

From modelization to simulation

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MathMods 2010

Introduction : Why we need computation?

To enjoy and understand!



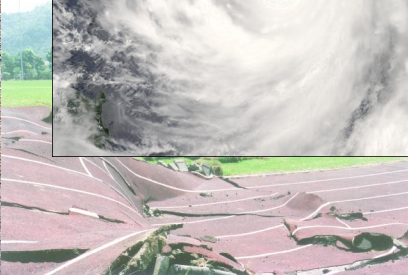
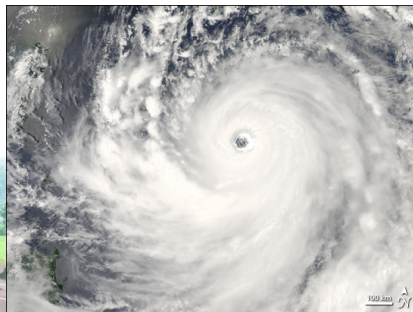
Introduction : Why we need computation?



Dryden Flight Research Center EC92- 1284 Photographed 1992
SR-71B take-off with "shock diamonds" in the exhaust. NASA photo

To prevent some humanity disaster, at least we hope so!

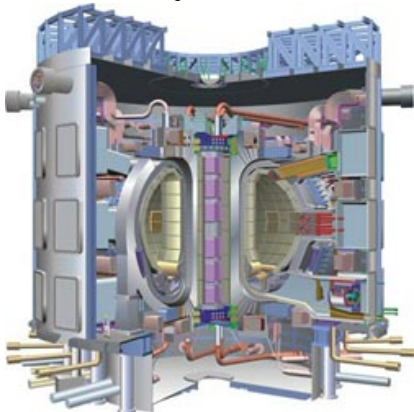
Introduction : Why we need computation?



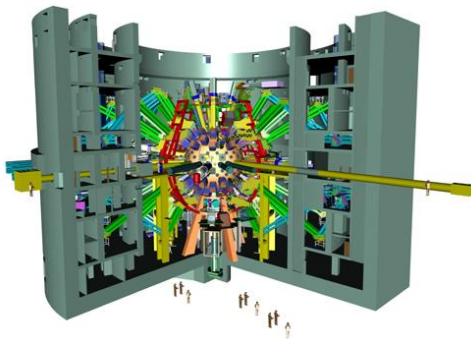
To prevent consequences of some natural disaster!

Introduction : Why we need computation?

ITER Int. Project.



LMJ & NIF : Laser/plasmas



To help meet mankind's future energy needs : Fusion

Are computations possibles?

Yes, Because we have

Fundamental Laws

Conservation of **mass**,
Momentum, **Energy**.

Laws of the Thermodynamics:
(1st, 2nd, 3th) Gauss, Ampère's,
Faraday Laws

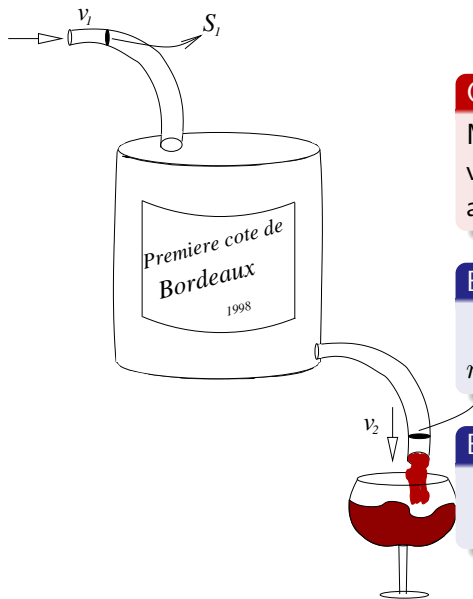
Computers are efficient

Tera-FLOPS computers
available **10^{12} Floating point
Operations Per Second**.

Numerical approximation strategies

Finite volume, Finite element, Finite difference, Particles In Cells,
..., structured/unstructured mesh, Parallel programming (MPI),

Balance “relations” or equations!



Conservation Law: for Mass

Mass fluctuation, in a control volume, is the sum of outgoing and incoming mass:

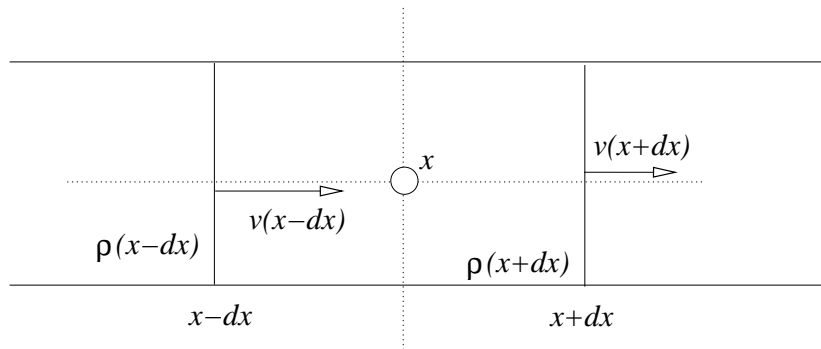
Balance Relation

$$m(t+dt) = m(t) + \rho_1 S_1 v_1 - \rho_2 S_2 v_2$$

Balance equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

Balance “relations” or equations!

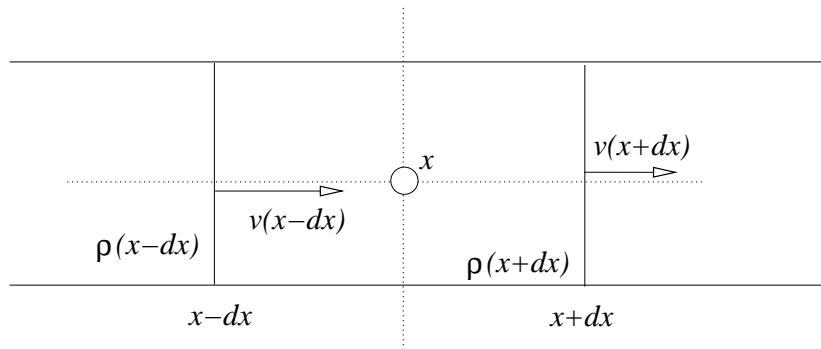


From relations to equations

$$m(x, t + dt) = m(x, t) + S \int_t^{t+dt} f(x - dx, s) ds - S \int_t^{t+dt} f(x + dx, s) ds$$

where the flux is defined by $f(x, t) = \rho(x, t)v(x, t)$

Balance “relations” or equations!



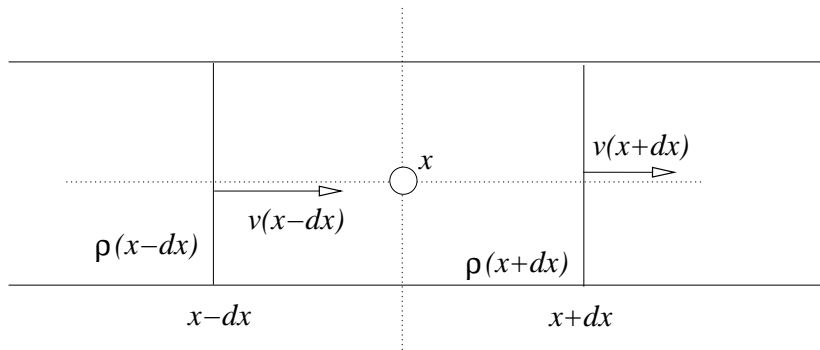
From relations to equations

$$m(x, t + dt) = m(x, t) + Sdt f(x - dx, t) - Sdt f(x + dx, t)$$

$$m(x, \cdot) = 2Sdx\rho(x, \cdot)$$

where the flux is defined by $f(x, t) = \rho(x, t)v(x, t)$

Balance “relations” or equations!

