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HZDR
13th October, 2020

NUMERICS AND HPC

NE's grand challenge HPC list



Strong Field QED

1. Electron-positron cascade
2. QED+Relativistic plasma effects
3. Vacuum birefringence

8D based integro-differential equation
PIC+QED Monte-Carlo (sub-optimal)

Laser & thin foils

1. Molecular dynamics
2. Continuum-kinetic (2T+Boltzmann)
3. Relativistic effects (PIC)

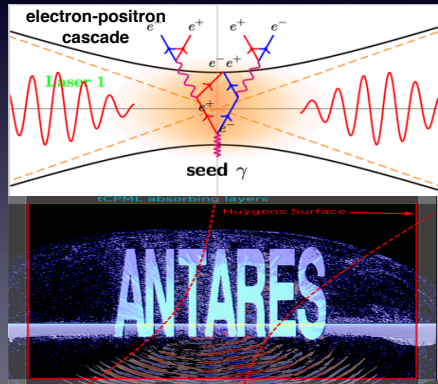
Composite multi-physics
application

Particle-in-Cell Code PIC-ANTARES

Kinetic plasma turbulence:

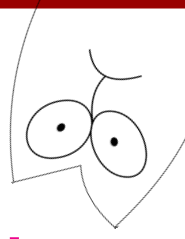
1. Anomalous resistivity
2. Fast magnetic reconnection
3. Multi-scale model of solar flares

6D based Vlasov+Maxwell solver

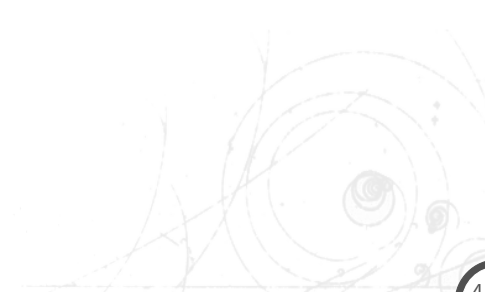


Agenda

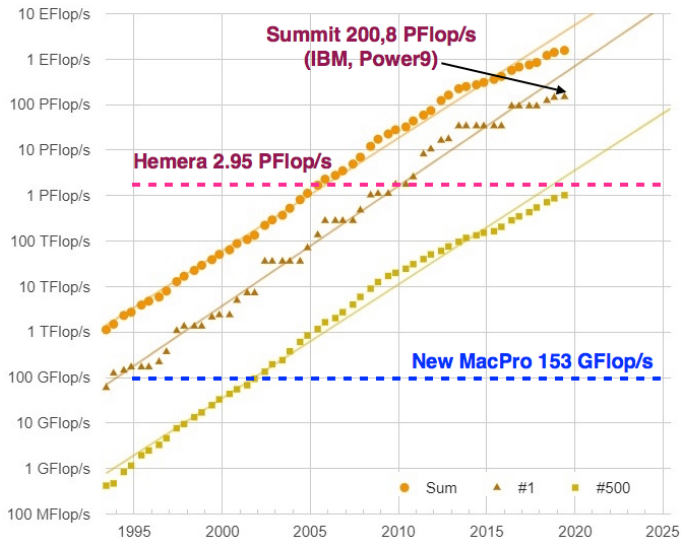
- Trends in HPC
 - Amdahl's law
 - Roof line model
 - Arithmetic intensity of methods
-
- Numerics vs. Asteroids
 - 'Explitization' of methods for parallel codes
 - Smoothed Particle Hydrodynamics
 - Hydrodynamic model of surface ablation
- Hardware
 - Numerics



Parallel World!

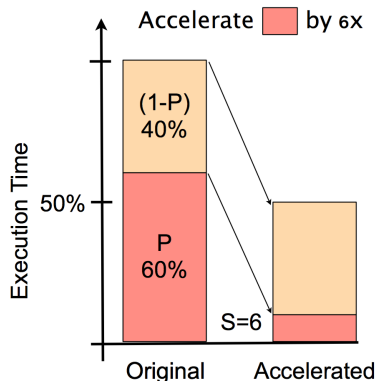


Moore's Law and Top500



Amdahl's Law

$$S = \frac{1}{(1 - P) + P/S}$$

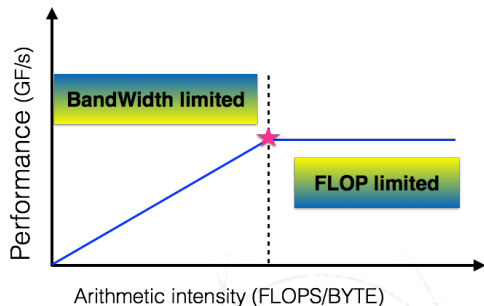


- Sequential parts
 - initialization
 - sequential I/O
 - Synchronization, Barriers
- Reduce/optimize sequential part 'S'
- **Increase parallel part 'P'**
- Asynchronous and one-sided communications
- **Use memory hierarchy to reach super-linear scaling**

