

# Some numerical strategies to be improved for controlled fusion designed.

B. Nkonga,  
*with*

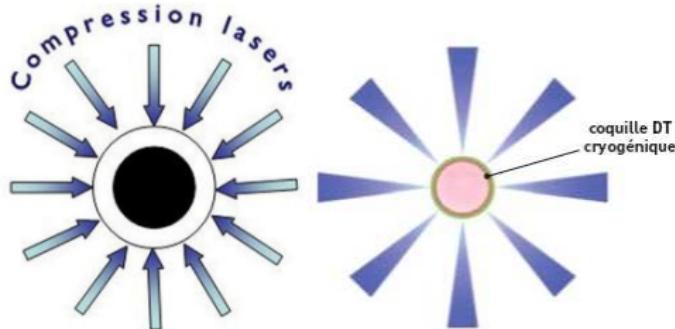
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P.H. Maire, V. Tikhonchuk, ...

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1ères journées du GDR Calcul : 9-10 novembre 2009

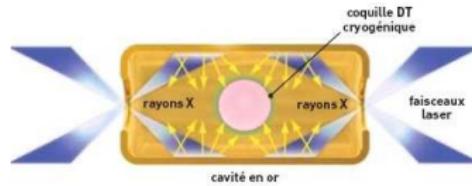
# Inertial Confinement Fusion : Compression Ignition

- Ignition by lasers compression



Needs : Lagrangian Hydrodynamics Scheme...

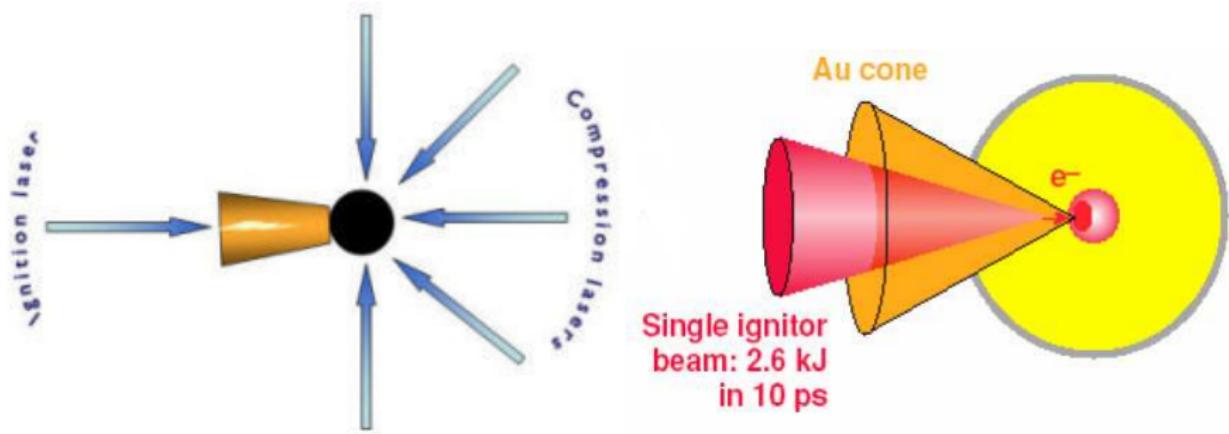
- Ignition by X-rays compression



Needs : Compute Focusing Beams interactions...

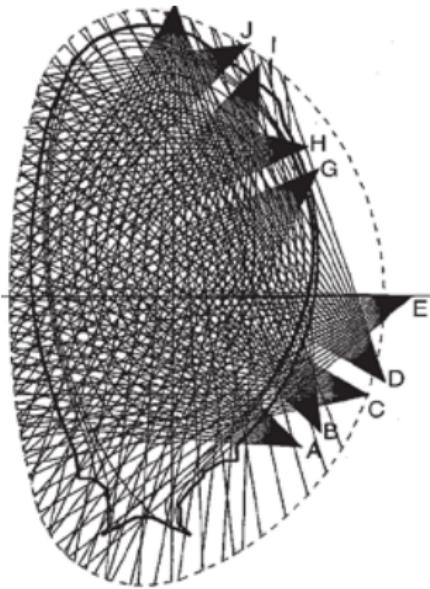
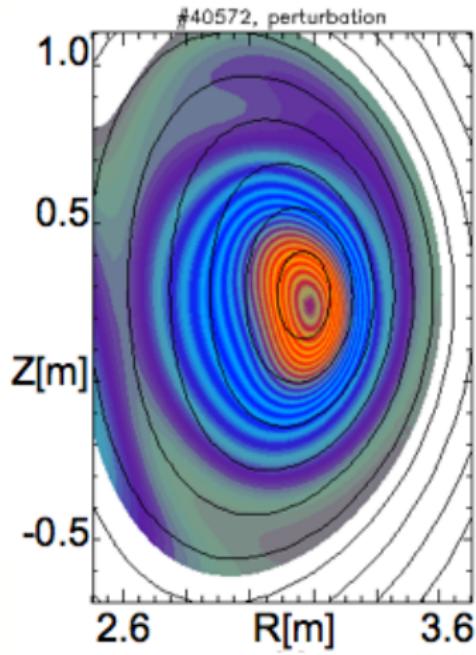
- Interfaces flow
- Large ratio computational domain change.

# Inertial Confinement Fusion : Fast laser ignition



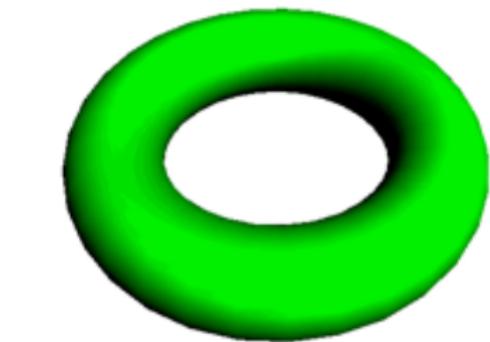
Need : Nonlinear laser/plasmas model, non-local Transport...

# Tokamak Plasma : Avoid large scale instabilities.

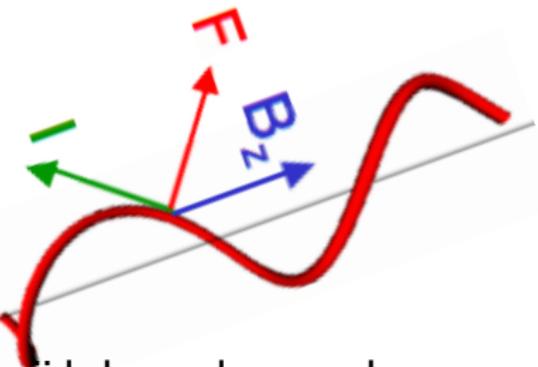
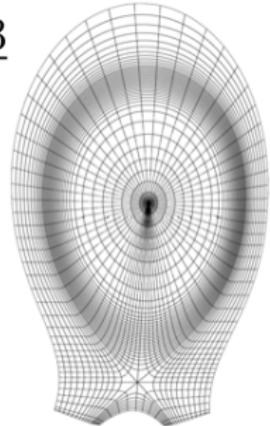


Tomographic reconstruction of X-ray emission. JET SXR cameras (1998).

