

Simulation de plasmas cinétiques

De la physique à l'optimisation numérique

LLR

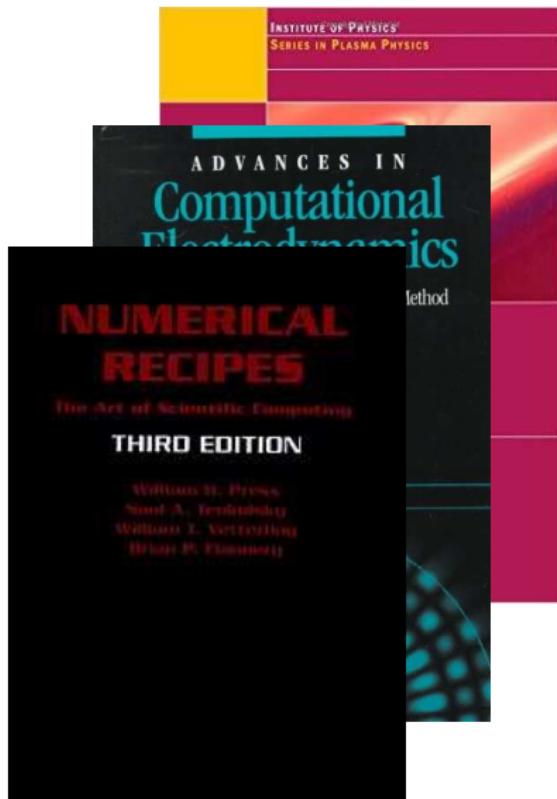


References

Plasma Physics via Computer Simulation
C. K. Birdsall & A. B. Langdon

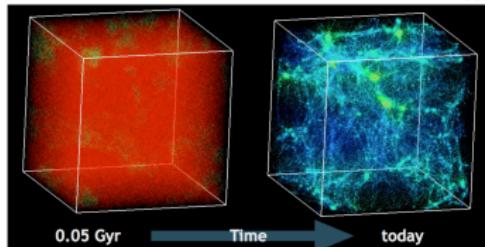
Computational Electrodynamics
A. Taflove

Numerical Recipies
W. H. Press *et al.*



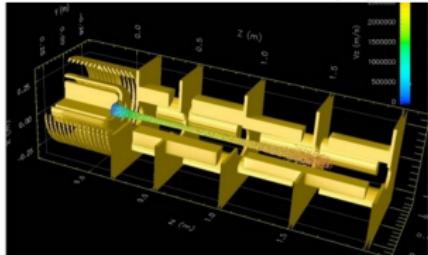
The Particle-In-Cell (PIC) method is a central tool for simulation over a wide range of physics studies

Cosmology



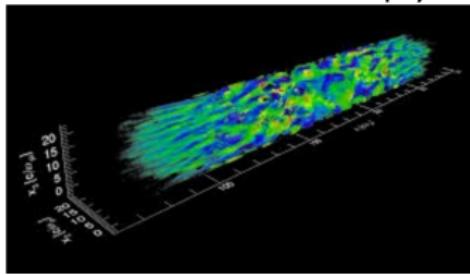
source: K. Heitmann, Argonne National Lab

Accelerator physics



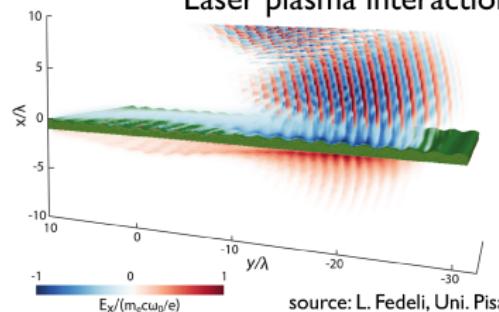
source: WARP , Berkeley Lab

Relativistic astrophysics



source: F. Fiuzza, Livermore National Lab

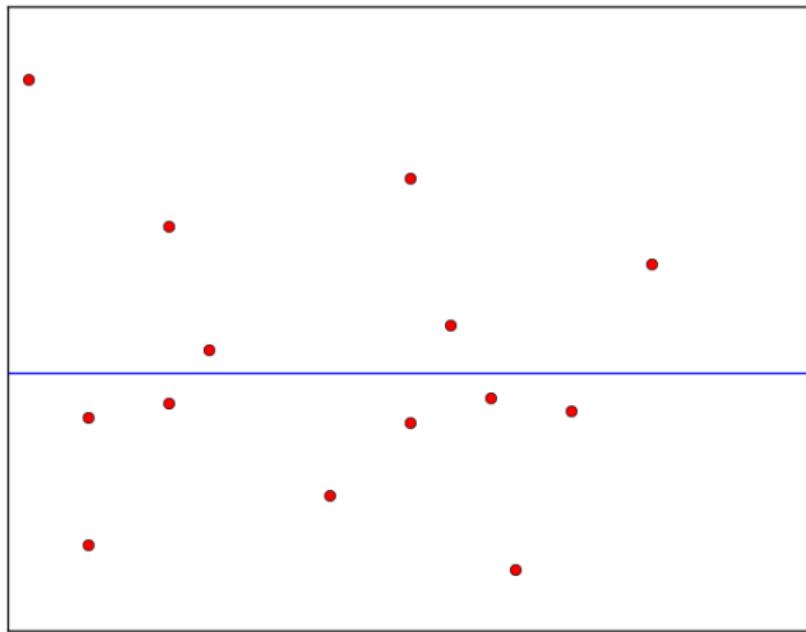
Laser plasma interaction



source: L. Fedeli, Uni. Pisa

- Conceptually simple
- Efficiently implemented on (massively) parallel super-computers