Roofline Model¹

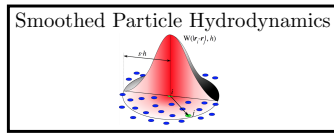
Performance is bounded by

- the peak flop rate
- the streaming bandwidth



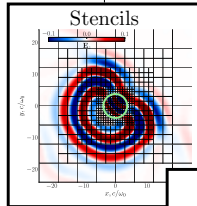
¹Williams et.al, 2009

Classification of methods by arithmetic intensity



ARITHMETIC INTENSITY

Sparse Matrices

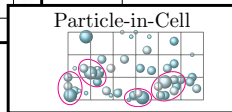


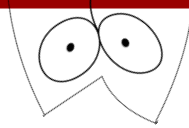
FFT

Fast Multipole Method

Dense Matrices

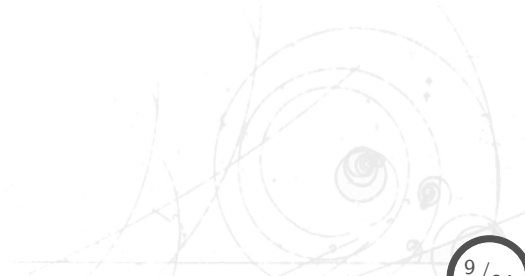
True Molecular Dynamics





and now for something completely different:

Numerics&Asteroids



99942 Apophis

discovered: 2004
fly by: 2012
next visit 13.04.2029
?? 2036
??? 2068

450 m

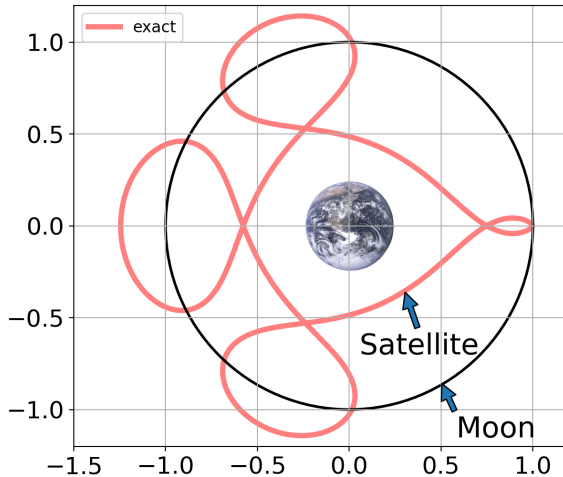
Numerics&HPC

- 1. Estimate Chances: Prediction of orbit**
- 2. Worst-case: Impact and Megatsunami**
- 3. Best-case: push asteroid away with lasers**

simulations done on Hemera

object	size	how often	crater size	outcome
dust grain	0.5m	all the time	none	make a wish
	<30m	1y	none	a big wish :)
	~30m	250y		Tunguska Arizona
	~100m	3000y	2km	Local DD
	1km	1Ma	20km	Global DD
Game Over	>10km	100Ma	 	

Orbit benchmark: restricted 3-body problem ²



²aka Arenstorf's problem

Explicit methods

Semi-implicit

Implicit

- Runge-Kutta (RK4)
- Partitioned RK (leap frog, Verlet)
- nested methods
RK-Fehlberg
- RK-Nyström
- Pseudo-symplectic

- IMEX (implicit-explicit)
(MHD, Multi-Fluid)
- Diagonally implicit
- Rosenbrock
- **Iterated Crank-Nicolson**
SPH, PIC

- Gauss-Legendre-RK
(QED, ultra-relativistic)
- Gauss-Lobatto-RK
- Keller box
(Wave/Maxwell)
- **Crank-Nicolson**

Extra-techniques: adaptive times stepping, arc-length, Richardson extrapolation, stiffness estimators, **strong stability preserving** (hyperbolic PDEs), symplectic, **low-storage**, extended stability RK-Chebyshev