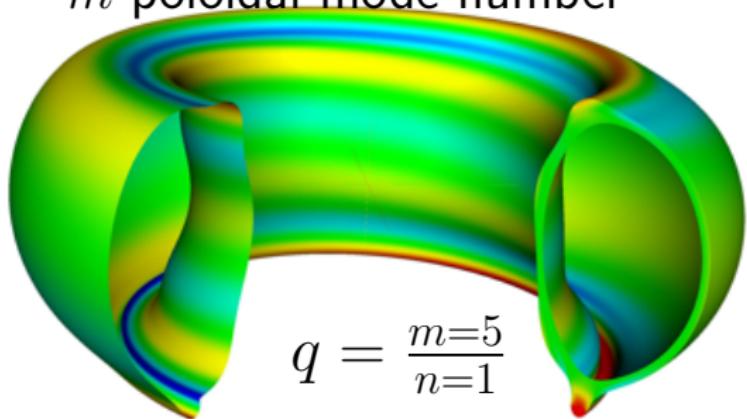
# Tokamak Plasma : Kink instability (MHD, Jorek).



$$q = \frac{m=3}{n=1}$$



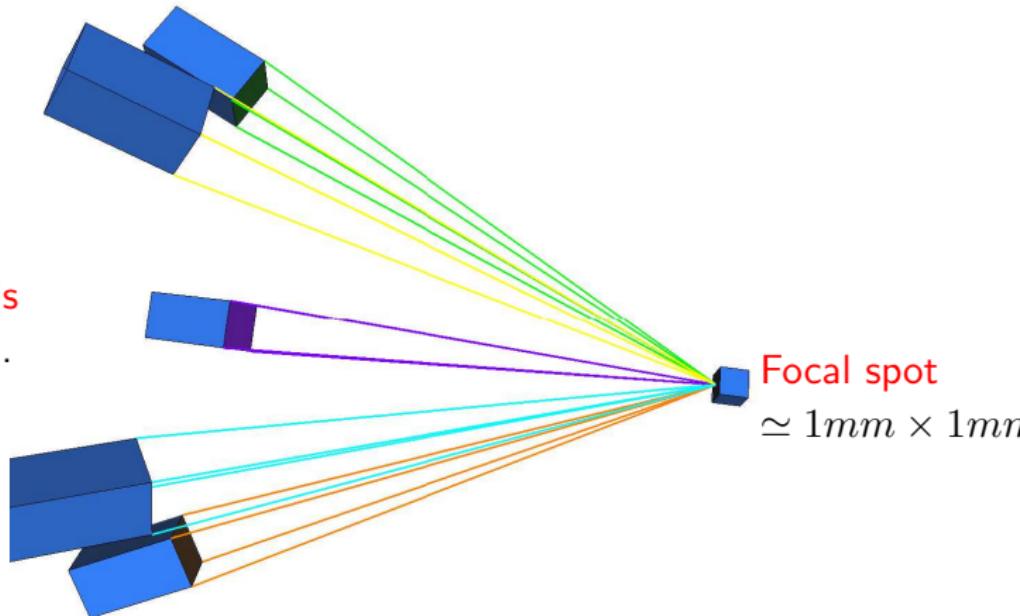
$n$  toroidal mode number  
 $m$  poloidal mode number



$$q = \frac{m=5}{n=1}$$

# Laser focusing (ICF): Huygens-Fresnel Theorem.

$\simeq 30$  Laser Quads  
 $4(40\text{cm} \times 40\text{cm})$ .



$$\mathbf{E}(t, \mathbf{x}) = \int_{\mathbb{R}^2} d\boldsymbol{\theta} \int_{\mathbb{R}} d\omega \hat{\mathcal{E}}(\boldsymbol{\theta}, \omega) \exp \left[ i \left( \boldsymbol{\theta} \cdot \boldsymbol{\xi}(\mathbf{x}) + k_0 n_0(\mathbf{x}) - \omega t \right) \right]$$

# Focusing Laser : Approximations and Computations.

$$\mathbf{E}(\mathbf{x}, t) = \sum_{\ell=1}^{N_\ell} \sum_{m=1}^{N_w} \sum_{i=1}^{Nk_x} \sum_{j=1}^{Nk_y} \mathcal{E}_{\ell,i,j,m} \mathcal{G}_{\ell,h}(t, \mathbf{x}, \omega_m, \boldsymbol{\theta}_{ij}) e^{i\Phi_{\ell,i,j,m}} e^{i\omega_m(t - \frac{n_\ell(\mathbf{x})}{c})}$$

where  $\Phi_{\ell,i,j,m} = \boldsymbol{\beta}_\ell(\mathbf{x}) \cdot \mathbf{k}_\ell(\boldsymbol{\theta}_{ij}, \omega_m) + \frac{\omega_m n_\ell(\mathbf{x})}{c}$

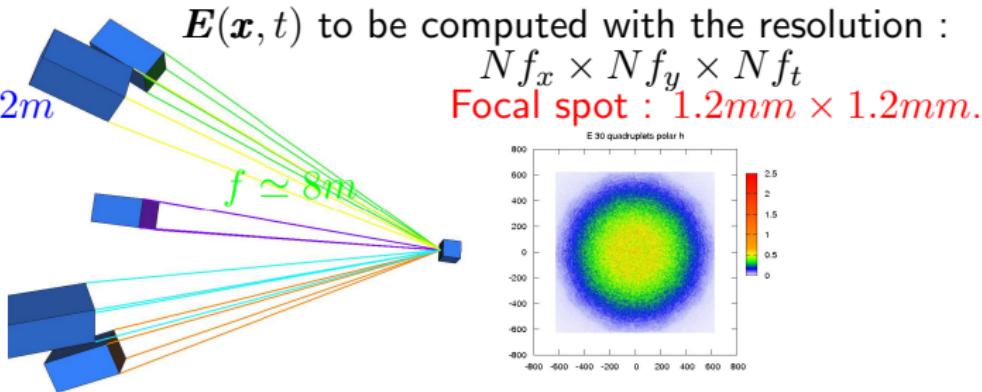
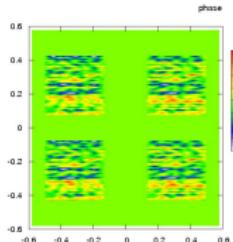
$$\mathbf{k}_\ell(\boldsymbol{\theta}, \omega) = k_{0,\ell}(\boldsymbol{\theta}, \omega) \mathbf{n}_{0,\ell} + \theta_{1,\ell} \mathbf{n}_{1,\ell} + \theta_{2,\ell} \mathbf{n}_{2,\ell}$$

$$\boldsymbol{\beta}_\ell(\mathbf{x}) = \mathbf{x} - \mathbf{x}_\ell = n_\ell(\mathbf{x}) \mathbf{n}_{0,\ell} + \xi_{1,\ell}(\mathbf{x}) \mathbf{n}_{1,\ell} + \xi_{2,\ell}(\mathbf{x}) \mathbf{n}_{2,\ell}$$

Given  $\mathcal{E}_{\ell,i,j,m}$

$N_l = 30$  quads

Quad  $\simeq 1.2m \times 1.2m$



# Focusing Laser Beams : CPU Consuming

Mega Joule Laser (Bordeaux) : Input and Operations

$$N_w \simeq 10^3, \quad Nk_x \simeq Nk_y \simeq 10^3 \quad N_\ell \simeq 30 \text{ quads}$$

$$\text{Total of Floating Operations} = \text{Flop} \simeq 3 \times 10^{10} \times \mathcal{R}_f$$

$\mathcal{R}_f = Nf_x \times Nf_y \times Nf_t$  is the focal spot resolution

CPU Time for  $\mathcal{R}_f = 2048 \times 2048 \times 1000 \simeq 4 \times 10^9$

$\text{Flop} \simeq 10^{20} = 10^8 \text{Tera} \implies \underline{28 \times 10^3 \text{ H with a Tera computer}} \equiv 3 \text{ years}$

Parallel Computing unavoidable !  
Need of mathematical approximations!