A l'IN2P3 : l'accélération laser plasma



Structure

1 La méthode PIC

2 L'implémentation dans SMILEI

3 La communauté

Cours de l'exposé

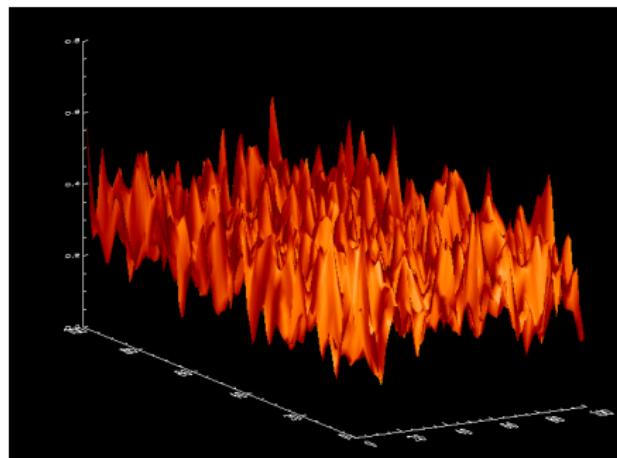
1 La méthode PIC

2 L'implémentation dans SMILEI

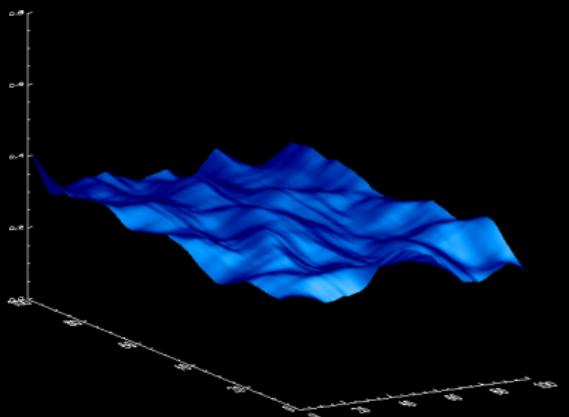
3 La communauté

Approche statistique de champ moyen : représentation Vlasovienne

L'approche 'Vlasov' : les champs électriques sont des champs moyens et lisses produits par des effets collectifs et auto-consistants avec la dynamique des particules.



Champ électrique 'réel'



Champ électrique 'Vlasov'

Les équations à résoudre

$f_s(\mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v}$ is the probability to find a particle of species s in the phase space point (\mathbf{x}, \mathbf{v}) around $d\mathbf{x} d\mathbf{v}$.

Vlasov equation

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \frac{\partial f_s}{\partial \mathbf{x}} + q_s/m_s (\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c}) \cdot \frac{\partial f_s}{\partial \mathbf{v}} = 0 \quad \text{No collisions}$$

Maxwell's equations

$$\begin{cases} \nabla \cdot \mathbf{E} = 4\pi\rho \\ \nabla \cdot \mathbf{B} = 0 \\ \nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \\ \nabla \times \mathbf{B} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \mathbf{J} \end{cases}$$

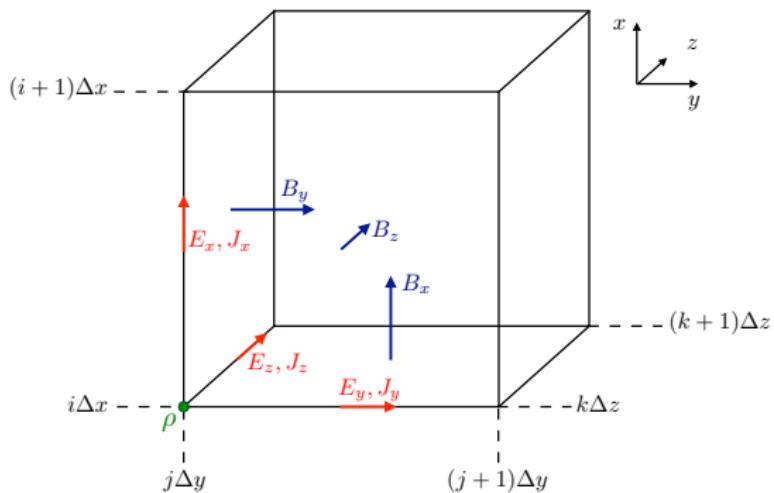
Moments equations

$$\rho = \sum_s^{n_s} q_s \int f_s d\mathbf{v}$$
$$\mathbf{J} = \sum_s^{n_s} q_s \int \mathbf{v} f_s d\mathbf{v}$$

Difficulté ==> les équations sont couplées !

Comment fait on pour les champs ?

Les champs sont 3D (x, y, z). Pour les discréteriser, il faut discréteriser l'espace.



