# Multiphase code development for simulation of PHELIX experiments

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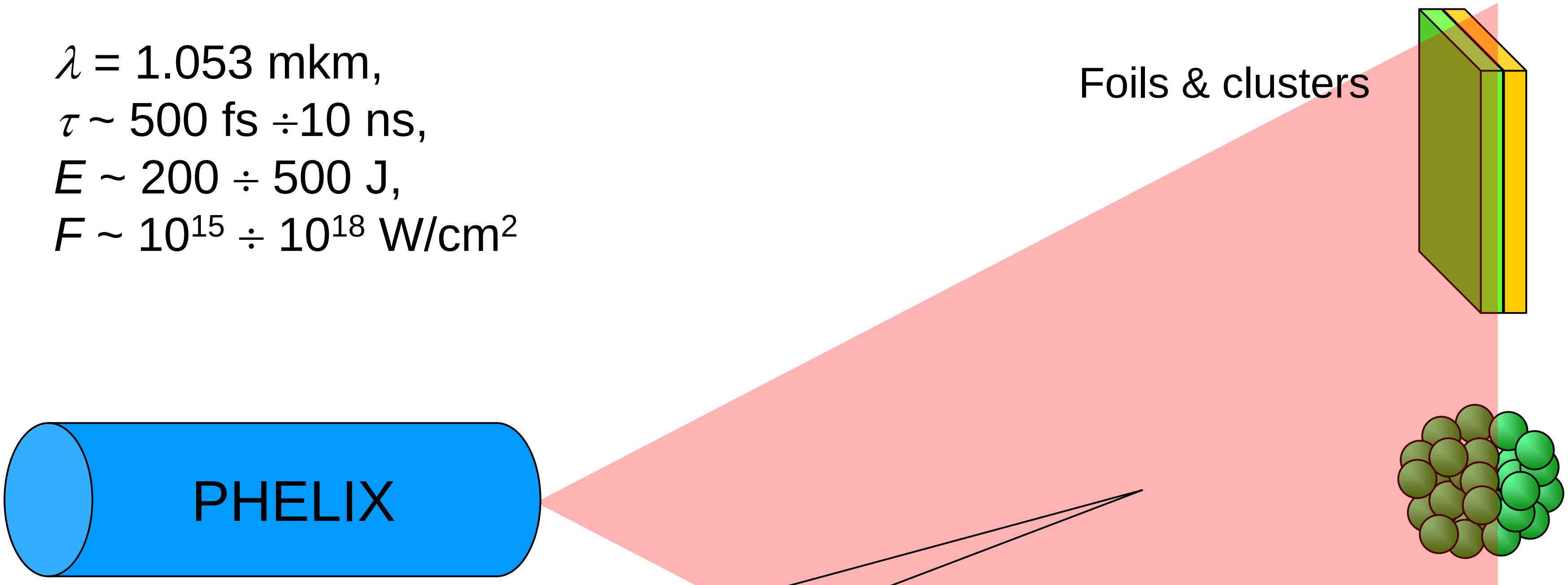
# Outline

- Motivation
- PHELIX setup parameters and targets
- Model and problems of realization
  - — Multiscale and multistage tasks
  - — Adaptive mesh refinement
  - — Summary of our model
- Preliminary results
- Conclusions and future plans
- Discussion

