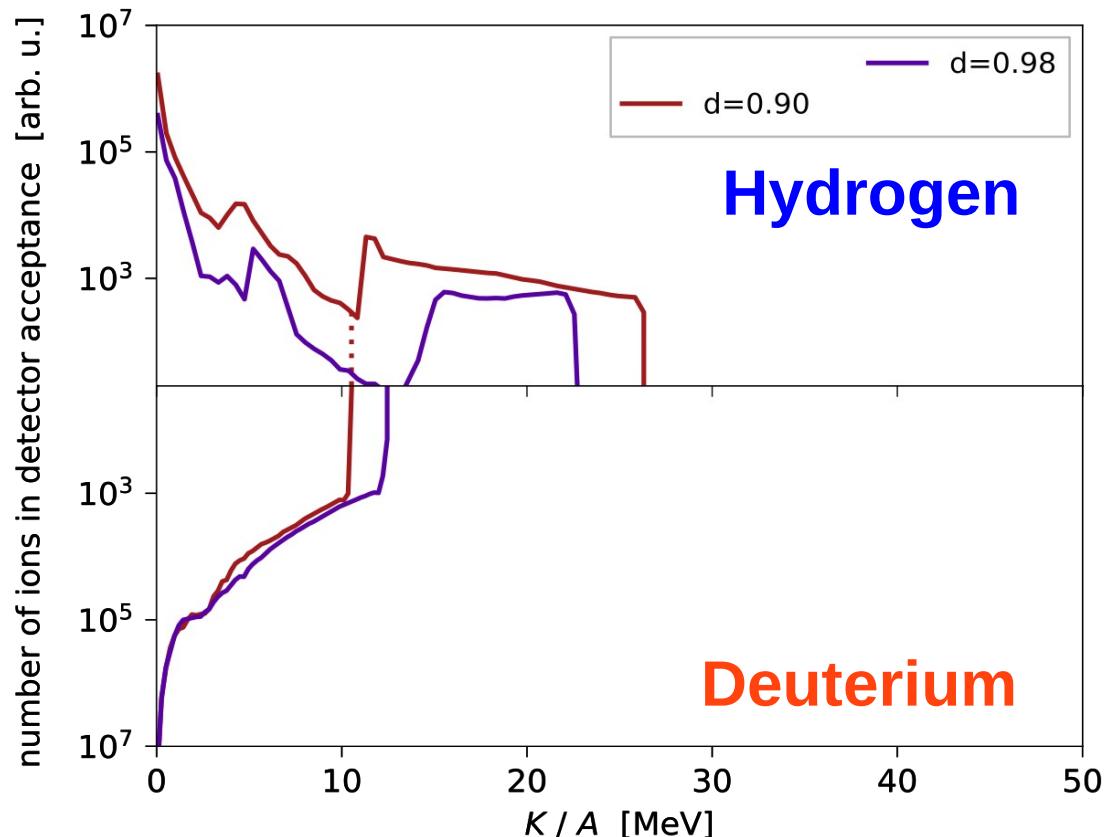
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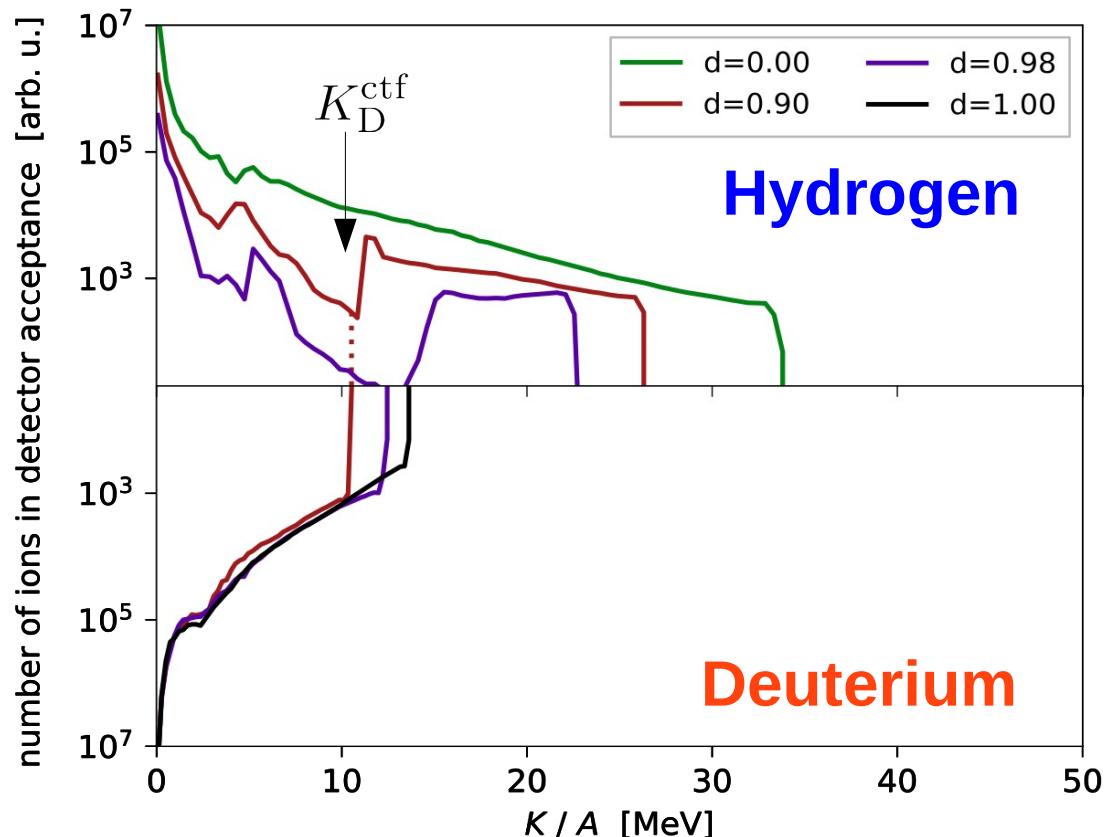
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