Les équations de Maxwell sont discréétisées par différences finies et résolues sur cette grille.

Comment fait on pour la fonction de distribution ?

f est 6D (x, y, z, v_x, v_y, v_z).

Pour la discréteriser il nous faut discréteriser l'espace des phases.



Un maillage 6D est très coûteux !

L'astuce

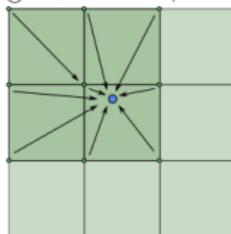
On échantillonne l'espace des phases avec des macro-particules qui sont des objets qui ressemblent à des particules (position & vitesse) mais qui ont une forme et représentent un petit morceau d'espace des phases.

$$f = \sum_{p=0}^{N-1} f_p$$

PIC = Particle In Cell

Les étapes d'un code PIC explicite

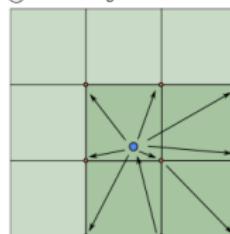
① Scatter E & B fields to particles



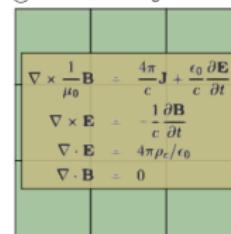
② Move particles



③ Gather charges and currents



④ Solve Maxwell on grid



Étapes

- ① Interpolation
- ② Pousseur
- ③ Projection
- ④ Maxwell

Problèmes

- Accès aléatoires en mémoire.
- Équilibrage de charge.

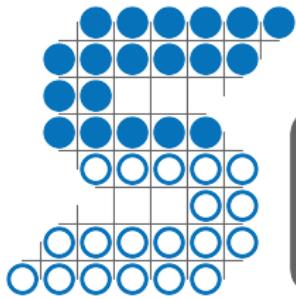
Cours de l'exposé

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«A collaborative, open-source, multi-purpose PIC code
for the next generation of super-computers»

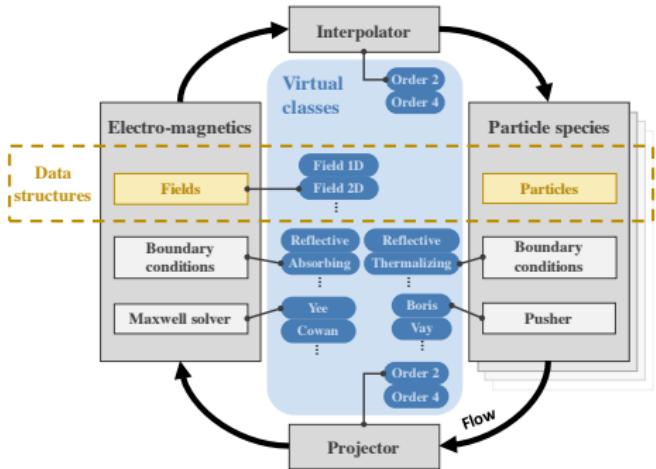


milei)



[www.maisondelasimulation.fr / milei](http://www.maisondelasimulation.fr/milei)

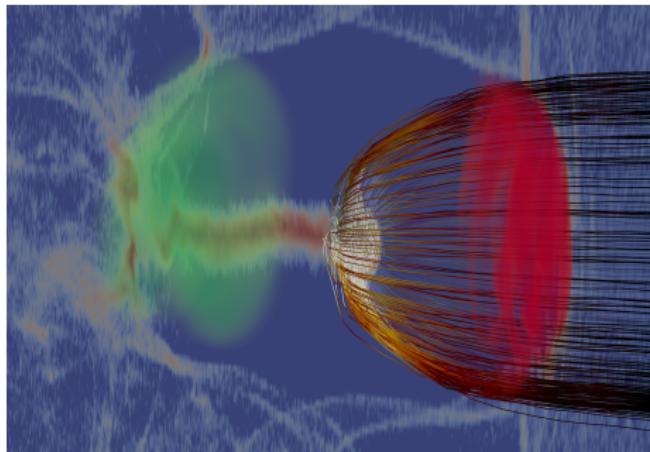
Code C++ structure



- ① Performances
- ② Multi-purpose capability
- ③ Maintainability
- ④ Ease of evolution

To achieve these objectives it is important to separate the physics from the computing aspects. It is not an easy task and the C++ structure helps.
SMILEI uses many virtual classes and STL : :vectors for objects and memory structures.

L'accélération laser-plasma : un challenge numérique



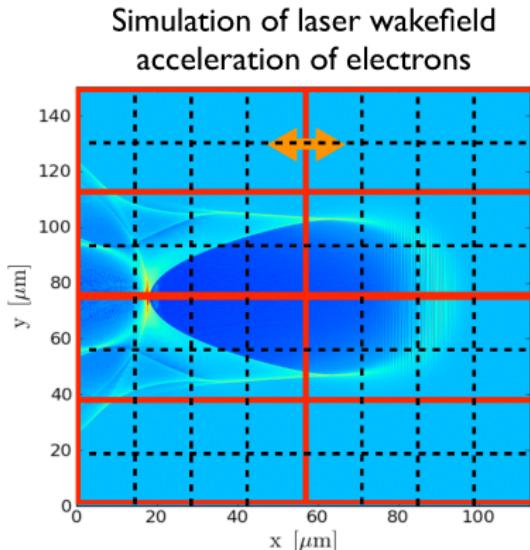
- Les simulations 3D sont LOURDES !
 $\simeq 10^9$ cellules, 8 particules/cellule,
 $\simeq 10^7$ itérations ==> 10^{19} opérations
<==> **300 siècles de calcul**
- Soit **255 Mheures CPU**.
- 1 TB RAM.

