Uncovering the secrets of extreme physics with large scale numerical plasma simulations (and lasers)

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Accelerates ERC-2010-AdG 267841

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Acknowledgments

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🖗 Everyone at



- Work in collaboration with:
 - W. B. Mori, C. Joshi (UCLA)
- Simulation results obtained at the epp and IST Clusters (IST), Dawson Cluster (UCLA), Franklin (NERSC), Intrepid (Argonne), Jugene (FZ Jülich), and Jaguar (ORNL)



Tech developments have triggered a revolution

Lasers and supercomputers





In the project Manhathan (c. 1940) the cost of one floating point operation was ~ $10^{-3} \in$

Operations performed in mechanical calculators. Cost of labour ~ 4 €/hour, assuming one operation per second. Total number of operation corresponding to 4 € = 1 flop/s 60 × 60 s

Today, in a graphics processor unit each floating point operation costs ~ | 0^{-|8}€

GPU performs 0.5 Tflop/s and costs ~ 2000 euros. We assume a 3 year lifetime. Neglect the cost of electricity. Total number of operation for 2000 euros = 0.5×10^{12} flop/s $\times 3 \times 365 \times 24 \times 60 \times 60$ s

How can we describe the plasma physics?

Hierarchy of descriptions (ignoring quantum effects)

- Klimontovich equation ("exact").
- Ensemble average the Klimontovich equation
 - Leads to Vlasov Fokker Planck equation (approximate)
- \blacktriangleright Take the limit that N_D is very very large
 - Vlasov equation
- Take moments of the Vlasov or Vlasov Fokker Planck equation
 - "Two" fluid (transport) equations
- Ignore electron inertia
 - Single fluid or MHD equations

What is the particle-in-cell model?

Is it an efficient way of modeling the Vlasov equation? No, it is a Klimontovich description for finite size (macro-particles)

Klimontovich eq. of macro-particles	Maxwell's equations	
$\frac{D}{Dt}F = 0$	$\frac{\partial}{\partial t}\vec{E} = \nabla\times\vec{B} - \frac{4\pi}{c}\vec{J}$	
$F(\vec{x}, \vec{v}; t) = \sum_{i}^{N} S_p(\vec{x} - \vec{x}_i(t))\delta(\vec{v} - \vec{v}_i(t))$	$\frac{\partial}{\partial t}\vec{B} = -\nabla\times\vec{E}$	
$\left[\frac{D}{Dt} \equiv \partial_t + \vec{v} \cdot \nabla_x + \vec{a} \cdot \nabla_v\right]$	$ec{J}(ec{x},t) = \int dec{v} \; qec{v} \; F(ec{x},ec{v},t)$	
$\vec{a} \equiv \frac{d}{dt}\vec{v} = \frac{q}{m}\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right)$	J	

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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

~ 10¹⁰ particles ~ (1000)³ cells

RAM ~ I Gbyte - 5 TByte Run time: hours to months Data/run ~ few MB - 10s 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

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







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The particle-in-cell methodology



Modeling kinetic physics

- Particle simulations
 - (# operations $\propto N^2$)
- Particle-Mesh simulations(# operations ~ N)
 - Fields + densities
 - Long range interactions
- Additional MC binary Coulomb collision module can model short range interactions





* Dawson, Buneman, 1960's; Birdsall and Langdon, Plasma Phys. via Comp. Simulation (1985) L. O. Silva | PlasmaSurf 2016 | Oeiras, July 11 2016

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Particle-in-cell methodology*



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The particle-in-cell methodology



Modeling kinetic physics

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MC binary Coulomb collisions*



* Takizuka & Abe JCP 1977

OSIRIS 2.0





osiris framework

- Massivelly Parallel, Fully Relativistic
 Particle-in-Cell (PIC) Code
- Visualization and Data Analysis Infrastructure
- Developed by the osiris.consortium \Rightarrow UCLA + IST

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http://cfp.ist.utl.pt/golp/epp/ http://exodus.physics.ucla.edu/



New Features in v2.0



- Bessel Beams
- Binary Collision Module
- Tunnel (ADK) and Impact Ionization
- Dynamic Load Balancing
- PML absorbing BC
- Optimized higher order splines
- Parallel I/O (HDF5)
- Boosted frame in 1/2/3D

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Particle-in-cell loop in osiris 2.0



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Taking advantage of the largest machines in the World



10¹² particles0.78 Pflop/s33% peak performance

- Jaguar (jaguarpf)
 - 18688 compute nodes
 - dedicated service/login nodes
 - SeaStar2+ network

- XT5 Compute node
 - Dual hex-core AMD Opteron 2435 (Istanbul) at 2.6 GHz
 - I6GB DDR2-800 memory

Complete system
 224256 processing cores
 300 TB of memory
 Peak performance 2.3 PFlop/s

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What challenges lie ahead?