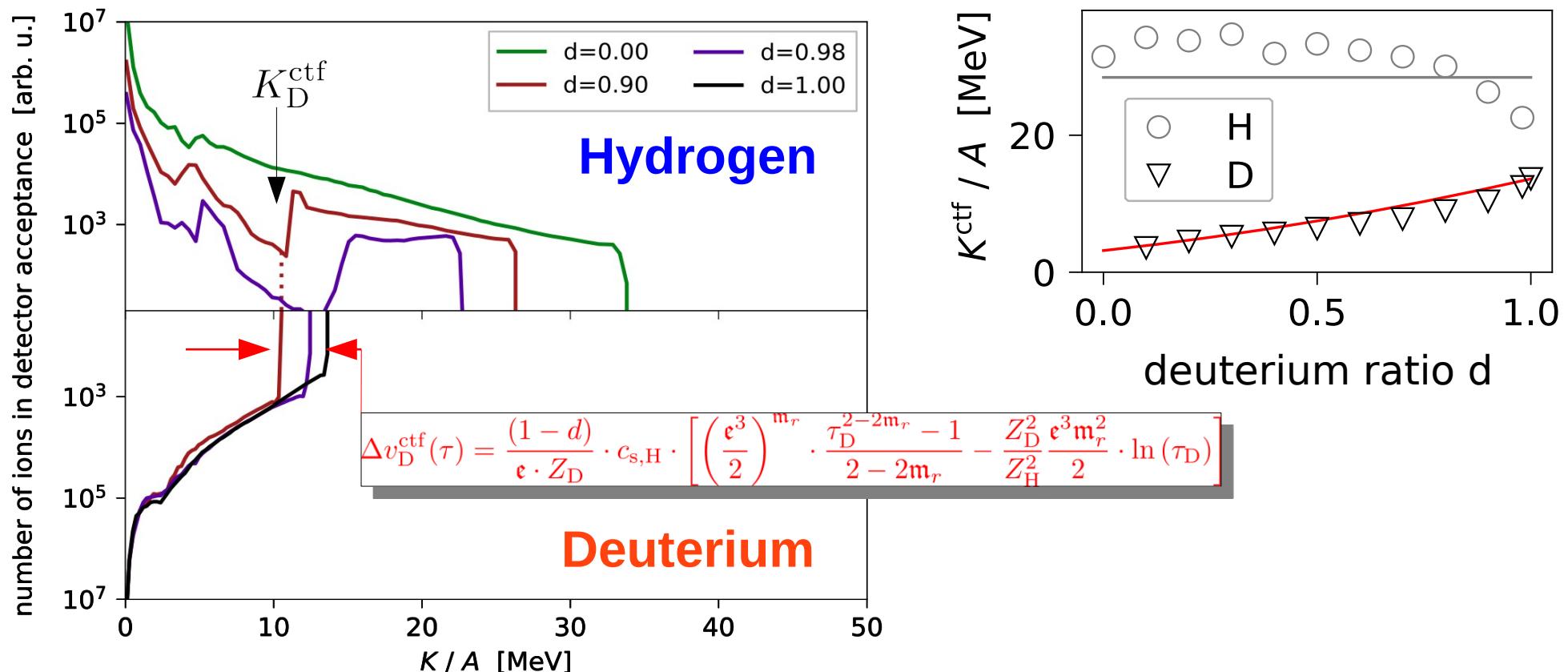
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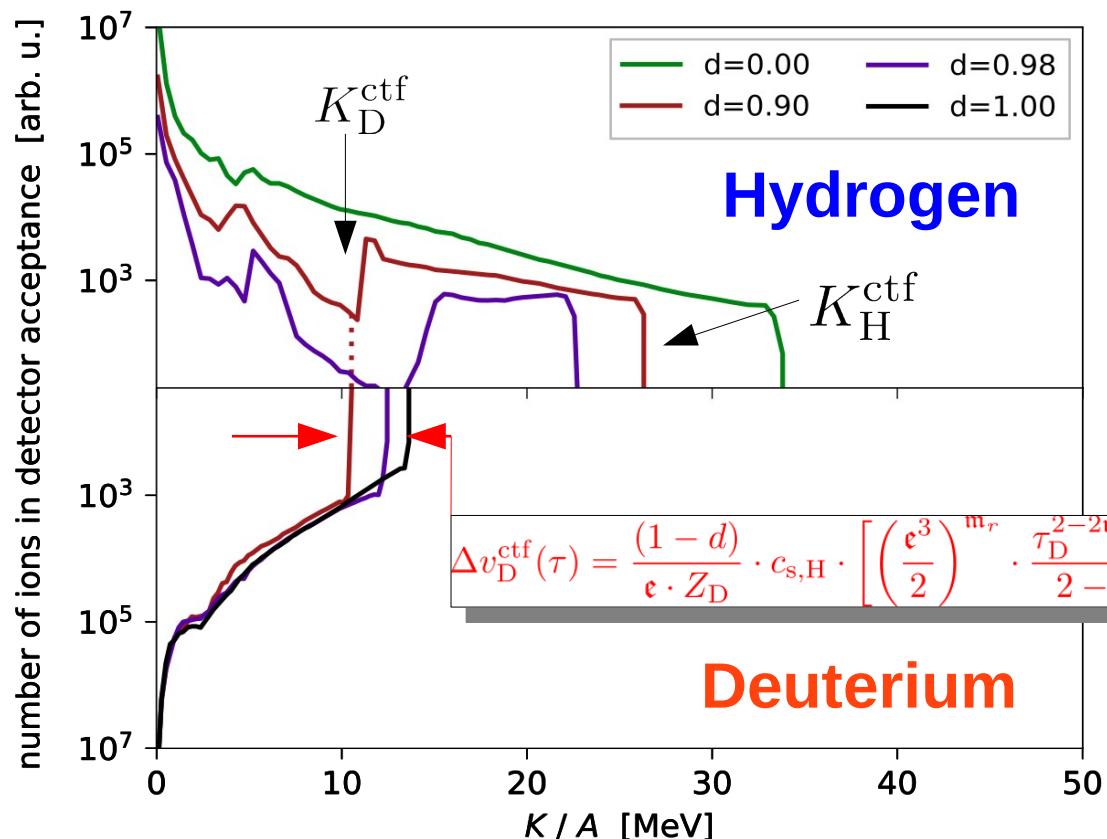
