In silico plasmas under extreme conditions: from particle accelerators to pair plasmas in pulsars

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Acknowledgments


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Simulation results obtained at the Accelerates Cluster (IST), Dawson2 (UCLA), Jugene/Juqueen (FZ Jülich), SuperMUC (Münich), Sequoia (LLNL)

Many extreme plasma physics scenarios (field intensities in excess of $10^{23}$ W/cm$^2$ in the laboratory or in astrophysics) can only be fully explored in silico.

Several fundamental questions on plasma physics under extreme conditions can now be answered with ab initio petascale simulations + theory + experiments with intense beams.

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Outline

Particle in cell simulations towards the exascale

Laser particle acceleration and exotic beams

Exploring fundamental plasma processes for lab and astro

Moving to ultra high intensities

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In the project Manhattan (c. 1940) the cost of one floating point operation was $\sim 10^{-3}\text{€}$

Operations performed in mechanical calculators.
Cost of labour $\sim 4\text{ €/hour}$, assuming one operation per second.
Total number of operation corresponding to $4\text{ €} = 1\text{ flop/s} \times 60 \times 60$ s
Today, in a graphics processor unit each floating point operation costs $\sim 10^{-18}$ €.

GPU performs 0.5 Tflop/s and costs $\sim$ 2000 euros. We assume a 3 year lifetime. Neglect the cost of electricity.

Total number of operation for 2000 euros = $0.5 \times 10^{12}$ flop/s $\times$ 3 $\times$ 365 $\times$ 24 $\times$ 60 $\times$ 60 s
Particle-in-cell simulations

Solving Maxwell’s equations on a grid with self-consistent charges and currents due to charged particle dynamics

**State-of-the-art**

~ $10^{12}$ particles
~ $(12000)^3$ cells

RAM ~ 1 Gbyte - 100 TByte
Run time: hours to months
Data/run ~ few MB - 100s TByte

One-to-one simulations of plasma based accelerators & cluster dynamics
Weibel/two stream instability in astrophysics, relativistic shocks, fast igniton/inertial fusion energy, low temperature plasmas

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Particle-in-cell (PIC) - (Dawson, Buneman, 1960’s)
Maxwell’s equation solved on simulation grid
Particles pushed with Lorentz force

Osiris 3.0

Osiris framework
- Massively Parallel, Fully Relativistic Particle-in-Cell (PIC) Code
- Visualization and Data Analysis Infrastructure
- Developed by the osiris.consortium ⇒ UCLA + IST

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TÉCNICO
LISBOA

UCLA

code features
- Scalability to ~ 1.6 M cores
- SIMD hardware optimized
- Parallel I/O
- Dynamic Load Balancing
- QED module
- Particle merging
- GPGPU support
- Xeon Phi support
Integration of equations of motion:
moving particles
\[ \frac{dp}{dt} = F_p \rightarrow u_p \rightarrow x_p \]

Integration of field equations:
updating fields
\[ \frac{\partial E}{\partial t} = c \nabla \times B - 4\pi j \]
\[ \frac{\partial B}{\partial t} = -c \nabla \times E \]

Deposition:
calculating current on grid
\[ (x, u)_p \rightarrow j_i \]

Interpolation:
evaluating force on particles
\[ (E, B)_i \rightarrow F_p \]

Emission of photons
Probability of pair creation
\[ \rightarrow \text{new particles} \]

Probabilistic
Extended to include QED effects

**Emission Rate**

\[
\frac{dP}{dt} = \int_0^{\chi_e} d\gamma \frac{d^2 P}{dtd\gamma}
\]

\[
\tau_e = \frac{\hbar}{mc^2}
\]

**Pair creation rate**

\[
dP / dt = \int_0^{\chi_e} dx \gamma \frac{d^2 P}{dtd\gamma}
\]

**Additions to the PIC loop**
- Quantum radiation reaction / photon emission
- Photon propagation / Pair Creation

**Study extreme lab / astrophysical scenarios**
- Merge algorithm critical

Seeded QED cascades in counter propagating laser pulses

Linear Polarization


Double clockwise polarization
These particles are close
- in real space
- in momentum space

\[
\begin{align*}
\Delta \mathbf{p} &= \Delta p_x \mathbf{e}_x + \Delta p_y \mathbf{e}_y + \Delta p_z \mathbf{e}_z \\
\end{align*}
\]