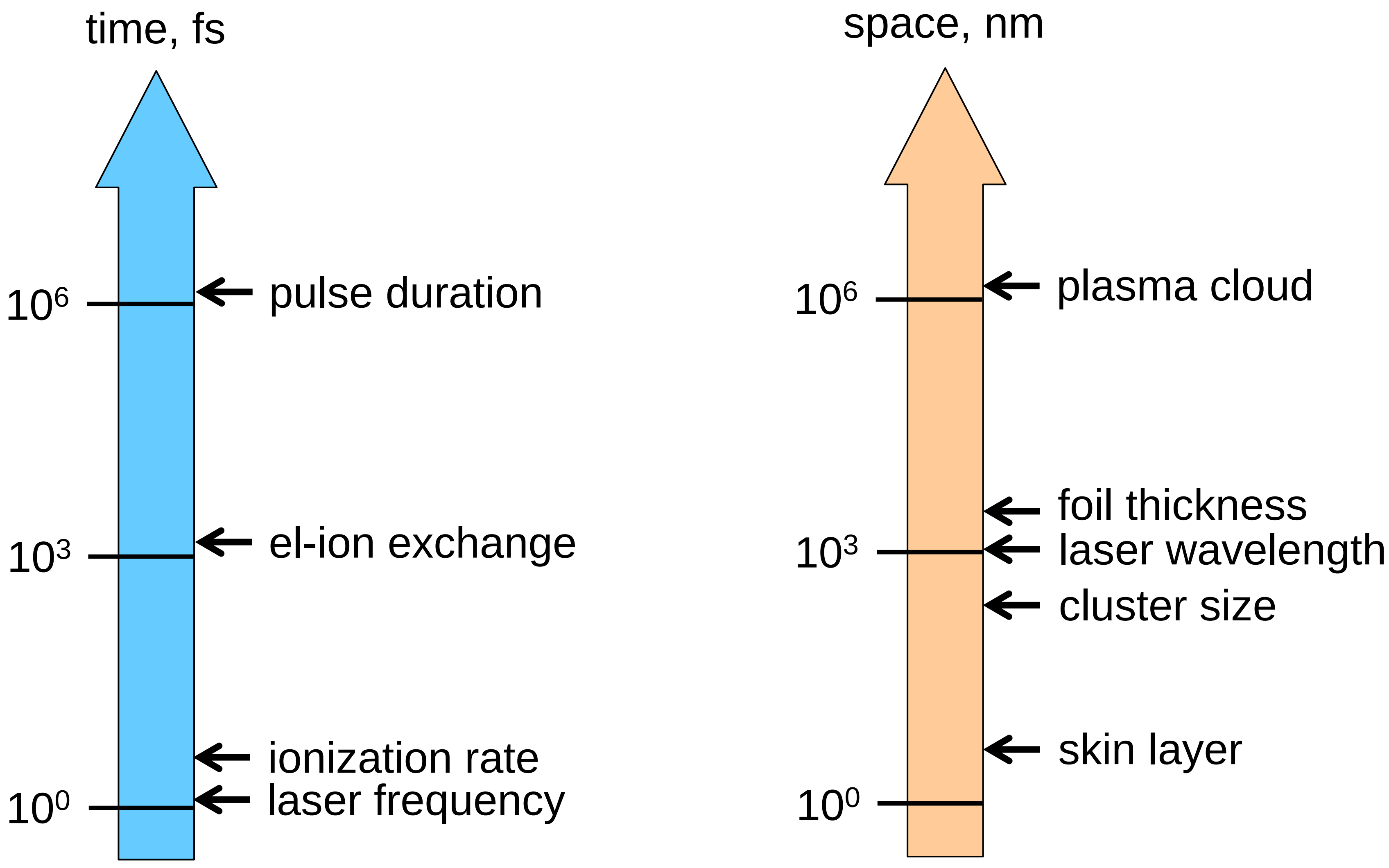
# Setup parameters & tasks

$\lambda$ = 1.053 mkm,
$\tau$ ~ 500 fs ÷10 ns,
$E$ ~ 200 ÷ 500 J,
$F$ ~ $10^{15}$ ÷ $10^{18}$ W/cm$^2$




Actual questions:
- warm dense matter
- increase absorption efficiency
- high temperature and ionization
- radiation loss