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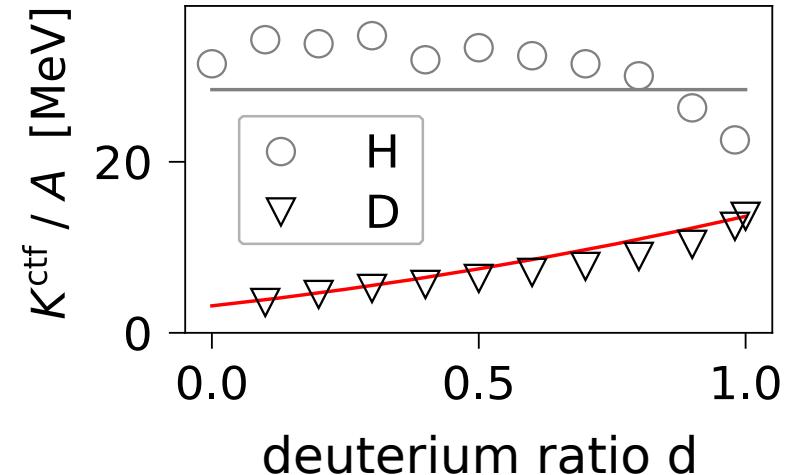
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$$c_{s,i} = c_{s,i}(\langle T_e \rangle)$$