Equations to satisfy
\[
\begin{align*}
w_t &= w_a + w_b \\
\mathbf{p}_t &= w_a \mathbf{p}_a + w_b \mathbf{p}_b \\
\epsilon_t &= w_a \epsilon_a + w_b \epsilon_b \\
\end{align*}
\]
Scaling Tests

- Scaling tests on LLNL Sequoia
  4096 → 1572864 cores (full system)
- Warm plasma tests
  Quadratic interpolation
  $u_{th} = 0.1 \, c$
- Weak scaling
  Grow problem size
  cells = $256^3 \times (N_{\text{cores}} / 4096)$
  $2^3$ particles/cell
- Strong scaling
  Fixed problem size
  cells = $2048^3$
  16 particles / cell

R. A. Fonseca et al. PPCF 55, 4011 (2013)
Similiar progress in supercomputers and intense lasers

Lasers and supercomputers

'14 Peak laser intensity ~ $10^{23}$ W/cm$^2$

'14 Peak computing power > 10 Pflop/s

Top System Performance [MFlop/s]

Mourou, Tajima, Bulanov (2006)

Source: top500.org
Similar intensities are present in particle beams

<table>
<thead>
<tr>
<th>Existing or planned particle beams</th>
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</table>
| **LHC @ CERN** I $\sim 2.5 \times 10^{19}$ W/cm$^2$  
100 kJ, 7 TeV per proton, $10^{11}$ protons per beam; 10 cm long bunch; 200 microns spot |
| **SPS @ CERN** I $\sim 1.5 \times 10^{18}$ W/cm$^2$  
$\sim$7 kJ, 0.5 TeV per proton, $10^{11}$ protons per beam; 10 cm long bunch; 200 microns spot |
| **ILC** I $\sim 1.5 \times 10^{24}$ W/cm$^2$  
1.6 kJ, 0.5 TeV per electron/positron, $2 \times 10^{10}$ electrons/positrons; $< 10$ nm width in x; $< \sim 100$ nm width in y; 6 mm long |
| **SLAC** I $\sim 1.2 \times 10^{19}$ W/cm$^2$  
160 J, 50 GeV per electron/positron, $2 \times 10^{10}$ electrons/positrons; $\sim 50$ microns long; $\sim 50$ microns spot |
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Can (laser) plasma accelerators reach the energy frontier?

Next generation of lasers @ 10+ PW

Vulcan Laser Facility
- USER Facility
- 8 Beam CPA Laser
- 3 Target Areas
- 3 KJ Energy
- 1 PW Power
Blow-out regime of laser wakefield acceleration

Self-injection, Dephasing, and Depletion

\[ a_0 \approx 0.8 \frac{\lambda \mu m}{\text{Intensity/10}^{18} \text{W/cm}^2}^{1/2} \]

\[ W_0 \text{ spot size} \]

\[ T_{\text{laser}} \text{ pulse duration} \]

Window co-moving with laser pulse @ speed of light
### Extreme blowout :: $a_0=53$

- Very nonlinear and complex physics
- Bubble radius varies with laser propagation
- Electron injection is continuous $\Rightarrow$ very strong beam loading
- Wakefield is noisy and the bubble sheath is not well defined

### Controlled self-guided :: $a_0=5.8$

- Lower laser intensity $\Rightarrow$ cleaner wakefield and sheath
- Loaded wakefield is relatively flat
- Blowout radius remains nearly constant
- Three distinct bunches $\Rightarrow$ room for tuning the laser parameters

### Channel guided :: $a_0=2$

- Lowest laser intensity $\Rightarrow$ highest beam energies (less charge)
- External guiding of the laser $\Rightarrow$ stable wakefield
- Tailored electron beam that initially flattens the wake
- Controlled acceleration of an externally injected beam to very high energies

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S. Gordienko and A. Pukhov PoP (2005); W. Lu et al. PR-STAB (2007)
S. F. Martins et al., Nature Physics (2009)
The orbital angular momentum of light is an unexplored degree of freedom for laser-plasma interactions.