Orbit benchmark: numerical integration

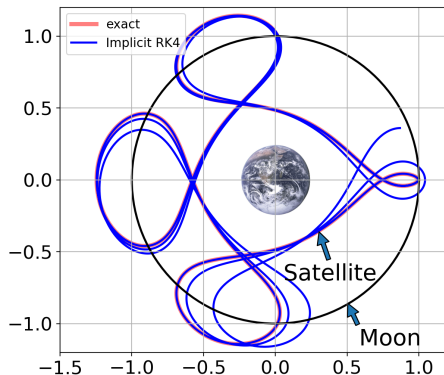
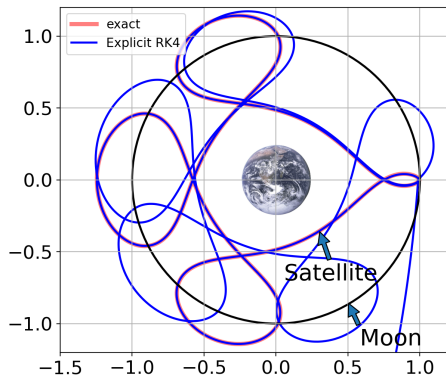
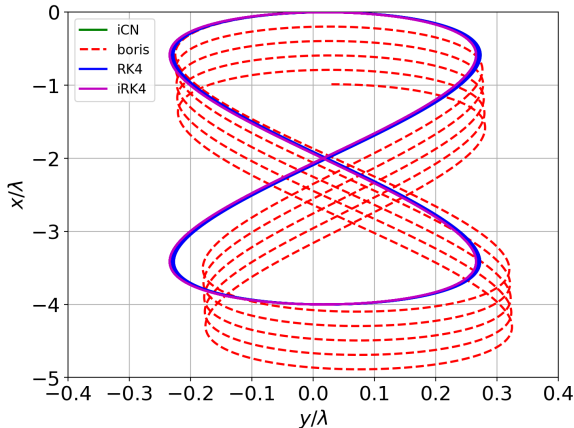
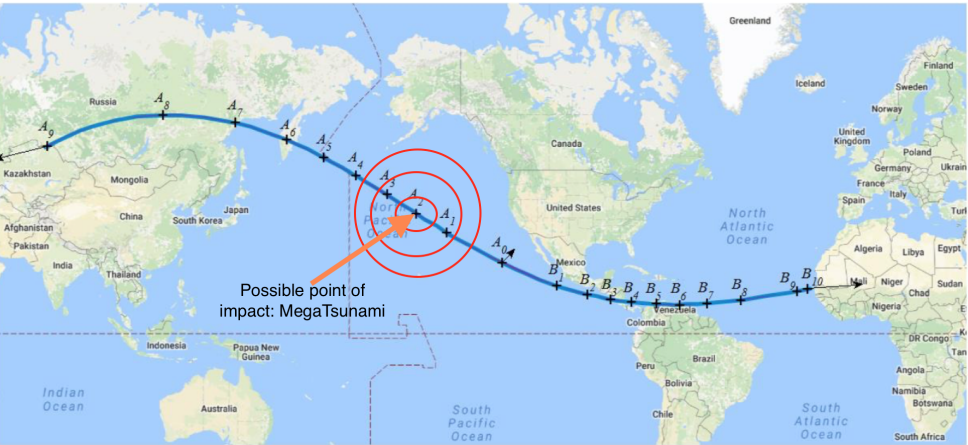


figure-8) motion: relevant to particle-in-cell codes ³



³particle in EM wave, $a_0 > 1$; Boris's method shows a significant drift

Impact path risk of APOPHIS⁴



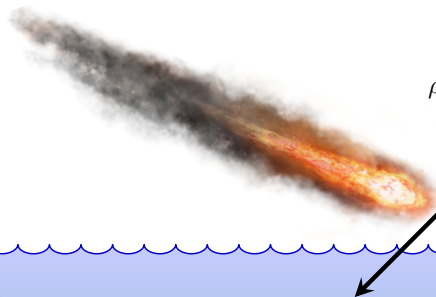
⁴[Guo&Ivashkin, 2017]

MegaTsunami: Smoothed Particle Hydrodynamics

Navier-Stokes equations

$$\rho \left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla \right) \vec{u} = -\nabla p + \mu \nabla \cdot (\nabla \vec{u}) + \vec{f}$$

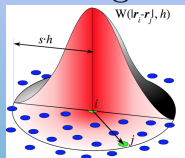
$$\nabla \cdot \vec{u} = 0 \quad \text{incompressibility}$$