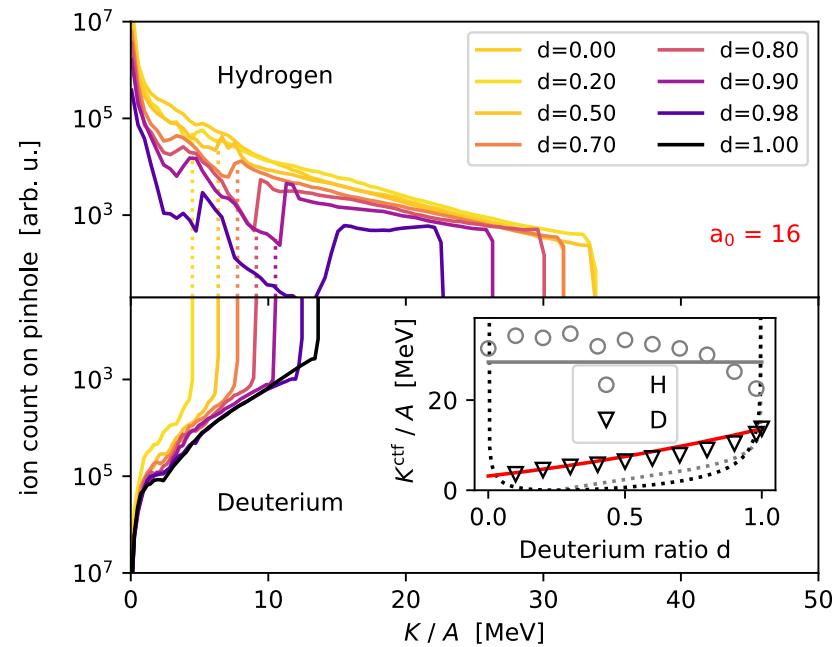
$$\tau_D = \tau_D(n_e)$$

$$K_D^{\text{ctf}}(d) = K_D^{\text{ctf}}(\langle T_e \rangle, n_e)$$

$$K_H^{\text{ctf}} = K_H^{\text{ctf}}(\langle T_e \rangle, n_e)$$

Ensemble Studies for the Draco Laser