**Applications**
- Astrophysics
- Ultrafast optical communications
- Nano particle manipulation

**Laser-plasma accelerators**
- Shaped electron/x-ray beams
- Ion acceleration (maybe reduce divergence)
  - High gradient positron acceleration
Laguerre-Gaussian lasers drive exotic (e.g. doughnut like) plasma waves in strongly non-linear regimes

**Linear doughnut wakefields**

- Laguerre-Gaussian laser
- Doughnut plasma wave

J. T. Mendonça and J. Vieira, PoP 21, 033107 (2014)

**Non-linear doughnut bubbles**

- Hollow electron bunch
- Hollow bubble

e-e+ fireballs from laser generated beams in solids

Experimental results demonstrate formation of e-e+ fireball

G. Sarri et al., Nature Communications (2015)
e-e+ plasma
Additional source of secondary radiation (e.g. gamma rays)
Platform to understand microinstabilities of relevance in astrophysics
“Dark electromagnetism”

\[
\sigma_x = \sigma_y = 2\sigma_z = 20 \mu m \\
\text{Emittance} = 10^{-5} \text{ mrad}
\]

Dephasing technique to overlap beams
Typically used in PWFA to reduce bunch
distance to ~100 microns

P. Muggli et al., arXiv:1306.4380
Interaction of fireball beam with plasma generates current filamentation instability (CFI)

### Beam density

- Filament size $\sim 0.5 \lambda_{pe}$
- Distance: 1.5 cm

### Growth of B3-field

- (a) Isosurfaces of $E_{dy}$ (red density; projections correspond to the baseline density for the normalization). The dotted line indicates the separation between the fireball beam and the baseline density case (solid line): the filaments are tilted, which in a plasma with a single magnetic filament of index $n = 2$, the orbit amplitude. The $B_0$-field associated with the filaments of opposite reference of the order of the plasma wavelength (plotted in units of $\lambda_{pe}$).

- (b-c) 2D density case (Fig. 2): the filaments are tilted, which in a plasma with $n = 2$ the orbit amplitude. The $B_0$-field associated with the filaments of opposite reference of the order of the plasma wavelength.

- (d) Integral of transverse motion and radiation (vectors represent $B$-field to a lower current and thus to a lower saturated $B$-field. This indicates that the particles can detrapping more easily, leading to a reduction in the $B$-field strength parameter.

- (e) The mixed mode has clearly developed more strongly in the high density scenario. The coupling of the excited longitudinal to the $B$-field.

Onset of CFI is determined by the balance between the beam emittance and CFI growth rate

- Rate of beam expansion can be expressed by the envelope equation as the function of beam emittance
  \[
  \frac{1}{\sigma_b} \frac{d\sigma_b}{dt} = \frac{t}{\sigma_{b0}^2 \gamma_b^2} 
  \]
  where \(\sigma_b\) is the beam radius, \(\gamma_b\) is relativistic factor and \(\varepsilon_N (= p_r \gamma_b)\) is normalised beam emittance.

- The criteria for CFI growth is that the beam expansion rate is much smaller than the CFI growth rate
  \[
  \theta \ll \left( \frac{\Gamma_{CFI} \sigma_{b0}^2}{L_{growth} c} \right)^{1/2}
  \]
  where \(\theta = \langle p_\perp \rangle / \gamma_b\) and we have considered that \(t \sim L_{growth} / c\), \(L_{growth}\) is the growth length of CFI.
Going from short beam to longer beam

Density ratio is decreased i.e. for longer beam the plasma is overdense $\omega_{pe} \gg \omega_{be}$

The growth rate of the two-streaming instability can be significant

\[
\begin{align*}
\Gamma_{OBI} & \approx \frac{\sqrt{3}}{2^{4/3}} \frac{\alpha^{1/3}}{\gamma b_0} ;
\Gamma_{CFI} \approx \sqrt{\frac{\alpha}{\gamma b_0}} \\
\frac{\Gamma_{OBI}}{\Gamma_{CFI}} & = \frac{\sqrt{3}}{2^{4/3}} \frac{1}{\beta_b} \left( \frac{\gamma b}{\alpha} \right)^{1/6}
\end{align*}
\]

where $\alpha = n_{b0}/n_{p0}$

Far smaller density ratio, oblique instability may be greater or comparable to the CFI
Three dimensional simulations confirm the growth of the OBI for smaller density ratios.