Stationary phase approximation : asymptotic of oscillatory integrals

# Focusing Laser Beams : Parallel strategy (simple)

- Scatter the Flop:

$$\mathbf{E}(\mathbf{x}, t, \text{me}) = \sum_{\ell} \sum_{m_1(\text{me})}^{m_N(\text{me})} \sum_{i_1(\text{me})}^{i_N(\text{me})} \sum_{j_1(\text{me})}^{j_N(\text{me})} \mathcal{E}_{\ell, i, j, m} \mathcal{G}_{\ell, h} e^{i\Phi_{l, i, j, m}} e^{i\omega_m t}$$

- Gather the solution :

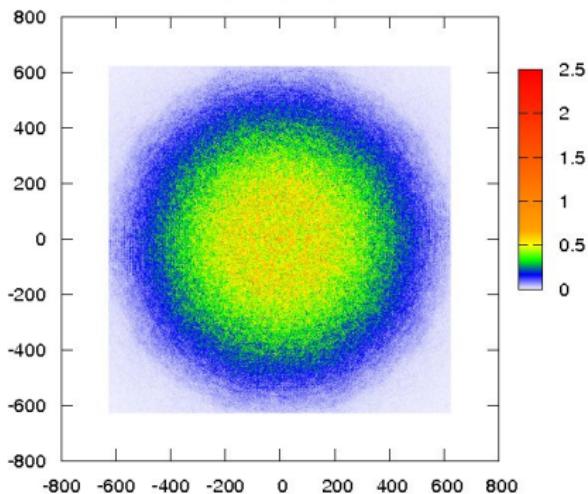
$$\mathbf{E}(\mathbf{x}, t) = \bigoplus_{\text{me}=0}^{N_p-1} \mathbf{E}(\mathbf{x}, t, \text{me})$$

FFTW + MPI

# Focusing Laser Beams : Computed focal spot and zoom.

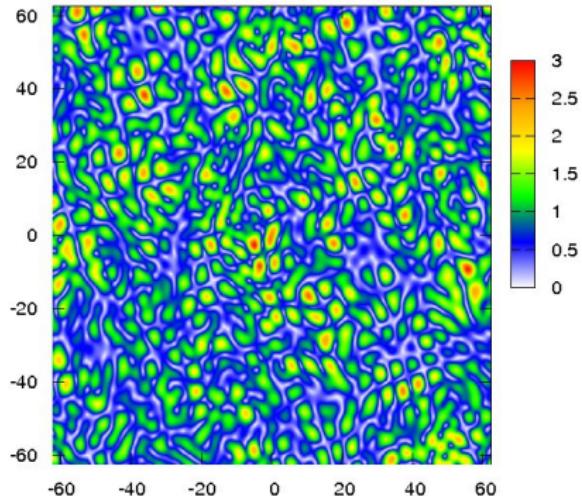
$$\|E(\mathbf{x}, t)\|$$

E 30 quadruplets polar h



$$\|E(\mathbf{x}, t)\|$$

2048

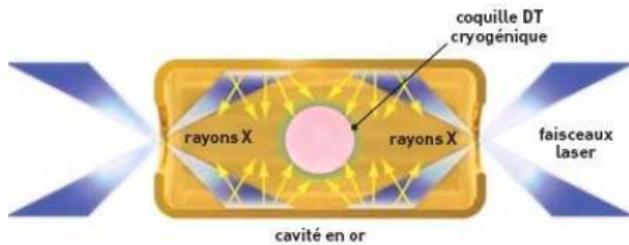


21H CPU with 1936 cores : 30 quads = 120 (40cm x 40cm )

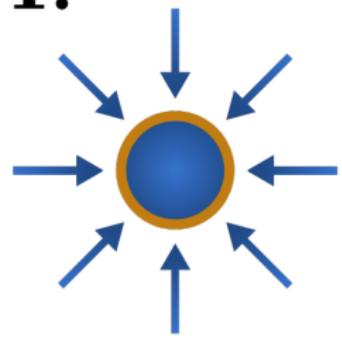
Nodes : 4 Intel®Itanium® II, Dual-Core, 1.6 Ghz, 128 Go

$N_w = Nf_t = 1$ ,  $Nk_x = Nk_y = 2048$  and  $Nf_x = Nf_y = 2048$

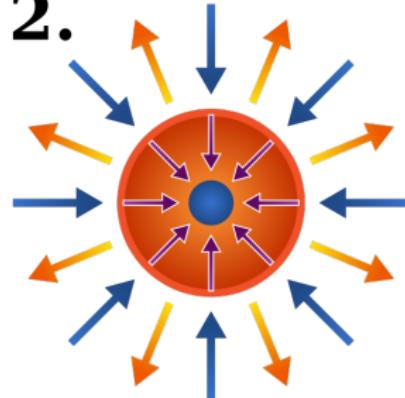
# From the focal spot to Lagrangian Hydrodynamics



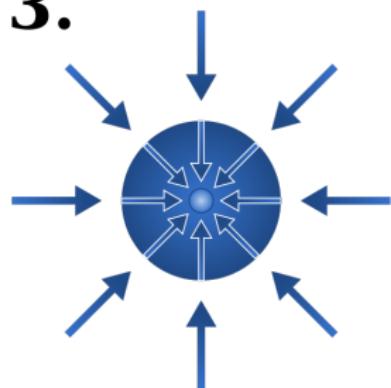
1.



2.



3.



# Weak formulation of Conservation Law

Integral form in arbitrary coordinates

$$\left\{ \begin{array}{lcl} \frac{d}{dt} \int_{\mathcal{C}(t)} \rho \, d\mathbf{x} + \int_{\partial\mathcal{C}(t)} \rho (\mathbf{u} - \boldsymbol{\kappa}) \cdot \mathbf{n} \, dS & = & 0, \\ \frac{d}{dt} \int_{\mathcal{C}(t)} \rho \mathbf{u} \, d\mathbf{x} + \int_{\partial\mathcal{C}(t)} \rho \mathbf{u} (\mathbf{u} - \boldsymbol{\kappa}) \cdot \mathbf{n} \, dS & = & - \int_{\partial\mathcal{C}(t)} p \mathbf{n} \, dS, \\ \frac{d}{dt} \int_{\mathcal{C}(t)} \rho \mathbf{e} \, d\mathbf{x} + \int_{\partial\mathcal{C}(t)} \rho \mathbf{e} (\mathbf{u} - \boldsymbol{\kappa}) \cdot \mathbf{n} \, dS & = & - \int_{\partial\mathcal{C}(t)} p \mathbf{u} \cdot \mathbf{n} \, dS. \end{array} \right.$$

Lagrangian control volume :  $\boldsymbol{\kappa} = \mathbf{u}$  on  $\partial\mathcal{C}(t)$

- $\tilde{m}_C \frac{d}{dt} \tilde{\mathbf{u}}_C = - \int_{\partial\mathcal{C}_C(t)} p \mathbf{n} \, dS,$
  - $\tilde{m}_C \frac{d}{dt} \tilde{e}_C = - \int_{\partial\mathcal{C}_C(t)} p \boldsymbol{\kappa} \cdot \mathbf{n} \, dS.$
- where      •  $\frac{d}{dt} \tilde{m}_C = 0,$

Coupling between averaged(mesh scale) and subscale states.