Demonstrate 10s GeV e- and 200 MeV protons with lasers

Make nuclear fusion (with lasers) a viable alternative for energy production

Determine the conditions & observe Fermi acceleration in the laboratory

"Boil the vacuum"



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Particle accelerators: rich science and applications

From compact to country size

Large

- Verified Standard Model of Particle Physics
- 🏺 W, Z bosons
- Quarks, gluons and quark-gluon plasma
- Solution Asymmetry of matter and anti-matter
- 🖗 In pursuit of the Higgs boson

Compact

- Medicine
 - sancer therapy, imaging

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- 🏺 Industry
 - 🏺 lithography
- Light sources (synchrotrons)
 - 🏺 bio imaging
 - condensed matter science



Plasma Accelerator Progress and the "Accelerator Moore's Law"



Courtesy: Tom Katsouleas (Duke) / Physics Today 2004

NETWORKING IN THE IMMUNE SYSTEM • NANOTECH BATTERIES

SCIENTIFIC AMERICAN

How to Protect New Orleans from Future Storms

FEBRUARY 2006 WWW.SCIAM.COM

Big Physics Gets Small

Tabletop Accelerators Make Particles Surf on Plasma Waves

How to Stop Nuclear Terrorists

Guess Who Owns Your Genes?

CSI: Washington (George, that is)

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Electrons hang ten on laser wake

Thomas Katsouleas

Electrons can be accelerated by making them surf a laser-driven plasma wave. High acceleration rates, and now the production of well-populated, high-quality beams, signal the potential of this table-top technology.

PLASMA ACCELERATORS

A new method of particle acceleration in which the particles "surf" on a wave of plasma promises to unleash a wealth of applications

By Chandrashekhar Joshi

www.sciam.com

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Accelerating particles in plasma wakes



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Recent progress has put plasma acceleration at the forefront of Science

Simulations + lasers + sources directly impacted this progress



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Why plasmas?



Plasmas do not "break" under very large electric fields

RF cavities sustain 50 MeV/m



x 20 000 for ILC



Maximum accelerating electric field determined by disruption of RF cavity walls

Plasmas can sustain 10's GeV/m



 E_0 [V/cm] $\approx 0.96 n_0^{1/2}$ [cm⁻³] $n_0 = 10^{18} \text{ cm}^{-3} \rightarrow E_0 \approx 1 \text{ GV/cm}$

Plasmas can sustain waves with very large electric fields with relativistic phase velocities

Pioneering work in 70s - 80s opened a brand new field

Plasma based accelerators



Pre-2004 results demonstrated relativistic plasma wave excitation

Electron acceleration up to ~ 200 MeV

Relativistic plasma waves



Thermal-like spectrum up to 200 MeV

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2004 results confirm potential of laser-plasma accelerators

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Monoenergetic beams of self-injected electrons



Courtesy: V. Malka (LOA), K. Krushelnick (IC/RAL), W. Leemans (LBL)

Can LWFA reach the energy frontier with the next generation of lasers?



Next generation of lasers @ 10 PW



Blow-out regime of laser wakefield acceleration



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Petascale modelling of LWFA

LWFA Performance

- 7.09×10¹⁰ part / s
- 3.12 µs core push time
- 77 TFlops (3.3 % of R_{peak})
- Limited by load imbalance

Peak Performance

- I.86 × IO¹² particles
- I.46 × I0¹² particles / s
- 0.74 PFlops
- 32% of Rpeak (42% of Rmax)



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Challenge: Parameter range for a 300J laser

		Self-guiding		External-guiding	
Laser		Self Injection I*	Self Injection II**	Self Injection**	External Injection**
	a0	43	5.8	3.5	2
	Spot [µm]	9	50	70	101
	Duration [fs]	30	110	155	224
Ρ	lasma				
	Density [cm ⁻³]	1.5×10 ¹⁹	2.7×10 ¹⁷	8.2×10 ¹⁶	2.2×10 ¹⁶
	Length [cm]	0.25	22	100	500
e	Bunch				
	Energy [GeV]	4	13	25	53
	Charge [nC]	14	2	1.8	1.5
Si	mulation				
time [days in 512CPUs]			400	2,500	12,000

* S. Gordienko and A. Pukhov PoP (2005) ** W. Lu et al. PR-STAB (2007)

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Boosted Frames in LWFA simulations