# Time & space scales for PHELIX setup



# Limitations of modeling

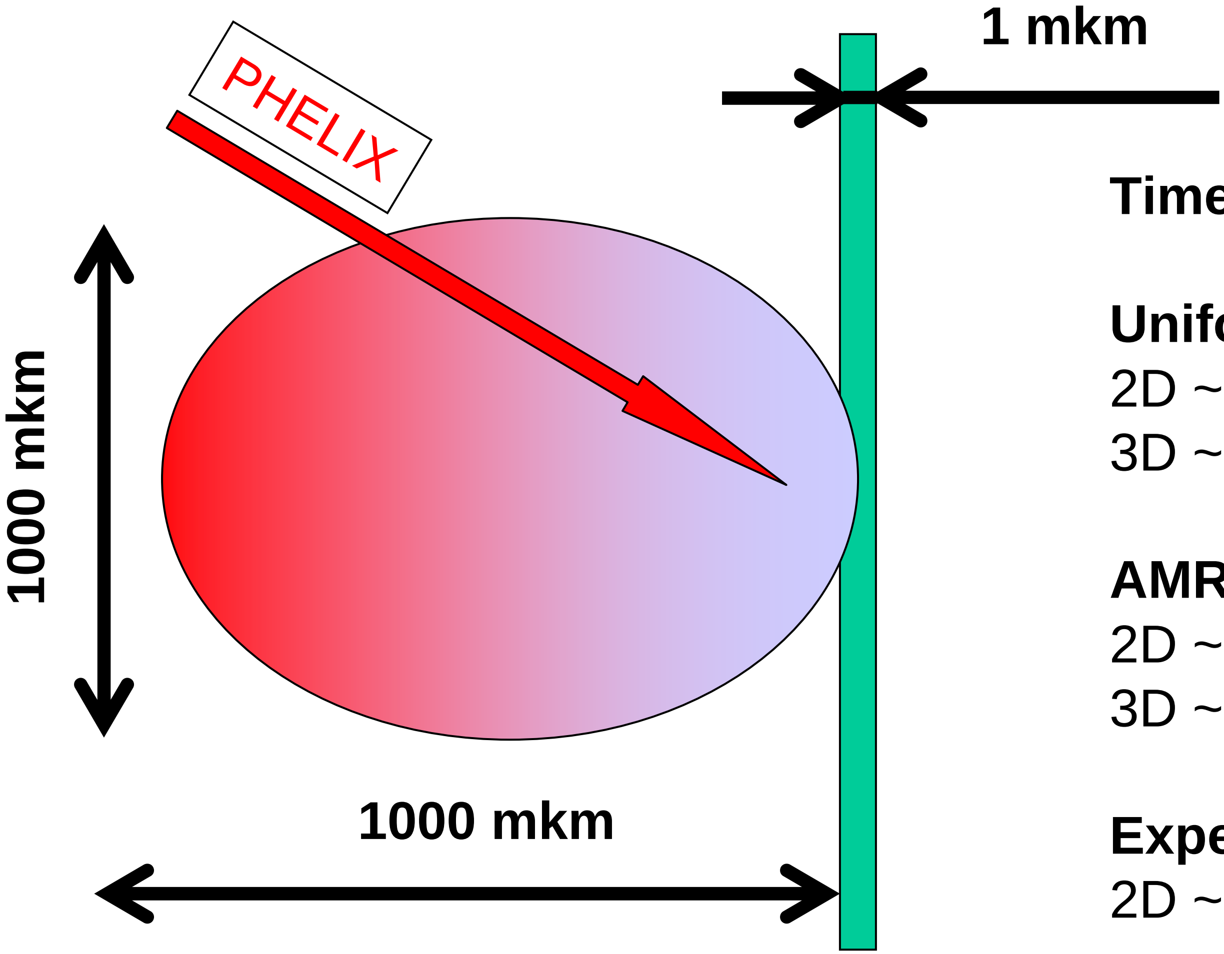
**QMC** ~ 100 particles

**MD** ~ 1 mkm$^3$ (~$10^5$ processors, Blue Gene etc.)

**Hydrodynamics** – real size systems, but…

…kinetic models

# Multiscale problem




**Time steps ~ $10^5$**

**Uniform mesh**

2D ~ $10^6 \div 10^8$ cells

3D ~ $10^9 \div 10^{12}$ cells

**AMR**

2D ~ $10^5 \div 10^7$ cells

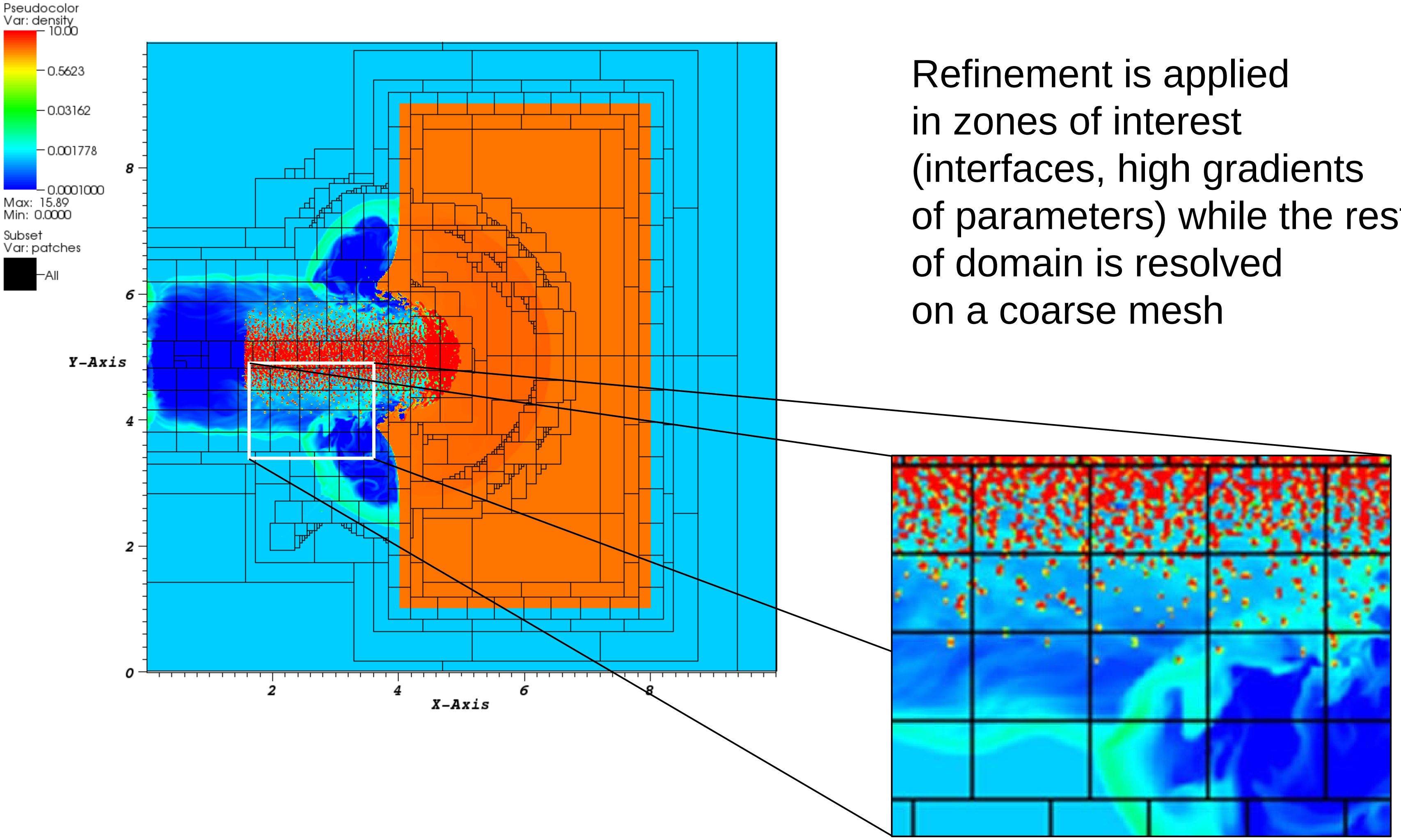
3D ~ $10^7 \div 10^{10}$ cells

**Expecting AMR profit**

2D ~ 10 times

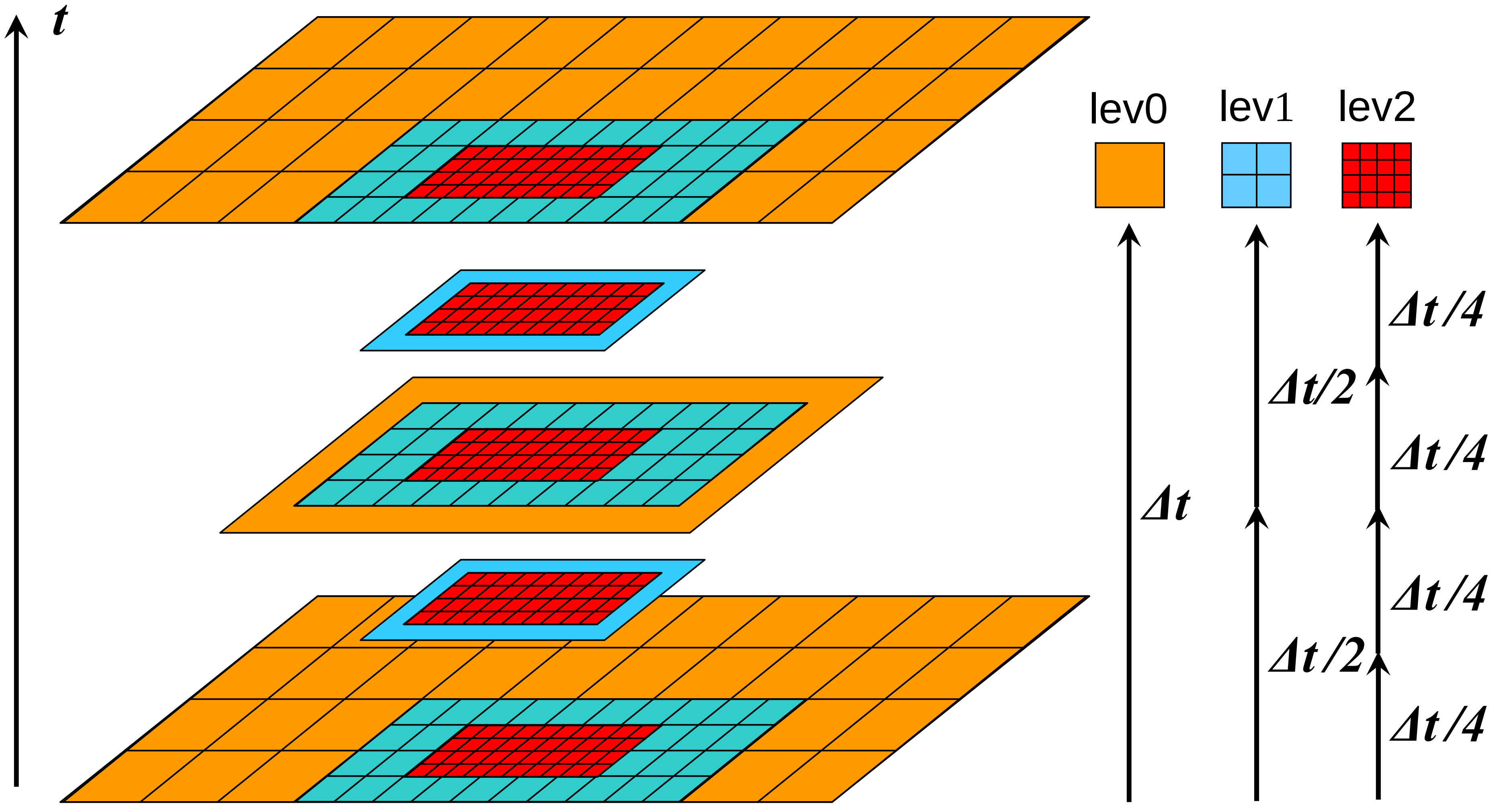
3D ~ 100 times

# Adaptive mesh refinement




Refinement is applied in zones of interest (interfaces, high gradients of parameters) while the rest of domain is resolved on a coarse mesh

# Advance in time (3 levels of AMR)



# Multiscale problem

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**Expected AMR profit**
**2D ~ 10 times**
**3D ~ 100 times**

# Two-temperature multi-material Eulerian hydrodynamics

## Basic equations

$$\frac{\partial f^\alpha}{\partial t} + \nabla\cdot(f^\alpha \mathbf{u}) = \frac{f^\alpha \overline{K}_S}{K_S^\alpha}\nabla\cdot\mathbf{u}$$

$$\frac{\partial (f^\alpha \rho^\alpha)}{\partial t} + \nabla\cdot(f^\alpha \rho^\alpha \mathbf{u}) = 0$$

$$\frac{\partial\left(\overline{\rho}\mathbf{u}\right)}{\partial t} + \nabla\cdot(\overline{\rho}\mathbf{u}\otimes\mathbf{u}) + \nabla\overline{P} = 0$$