# Multiscale formulation and approximation

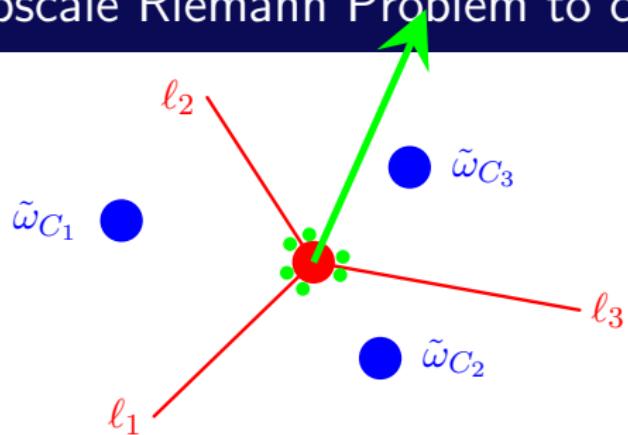
## Mesh scale equations

- $\tilde{m}_C \frac{d}{dt} \tilde{\mathbf{u}}_C = - \int_{\partial \mathcal{C}_C(t)} p \mathbf{n} \, dS,$
  - $\tilde{m}_C \frac{d}{dt} \tilde{e}_C = - \int_{\partial \mathcal{C}_C(t)} p \boldsymbol{\kappa} \cdot \mathbf{n} \, dS.$
- where •  $\frac{d}{dt} \tilde{m}_C = 0,$

sub-scale  $\mathcal{K}_{j,C}^\epsilon \subset \mathcal{C}_C$  and  $\mathcal{K}_{j,C}^\epsilon \subset \mathcal{K}_j^\epsilon :: \epsilon \mapsto 0$

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{K}_j^\epsilon(t)} \rho \boldsymbol{\kappa} \, d\mathbf{x} &= - \int_{\partial \mathcal{K}_j^\epsilon(t)} p \mathbf{n} \, dS, & |\mathcal{K}_j^\epsilon| &\simeq O(\epsilon) \\ \frac{d}{dt} \int_{\mathcal{K}_{j,C}^\epsilon(t)} \rho \boldsymbol{\kappa} \, d\mathbf{x} &= - \int_{\partial \mathcal{K}_{j,C}^\epsilon(t)} p \mathbf{n} \, dS, & |\mathcal{K}_{j,C}^\epsilon| &\simeq O(\epsilon) \end{aligned}$$

## Subscale Riemann Problem to compute $p_{C,\ell,j}^*$ and $\kappa_j$



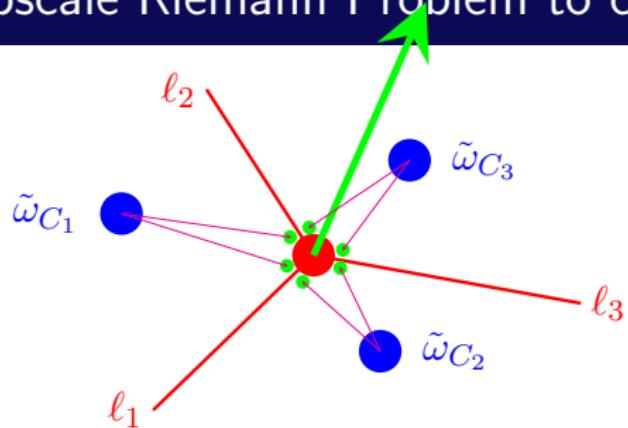
Half Riemann Solver for  $\kappa_j$  fixed: Godunov-type method

$$p_{C,\ell,j}^* = p_\ell^*(\tilde{\omega}_C, \kappa_j) = p_C + Z_{C,j}(\tilde{u}_C - \kappa_j) \cdot \frac{\mathbf{m}_{C,\ell,j}}{\|\mathbf{m}_{C,\ell,j}\|}$$

Subscale compatibility: The local system can be nonlinear:  $\hookrightarrow \kappa_j$

$$\sum_{\ell \in \vartheta(j)} r_\ell (p_{C_1,\ell,j}^* - p_{C_2,\ell,j}^*) \mathbf{n}_{C_1,\ell} = 0$$

## Subscale Riemann Problem to compute $p_{C,\ell,j}^*$ and $\kappa_j$



Half Riemann Solver for  $\kappa_j$  fixed: Godunov-type method

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Subscale compatibility: The local system can be nonlinear:  $\hookrightarrow \kappa_j$

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# Numerical Scheme : Linear mapping for $\psi_{\ell,j}(\xi)$

$$p_{\ell}^*(\tilde{\omega}_C, \boldsymbol{\kappa}_j) = p_C + Z_{C,j} (\tilde{\mathbf{u}}_C - \boldsymbol{\kappa}_j) \cdot \mathbf{m}_{C,\ell,j}$$

Explicit scheme :  $\left[ \mathcal{A}_j \left( \tilde{\omega}_*^n, \boldsymbol{\kappa}_*^n \right) \right] \boldsymbol{\kappa}_j^* = \mathbf{g}_j \left( \tilde{\omega}_*^n, \boldsymbol{\kappa}_*^n \right) \longrightarrow \mathbf{x}^{n+\theta}$

$$\boldsymbol{\kappa}_{\ell}(\mathbf{x}) = \sum \varphi_{\ell,j}(\mathbf{x}) \boldsymbol{\kappa}_j^*, \quad p_{C,\ell}(\mathbf{x}) = \sum \psi_{\ell,j}(\mathbf{x}) p_{\ell}^*(\tilde{\omega}_C^n, \boldsymbol{\kappa}_j^*)$$

$$\tilde{m}_C \frac{d}{dt} \tilde{\mathbf{u}}_C = - \sum_{\ell \in \partial C} \int_{\ell} p_{C,\ell}(\mathbf{x}) \mathbf{n}(\boldsymbol{\kappa}_*^n) d\ell,$$

$$\tilde{m}_C \frac{d}{dt} \tilde{e}_C = - \sum_{\ell \in \partial C} \int_{\ell} p_{C,\ell}(\mathbf{x}) \boldsymbol{\kappa}_{\ell}(\mathbf{x}) \cdot \mathbf{n}(\boldsymbol{\kappa}_*^n) d\ell.$$

Orthogonality constraint  
for interpolation gives

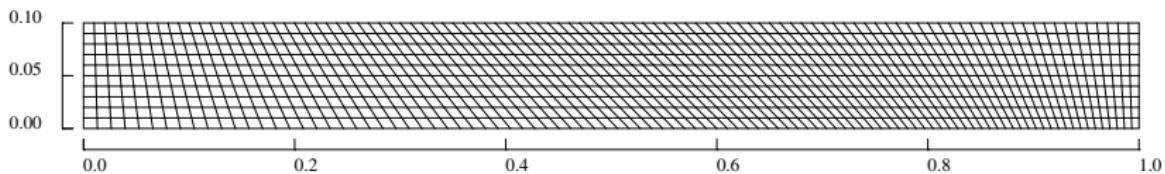
$$\psi_{\ell,j}(\xi) = (d+1)\varphi_{\ell,j}(\xi) - 1 \quad \text{and} \quad \int_{\ell} \psi_{\ell,i} \varphi_{\ell,j} d\ell = \frac{\|\ell\|}{d} \delta_{i,j}$$

Therefore we have analitical formula for the right hand side to compute  
 $\hookrightarrow \mathbf{u}^{n+\theta}, \mathbf{e}^{n+\theta}, \mathbf{p}^{n+\theta}, p^{n+\theta} \hookrightarrow \tilde{\omega}^{n+\theta}$