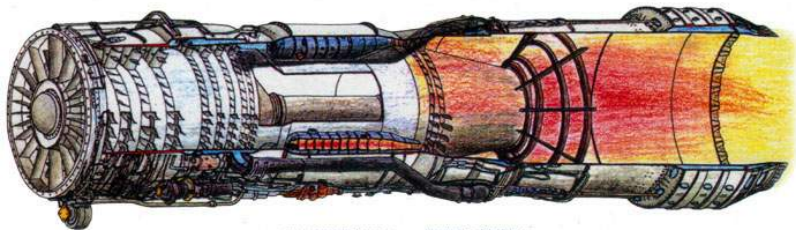


From relations to equations $dx \rightarrow 0$ and $dt \rightarrow 0$

$$\frac{\rho(x, t + dt) - \rho(x, t)}{dt} = - \frac{f(x + dx, t) - f(x - dx, t)}{2dx}$$
$$\implies \frac{\partial \rho}{\partial t} + \frac{\partial f}{\partial x} = 0 \implies \frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial x} = 0$$

where the flux is defined by $f(x, t) = \rho(x, t)v(x, t)$

Balance equations : general 1D case



www.aerostories.org

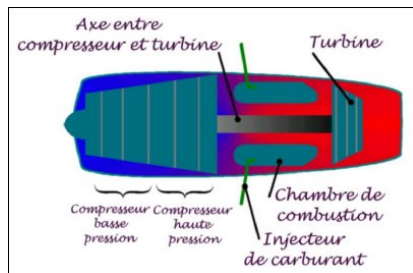
Illustration Ph. Ricco

$$\frac{\partial \omega}{\partial t} + \frac{\partial f(\omega)}{\partial x} = \mathcal{S}$$

where \mathcal{S} can be defined, for example, by the chemistry process, geometrical topology ...

$$\omega(x, t) = \begin{pmatrix} \rho \\ \rho Y \\ \rho u \\ E \end{pmatrix} \quad \text{and} \quad f(\omega) = \begin{pmatrix} \rho u \\ \rho Y u \\ \rho u^2 + p \\ (E + p)u \end{pmatrix}$$

Balance equations : general 1D case

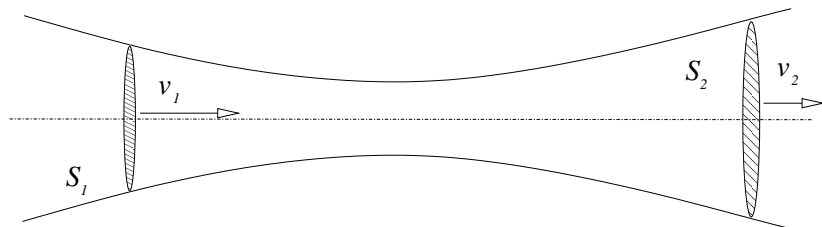


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Balance equations : general 1D case



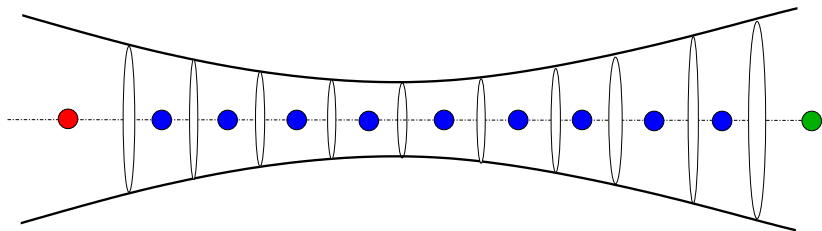
$$\frac{\partial \omega}{\partial t} + \frac{\partial f(\omega)}{\partial x} = \mathcal{S}$$

where \mathcal{S} can be defined, for example, by the chemistry process, geometrical topology ...

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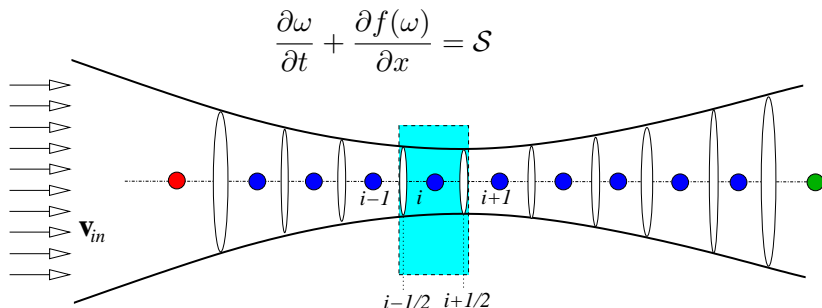
Finite volume Scheme: 1D case

$$\frac{\partial \omega}{\partial t} + \frac{\partial f(\omega)}{\partial x} = S$$



Mesh and Control volumes

Finite volume Scheme: 1D case



$$\frac{\omega_i^{n+1} - \omega_i^n}{t^{n+1} - t^n} + \frac{\phi_{i+1/2}^m - \phi_{i-1/2}^m}{x_{i+1/2} - x_{i-1/2}} = S_i^m$$

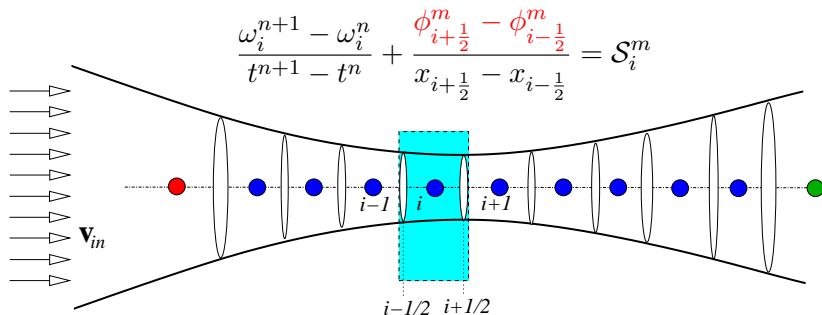
Balance relations on a Control volume

Finite volume Scheme: 1D case

$$\frac{\omega_i^{n+1} - \omega_i^n}{t^{n+1} - t^n} + \frac{\phi_{i+\frac{1}{2}}^m - \phi_{i-\frac{1}{2}}^m}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}} = \mathcal{S}_i^m$$

How to define the numerical
flux $\phi \simeq f$

Finite volume Scheme: 1D case

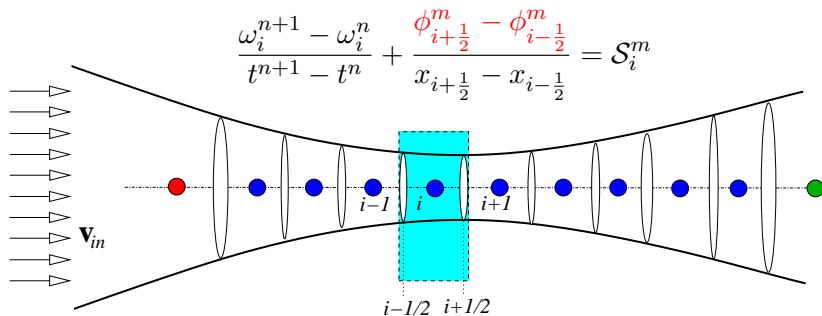


Centered scheme:

$$\phi_{i+\frac{1}{2}} = \frac{f_i + f_{i+1}}{2}$$

Accurate but **Unstable!**

Finite volume Scheme: 1D case

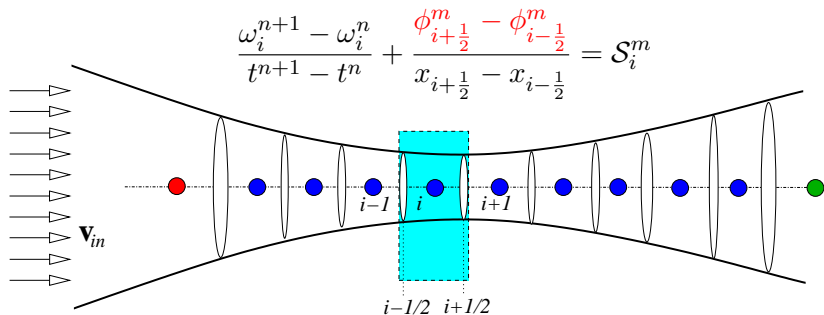


Upwind scheme (in this case):

$$\phi_{i+\frac{1}{2}} = f_i \quad \text{and} \quad \phi_{i-\frac{1}{2}} = f_{i-1}$$

Less accurate but **Stable** ✓

Finite volume Scheme: 1D case

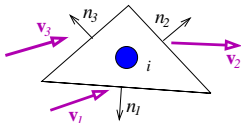
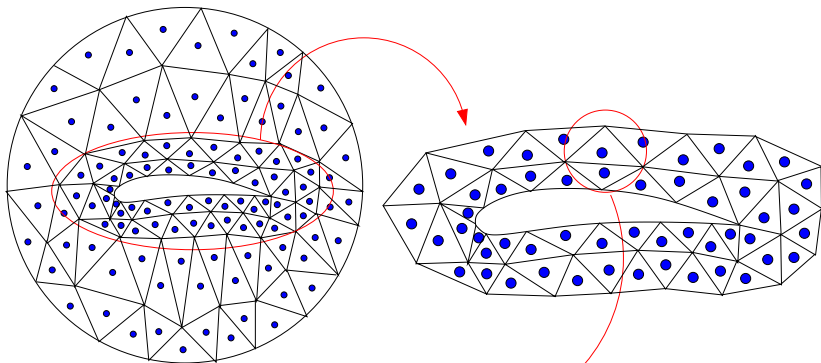


General rule:

The numerical flux should be consistent with the physics

Upwind : Follows informations traveling in the correct direction.