$$\frac{\partial}{\partial t}\left[f^\alpha\rho^\alpha\left(E_e^\alpha + \frac{|\mathbf{u}|^2}{2}\right)\right] + \nabla\cdot\left[f^\alpha\rho^\alpha\left(E_e^\alpha + \frac{|\mathbf{u}|^2}{2}\right)\mathbf{u}\right] + \frac{f^\alpha\rho^\alpha}{\overline{\rho}}\nabla\overline{P}\cdot\mathbf{u} =$$
$$-\overline{P}_e\frac{f^\alpha\overline{K}_S}{K_S^\alpha}\nabla\cdot\mathbf{u} - f^\alpha Q_{ei}^\alpha + Q_L^\alpha + \frac{f^\alpha\rho^\alpha C_e^\alpha}{\overline{\rho}\overline{C}_e}\nabla\cdot(\overline{\kappa}_e\nabla\overline{T}_e) + f^\alpha Q_J + f^\alpha Q_{rad}$$

$$\frac{\partial\left(f^\alpha\rho^\alpha E_i^\alpha\right)}{\partial t} + \nabla\cdot(f^\alpha\rho^\alpha E_i^\alpha\mathbf{u}) = -\overline{P}_i\frac{f^\alpha\overline{K}_S}{K_S^\alpha}\nabla\cdot\mathbf{u} + f^\alpha Q_{ei}^\alpha$$

$$F_i^\alpha(\rho, T_i) \Rightarrow E_i^\alpha, C_i^\alpha, P_i^\alpha, K_{iS}^\alpha$$
$$F_e^\alpha(\rho, T_e) \Rightarrow E_e^\alpha, C_e^\alpha, P_e^\alpha, K_{eS}^\alpha$$

## Mixture model

$$\sum_\alpha f^\alpha = 1$$

$$\overline{\rho} = \sum_\alpha f^\alpha\rho^\alpha$$

$$\overline{C}_e = \frac{1}{\overline{\rho}}\sum_\alpha(f^\alpha\rho^\alpha C_e^\alpha)$$

$$1/\overline{K}_S = \sum_\alpha(f^\alpha/K_S^\alpha)$$

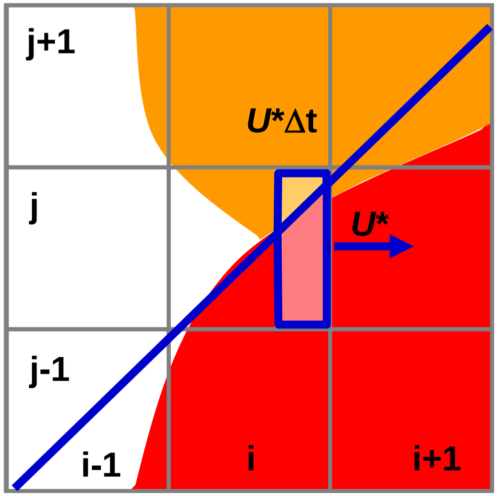
$$\overline{P} = \sum_\alpha\frac{f^\alpha P^\alpha}{K_S^\alpha}\Big/\sum_\alpha\frac{f^\alpha}{K_S^\alpha}$$

$$\overline{\rho}\overline{C}_e/\overline{\kappa}_e = \sum_\alpha(f^\alpha\rho^\alpha C_e^\alpha/\kappa_e^\alpha)$$

$$\overline{T} = \sum_\alpha f^\alpha\rho^\alpha C^\alpha T^\alpha\Big/\sum_\alpha f^\alpha\rho^\alpha C^\alpha$$