## Saltzman problem

Computational domain  $(x, y) \in [0, 1] \times [0, 0.1]$  with  $(n_x, n_y) = (100, 10)$  skewed by the map

$$x_{\text{sk}} = x + (0.1 - y) \sin(\pi x), \quad y_{\text{sk}} = y.$$

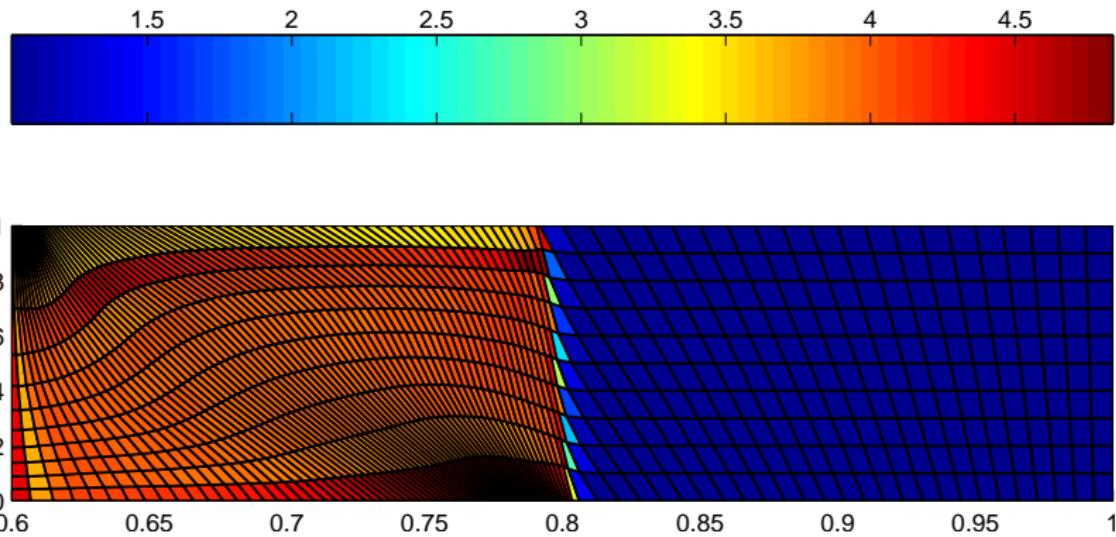


Initial conditions:  $(\rho^0, P^0, \mathbf{U}^0) = (1, 10^{-6}, 0)$

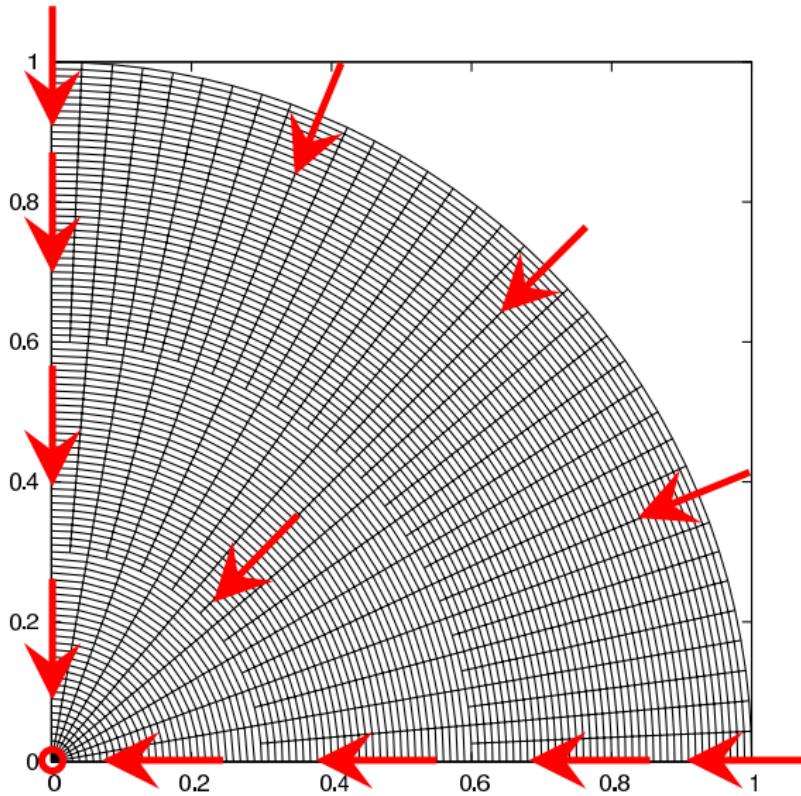
Materials: gamma law gas with  $(\gamma = 5/3)$

Boundary conditions: inflow velocity  $U^* = 1$  at  $x = 0$ .

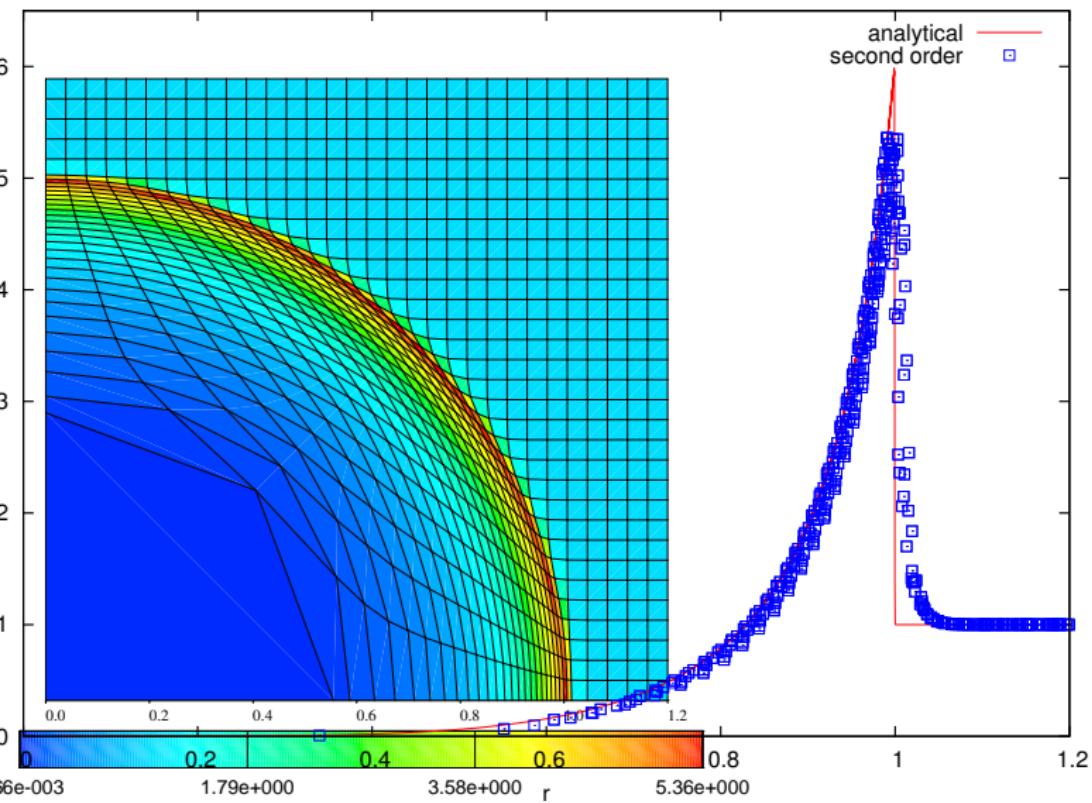
# *Saltzman problem : Density at t = 0.6*



# Cylindrical Noh Problem: non-conformal, 2250 cells

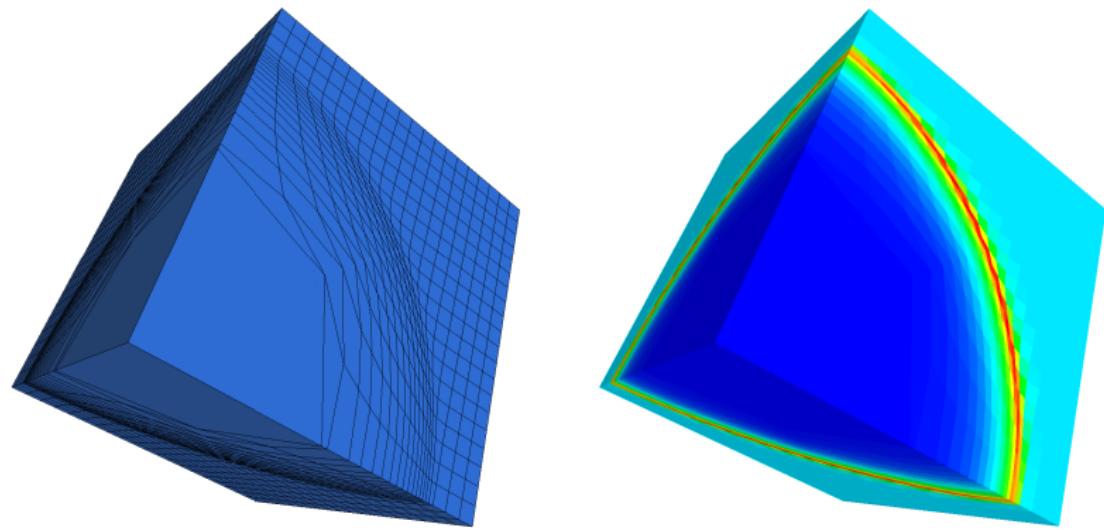


# Sedov-Taylor blast wave: $31 \times 31$ Cartesian grid



Density map (left) and density in all the cells (right) at  $t = 1$ .