Finite volume Scheme: 2D case



$$a_i \frac{\omega_i^{n+1} - \omega_i^n}{t^{n+1} - t^n} = - \sum_{j \in \vartheta(i)} \Phi_{i,j}$$

$\phi_{i,j}$ is now the flux crossing an interface from the cell i to j .

Need properties for $\phi_{i,j}$

$$\phi_{i,j} = \phi(\omega_i, \omega_j)$$

can be obtained by the resolution of a simplify problem:
Riemann Problem.

Properties we want the numerical flux to satisfy

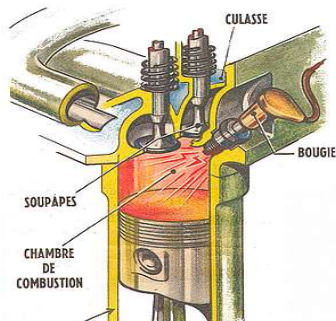
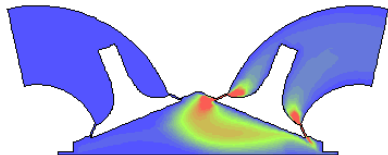
- Consistency, Stability, Convergence
- Positivity and maximum principles $\rho \geq 0, ||v|| \leq c.$
- Second thermodynamic law (entropy production).
- Accuracy : have a better result with a given mesh.

Lax Theorem for conservative systems

Consistency + Stability = Convergence

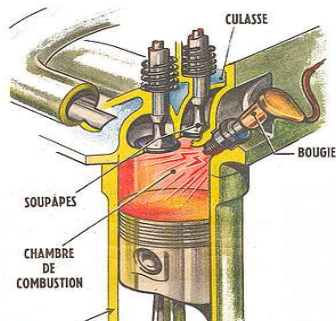
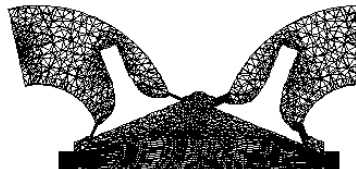
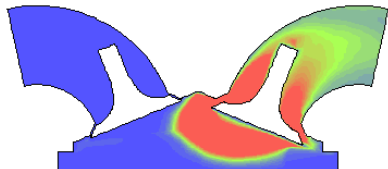
Four valves Diesel engine flow : Moving Boundaries

B. Nkonga (97).



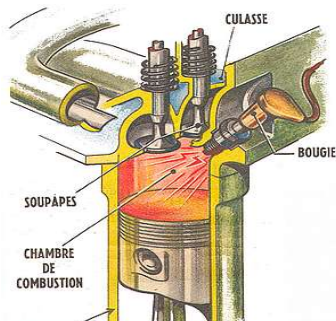
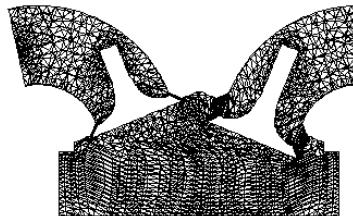
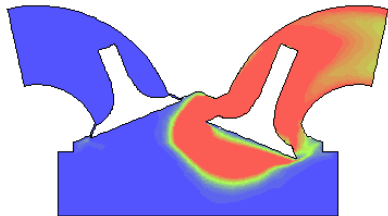
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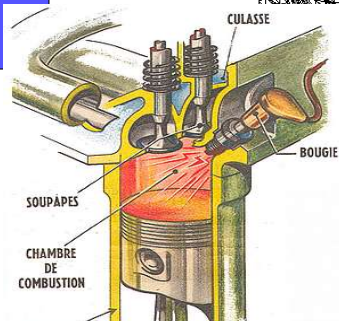
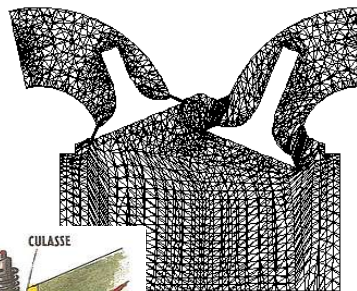
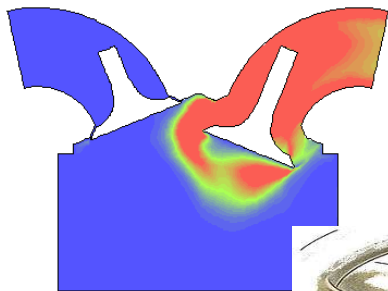
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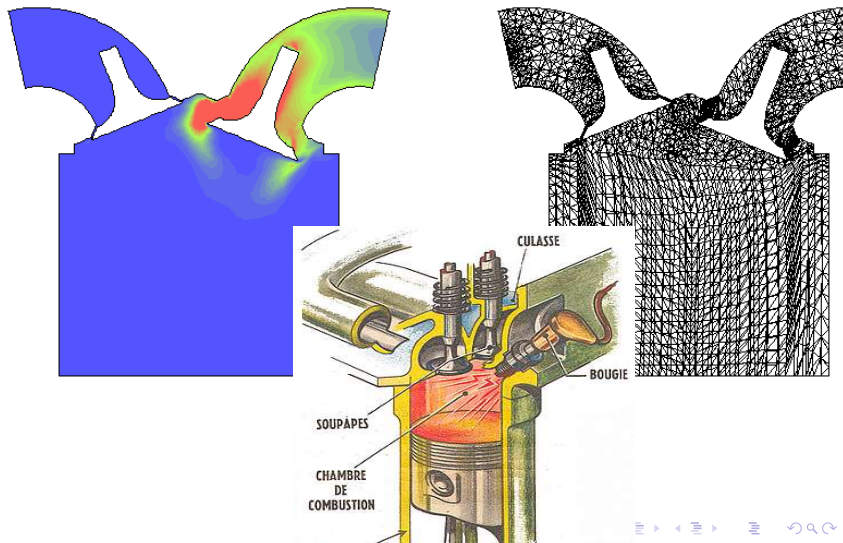
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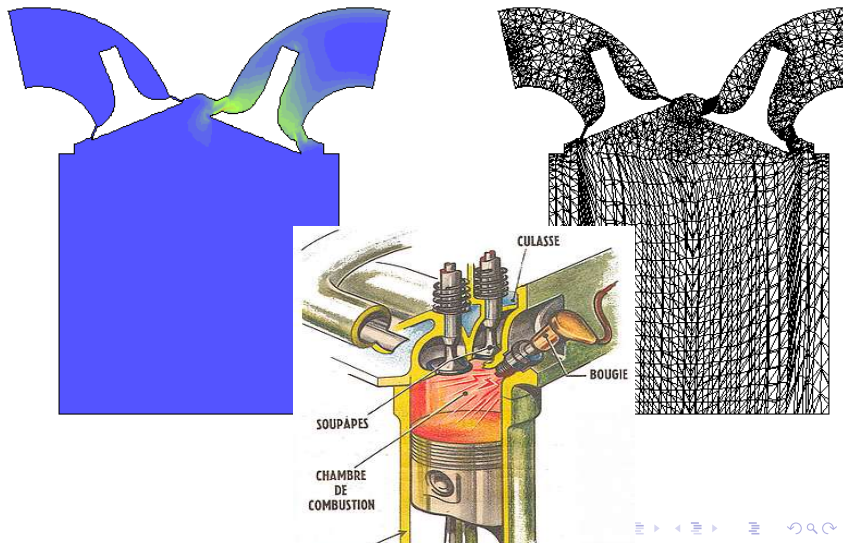
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Four valves Diesel engine flow : Moving Boundaries

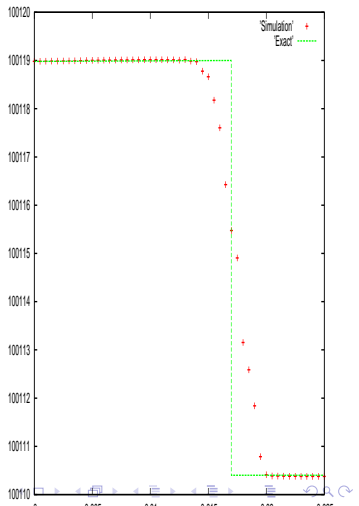
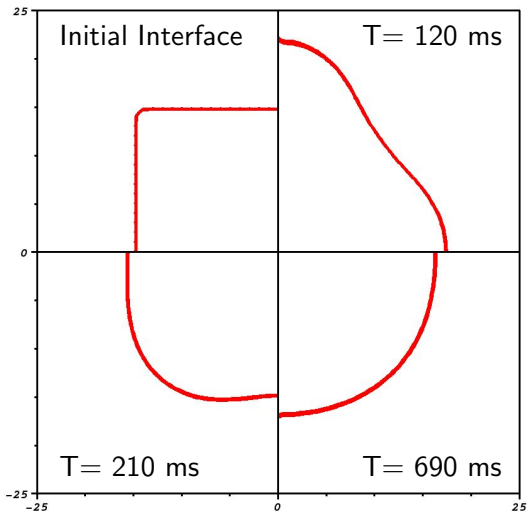
B. Nkonga (97).