# Interface reconstruction algorithm

2D

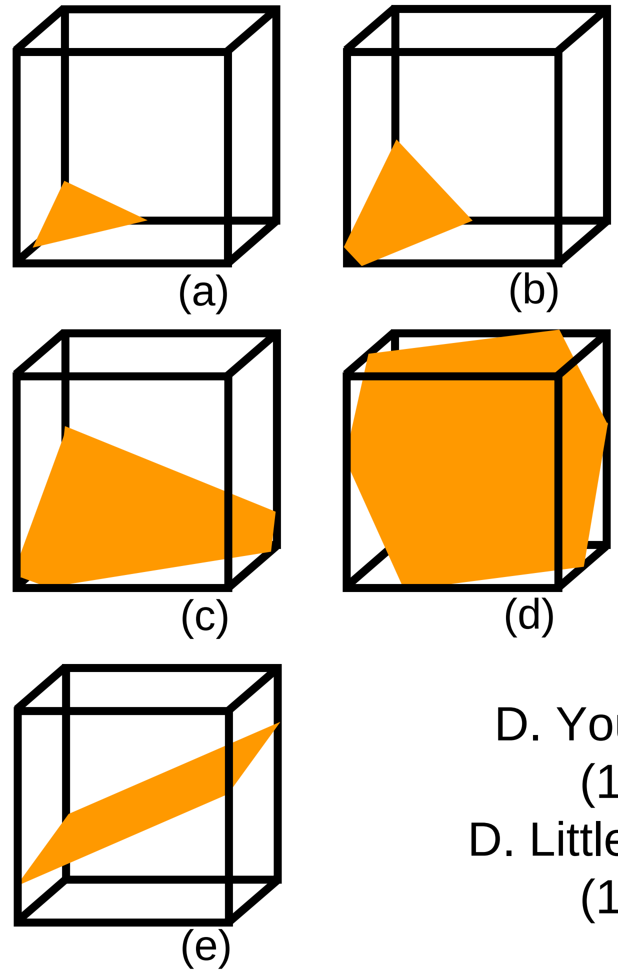



$$\min \sum_{l=i-1}^{i+1} \sum_{m=j-1}^{j+1} \left(f^{*\alpha}_{l,m} - f^{\alpha}_{l,m}\right)^2$$

$$f^{*\alpha}_{i,j} \equiv f^{\alpha}_{i,j}$$

Symmetric difference approximation or some norm minimization is used to determine unit normal vector