La parallelisation massive est absolument nécessaire. Il faut viser les TGIR de calcul intensif (TGCC, CINES, IDRIS).

R. Fonseca *et al*, *Exploiting multi-scale parallelism for large scale numerical modeling of laser wakefield accelerators*, Plasma Phys. Control. Fusion (2013)

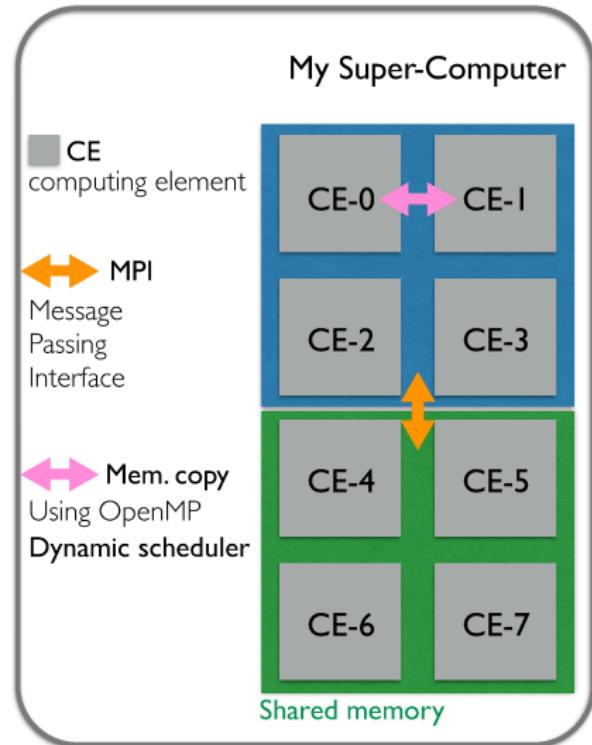
A. Beck *et al*, *Load management strategy for Particle-In-Cell simulations in high energy particle acceleration*, Nucl. Instrum. Methods in Phys. Res. A (2016)

PIC code are ‘easily’ parallelized using domain decomposition



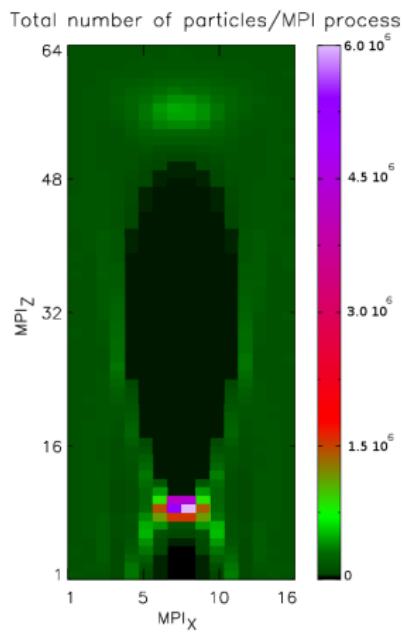
Domain decomp. is not enough!!!

- workload not optimally shared
- not adapted to new architectures!



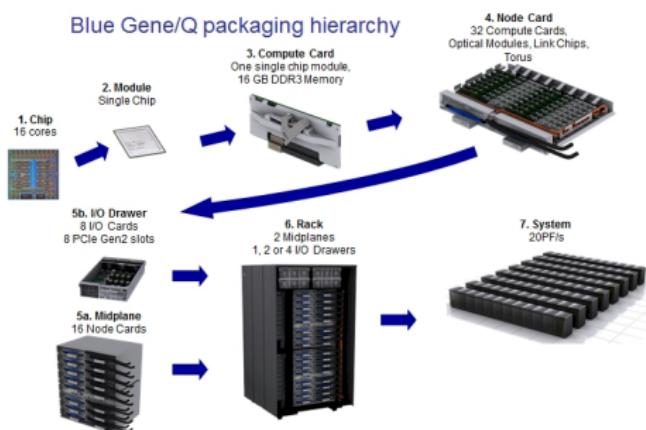
The load balancing problem in LWFA simulations

Photon-Plasma¹ code in full 3D.



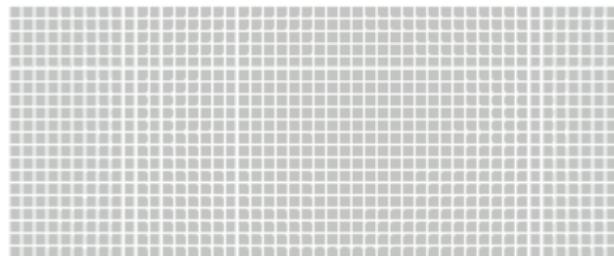
2048 nodes BG/Q.
16X16X64 MPI processes.
8 openMP threads.
Imbalance of 40X.