Low Mach interface flow with surface Tension

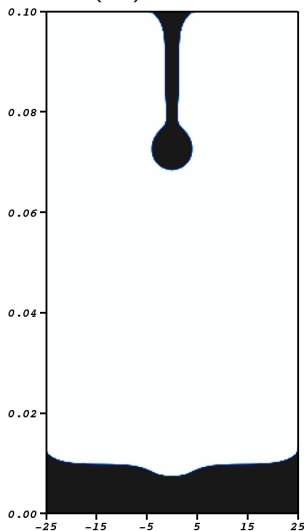
B. Nkonga & B. Braconnier (07)

Laplace Law Recovered : $\delta p = \sigma \kappa$



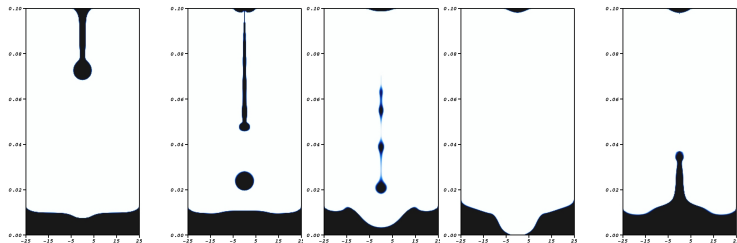
Water drop in air, gravity and Surface tension

B. Nkonga & B. Braconnier (07)



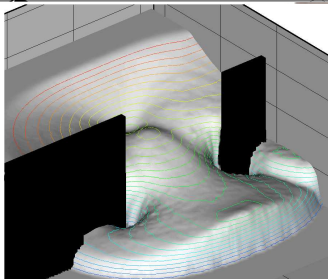
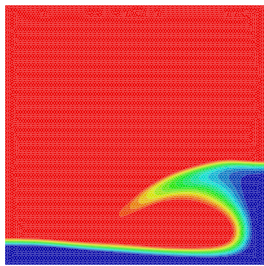
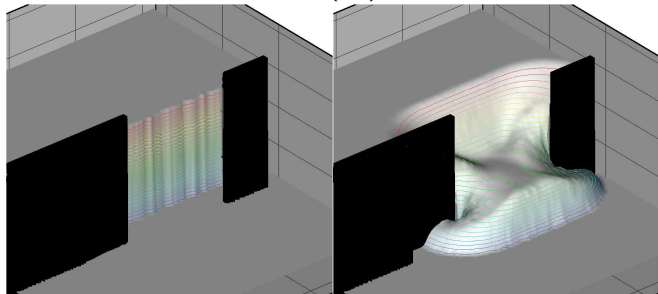
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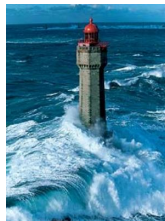
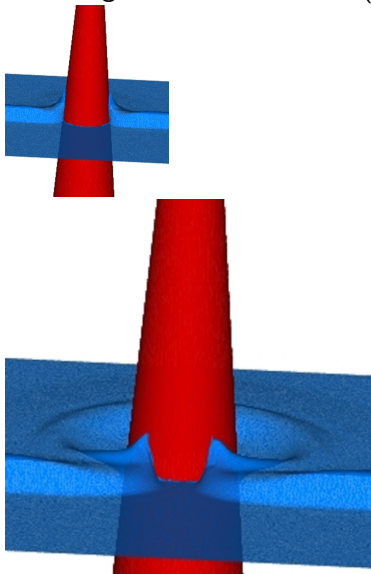
Dam Break : Shallow water and Multiphase flow

R. Abgrall & M. Ricchiuto (05)



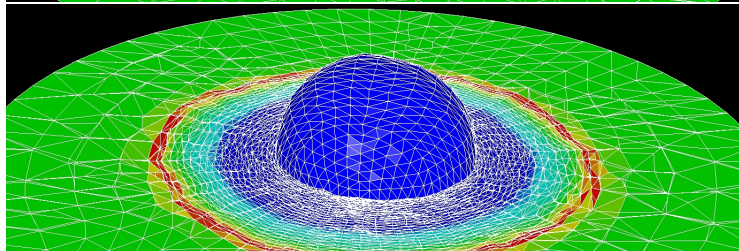
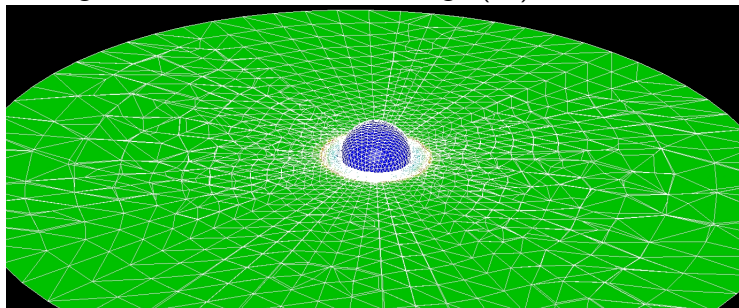
Shallow water and Multiphase flow

R. Abgrall & M. Ricchiuto (05)



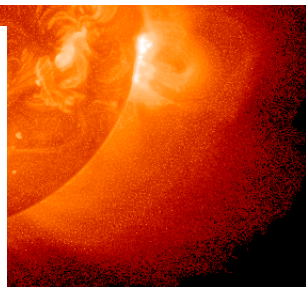
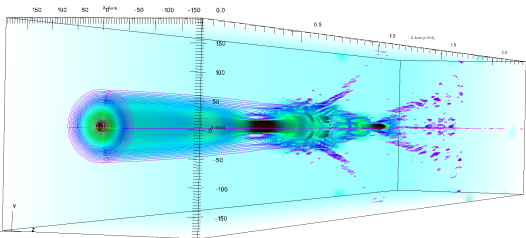
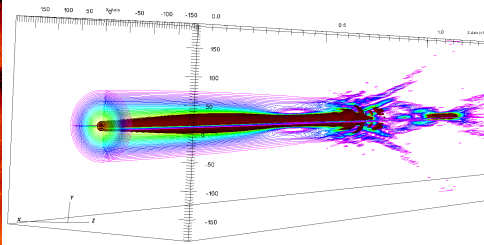
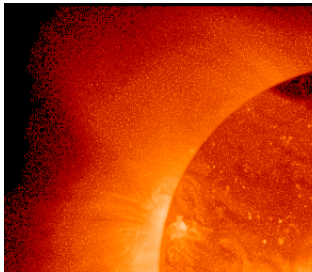
Explosion and propagation : Mesh follows the shock front.