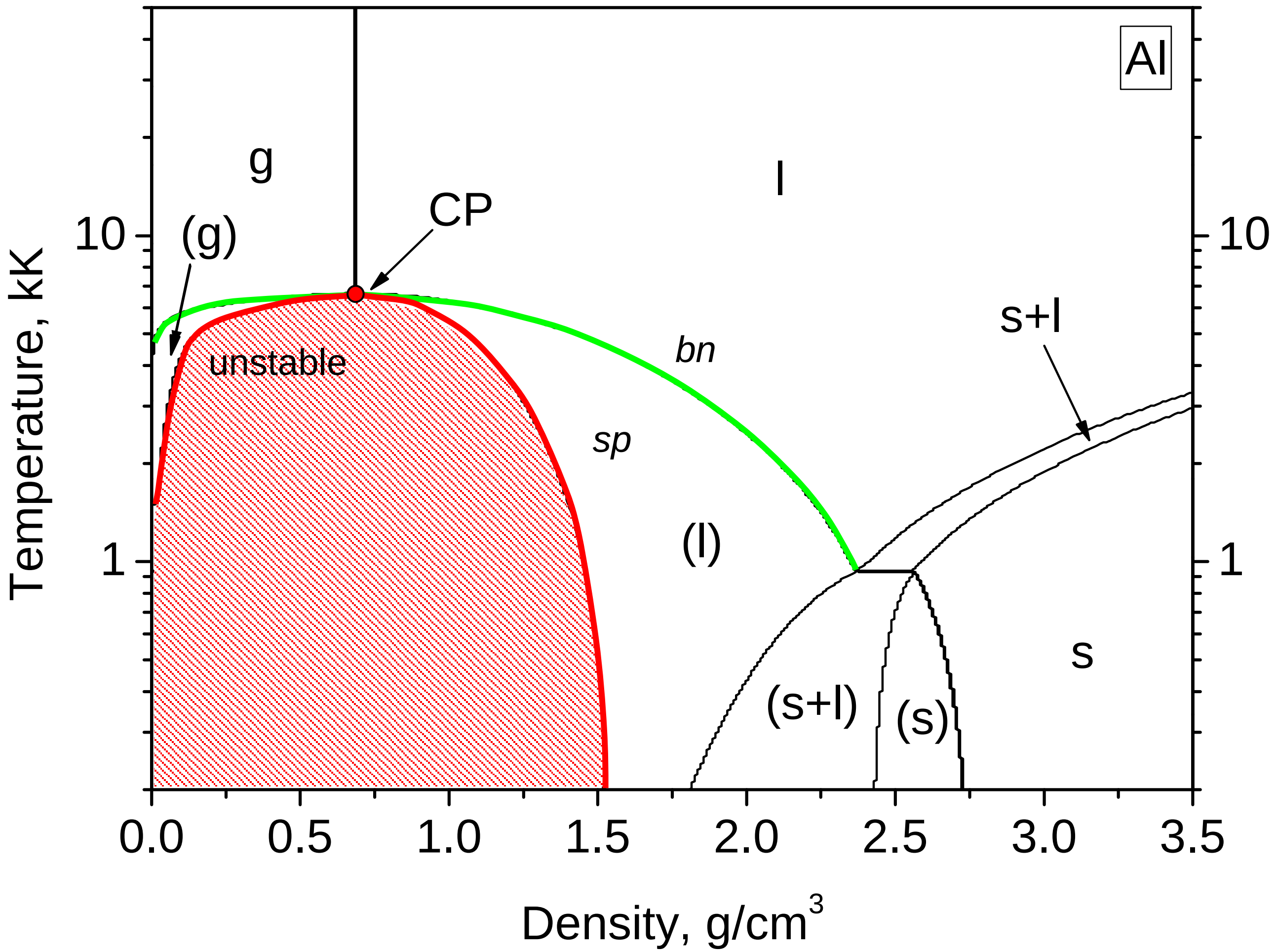
3D



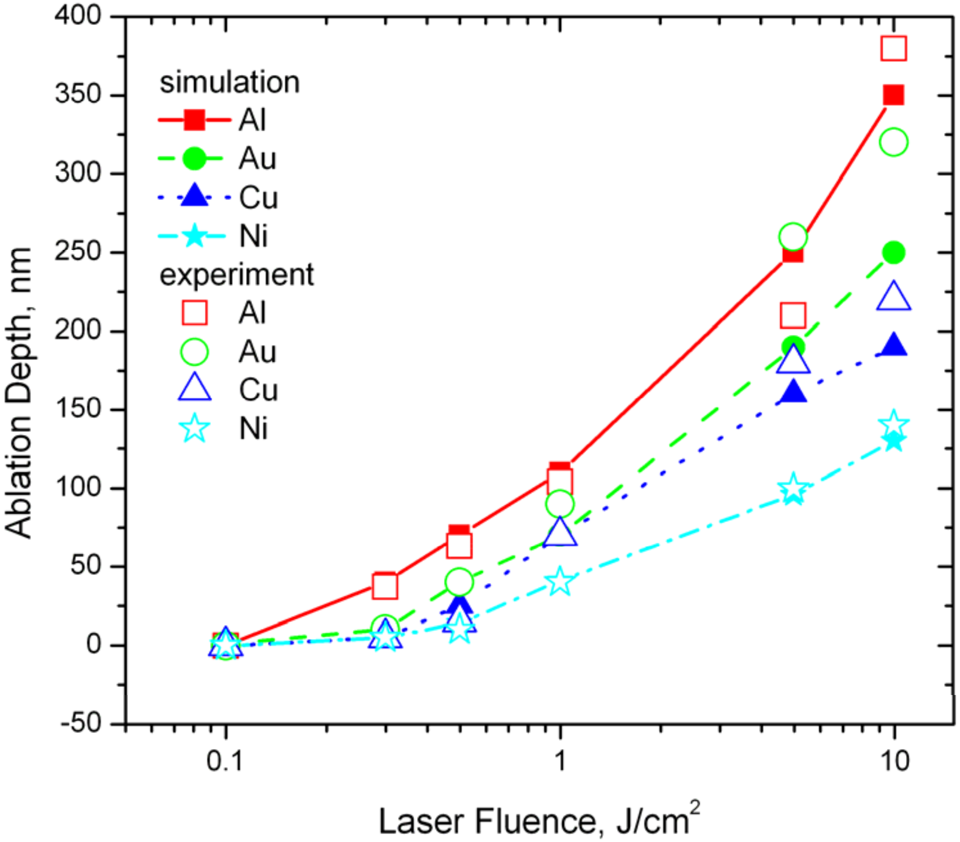

D. Youngs (1987)
D. Littlefield (1999)

Specific corner and specific orientation choice makes only five possible intersections of the cell

# Two-temperature semi-empirical EOS



# Ablation of metal targets by fs pulses

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M. E. Povarnitsyn *et al.* // Appl. Surf. Sci. **253**, 6343 (2007)
M. E. Povarnitsyn *et al.* // Appl. Surf. Sci. (in press, 2008)

# Extra effects in hot plasma

$$\nu_e = \min\left\{ \nu_{met}, \frac{\sqrt{\upsilon_F{}^2 + k_B T_e / m}}{r_0}, \nu_{hot} \right\}$$

$$Q_{ei} = \frac{3mk_B}{m_i} n_e \nu_e (T_e - T_i)$$

$$Q_L = I_L k_0 \operatorname{Im}\{\varepsilon\} \, | E / E_L |^2$$

$$Q_{rad} = \left( \frac{2\pi k_B T_e}{3m} \right)^{1/2} \frac{16\pi e^6}{3\pi\hbar mc^3} Z n_e^2$$

$$S_e = k_i n_e n_i \left( 1 - \frac{Z}{Z_{eq}} \right) \qquad k_i = A_3 \left( \frac{I_H}{I} \right)^{3/2} \exp\left( -\frac{I}{T_e} \right) \left( \frac{I}{T_e} \right)^{1/2} \left( 1 + \frac{I}{T_e} \right)^{-1}$$