Blue Gene/Q packaging hierarchy

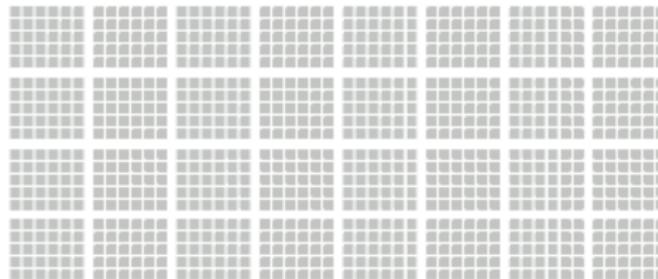


1. T. Haugbølle, J. Trier Frederiksen, Å.Nordlund, Phys. Plasmas 20 (2013) 062904.

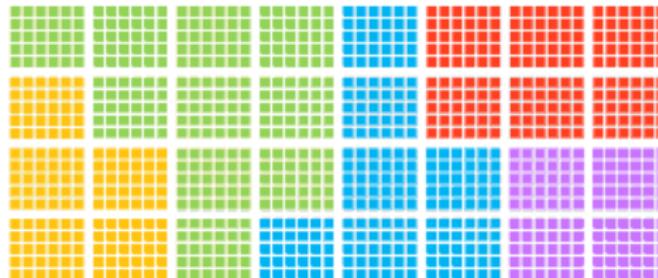
Patched base data structure



960 cells

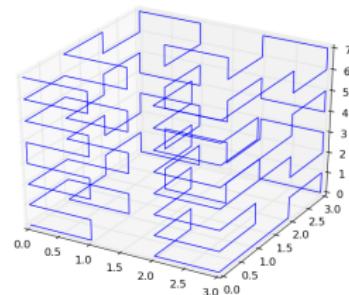
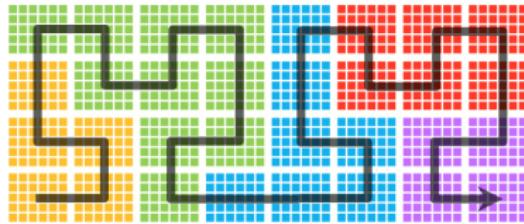


32 patches



5 MPI regions

Hilbert ordering

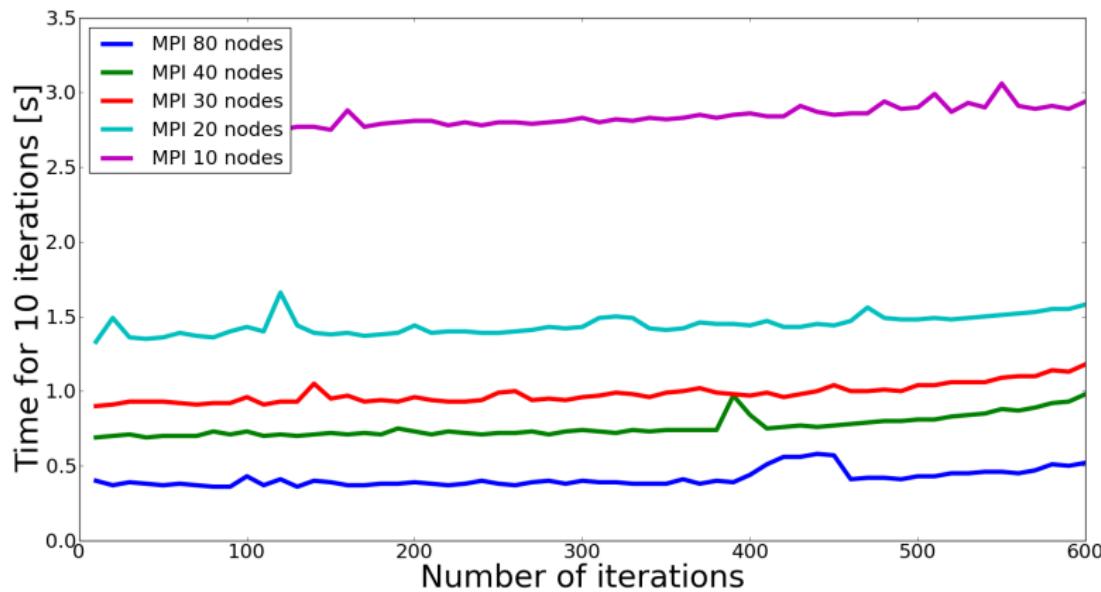


We need a policy to assign patches to MPI processes. To do so, patches are organized along a one dimensional **space-filling curve**.

- ➊ Continuous curve which goes across all patches.
- ➋ Each patch is visited only once.
- ➌ Two consecutive patches are neighbours.
- ➍ In addition we want compactness !

So you think you can scale ?