150 TW to PW-Scale ($a_0=8 - 42$, $\tau_0=30$ fs)

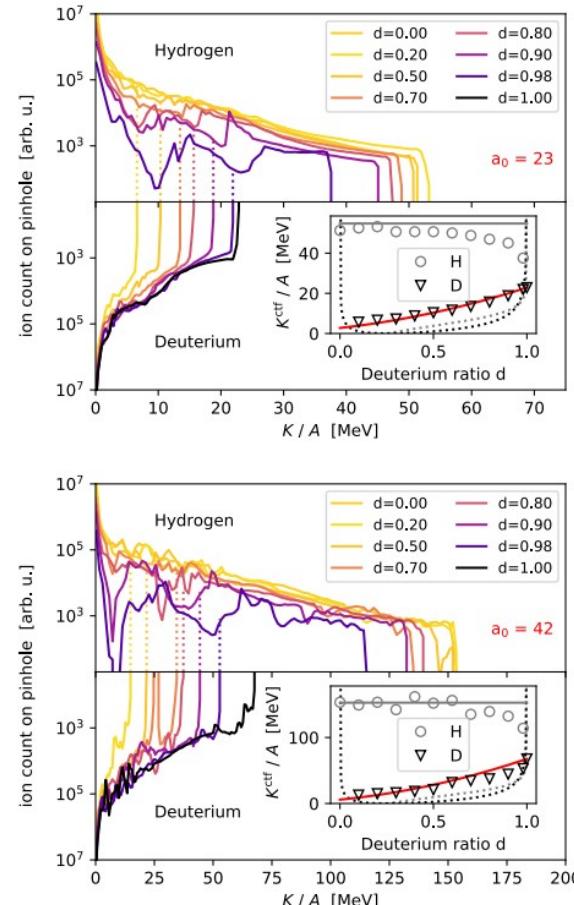
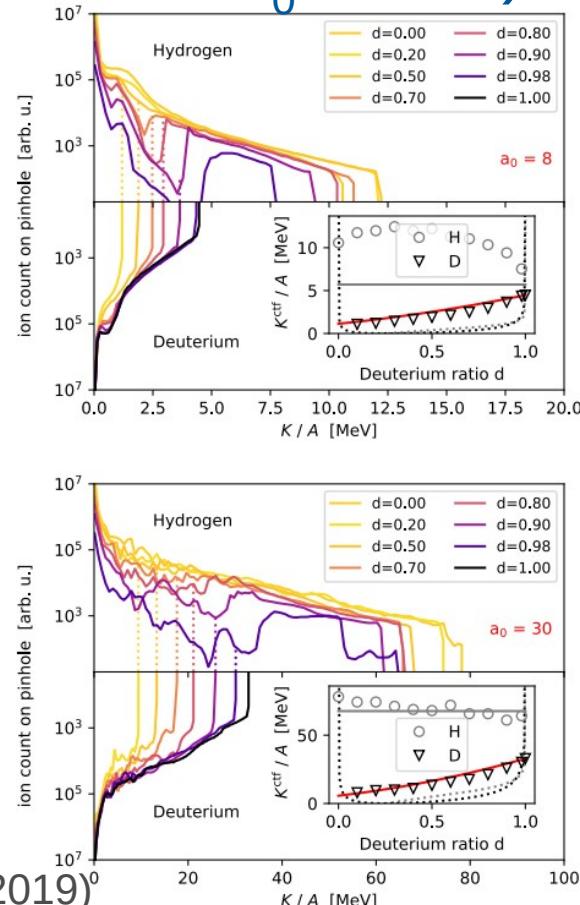
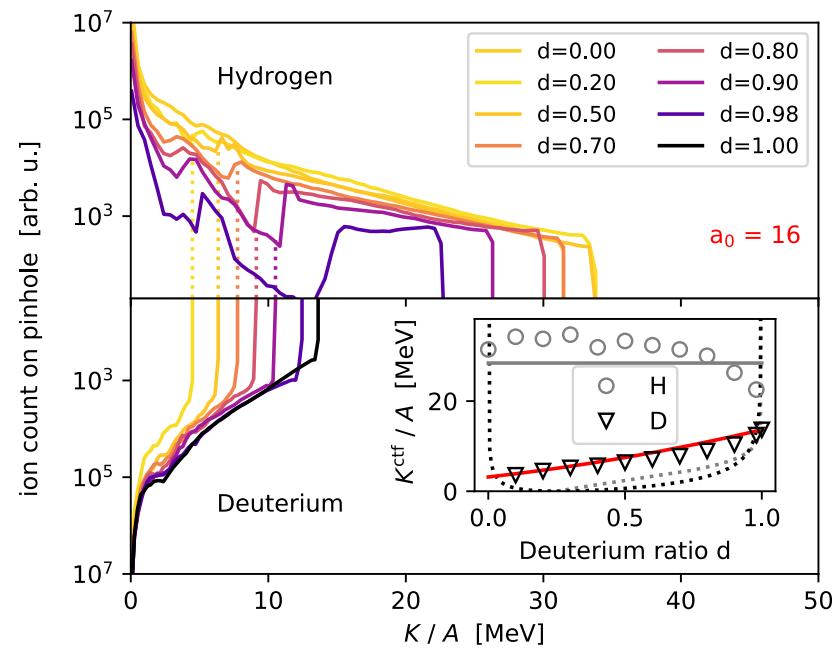


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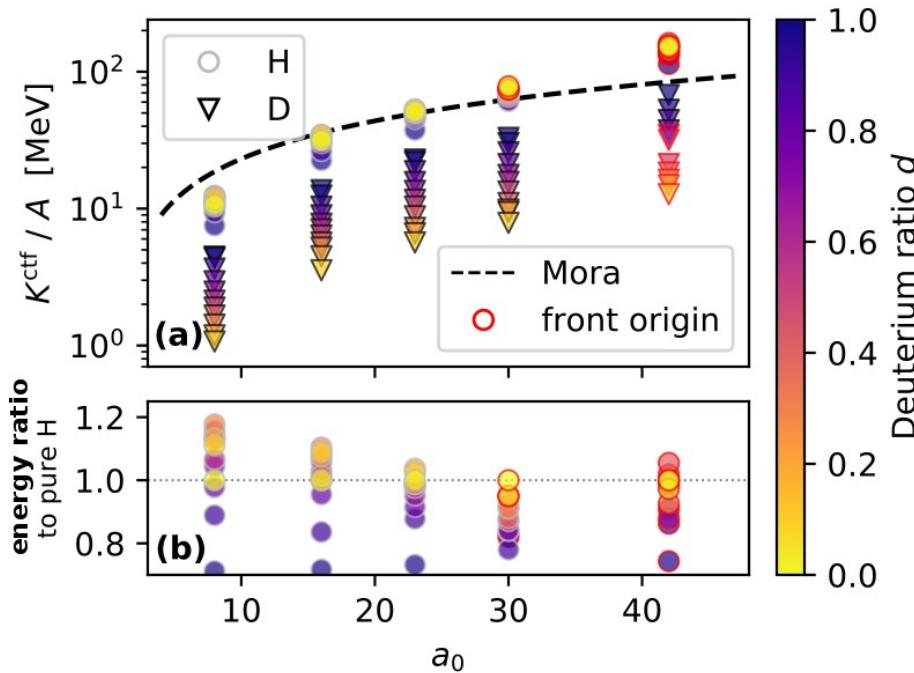