Grid resolution in Laboratory and Boosted frame



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~2GeV self-injection in strongly nonlinear regime



S.F. Martins et al., Nat Phys (2010)

+10GeV self-injection in nonlinear regime



S.F. Martins et al., Nat Phys (2010)

>IOGeV simulation for next generation lasers

Injected bunches properties



Energy spectrum & Emittance



+40GeV with externally injected beams



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Applications for LWFA beams

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HEP Collider & radiation


Betatron radiation in plasma wakefield acceleration

UCLA/SLAC/USC have demonstrated x-ray betatron radiation with SLAC beam (28 GeV)



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Betatron sources & table top synchrotrons



Advanced radiation diagnostic

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S. Kneip, C. McGuffey, J. L, Martins et al., Nature Phys., 2010

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Laser driven ion beams hold promising applications

Laser-plasma accelerators



Compact sources



lon beam driven inertial fusion

Medical applications

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Quest is driven by medical applications

Ion beams can have a localized energy deposition in deep-seated tumors



The quest for high-quality mono-energetic proton beams



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Shock acceleration can potentially lead to mono-energetic beams



J. Denavit PRL 69, 3052 (1992) L. O. Silva et al. PRL 102, 015002 (2004)



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n_{cr} targets allow for high-quality shock accelerated beams



Requirements for high-quality shock acceleration

- High Mach number shocks in different density/temperature plasmas^{*}
- Shock acceleration must dominate over TNSA fields^{**}
- When shock is formed:***

$$\mathbf{v}_{\rm sh} > \mathbf{v}_{\rm ions} \Rightarrow \quad L_g > \frac{20\pi}{\omega_{pi}} \frac{C_{s0}^2}{v_{sh}}$$

• When shock crosses back of target:

$$\mathbf{v}_{\rm sh} > \mathbf{v}_{\rm ions} \Rightarrow \quad L_g \ll \frac{v_{sh}}{\omega_{pi}} \left(e^{\frac{v_{sh}}{2C_{s0}}} - 20\pi \right)$$

• For optimal absorption $(n_p \sim n_c)$, optimal thickness $L_g \sim 20 l_0$

Near n_{cr} targets are optimal

 CO_2 lasers in mm scale gas jet targets (n_c) at high repetition rates

- * G. Sorasio et al. PRL 2006
- ** T. Grismayer & P. Mora Phys. Plasmas 2006
- ^{***} shock formation time ~ 20p w_{pi}^{-1} (D.W. Forslund & C. R. Shonk PRL 1970)

Interplay between shock acceleration and TNSA is critical If





Previously I MeV, rms $\Delta E/E \sim 4\%$ had been measured (C. Palmer PRL 2011)

D. Haberberger et al., Nature Physics, January 2012



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Low beam emittance has been measured





Shock acceleration is extensible to ultrahigh energies

Favorable scaling provides proton beams for medical applications (200 MeV) with readily available lasers (a0 ~ 10)



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Proton driven wakefield accelerator @ CERN



CERN, DESY, MPI, UCLA, USC, BNL, TH, D, IST, UCL, IC, IPP, RAL



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A WAKE

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Nuclear fusion with lasers @ NIF



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Indirect drive nuclear fusion



National Ignition Facility Target (~ I cm long)

Advanced concepts: fast ignition concept*



The fast ignition concept



^{*} R. Kodama et al., Nature **412**, 798 (2001); R. Kodama et al., Nature **432**, 1005 (2004)

L. O. Silva | PlasmaSurf 2013 | Oeiras, July 8 2013

The fast ignition concept



* G. Li et al., Phys. Rev. Lett. 100, 125002 (2008)

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Modeling is extremely demanding due to different scales involved

Typical HED compressed target



Computational requirements for PIC

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Physical size

Box size: 1 mm Cell size: 5 Å Duration: 10 ps Time step: 1 as (10⁻¹⁸ s)

Numerical size

cells/dim: 2x10⁶ # particles/cell: 100 (1D); 10 (2D); 1 (3D) # time steps: 10⁶

Particle push time: I ms

Computational time

ID - $2x10^3$ CPU days 2D - $5x10^8$ CPU days ~ 10^6 CPU years 3D - $2x10^{11}$ CPU days ~ $7x10^8$ CPU years

F. Fiúza et al

New hybrid-PIC algorithm for HEDP modeling*





Full-PIC code

- Full Maxwell's equations
- Kinetic species
- $n_0 < 10^{23} \text{ cm}^{-3}$
- $\omega_p \Delta t < O(1)$
- $\Delta x \omega_p / c < O(1)$
- $c\Delta t/\Delta x < I$