R. Abgrall & P-H Maire & B. Nkonga (08)

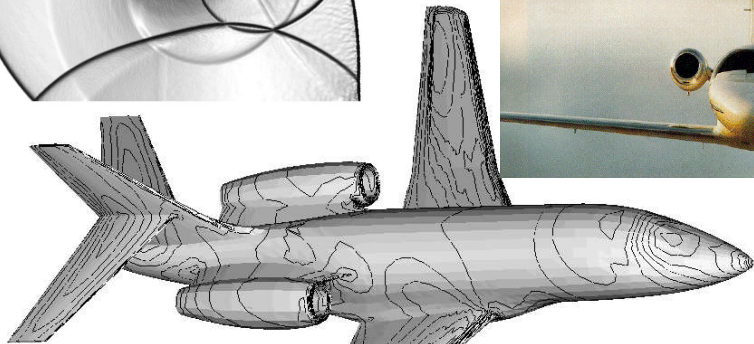
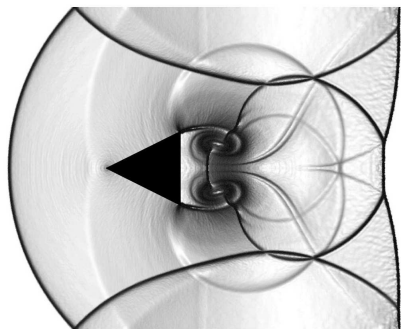


Laser / Plasmas Interactions for Nuclear Fusion

A. Bellue & A. Bourgeade & B. Nkonga & S. Weber (08)

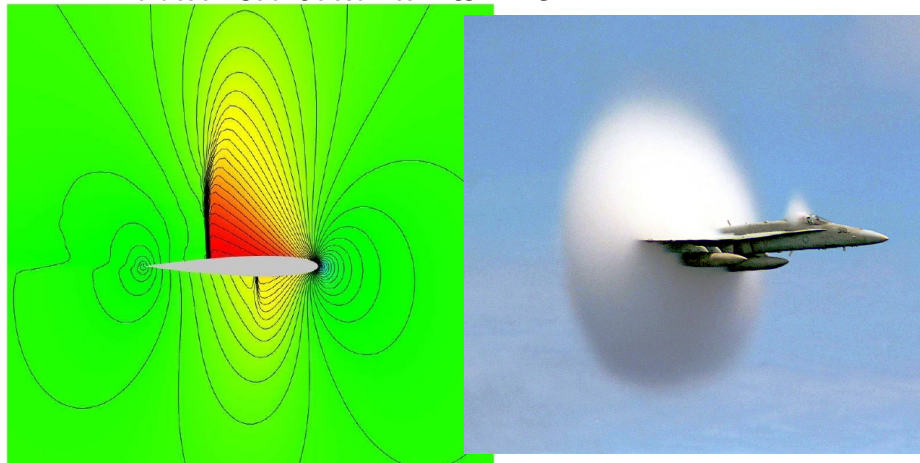


Computation and reality : Aerodynamic flow



High speed aerodynamics : Choc and condensation

INRIA Bordeaux Sud-Ouest Team & ADIGMA

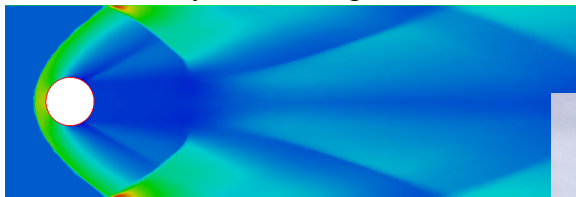


Condensation gives a view
of the choc wave profile.

Shock waves interactions : Diamond structure

C. Dobrisinsky & B. Nkonga & M. Ricchiuto (07)

FluidBox

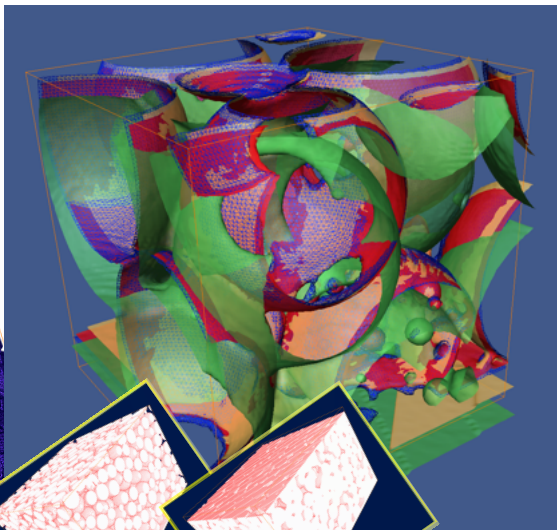
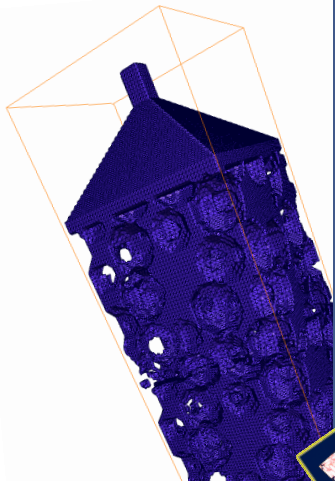


Dryden Flight Research Center EC92-1284 Photograph SR-71B take-off with "shock diamonds" in the exhaust.



Material & Numerics

(P. Charrier, D. Bernard, B. Nkonga, M. Ricchiuto, G. Vignoles)



From modelization to simulation

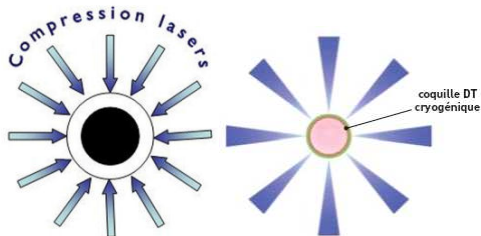
B. Nkonga

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Inertial Confinement Fusion : Compression Ignition

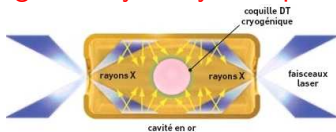
- Ignition by lasers compression



- Interfaces flow
- Large ratio computational domain change.

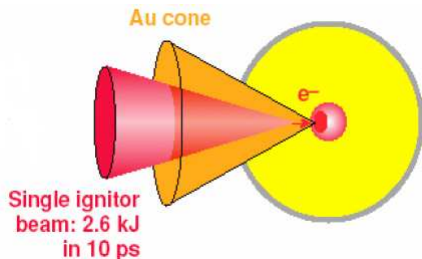
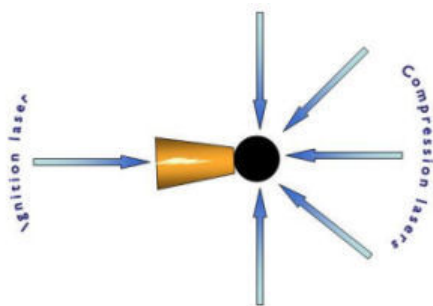
Needs : Lagrangian Hydrodynamics Scheme...

- Ignition by X-rays compression



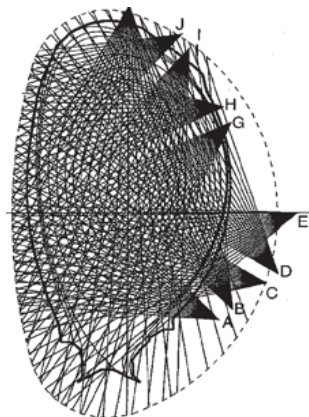
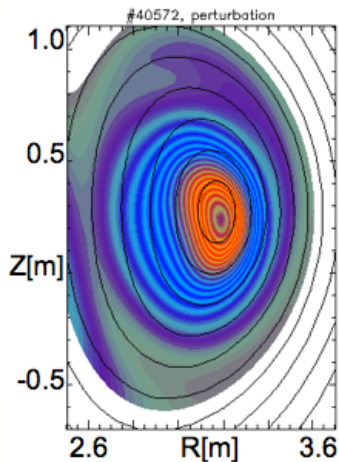
Needs : Compute Focusing Beams interactions...

Inertial Confinement Fusion : Fast laser ignition



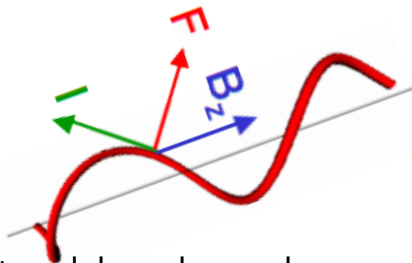
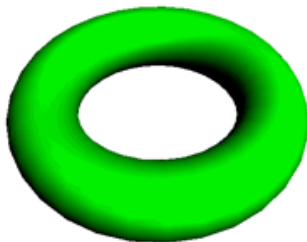
Need : Nonlinear laser/plasmas model, non-local Transport...

Tokamak Plasma : Avoid large scale instabilities.