# Sedov-Taylor blast wave: 3D hexahedra mesh



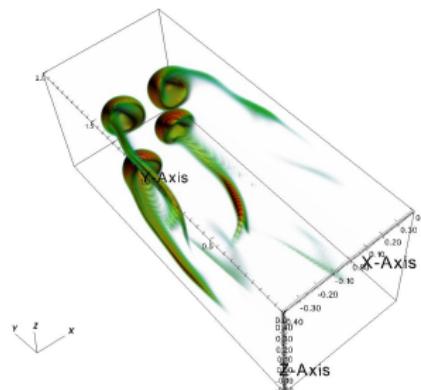
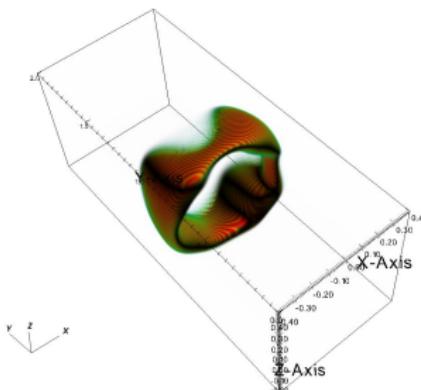
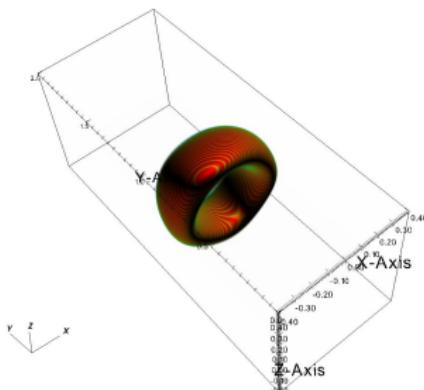
- Initial high pressure in only one cell.
- Symmetry boundary conditions

# Multifluid Hydrodynamic 3D : $8 \times 10^6$ unknowns

$$\omega = (\alpha, \rho_1, \rho_2, \rho \mathbf{u}, E)^T$$

Implicit Low mach scheme, Surface tension, Gravity.

$1.3 \times 10^6$  Cells, Time Steps = 14 610, Final Physical Time = 3.59s,  
RAM used = 1.35Go/Core  $\simeq$  11 Go, CPU = 12 days  $\times$  8Pe



Pe : 2x3GHz Quad-core Intel Xeon

RAM: 16 Go 667MHz DDR2 FB-DIMM

# Multifluid Hydrodynamic 3D : $8 \times 10^6$ unknowns

Explicit scheme : CFL 0.9

$$\frac{T_{phys}}{T_{cpu}} \simeq 1.7 \times 10^{-4}$$

RAM used = 0.45Go/Core  $\simeq$  3.6Go

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Implicit scheme : CFL 40 (GS Relaxations  $\leq$  25,  $\varepsilon = 10^{-5}$ )

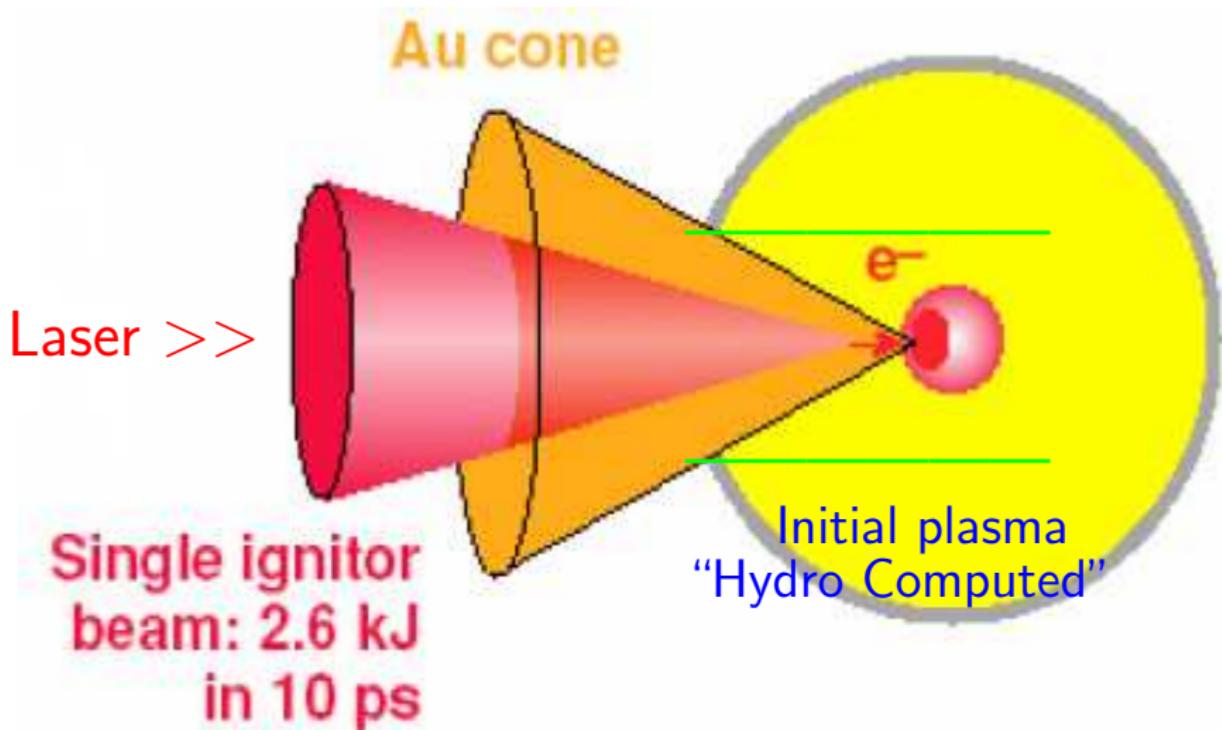
$$\frac{T_{phys}}{T_{cpu}} \simeq 15 \times 10^{-4}$$

RAM used = 1.35Go/Core  $\simeq$  11 Go

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$$\mathcal{E}_{cpu} = \frac{15}{1.7} \simeq 9 \quad \mathcal{E}_{ram} = \frac{11}{3.6} \simeq 3$$

# From Lagrangian Hydrodynamics to Nonlinear Laser/plasmas interaction



# Laser/plasma interaction : Physical Model

- Paraxial approximation:

$$\frac{2i\omega_0}{c^2} \partial_t \mathbf{E} + 2ik_0 \partial_z \mathbf{E} + \left( i\partial_z k_0 - \frac{\omega_0^2}{c^2} \frac{n_e - n_{e0}}{n_c} + i\frac{\nu_{ei}\omega_0}{c^2} \frac{n_{e0}}{n_c} \right) \mathbf{E} + \left( \frac{2\nabla^2}{1 + \sqrt{1 + \nabla^2/k_0^2}} \right) \mathbf{E} = 0.$$

