Radiation imprint of ultra-intense laser heating of solids

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We acknowledge PRACE for awarding us access to Piz Daint at CSCS, Switzerland.

15\textsuperscript{th} PRACE call, Project ID 2016163983.
Conventional ion acceleration at extreme scales

CERN Large Hadron Collider

- **Circumference**: 27 km
- **Particle energy**: 6.5 TeV
Conventional ion accelerators for medical application

Heidelberg Ion-Beam Therapy Center HIT
- **Construction cost:** 120 million €
- **Particle energy:** 50-430 MeV/nucleon
Laser-driven proton sources for applications

- Breakdown-limit of conventional accelerators at ~50 MV / m
  → long accelerating structures
- Concrete radiation shielding
  → high construction cost

Alternative: Compact, laser-driven ion sources?

- Energy gain: MeV / µm
- Field strength: TV / m instead of ~10 MV / m

"... for their method of generating high-intensity, ultra-short optical pulses."
Laser-driven proton sources for applications

Beams of high dose (~ 1 Gy) + ultra-short (~ 1 ps) duration desirable for

- High-dose radiobiology
- Translational research in radiooncology
- Proton radiography
- Materials research

Target-normal sheath acceleration (TNSA) of Ions

Absorption and electron acceleration
fs - time scale

Electron transport and forming of Debye sheath

Expansion of electron-proton plasmas into vacuum
ps – time scale

Acc. field
E ~ TV/m

Currents of 10^6-10^9 A
C, H, O contaminant

~ nm-µm
Laser-driven ion acceleration - status

What limits the performance?

Proton acceleration – stability in experiment

- “cleaning” of temporal contrast with plasma mirror techniques
  → can shoot thinner targets

- Best performance ≠ usual
- Key could be temporal pulse shape of the **last picosecond**
Laser pulse leading edge

- Measured laser contrast underlies limits in time resolution and dynamic range
- Shot-to-shot fluctuation


- Extract characteristic features
- Understand interaction systematically
Simulation of plasma dynamics with particle-in-cell codes

**Particle-in-cell algorithm:**

- One complete cycle corresponds to one time step.
- Repeated cycles allow simulating longer time durations.
- Local operations only: well suited for parallelization.

**Force Calculation**
$$\vec{F} = q \cdot (\vec{E} + \vec{v} \times \vec{B})$$

**Particle Push**
$$\vec{p}_{i+1} = \vec{p}_i + \Delta t \cdot \vec{F}$$

**Field Evolution**
$$\frac{\partial \vec{E}}{\partial t} = -\vec{v} \times \vec{E}$$
$$\frac{\partial \vec{B}}{\partial t} = c^2 (-\mu \vec{j} + \vec{v} \times \vec{B})$$

**Current Deposition**
$$\vec{j} = \int q \cdot \vec{v} \cdot f(\vec{r}, \vec{v}) dV$$
2D Simulation pre-study at HZDR

- optimal thickness does not shift much with laser contrast

![Graph showing $E_{\text{max}}$ (MeV) vs. thickness ($d$) in nm]

- perfect contrast $\rightarrow$ perfectly sharp target rear surface
  $\rightarrow$ best accelerating shield field

Would 3D simulations show the same trend?
3D simulation campaign on Piz-Daint

- PRACE Tier-0 1.6 million GPU hours
- ~4000³ cells @ 2400 GPUs
- > 10¹⁰ particles
- O(10⁴) GPU hours per simulation
- 13 TB / raw output step

Currently 5th largest cluster in the world & former 1st regarding GPUs until June ‘18

15th PRACE call, Project ID 2016163983.
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The Result of 1.6 Million GPU Hours & 4 PB of Data
Maximum proton energy – parameter scan

- Observe **optimum thickness** & **optimum leading edge at non-ideal contrast**

- Completely different from 2D simulation results!

Copper, $d_{\text{opt}} = 17 \text{ nm}$, $T = 60 \text{ fs}$, $E_{\text{Laser}} = 30 \text{ J}$
Acceleration mechanism

- 3D effects in pre-expansion and proton diffusion
- Pre-acceleration due to radiation pressure
Where do the differences come from?

2D and 3D are conceptionally different!

- **Circular** spot
- **Spherical** symmetry
  
  **laser focus**
  **acc. field**

- Equivalent to **line** focus
- **Cylindrical** symmetry
PIConGPU
our HPC work horse to run fast full 3D simulations
Particle-in-Cell Simulations for the Exascale Era

a fully relativistic 3D3V particle-in-cell code developed and maintained at HZDR

- open source development
- runs on any hardware
- scales on the largest clusters
- efficient parallel I/O
- in-situ data analysis avoids bandwidth bottleneck

http://picongpu.hzdr.de
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![Graph showing effective I/O throughput vs. number of nodes]

Key features:
- **open source development**
- **runs on any hardware**
- **scales on the large clusters**
- **efficient parallel I/O**
- **in-situ data analysis avoids bandwidth bottleneck**
The main issue is throughput

Writing **reduced data** is still required.

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K20x GPU (2013), $bw := 6 \text{ GByte} \cdot 10 \text{ Hz steps}$

PCI-Express: $6 \text{ GByte/s}$
- $1 / 10 \text{ th bw}$

I/O per node:
- $1 / 10 \text{ th} \cdot 1 / 200 \text{ th bw}$
  - 42 MByte/s (Titan)
  - 29 MByte/s (PizDaint)

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Summit (ORNL, 2018): ratio 4x **“worse”** - gap of $10^4$
The main issue is throughput

Writing reduced data is still required.

Compression does not help per se

Huebl A. et al., (2017) ISC High Performance (pp 15-29) DOI: 10.1007/978-3-319-67630-2_2
Reducing complex data requires computing:
This is not only true for simulations but for experiments as well.

- **Complexity (per event/data set/image and community):** Machines + detectors produce more and more complex data, more and more scientific communities are involved in analyzing this data.
Harvest the wealth or particle data: Data reduction via synthetic diagnostics

- Plasma dynamics encoded in emitted radiation
- Bremsstrahlung and synchrotron radiation do not just follow electron distribution
- Would require explicit trajectories → TB / s output … doable but unfeasible
- Instead simulate photons as well and record virtual detector signal
- Develop analytical model to predict signal in experiments
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radiation simulation:

live visualization:
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throughput equiv. to ~10 TB/s
Conclusion

- Optimum proton energies at non-optimal laser contrast
- Full 3D simulations become inevitable
- Efficient data throughput matters
- Enormous amounts of data require in-situ analysis and visualization
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