**Signature of Oblique mode**

**Drives wakefield structure**

**Tilting of B-field lines**

- \[ E_1 = 0.022 \, [m_0 c \omega_p/e] \]
- \[ E_1 = -0.02 \]

- \[ B_3 = 0.0033 \, [m_0 c \omega_p/e] \]
- \[ B_3 = -0.003 \]

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**B-fields generated by current filamentsation/Weibel in GRBs**
[Medvedev & Loeb, Gruzinov & Waxman, 99, Silva et al, 03]

**Fields in relativistic shocks are mediated by Weibel/current filamentation generated fields**
[Spiktovksy 08, Martins et al., 09]
Collision of two relativistic plasma slabs

Simulation apparatus

Wall reflection + Shock formation

“Cold” plasma $\gamma = 20$

- Gamma = 20
- Electrons + ions
- $m_i = 32 \, m_e$
- 1x2 particles per cell

Shock formation and evolution

Ion density

Strong shock structure and jump conditions verified

Ion density and shock profile

\[
\frac{n_2}{n_1} = \frac{\Gamma_{ad}}{\Gamma_{ad} - 1} + \frac{1}{\gamma_0 (\Gamma_{ad} - 1)} \approx 3.13
\]

\(n_2 \approx n_1 \times \lambda_{filaments}^{ad}
\]

Jump condition

Blandford & McKee (1976)
**Ab initio** Fermi acceleration determined by structure of the fields in the shock front [Spitkovsky 08, Martins et al, 09]

B-field amplification in upstream region via non-resonant “Bell” instability [Bell 04]

Connection with other B-field generation mechanisms (e.g. Biermann battery):
K. Schoeffler et al., PRL 2014
Filaments are stable over many plasma periods in electron-proton interpenetrating flows.
Electron trajectories follow the ExB drift in electron-ion magnetised flows

**Unmagnetized scenarios**

- **No preferential velocity direction**

**Magnetized**

- **e- rotation due to ExB drift**

\[(E_r \times B_0z)e_\theta\]
Calculating the radiation spectrum (and polarisation)

Energy deposition pattern and spectral features

Spectrum

\[
\frac{d^2 I}{d\omega dS} = \frac{e^2}{4\pi c} \left| \int_{-\infty}^{\infty} \tilde{n} \times \left[ \left( \tilde{n} - \tilde{\beta} \right) \times \tilde{\beta} \right] e^{i\omega(t' + R(t')/c)} dt \right|^2 / (1 - \tilde{n} \cdot \tilde{\beta})^2 R(t')^2
\]

Power

\[
\frac{dP}{dS} = \frac{e^2}{4\pi c} \frac{ \left| \tilde{n} \times \left[ \left( \tilde{n} - \tilde{\beta} \right) \times \tilde{\beta} \right] \right|^2}{(1 - \tilde{\beta} \cdot \tilde{n})^5 R(t')^2}
\]

Degree of Circular Polarization

\[
P_c = s_3/s_0; \quad s_3 = 2Im\langle E_x E_y^* \rangle; \quad s_0 = |E_x|^2 + |E_y|^2
\]

\[
P_c = \begin{cases} 1 & \text{RCP} \\ -1 & \text{LCP} \end{cases}
\]

CP photon flux

\[
\langle P_c \rangle_{\omega} = \frac{\int P_c I_{rad} d\omega}{\int I_{rad} d\omega}
\]

\[
\langle P_c \rangle = \frac{\iint P_c I_{rad} d\omega dS}{I_{rad} d\omega dS}
\]

J. L. Martins et. al., Proc. SPIE, 7390V, 2009b

Polarization depends on magnetization (external B field) in current filamentation instability