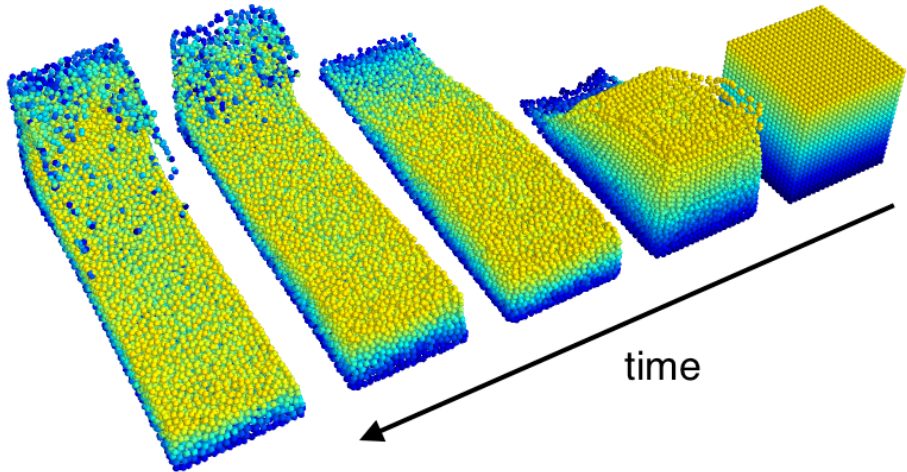
$$\frac{d\rho_i}{dt} = \sum_{j=1}^N m_j v_{ij}^{\beta} \frac{\partial W_{ij}}{\partial x_i^{\beta}}$$

$$\frac{dv_i^{\alpha}}{dt} = \sum_{j=1}^N m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right)$$