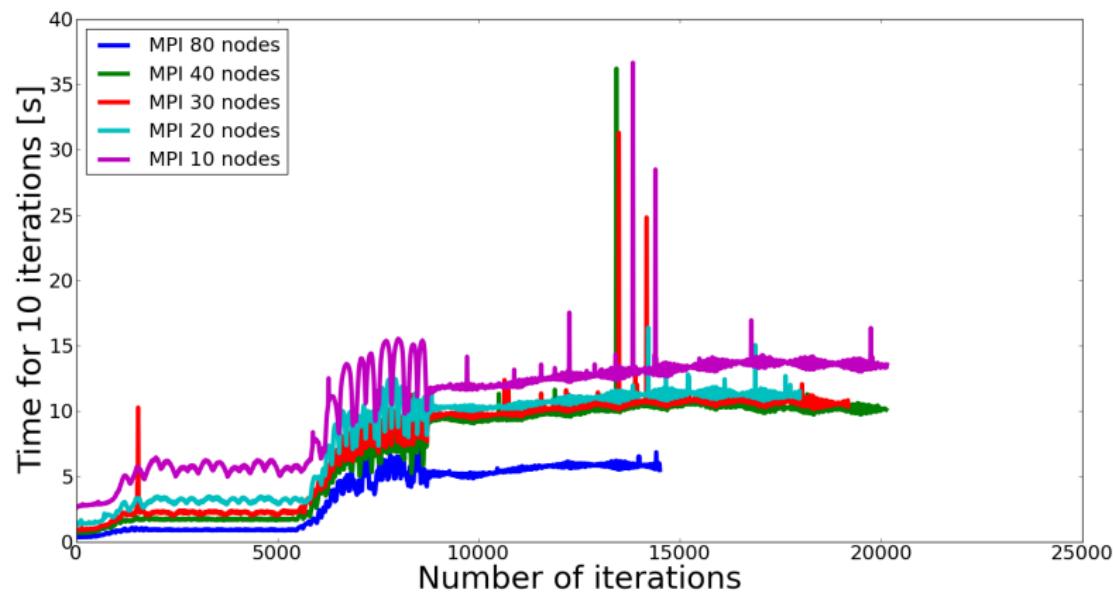
Strong scaling on a 10240×1280 cells domain. 24 MPI processes per node.



In trivial conditions, good strong scaling has been demonstrated up to 50k+ cores (OCCIGEN, system).

But for how long ?

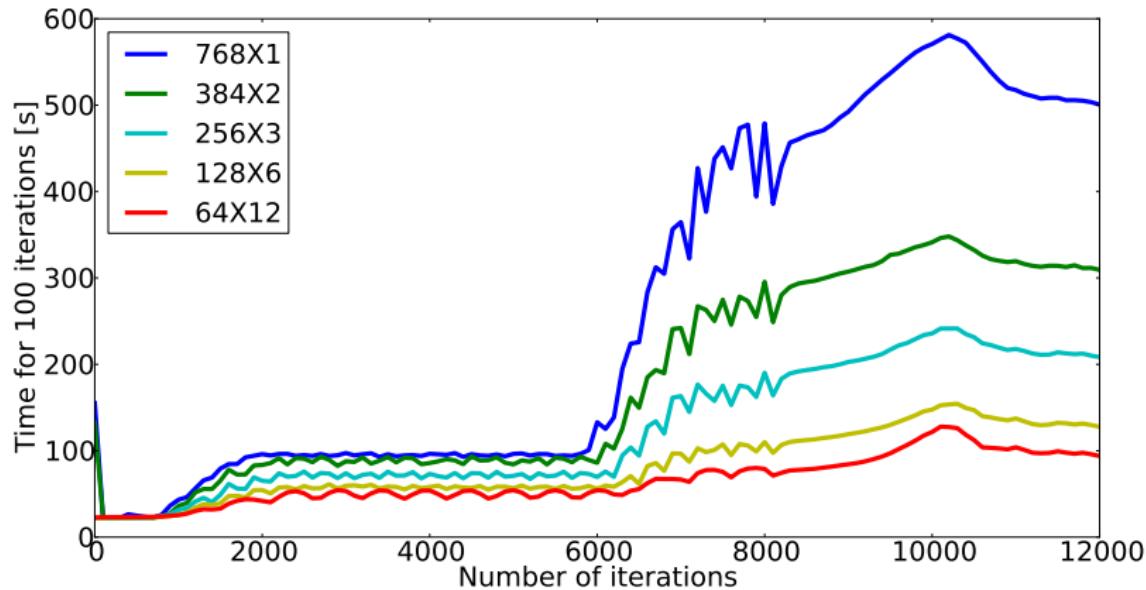
Strong scaling on a 10240×1280 cells domain. 24 MPI processes per node.



The hot spot is too small and you loose your scalability !