# Model & code features

1. Multi-material hydrodynamics (several substances + phase transitions)

2. Two-temperature model ($T_e \neq T_i$)

3. Two-temperature equations of state (Khishchenko)

4. Wide-range models of el-ion collisions, conductivity, heat conductivity ($\nu$, $\sigma$, $\chi$)

5. Model of laser energy absorption (electromagnetic field)

6. Model of ionization & recombination (metals, dielectrics)

7. Model of radiation loss (bremsstrahlung + spectral radiation)

8. Parallel realization with AMR

# Model & code features

1. Multi-material hydrodynamics (several substances + phase transitions)
2. Two-temperature model (Te $\neq$ Ti)
3. Two-temperature equations of state (Khishchenko)
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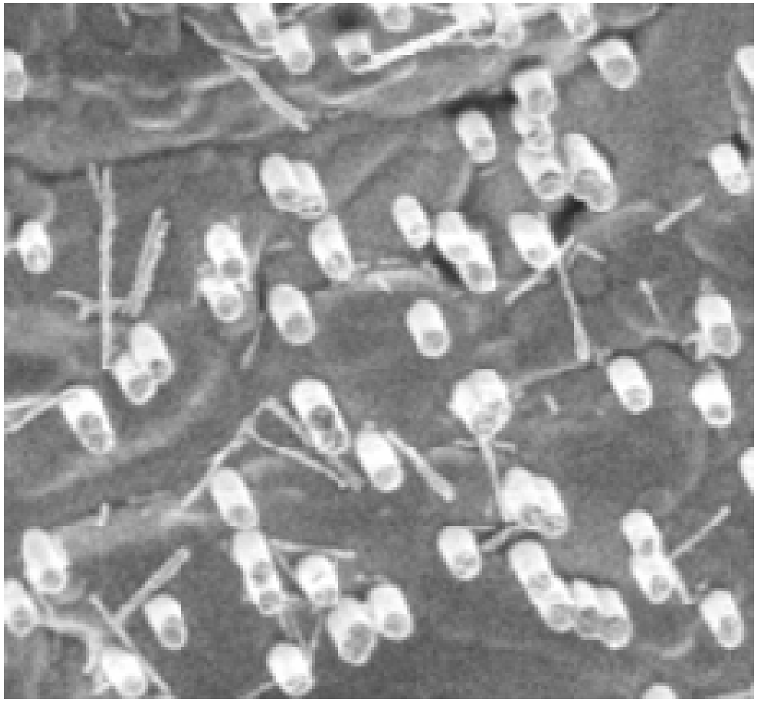
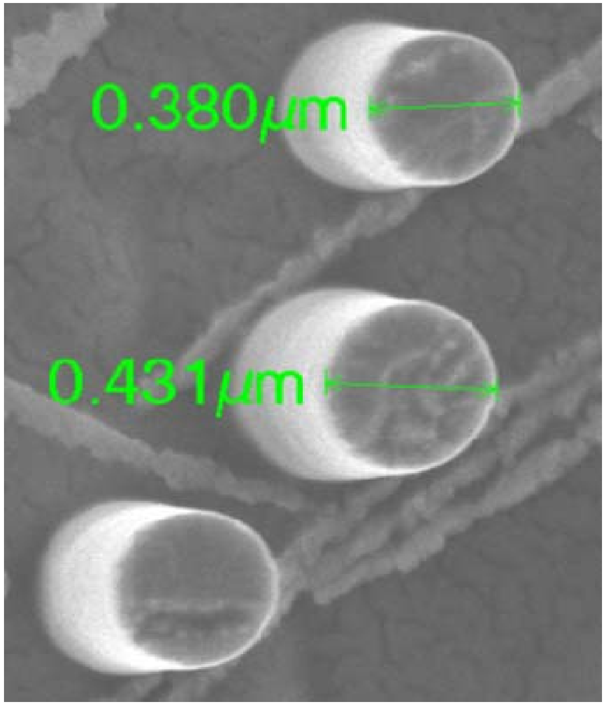
# Nanostructured Cu target





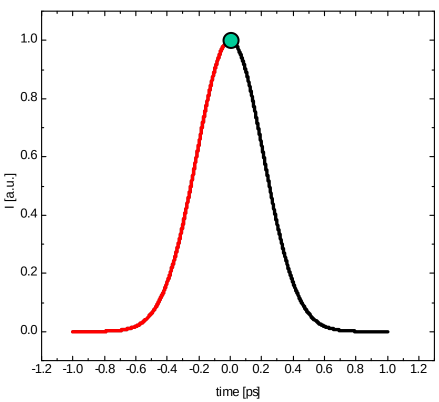

Material research Department GSI

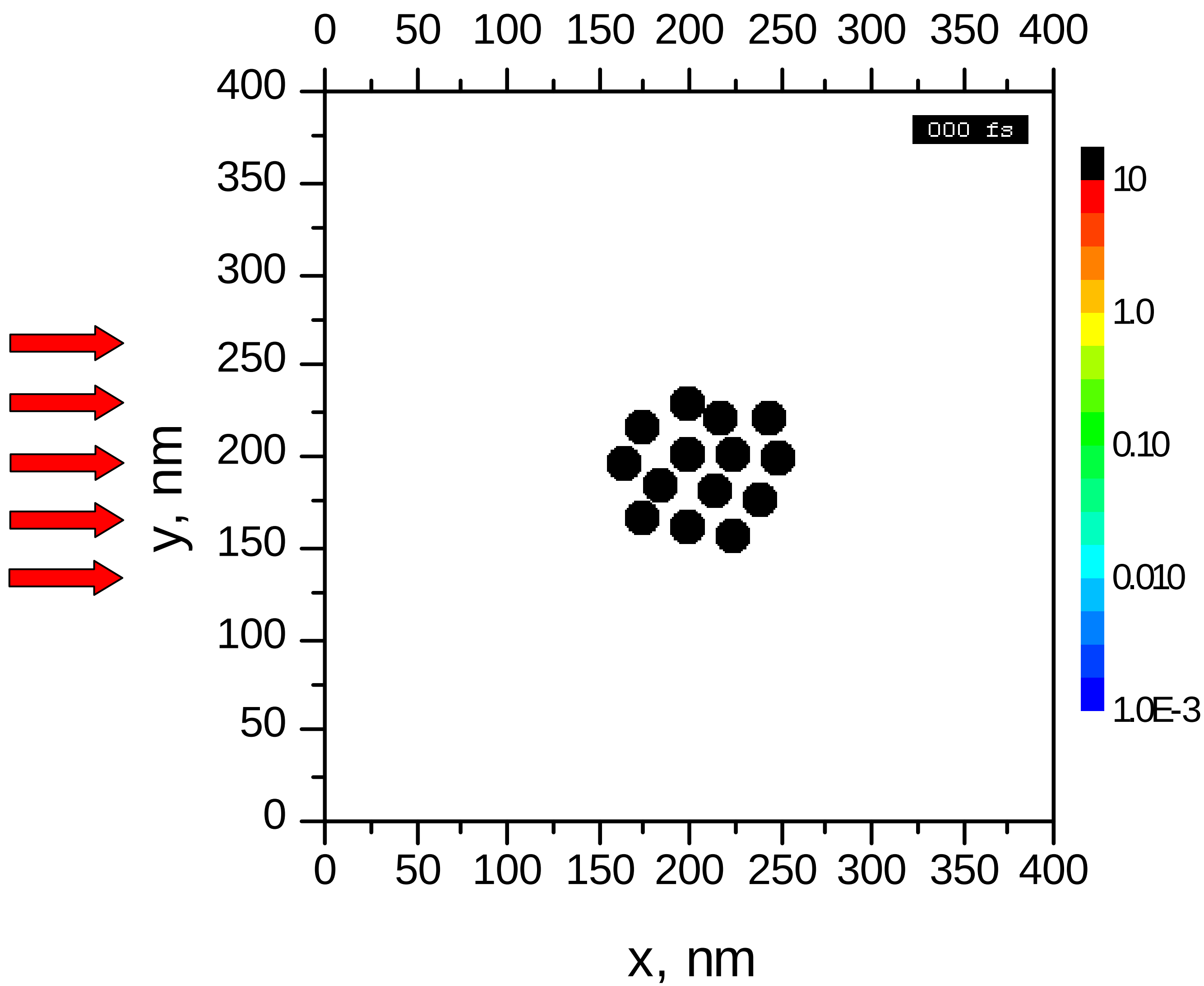
# Interaction with Cu clusters ($n_e/n_{cr}$)