If resistivity (Ohm's law) matches collisional model transition is natural and self-consistent



Hybrid-PIC code

- Maxwell's equations + Ohm's law (inertialess)
- Kinetic species
- $n_0 > 10^{23} \text{ cm}^{-3}$
- $v_{ei}\Delta t < O(1)$
- $c\Delta t/\Delta x < 1$

* B. Cohen, A. Kemp, L. Divol, JCP 229, 4591 (2010)

Accurate hybrid-PIC transition requires careful numerics



Advanced numerical techniques

- High-order splines
- MC binary Coulomb collisions
- Advanced smoothing
- PML boundary conditions



Stable and accurate transition



F. Fiuza et al. PPCF 53, 074004 (2011)

First full-scale FI modeling with realistic densities



Physical Parameters

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Laser

• $\lambda_0 = 1 \mu m$ • $I_0 = 2 \times 10^{20} \text{ W cm}^{-2} (100 \text{ kJ})$ • $W_0 = 30 \mu m$ • $\tau_0 = 15 \text{ ps}$ Plasma • $L = 450 \times 450 \mu m^2$ • $n_{e0} = 1 n_c - 2 \times 10^5 n_c$ • $m_i/m_e = 3672$

Numerical Parameters

- 42 cells/µm
- hybrid/full-PIC transition = 100 n_c
- Particles per cell = 64
- # time steps = 10^5
- cubic interpolation



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Fundamental questions on quantum electrodynamics Ji

The quantum vacuum and pair production with intense fields

QED at ultra high intensities is almost unexplored*



Intensities required to start to probe the quantum vacuum are within reach

Strong debate about this transition: 10²⁴ W/cm² or 10²⁶ W/cm²

Work done by the electric field over a Compton wavelength > electron rest mass determines the Schwinger field

*Physicists like perturbation theory around small quantities...

Adding radiation reaction force to the PIC loop



Adding radiation reaction force to the PIC loop



Unravelling the nature of radiation reaction

Understanding one of the oddest equations in physics

Lorentz-Abraham-Dirac equation has a third order derivative with respect to the position of a particle

laser wakefield accelerator in blowout regime provides GeV class beams second laser scatters on e- beam I ~ 10²¹ W/cm²

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M. Vranic, J. L. Martins et al., arXiv:1306.0766 (2013)

accelerated

electrons

QED cascades in counter propagating lasers



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QED cascades in counter propagating lasers



Time = $0.00 [1 / \omega_{p}]$



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Parameter range for QED cascade



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Colliding flows of plasmas are pervasive in astrophysics Jr



Pulsar Wind Nebulae



Crab nebula NASA/CXC/SAO

Supernova Explosion



Cassiopeia A X-ray: NASA/CXC/SAO; Optical: NASA/STScl; Infrared: NASA/JPL-Caltech

The landscape of collisionless astro/space shocks



Adapted from A. Spitkovsky

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Collision of two relativistic plasma slabs

Simulation apparatus



S. F. Martins et al., ApJ Lett (2009)

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Ab initio shock formation and evolution

lon density



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Ab initio Fermi acceleration

Trapped particle trajectories in the shock front - x l vs time



S. F. Martins et al, ApJ Lett (2009)

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OSIRIS simulation setup: shock generation in lab



Physical Parameters

Laser • $\lambda_0 = I \mu m$ • $I_0 = I0^{20} - I0^{22} W cm^{-2}$ • $\tau_0 = I ps$

Plasma • $L = 20 \times 100 \ \mu m^2 (W_{pi}^2)$ • $n_{e0} = 10 \ n_c - 100 \ n_c$

• $m_i/m_e = 1836$

Numerical Parameters

- $Dx = Dy = 0.25 \text{ c/w}_{pe}$
- 64 particles per cell
- I0⁹ particles
- ${\scriptstyle \bullet}$ cubic interpolation

F. Fiúza et al., PRL, 2012

Collisionless shock launched with ultraintense laser





F. Fiúza et al, PRL (2012)

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Similar underlying physics/results in 3D



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How about magnetized shocks?



* J. P. Knauer et al., Phys. Plasmas 17, 056318 (2010)

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Summary



The quest for ultra intense beams is driving technological advances in lasers and particle beams and computer simulations are opening these directions

Significant potential impact in many relevant societal questions

Potential to address fundamental questions in physics is also outstanding in regimes far from equilibrium



What challenges lie ahead?

Demonstrate 10s GeV e- and 200 MeV protons with lasers

Make nuclear fusion (with lasers) a viable alternative for energy production

Determine the conditions & observe Fermi acceleration in the laboratory

"Boil the vacuum"