First approach : openMP dynamic scheduler

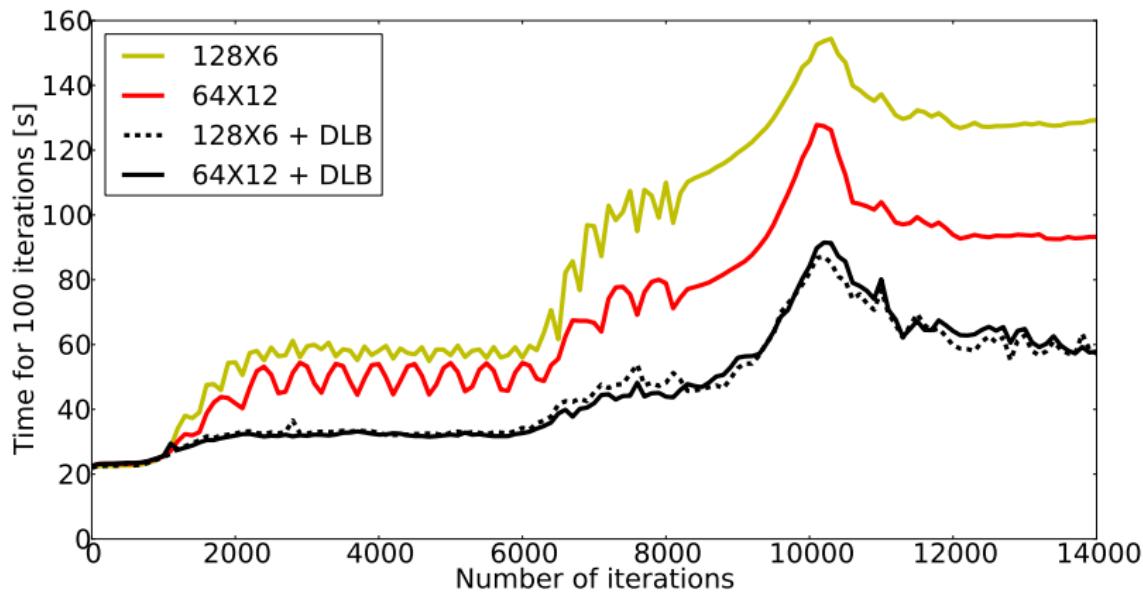
MPI × OpenMP



OpenMP dynamic scheduler is able to smooth the load but only at the node level.

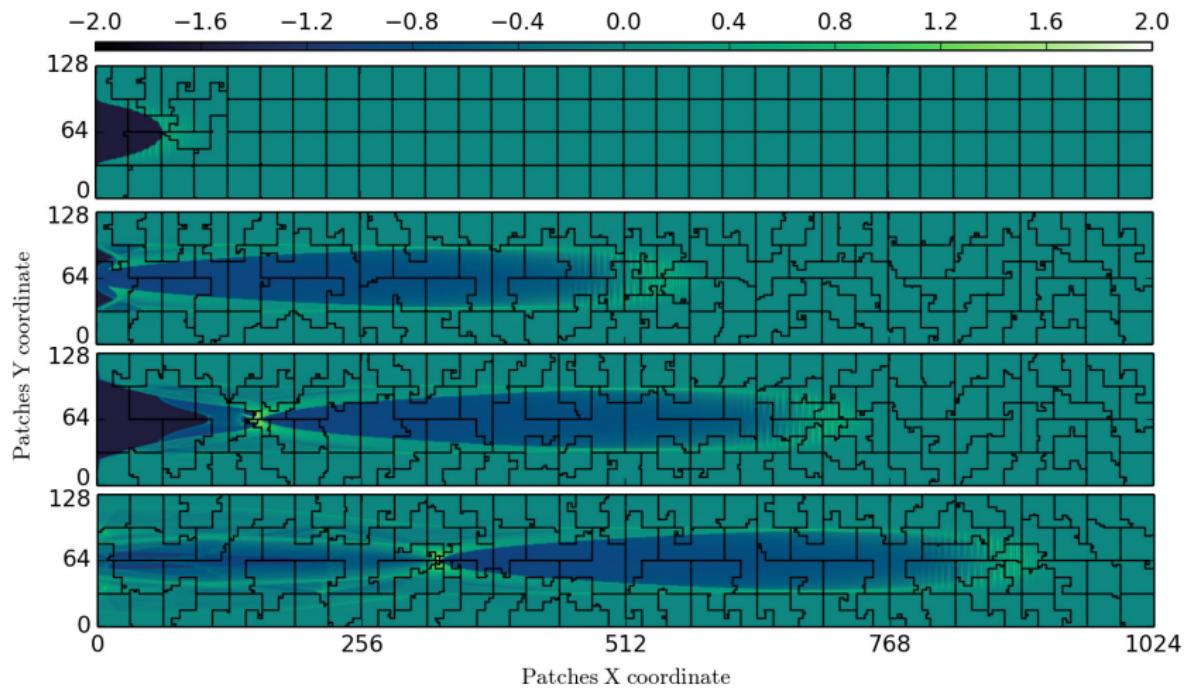
With dynamic load balancing activated

MPI × OpenMP



Yellow and red are copied from previous figure.