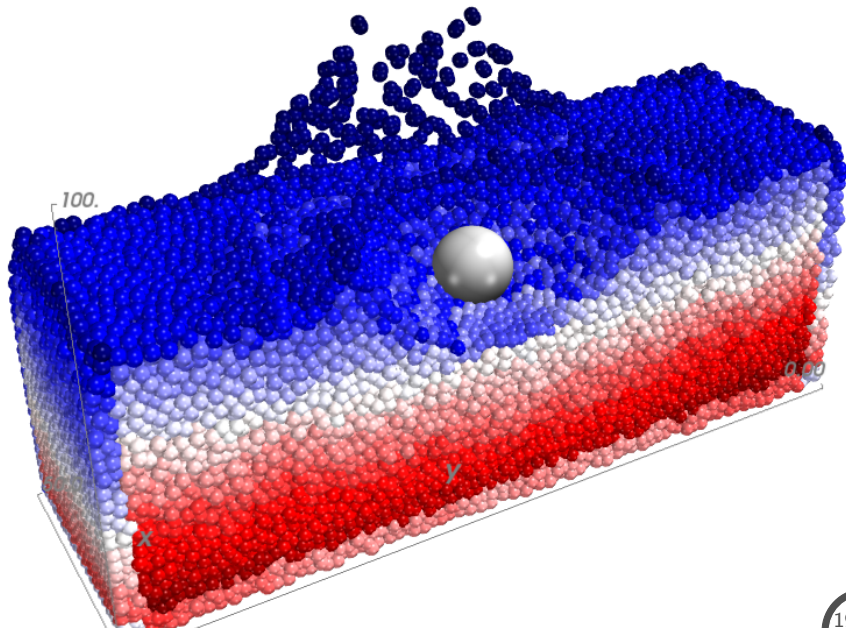
Smoothing kernel



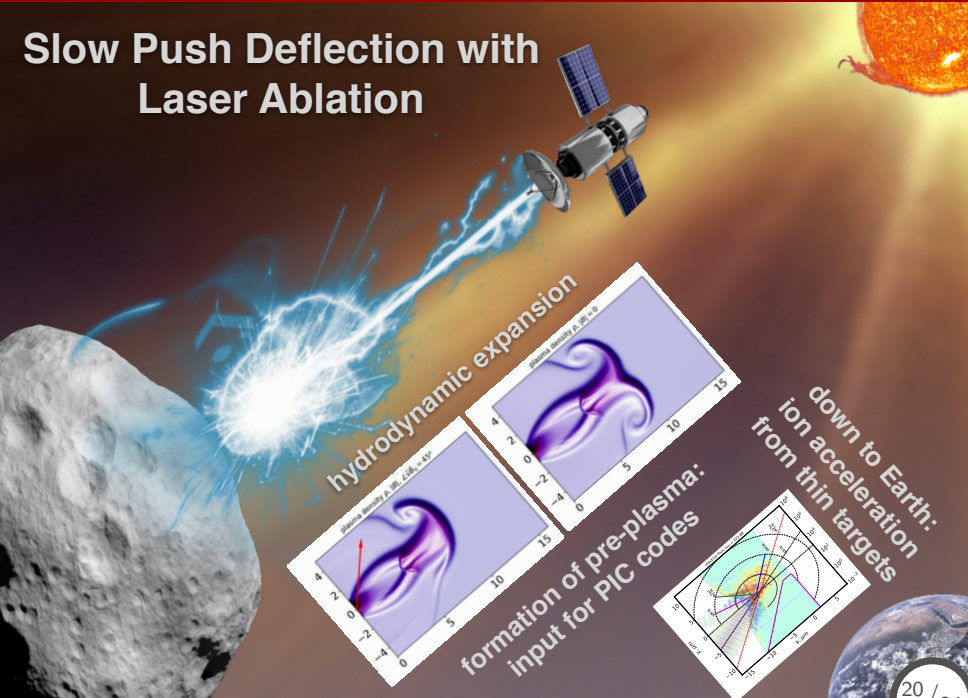
Benchmark SPH: collapsing dam



Water impact



Slow Push Deflection with Laser Ablation



Problems&Solutions in MHD simulations

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \vec{v} \\ \varepsilon \\ \varepsilon_\alpha \end{bmatrix} + \nabla \begin{bmatrix} \rho \vec{v} \\ \rho \vec{v} \vec{v}^T + (p + \frac{1}{2} B^2) I_{3 \times 3} - \vec{B} \vec{B}^T \\ (\frac{\gamma}{\gamma-1} p + \frac{1}{2} \rho v^2) \vec{v} - (\vec{v} \times \vec{B}) \times \vec{B} \\ (\rho \varepsilon_\alpha + p_\alpha) \vec{v} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -F \\ Q_{ei} + Q_{ea} \end{bmatrix}$$

magnetic induction

divergence free condition

$$\frac{\partial \vec{B}}{\partial t} = \nabla \times (\vec{v} \times \vec{B}),$$

$$\nabla \cdot \vec{B} = 0.$$

no magnetic monopoles!

Transport effects
Collisions
Heat Conduction
Ionisation etc.
requires small time step

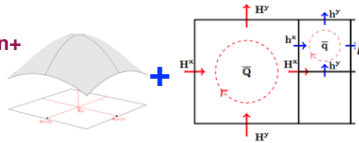
Method-of-Lines

$$\frac{d\vec{q}}{dt} + \frac{H^x_{i+1/2,j} - H^x_{i-1/2,j}}{\Delta x} + \frac{H^y_{i,j+1/2} - H^y_{i,j-1/2}}{\Delta y} = \vec{S}(\vec{q})$$

Implicit-Explicit ODE's solver

$$\begin{aligned} q^{(0)} &= q^n & + \frac{1}{4} \Delta t [S(q^{(0)})] \\ q^{(1)} &= q^n + \frac{1}{2} \Delta t (\mathcal{F}(q^{(0)})) & + \frac{1}{4} \Delta t [S(q^{(1)})] \\ q^{(2)} &= q^n + \frac{1}{2} \Delta t (\mathcal{F}(q^{(0)}) + \mathcal{F}(q^{(1)})) & + \frac{1}{3} \Delta t [S(q^{(0)}) + S(q^{(1)}) + S(q^{(2)})] \\ q^{n+1} &= q^n + \frac{1}{3} \Delta t (\mathcal{F}(q^{(0)}) + \mathcal{F}(q^{(1)}) + \mathcal{F}(q^{(2)})) & + \frac{1}{3} \Delta t [S(q^{(0)}) + S(q^{(1)}) + S(q^{(2)})] \end{aligned}$$

High-order reconstruction+ adaptive meshes



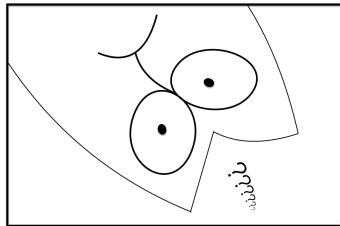
$$H_{i+1/2,j}(q^+, q^-) = \frac{a^x}{2} \left[f^x(q_{i+1/2,j}^-) + f^x(q_{i+1/2,j}^+) \right] - \frac{a^x}{2} (q_{i+1/2,j}^+ - q_{i+1/2,j}^-),$$

Divergence constraint

Constraints field (a kind of staggering), or auxiliary potentials

Summary&Conclusion

- Computational power is still on the rise
 - Heterogeneous architecture: CPU+GPU
 - Calculations vs. data movement
- Hardware
- Diverse and abundant
 - 'Explitisation' of implicit methods
 - 'Method-on-Demand' for HPC application
- Numerics



- What is the problems then?

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-

My answer from 1 year ago :)

new codes must be developed in a
production environment

partition -short

- Hardware
- Numerics,
Algorithms
- What is the
problems then?



**/*Thank You for
listening!*/**

**throw(questions?);
//angry comments?
//precios suggesions?**