**Finite circular polarisation**

\[
\langle P_c \rangle e^{-\frac{m_i}{m_e}}; \frac{m_i}{m_e} = 1836
\]

\[
\langle P_c \rangle e^{-\frac{m_i}{m_e}}; \frac{m_i}{m_e} = 918
\]

\[
\langle P_c \rangle e^{-\frac{m_i}{m_e}}; \frac{m_i}{m_e} = 1
\]

\[
\langle P_c \rangle e^{+\frac{m_i}{m_e}}; \frac{m_i}{m_e} = 1
\]

**Onset of circular polarisation**

- **Mass ratio**
  - \( m_i/m_e \gg 1 \)
  - Electron motion much faster than filament merging time

- **Magnetic fields**
  - Weak magnetisations (\( \sigma \ll 1 \)) yield 10-20% circularly polarised x-rays

- **Multiple sources**
  - No influence on final polarisation (random phase approximation)
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Identifying radiation reaction signatures in electron beam spectrum

- Laser wakefield accelerator in bubble regime
- Second laser $I \sim 10^{21}$ W/cm$^2$
- X-ray ($\gamma$-ray) detector
- Accelerated electrons

A. G. R. Thomas et al., PRX 2, 041004 (2012)
M. Vranic et al., PRL 113, 1348001 (2014)
~40% energy loss for 1 GeV beam at $10^{21}$ W/cm$^2$

Radiation reaction can be tested with state-of-the-art lasers in this configuration

3D full-scale parameter scan

M. Vranic et al., PRL 113, 1348001 (2014)
Pairs can be produced already at $\chi = 0.6$

~ 200 pairs obtained per 1 000 000 interacting electrons

- **Parameters**
  - Laser $l \sim 2 \times 10^{21}$ W/cm$^2$, 30 fs, 800 nm
  - Electron initial energy $\sim 3$ GeV

Electron beam energy spread and divergence:
M. Vranic et al., NJP (2016); ArXiv1511.04406
Capturing QED in PIC codes

Monte Carlo simulations showing **pair production via real photons per electron**

PIC simulations of QED cascade in various configuration (counter propagating laser, rotating field)

**Dense pair Plasmas and Ultra-Intense Bursts of Gamma-Rays from Laser-Irradiated Solids**


**Number of pairs produced**

**Picture of a cascade in rotating field**

Gamma rays from laser-irradiated solid
Modelling of QED cascades (& radiation cooling)

T. Grismayer et al.

Parameters
- absorbing boundaries
- $a_0 = 1000$
- $\lambda_0 = 1 \mu m$
- Linear polarization
- $W_0 = 5 \mu m$
- $\tau = 30 \text{ fs}$

Electromagnetic wave

electron

Electromagnetic wave

Time $= 0.00 \left[ 1/\omega_p \right]$

QED cascades in counter propagating electromagnetic fields

T. Grismayer et al.

Cascade

Time = 0.00 [1/ωₚ]

- photons
- positron
- electron

Optimal QED configurations with standing waves

This requires finding where the parameter

$$\chi = \frac{1}{E_S} \sqrt{\left( \gamma E + \frac{P}{mc} \times B \right)^2 - \left( \frac{P}{mc} \cdot E \right)^2}$$

reaches high values

<table>
<thead>
<tr>
<th>Linear</th>
<th>Double clockwise</th>
<th>Clockwise-anti clockwise</th>
</tr>
</thead>
<tbody>
<tr>
<td>• electron</td>
<td>• electron</td>
<td>• electron</td>
</tr>
<tr>
<td>• positron</td>
<td>• positron</td>
<td>• positron</td>
</tr>
<tr>
<td>• photon</td>
<td>• photon</td>
<td>• photon</td>
</tr>
</tbody>
</table>
Analytical growth rate model + 3D full scale parameter scan


Laser absorption via QED cascades absorption model + 2D/3D simulations


Possibility to achieve conditions close to the Goldreich-Julian density $e^{-}e^{+}$ density $\sim n_{cr} \sim$ Goldreich-Julian density

A. Gruzinov, Arxiv:1404.4615v1 (2014)
Heisenberg-Euler QED corrections

Physics below Schwinger limit

Relevance for extreme astrophysical scenarios?

Effect on laser properties as we reach Schwinger limit?