## Nonlinear nonlocal laser/plasma interaction

$$\begin{aligned} \partial_t \rho + \mathbf{u} \cdot \nabla \rho &= -\rho \nabla \cdot \mathbf{u} & , \\ \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\frac{1}{\rho} \nabla p & -\frac{Z \nabla (\|\mathbf{E}\|^2)}{2cn_c m_i} & + \frac{1}{\rho} \nabla \cdot (\eta \nabla \mathbf{u}), \\ \partial_t T_e + \mathbf{u} \cdot \nabla T_e &= -\frac{p_e}{\rho} \nabla \cdot \mathbf{u} & + \frac{\nu_{ei} \Gamma_e}{n_e c} \|\mathbf{E}\|^2 & + \frac{\Gamma_e}{n_e} \nabla \cdot (\kappa_e \nabla T_e), \\ \partial_t T_i + \mathbf{u} \cdot \nabla T_i &= -\frac{p_i}{\rho} \nabla \cdot \mathbf{u} & & + \frac{\Gamma_i}{n_i} \nabla \cdot (\kappa_i \nabla T_i). \\ \beta_z \partial_z \mathbf{E} &= -\beta_t \partial_t \mathbf{E} & -\mathcal{S}(\rho) \mathbf{E} & -\mathcal{L}(\nabla) \mathbf{E} \end{aligned}$$

# Numerical Approximation : $\mathbf{W} = (\rho, \mathbf{u}, T_e, T_i)^T$

$$\begin{cases} \partial_t \mathbf{W} + \mathcal{A}(\mathbf{W}) \nabla_{x,y} \mathbf{W} &= \mathcal{P}(\mathbf{W}, \mathbf{E}) + \mathcal{N}(\mathbf{W}), \\ \beta_z \partial_z \mathbf{E} &= -\mathcal{S}(\mathbf{W}) \mathbf{E} - \mathcal{L}(\nabla_{x,y}) \mathbf{E} \end{cases}$$

Given  $\mathbf{E}^n(z=0)$ ,  $\mathbf{W}^{n-\frac{1}{2}}(z + \frac{\delta z}{2})$  and set  $\mathcal{M}_{z+\frac{\delta z}{2}}^{n-\frac{1}{2}} = \mathcal{S}_{z+\frac{\delta z}{2}}^{n-\frac{1}{2}} + \mathcal{L}(\nabla_{x,y})$

- ① FFTW &  $\theta$ -scheme + MPI  $\Rightarrow \mathbf{E}^n(z + \delta z)$

$$\left[ \beta_z + \delta z \theta \mathcal{M}_{z+\frac{\delta z}{2}}^{n-\frac{1}{2}} \right] \mathbf{E}^n(z + \delta z) = \left[ \beta_z - \delta z (1 - \theta) \mathcal{M}_{z+\frac{\delta z}{2}}^{n-\frac{1}{2}} \right] \mathbf{E}^n(z)$$

- ② FV Second order accurate + MPI  $\Rightarrow \mathbf{W}_{i,j}^{(1)}(z + \frac{\delta z}{2})$

$$\mathbf{W}_{i,j}^{(1)} = \mathbf{W}_{i,j}^{n-\frac{1}{2}} + \frac{\delta t}{a_{i,j}} \left[ -\Phi_{i,j}^{n-\frac{1}{2}} + a_{i,j} \mathcal{P}_{i,j}^{n-\frac{1}{2}} \left( \frac{\mathbf{E}^n(z + \delta z) + \mathbf{E}^n(z)}{2} \right) \right]$$

- ③ FFTW &  $\theta$ -scheme + MPI  $\Rightarrow \mathbf{W}^{n+\frac{1}{2}}(z + \frac{\delta z}{2})$

$$\mathbf{W}_{i,j}^{n+\frac{1}{2}} - \delta t \theta \mathcal{N}_{i,j} \left( \mathbf{W}^{n+\frac{1}{2}} \right) = \mathbf{W}_{i,j}^{(1)} + \delta t (1 - \theta) \mathcal{N}_{i,j} \left( \mathbf{W}^{(1)} \right)$$

# Validation by a proton diagnostic.

- Incoming Electric field :  $I(t, \mathbf{r}) = I_{max} \exp\left(-\frac{2\mathbf{r}}{W_0^2} - \frac{t^2}{t_0^2}\right)$ .  
 $I_{max} = 3.7 \cdot 10^{14} W.cm^2$ ,  $W_0 = 60\mu m$ ,  $t_0 = 400ps$ .  $\lambda_0 = 1.053\mu m$ .
- Initial plasma (Helium:  $Z = 2$ ) :

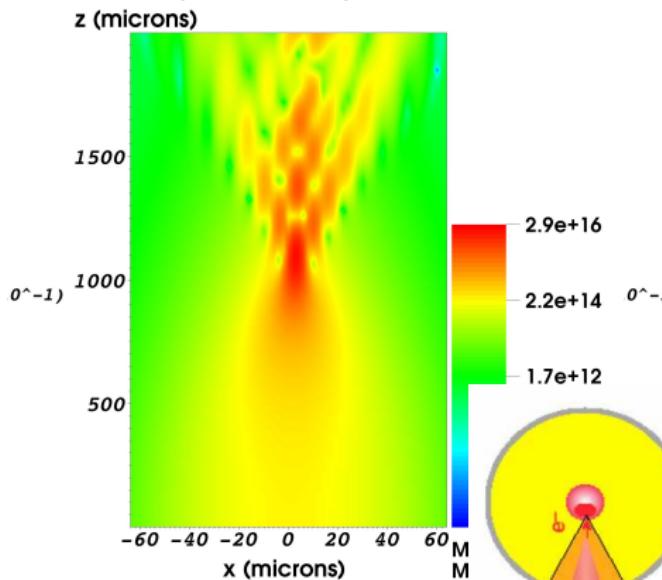
$$n_0 = 0.014n_c, T_{e0} = 100eV, T_{i0} = 30eV.$$

- Electron heat flux model:
  - Spitzer-Härm Conductivity, marginally valid for ICF :  
(non Maxwellian electrons density functions.)
  - Brantov (98) nonlocal Conductivity.  
Based on a linearised theory of Fokker-Planck  
Valid for an “arbitrary” collisionality.
- Braginskii viscosity & ion Landau damping  
--> ion heat conductivity. .

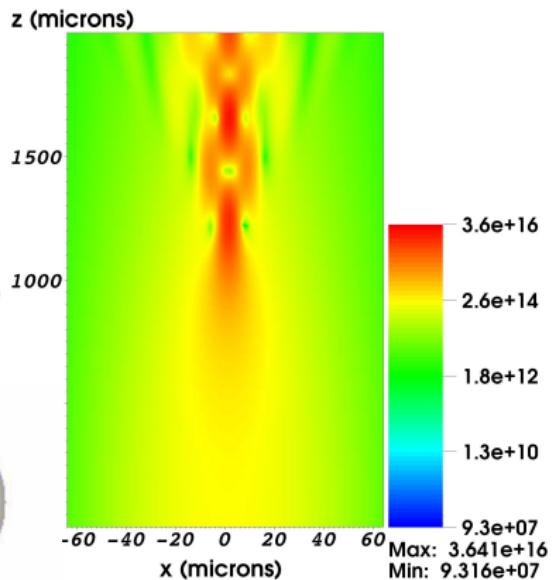
# Energy distribution (on a cut plane) at 550ps

Initial Density is constant in space

Brantov (non local)