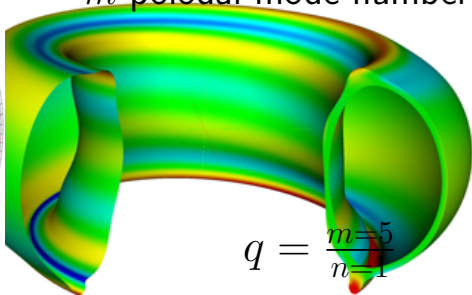
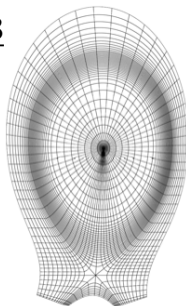
Tomographic reconstruction of X-ray emission. JET SXR cameras (1998).

Tokamak Plasma : Kink instability (MHD, Jorek).



n toroidal mode number
 m poloidal mode number

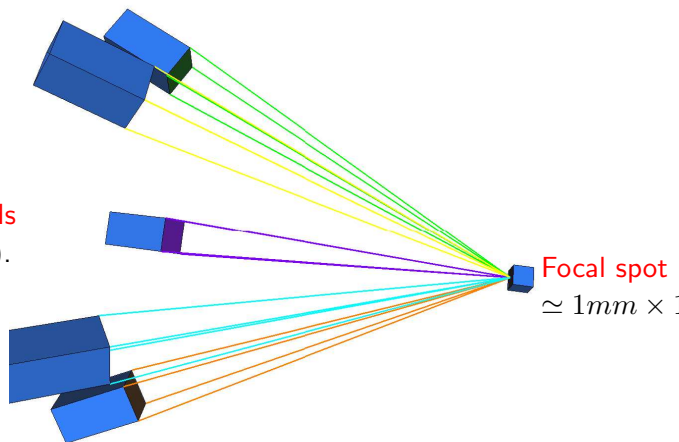
$$q = \frac{m=3}{n=1}$$



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

Laser focusing (ICF): Huygens-Fresnel Theorem.

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



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

Focusing Laser : Approximations and Computations.

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

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

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

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

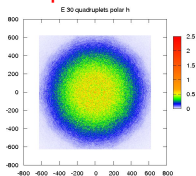
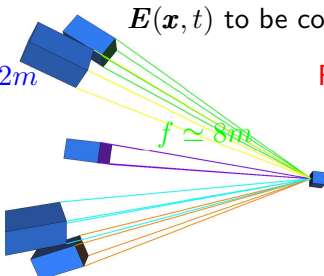
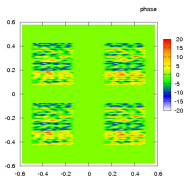
Given $\mathcal{E}_{\ell,i,j,m}$
 $N_{\ell} = 30$ quads

Quad $\simeq 1.2m \times 1.2m$

$\mathbf{E}(\mathbf{x}, t)$ to be computed with the resolution :

$Nf_x \times Nf_y \times Nf_t$

Focal spot : $1.2mm \times 1.2mm$



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:

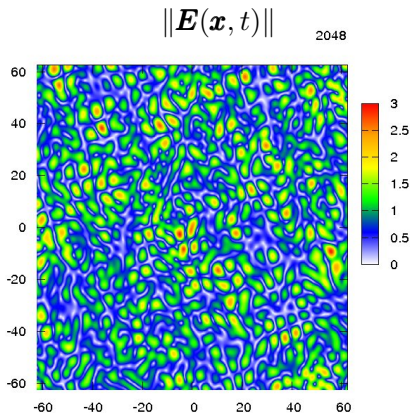
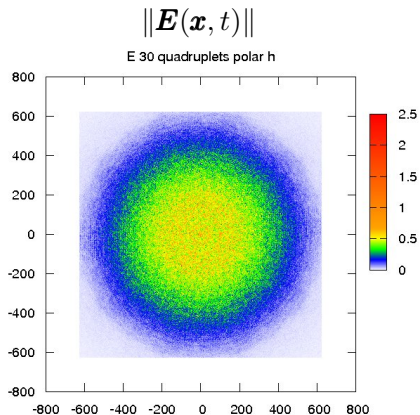
$$\mathbf{E}(\mathbf{x}, t, \mathbf{me}) = \sum_{\ell} \sum_{m_1(\mathbf{me})}^{m_N(\mathbf{me})} \sum_{i_1(\mathbf{me})}^{i_N(\mathbf{me})} \sum_{j_1(\mathbf{me})}^{j_N(\mathbf{me})} \mathcal{E}_{\ell, i, j, m} \mathcal{G}_{\ell, h} e^{i\Phi_{\ell, i, j, m}} e^{i\omega_m \tau}$$

- Gather the solution :

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

FFTW + MPI

Focusing Laser Beams : Computed focal spot and zoom.

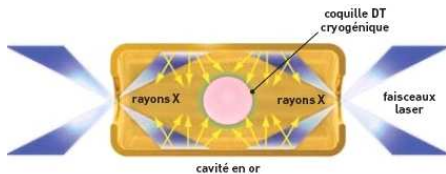


21H CPU with 1936 cores : 30 quads = 120 (40cm x 40cm)

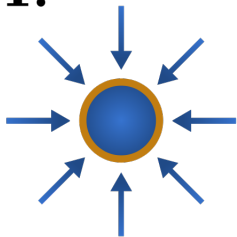
Nodes : 4 Intelltanium II, Dual-Core, 1.6 Ghz, 128 Go

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

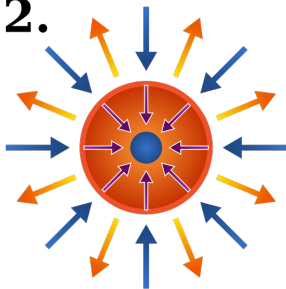
From the focal spot to Lagrangian Hydrodynamics



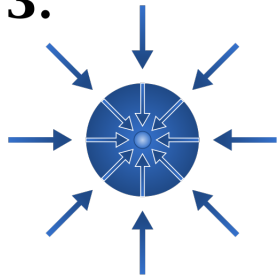
1.



2.



3.



Weak formulation of Conservation Law

Integral form of in arbitrary coordinates

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

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

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

Coupling between averaged(mesh scale) and subscale states.

Multiscale formulation and approximation

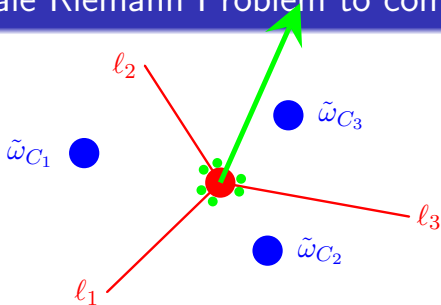
Mesh scale equations

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

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

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

Subscale Riemann Problem to compute $p_{C,l,j}^*$ and κ_j



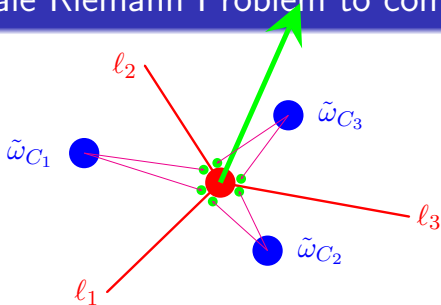
Half Riemann Solver for κ_j fixed: Godunov-type method

$$p_{C,l,j}^* = p_l^* \beta \tilde{w}_C, \quad \kappa_j = p_C + Z_{C,j} \beta \tilde{u}_C - \kappa_j \cdot \frac{\mathbf{m}_{C,l,j}}{\|\mathbf{m}_{C,l,j}\|}$$

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

$$\sum_{\ell \in \mathcal{V}(j)} r_\ell (p_{C_1,\ell,j}^* - p_{C_2,\ell,j}^*) n_{C_1,\ell} = 0$$

Subscale Riemann Problem to compute $p_{C,l,j}^*$ and κ_j



Half Riemann Solver for κ_j fixed: Godunov-type method

$$p_{C,l,j}^* = p_l^* \beta \tilde{\omega}_C, \quad \kappa_j = p_C + Z_{C,j} \beta \tilde{\mathbf{u}}_C - \kappa_j \cdot \frac{\mathbf{m}_{C,l,j}}{\|\mathbf{m}_{C,l,j}\|}$$

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

$$\sum_{\ell \in \mathcal{V}(j)} r_\ell (p_{C_1,\ell,j}^* - p_{C_2,\ell,j}^*) n_{C_1,\ell} = 0$$