Extract observable consequences of QED predictions.

Multi PW lasers combined with x-ray lasers will allow us to probe the dynamics of the Quantum Vacuum.

Heisenberg-Euler corrections to Maxwell’s Equations*

Electron-positron fluctuations give rise to an effective polarisation and magnetisation of the vacuum which can be treated in an effective form as corrections to Maxwell’s equations.

\[ \mathcal{L} = \mathcal{L}_M + \mathcal{L}_{HE} + \mathcal{L}_D \]

Valid for static inhomogeneous fields such that

\[ E << E_S \quad \omega << \omega_c \]

\[ E_S = \frac{m^2 c^3}{e \hbar} \quad \omega_c = \frac{mc^2}{2\hbar} \]

Effectively, we obtain a highly non linear, non dispersive vacuum (e.g. M.Soljačić and M. Segev Phys. Rev.A 62, 043817 (2000))

Higher order corrections include spatial and temporal derivatives of these corrections. May be neglected for:

\[ \omega << \omega_c \frac{E}{E_S} \]

Heisenberg-Euler QED corrections

Quantum vacuum corrections to Maxwell’s equations nonlinearly couple all field components

- Electron-positron fluctuations give rise to an effective polarisation and magnetisation of the vacuum which can be treated in an effective form as corrections to Maxwell’s equations*.

\[
\frac{\partial \vec{B}}{\partial t} + \vec{\nabla} \times \vec{E} = 0 \quad \vec{\nabla} \cdot \vec{B} = 0 \\
\vec{\nabla} \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = 0 \quad \vec{\nabla} \cdot \vec{D} = 0
\]

- with the constitutive relations,

\[
\vec{D} = \varepsilon_0 \vec{E} + \vec{P} \quad \vec{B} = \mu_0 \vec{H} + \vec{M}
\]

\[
\vec{P} = 2\xi \left[ 2(E^2 - c^2 B^2)\vec{E} + 7(\vec{E} \cdot \vec{B})\vec{B} \right] \\
\vec{M} = -2\xi \left[ (2E^2 - c^2 B^2)\vec{B} - 7(\vec{E} \cdot \vec{B})\vec{E} \right]
\]

\[
\xi = \frac{20\alpha^2 \varepsilon_0^2 \hbar^3}{45 m_e^4 c^5} \sim 10^{-51} \text{ [Fm/V}^2\text{]}\]

Effects of the quantum vacuum below the Schwinger limit

- Relevance for extreme astrophysical scenarios?
- Unprecedented intensities will allow to probe the quantum vacuum. What laser properties will be affected?
- Extract observable consequences of fundamental QED predictions.


**Ellipticity induced in x-ray probe propagating through birefringent vacuum**

T. Grismayer et al.

Simulation setup*: x-ray pulse probes birefringent vacuum created by optical laser. A measurement of ellipticity induced is a direct test of the Quantum vacuum

Using our QED solver, it is possible to simulate this setup in multidimensional and, via an electromagnetic treatment, obtain the ellipticity induces at various off-axis distances and for probe/pump parameters

**Simulation parameters**
- \( \xi = 10^{-6} \)
- \( \sigma = 30 \text{ fs probe duration} \)
- 1 keV x-ray probe
- \( I = 10^{23} \text{ W/cm}^2 \) pump
- \( \lambda = 1 \mu \text{m pump} \)
Multi mode mixing due to nonlinear vacuum corrections

Setup with 2 Gaussian pulses propagating in perpendicular directions ($a_0 = 100, \xi = 10^{-6}, \lambda = 1 \mu m$)

Combination of odd and even harmonics is generated; **After interaction**, imprint is left in both pulses as they now freely propagate.

P. Carneiro *et al.*, arXiv:1607.04224

To be explored e.g. at HIBEF (XFEL + ultra high intensity laser)
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Scenarios where all this comes together

Pulsar magnetospheres...

... in the laboratory?

INPAIRS
Summary

A wide range of extreme laboratory and astrophysical scenarios can now be explored and captured by ab initio simulations.

Continuous interplay between theory, multi scale models, and outstanding computational advances will continue to drive important advances in silico.

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