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Slight Variation of Laser Absorption

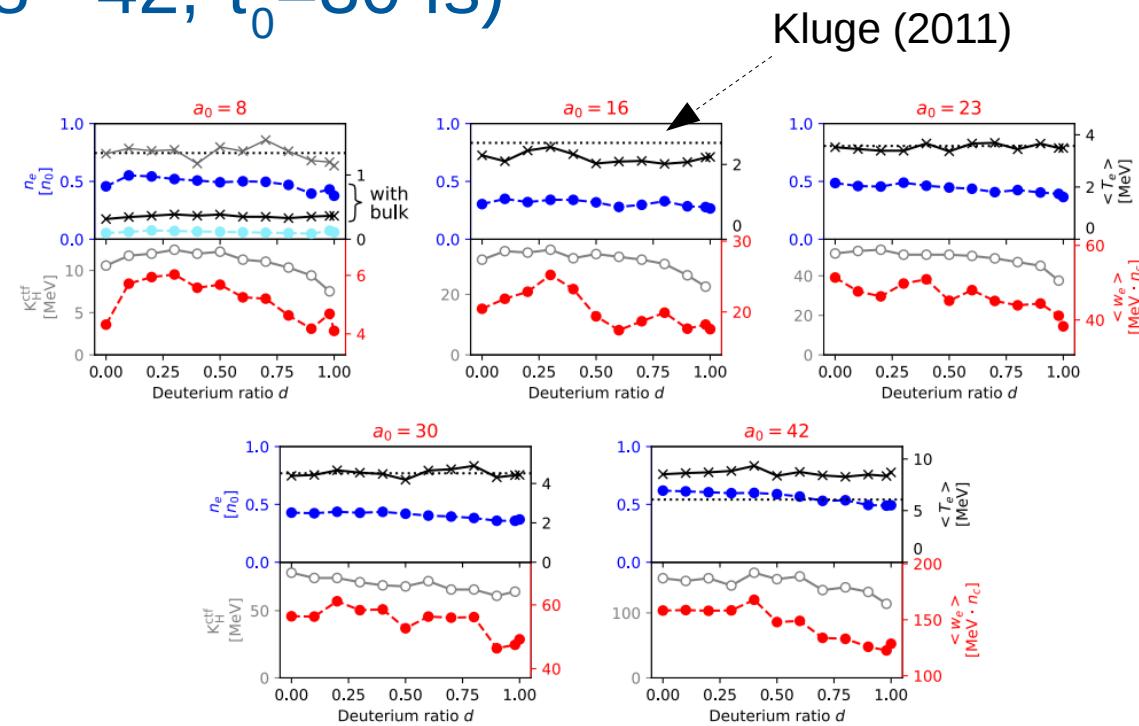
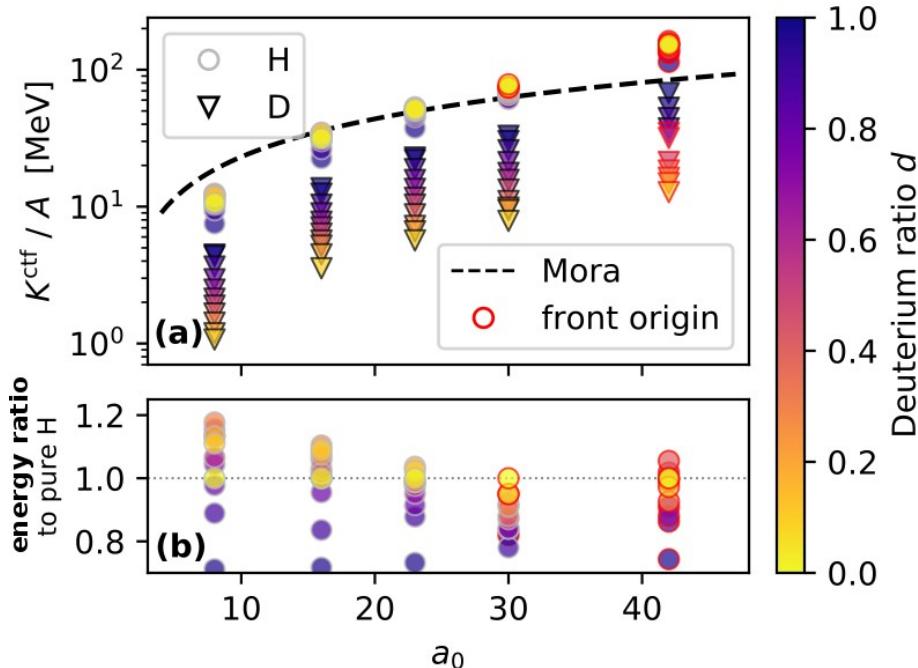
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T. Kluge et al., PRL **107**, 205003 (2011); K. Zeil et al., Nat. Comm. **3**, 874 (2012)
A. Huebl et al., arXiv:[1903.06428](https://arxiv.org/abs/1903.06428), submitted (2019)