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

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

Explicit scheme : $\left[\mathcal{A}_j \beta \tilde{\omega}_*^n, \kappa_*^n \right] \kappa_j^* = g_j \beta \tilde{\omega}_*^n, \kappa_*^n \longrightarrow \mathbf{x}^{n+\theta}$

$$\kappa_\ell(\mathbf{x}) = \sum \varphi_{\ell,j}(\mathbf{x}) \kappa_j^*, \quad p_{C,\ell}(\mathbf{x}) = \sum \psi_{\ell,j}(\mathbf{x}) p_\ell^* \beta \tilde{\omega}_C, \kappa_j^*$$

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

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

Orthogonality
constraint for
interpolation gives

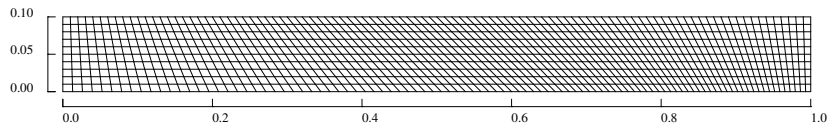
$$\begin{aligned} \psi_{\ell,j}(\xi) &= \\ & (d+1)\varphi_{\ell,j}(\xi) - 1 \\ & \text{and} \\ & \int_\ell \psi_{\ell,i} \varphi_{\ell,j} dl = \frac{\|\ell\|}{d} \delta_{i,j} \end{aligned}$$

Therefore we have analytical formula for the right hand side to

Saltzman problem

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

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

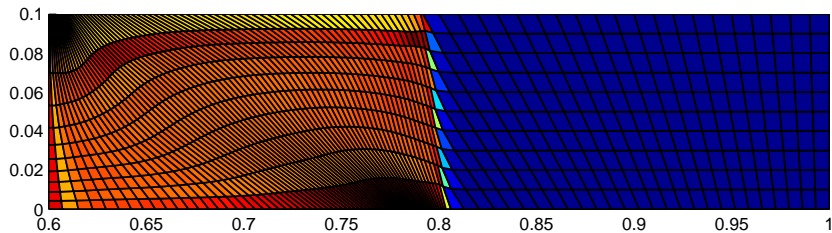


Initial conditions: $(\rho^0, P^0, \mathbf{U}^0) = (1, 10^{-6}, 0)$

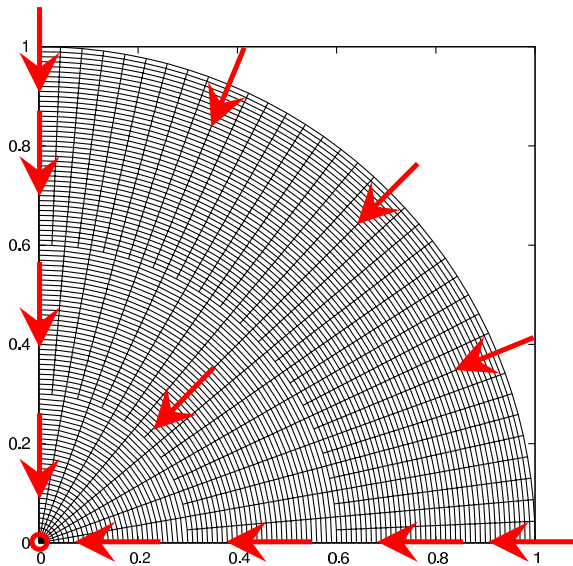
Materials: gamma law gas with $(\gamma = 5/3)$

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

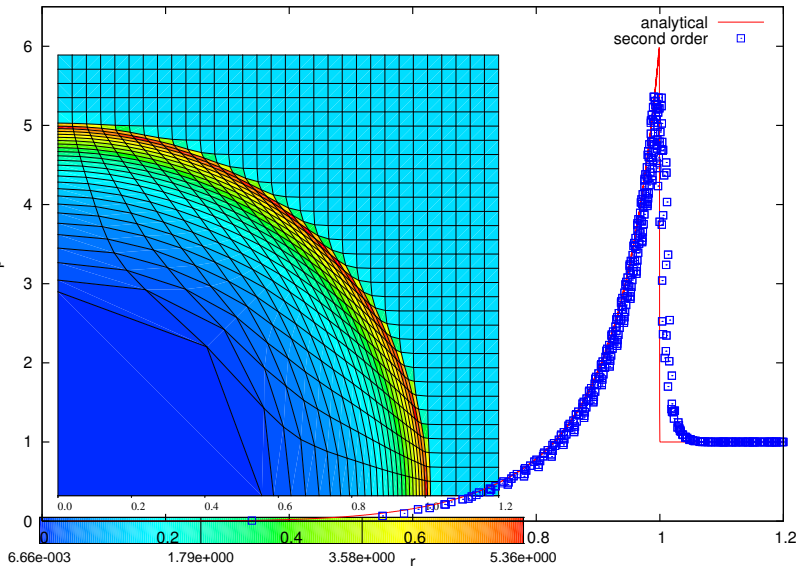
Saltzman problem : Density at $t = 0.6$



Cylindrical Noh Problem: non-conformal, 2250 cells

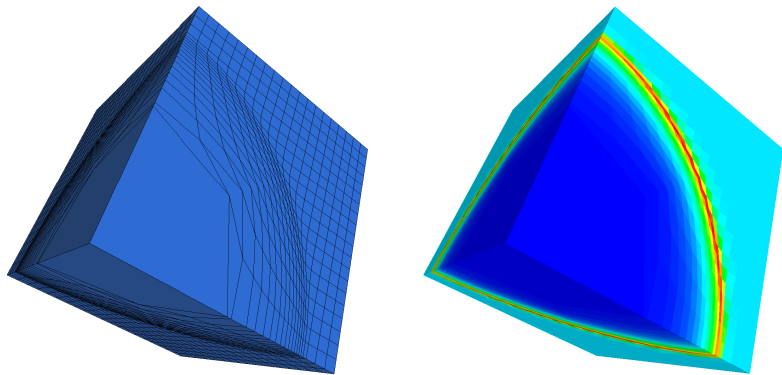


Sedov-Taylor blast wave: 31×31 Cartesian grid



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

Sedov-Taylor blast wave: 3D hexahedra mesh



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

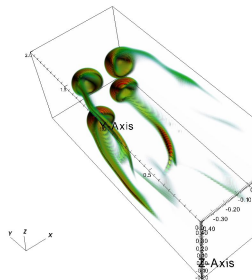
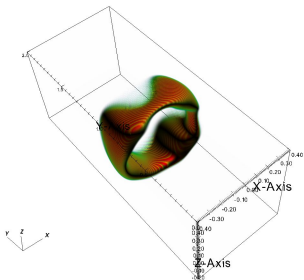
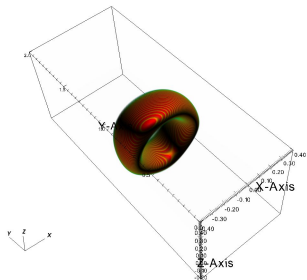
Multifluid Hydrodynamic 3D : 8×10^6 unknowns

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

Implicit Low mach scheme, Surface tension, Gravity.

1.3×10^6 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 : 8×10^6 unknowns

Explicit scheme : CFL 0.9

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

$$\text{RAM used} = 0.45\text{Go/Core} \simeq 3.6\text{Go}$$

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

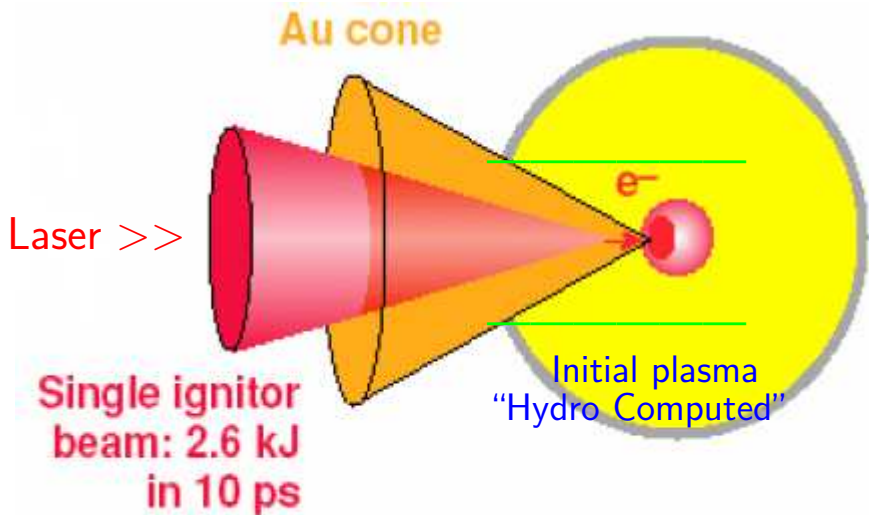
$$\frac{T_{phys}}{T_{cpu}} \simeq 15 \times 10^{-4}$$