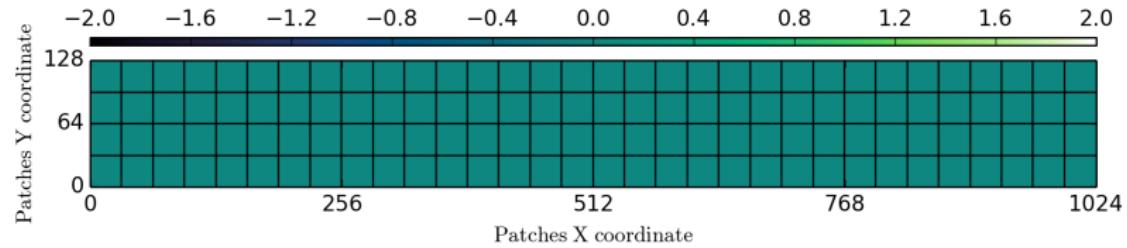
Dynamic evolution of MPI domains



Color represents the local patch computational load imbalance

$$I_{loc} = \log_{10} (L_{loc}/L_{av})$$

Dynamic evolution of MPI domains



Color represents the local patch computational load imbalance

$$I_{loc} = \log_{10} (L_{loc}/L_{av})$$

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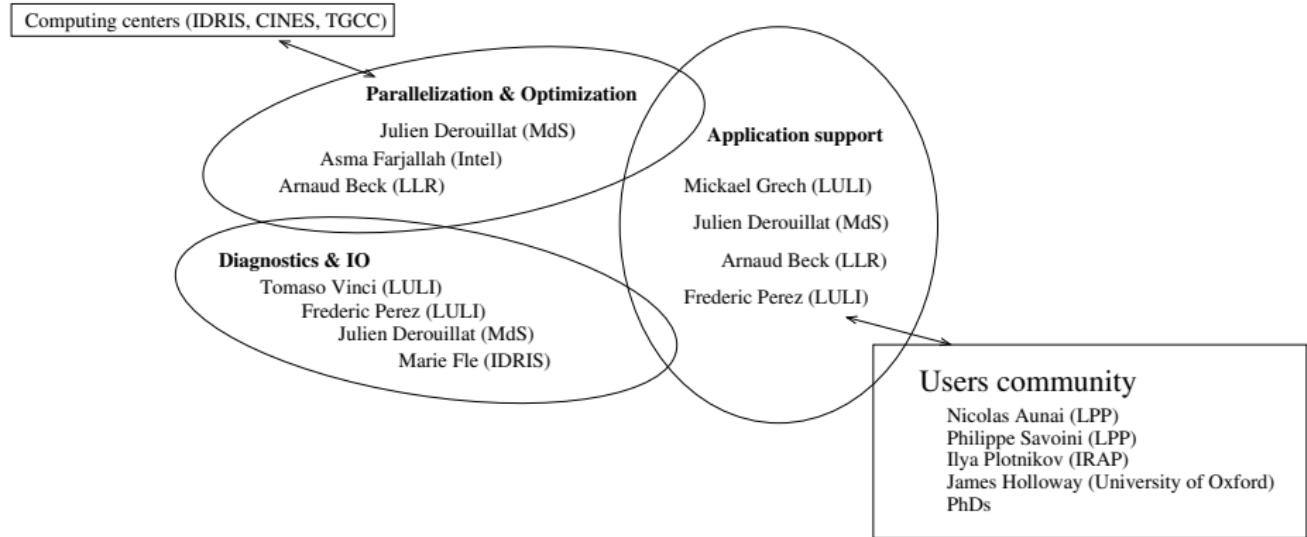


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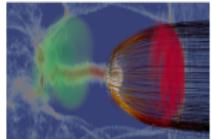
Staff organization



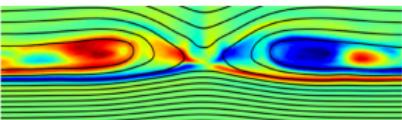
Dev meeting every month. Users are welcome to participate to report success or problems and suggest evolutions.

6 PhD ongoing, 1 incoming

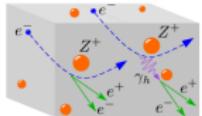
Coming soon (LLR), LWFA in cylindrical geometry



J. Dargent (LPP), *Magnetic reconnection*



F. Niel (LULI), *QED processes in laser-plasma interaction*

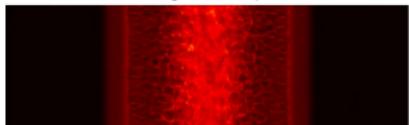


H. Kallala (MdS), *Spectral Solvers*

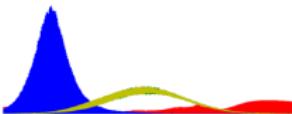
$$\tilde{\mathbf{E}}^{n+1} = \tilde{\mathbf{E}}^n + ic\Delta t \mathbf{k} \times \tilde{\mathbf{B}}^{n+1/2} - \Delta t \tilde{\mathbf{j}}^{n+1/2}$$

$$\tilde{\mathbf{B}}^{n+3/2} = \tilde{\mathbf{B}}^{n+1/2} - ic\Delta t \mathbf{k} \times \tilde{\mathbf{E}}^{n+1}$$

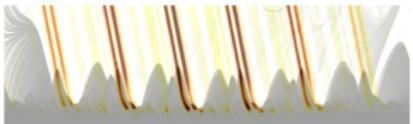
A. Grassi (LULI, Pisa), *Relativistic collisionless shocks in magnetised plasmas*



M. Chiaramello (LULI), *Amplification of short pulses using Brillouin scattering*



G. Bouchard (LIDyL), *High-harmonic generation in laser-solid interaction*



Website + full online documentation :

<http://www.maisondelasimulation.fr/Smilei>

gitHub :

<https://github.com/SmileiPIC/Smilei>

Paper :

arXiv:1702.05128 (soumis à Computer Physics Communication)