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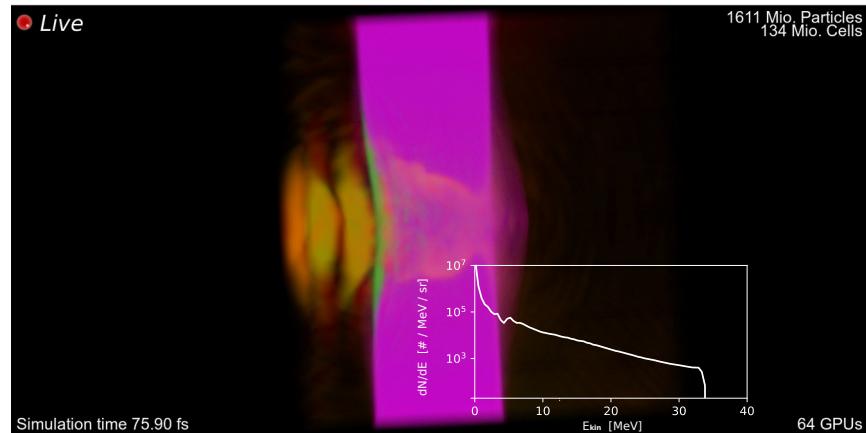
T. Kluge et al., PRL 107, 205003 (2011); K. Zeil et al., Nat. Comm. 3, 874 (2012)
A. Huebl et al., arXiv:1903.06428, submitted (2019)

Summary



- **Scalable Simulations**

- PIConGPU: fast, platform agnostic (CPU/MIC/GPU/Power), flexible, extensible, open source

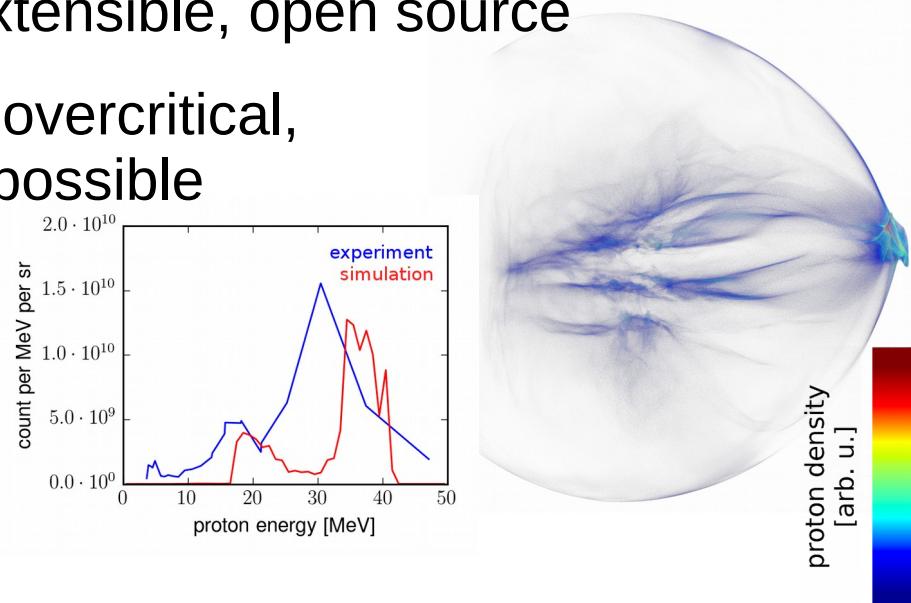
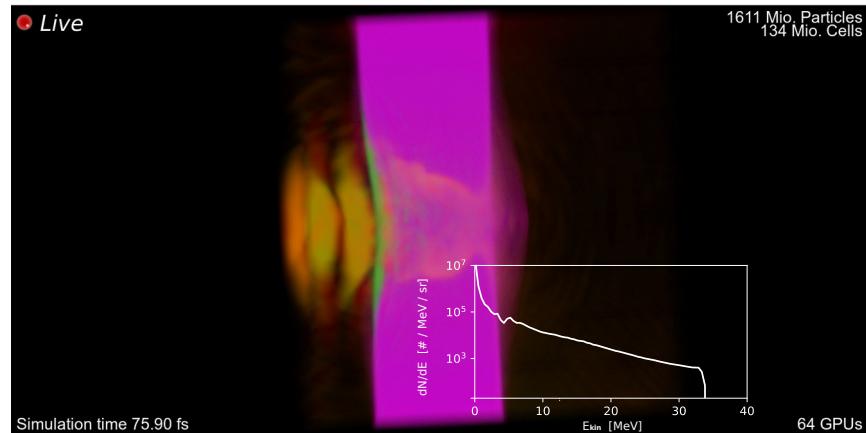