Spitzer-Härm



$$\delta x = \delta y = 2\mu m$$

$$N_x = N_y = 256$$

B. Nkonga et al.



$$\delta z = 5\mu m$$

$$N_z = 400$$

Numerics for Controlled Fusion

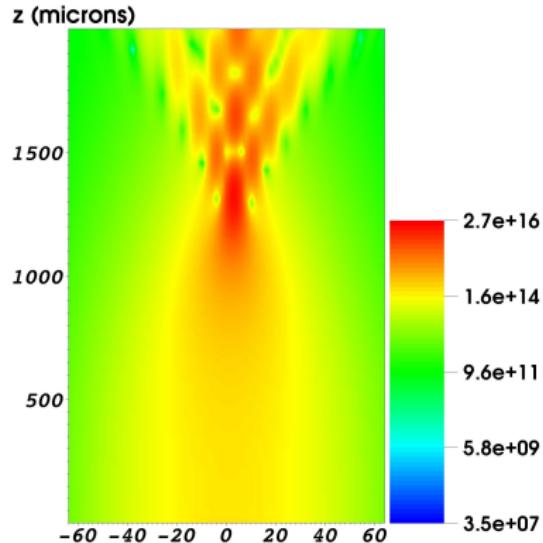
$$\delta t = 5 \cdot 10^{-2} \text{ ps}$$

GDR Calcul: Nov. 09

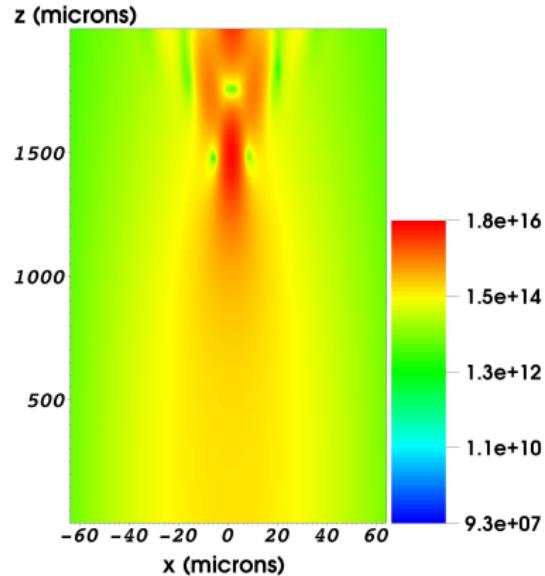
Energy after 550ps : $\delta x = \delta y = 2\mu m$ ,  $\delta z = 5\mu m$

## Initial Density is profiled in space

Brantov (non local)



Spitzer-Härm



Parallel computing : Quad Itanium® II, Dual-Core, 1.6 Ghz, 128 Go

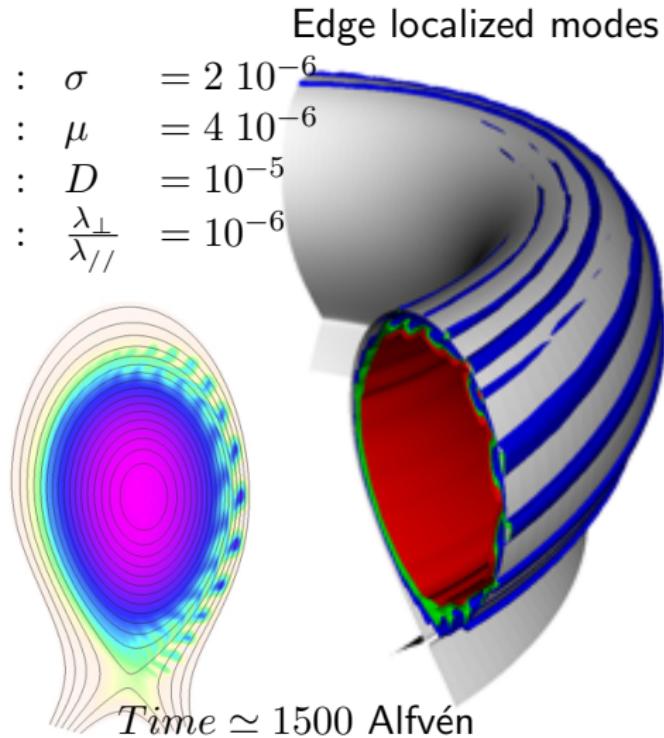
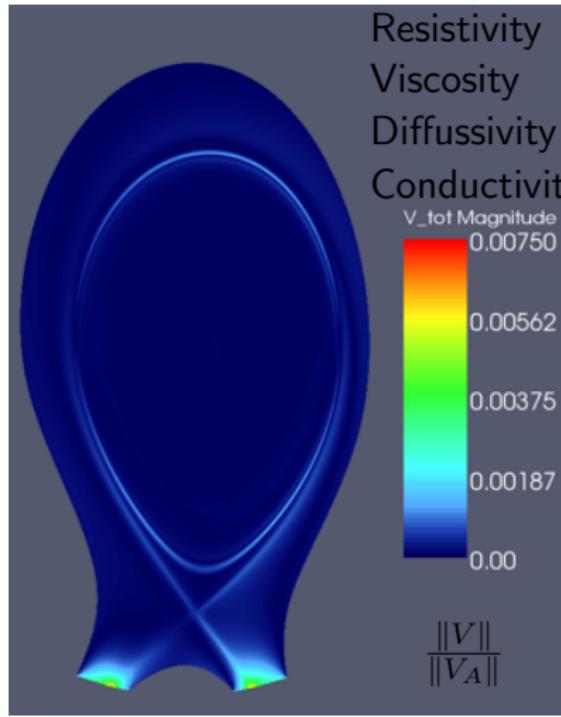
$\simeq 150 \times 10^6$  variables    $10^4$  time steps : 40H CPU with 32 cores

## Tokamak plasmas : KINETIC or/and FLUID ?

- What is the **range of applicability** of **fluids modelizations** for large Tokamaks plasmas ?
- Can we accurately take into account unresolved **kinetic and/or particles orbits effects** on large macroscopic scaled?
- What are **characteristic behaviors** of “Fluid like” modelizations, their stiffness and asymptotic?
- Can we design **appropriate, stable, accurate, efficient and scalable numerical** approximations that are able to simulate long time MHD instabilities for ITER and DEMO?

# Ballooning instability : Reduced MHD (Jorek)

Equilibrium: Flow  $\simeq 40 \text{ km/s}$



Temperature  $\simeq 10 \text{ kev}$ ,  $\|V_A\| \simeq 5000 \text{ km/s}$ , 18 Toroidal modes used

# Numerical Developments : ASTER (ANR-CIS.2006)

- ① Refinable cubic-Bezier FEM (O. Czarny, G. Huysmans).
- ② Direct/iterative parallel sparse matrix solver (P. Ramet, P. Henon, ...)
- ③ Optimized time-stepping algorithm ( G. Huysmans, B. Nkonga, ... )
- ④ Stabilised FEM, RD schemes (R. Abgrall, R. Huart, B. Nkonga,...)
- ⑤ Extended MHD model (E. van der Plas, G. Huysmans, B. Nkonga,...)
- ⑥ Boundary conditions (M. Becoulet, G. Huysmans, ...)

ANR program Intensive Computing and Simulation (ANR-CIS.2006)  
<http://aster.gforge.inria.fr/index.html>

# Open Questions: fluid “like” models for Hot plasmas

## ① Numerical schemes

- Dynamic mesh aligned with magnetic flux surfaces.
- High, i.e. realistic, (magnetic) Reynolds numbers
- Resolution of boundary layers (open field line and curved boundary )
- Long time integration: complete (internal disruption) ELM cycle (different ELM types).

## ② Non-linear evolution of MHD models

- Trigger of neoclassical transport (low collisionality, tearing modes).
- Extended MHD (Ti-Te + Generalized Ohm's law).
- Interaction with micromagnetic turbulence (anomalous transport).

## ③ Fast particles interaction with MHD modes (nonlocal transport).

## ④ Charge exchange neutrals, radiation, local heating, ...