$$\text{RAM used} = 1.35\text{Go/Core} \simeq 11 \text{ Go}$$

$$\mathcal{E}_{cpu} = \frac{15}{1.7} \simeq 9$$

$$\mathcal{E}_{ram} = \frac{11}{3.6} \simeq 3$$

From Lagrangian Hydrodynamics to Nonlinear Laser/plasmas interaction



Laser/plasma interaction : Physical Model

$$\begin{aligned}\partial_t \rho + \mathbf{u} \cdot \nabla \rho &= -\rho \nabla \cdot \mathbf{u} \\ \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\frac{1}{\rho} \nabla p \\ \partial_t T_e + \mathbf{u} \cdot \nabla T_e &= -(\gamma_e - 1) T_e \nabla \cdot \mathbf{u} \\ \partial_t T_i + \mathbf{u} \cdot \nabla T_i &= -(\gamma_i - 1) T_i \nabla \cdot \mathbf{u}\end{aligned}$$

with $\rho = \rho_e + \rho_i$, $p = p_e + p_i$, $n_e = Z n_i$, $\rho_e = m_e n_e$, $\rho_i = m_i n_i$,
 $p_e = n_e T_e$ and $p_i = n_i T_i$. Therefore, $\frac{\rho_e}{m_e} = Z \frac{\rho_i}{m_i}$

$$p_e = n_e T_e = \frac{\rho_e}{m_e} T_e = \frac{\rho T_e}{m_e \beta \mathbf{1} + \frac{m_i}{m_e Z}} = \frac{\rho Z T_e}{m_i + Z m_e}$$

$$p_i = n_i T_i = \frac{\rho_i}{m_i} T_i = \frac{\rho T_i}{m_i \beta Z \frac{m_e}{m_i} + 1} = \frac{\rho T_i}{m_i + Z m_e}$$

Laser/plasma interaction : Physical Model

- Paraxial approximation:

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

Nonlinear nonlocal laser/plasma interaction

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

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

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

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

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

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

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

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

- ③ FFTW & θ -scheme + MPI $\implies \mathbf{W}^{n+\frac{1}{2}} \beta z + \frac{\delta z}{2}$

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

Validation by a proton diagnostic.

- Incoming Electric field : $I(t, \mathbf{r}) = I_{max} \exp \beta - \frac{2\mathbf{r}}{W_0^2} - \frac{t^2}{t_0^2}$.

$$I_{max} = 3.7 \cdot 10^{14} \text{W.cm}^2, W_0 = 60 \mu\text{m}, t_0 = 400 \text{ps}.$$
$$\lambda_0 = 1.053 \mu\text{m}.$$

- Initial plasma (Helium: $Z = 2$) :

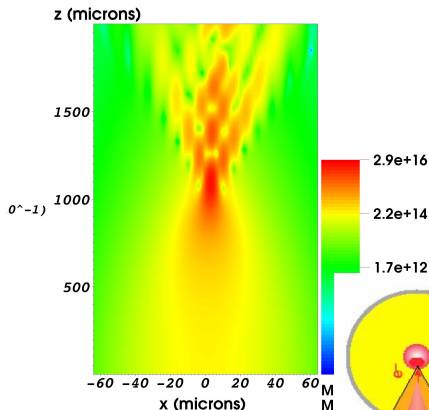
$$n_0 = 0.014 n_c, T_{e0} = 100 \text{eV}, T_{i0} = 30 \text{eV}.$$

- 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. .

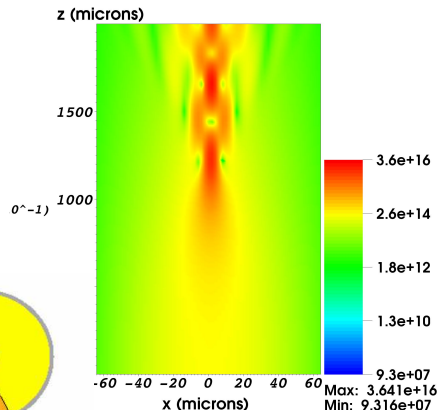
Energy distribution (on a cut plane) at 550ps

Initial Density is constant in space

Brantov (non local)



Spitzer-Härm



$$\delta x = \delta y = 2\mu\text{m} \quad \delta z = 5\mu\text{m}$$

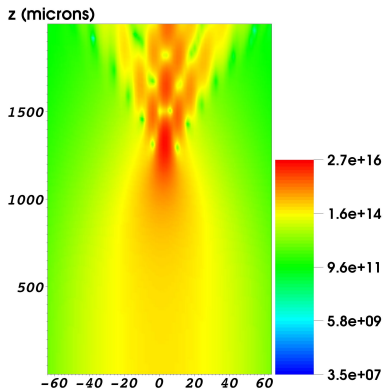
$$N_x = N_y = 256 \quad N_z = 400$$

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

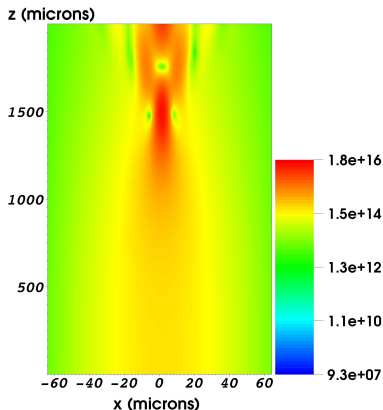
Energy after $550ps$: $\delta x = \delta y = 2\mu m$, $\delta z = 5\mu m$

Initial Density is profiled in space

Brantov (non local)



Spitzer-Härm

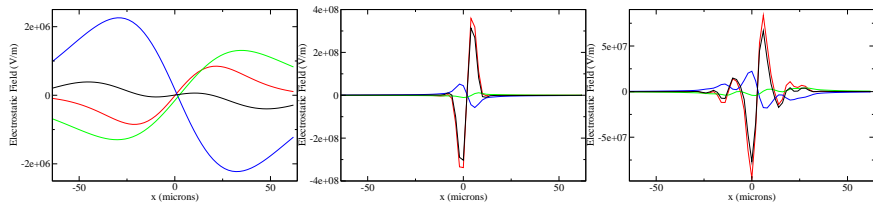


Parallel computing : Quad Itanium II, Dual-Core, 1.6 Ghz, 128 Go

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

Electrostatic fields at 500, 1300, 1700 μm

$$\mathbf{E} = k_1 \nabla I + k_2 \nabla T + k_3 \nabla n$$

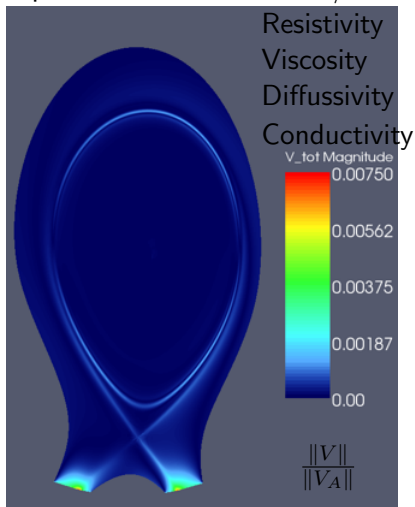


Tokamak plasmas : KINETIC or/and FLUID ?

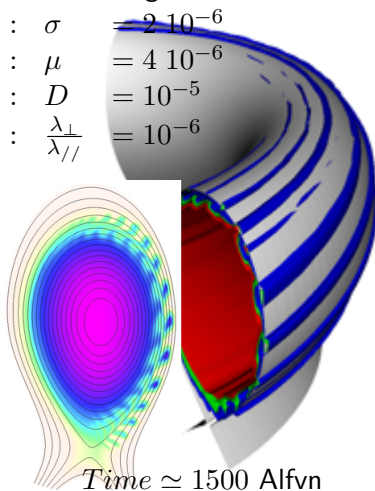
- What is the **range of applicability** of **fluids modelizations** for large Tokamaks plasmas ?
- Can we accurately take into account unresolved **kinetic and/or particles orbits effects** on large macroscopic scaled?
- What are **characteristic behaviors** of “Fluid like” modelizations, their stiffness 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 $\simeq 40\text{km/s}$



Edge localized modes



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, ...