Summary



▪ Scalable Simulations

- PIConGPU: fast, platform agnostic (CPU/MIC/GPU/Power), flexible, extensible, open source
- systematic, full-resolution, near- to overcritical, 3D ensemble simulations become possible
- bridging macroscopic observations and microscopic physics



Summary

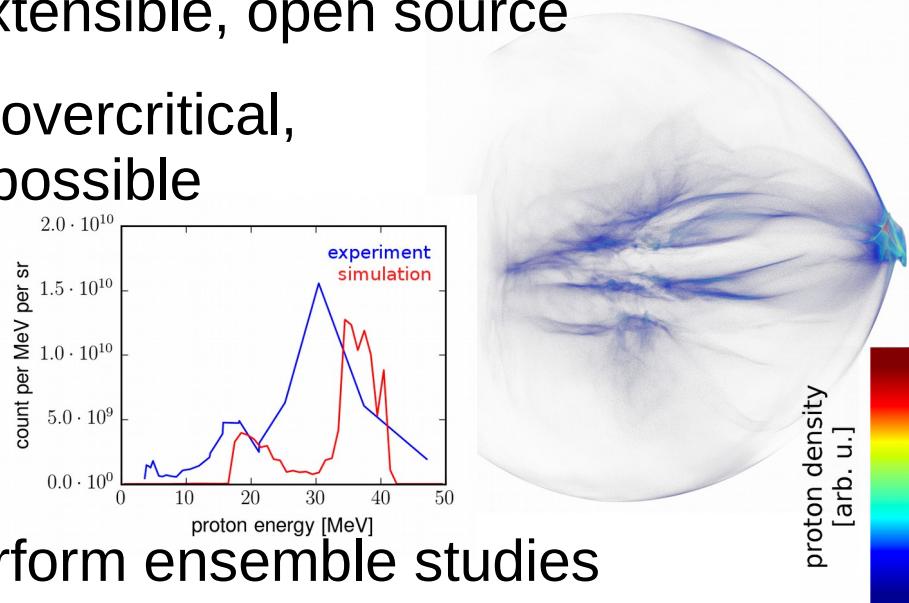
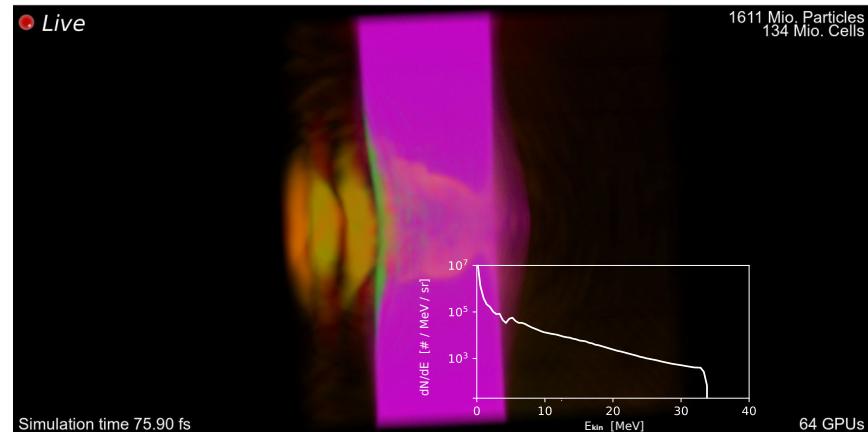


▪ Scalable Simulations

- PIConGPU: fast, platform agnostic (CPU/MIC/GPU/Power), flexible, extensible, open source
- systematic, full-resolution, near- to overcritical, 3D ensemble simulations become possible
- bridging macroscopic observations and microscopic physics

▪ Ion Energy Signatures

- spectral shapes are not unique, perform ensemble studies
- novel analytical model for multi-species signatures for arbitrary material compositions



proton density
[arb. u.]

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github.com/ComputationalRadiationPhysics



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