$\lambda$ = 1.053 mkm

$I_0 = 10^{17}$ W/cm$^2$

$\tau$ = 500 fs




| | #14 |
|---|---|
| ρ [g/cc] | 2.8 |
| $T_e$ [ev] | 620 |
| $T_i$ [ev] | 75 |

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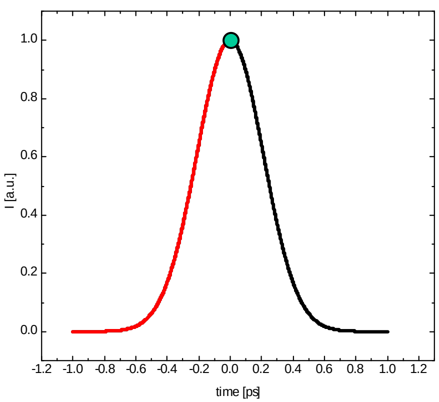


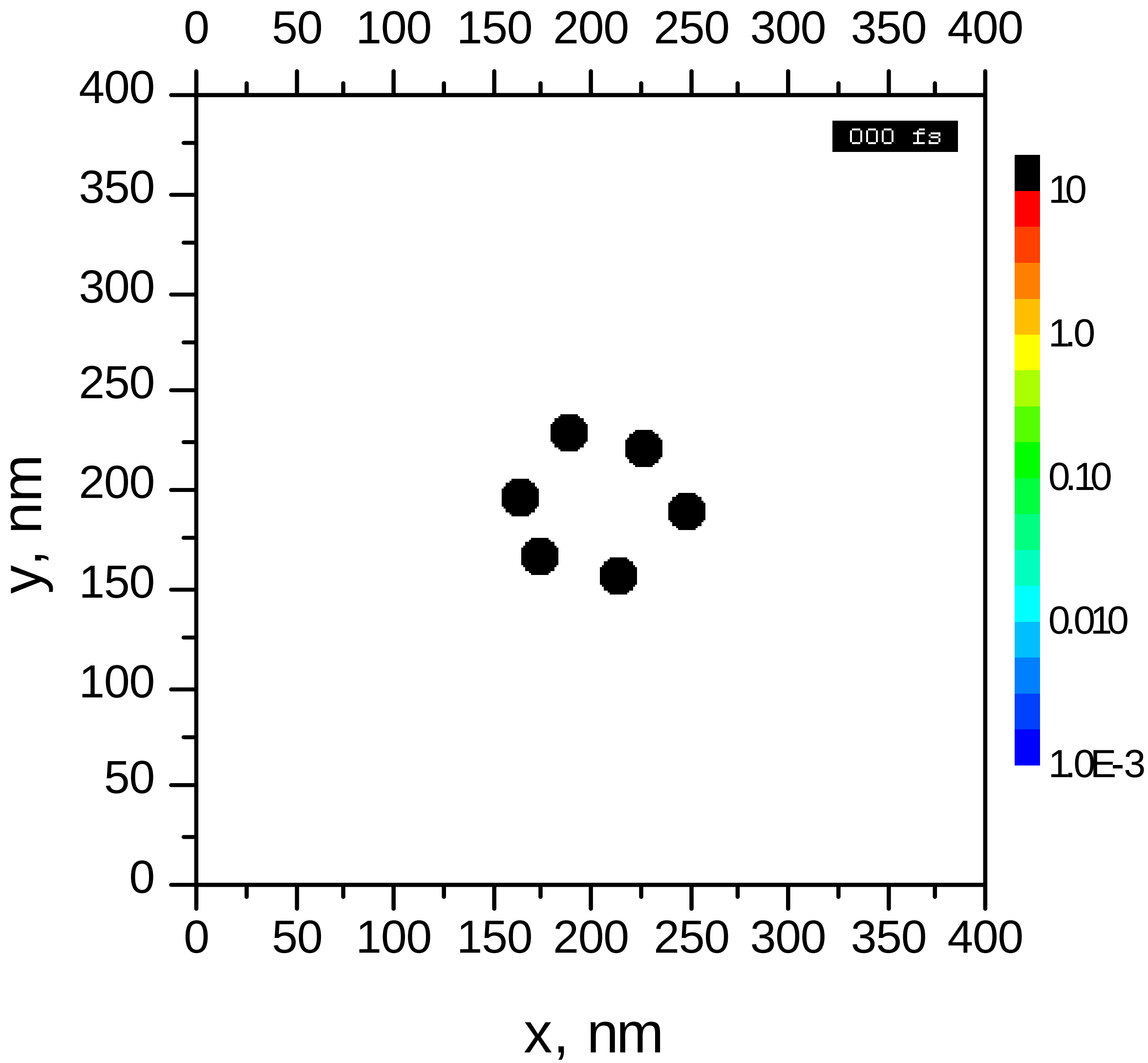


| | #14 | #6 |
|---|---|---|
| $\rho$ [g/cc] | 2.8 | 1 |
| $T_e$ [ev] | 620 | 970 |
| $T_i$ [ev] | 75 | 60 |

# Conclusions and Outlook

- Simulation results are sensitive to the models used: absorption, thermal conductivity, electron-ion collisions, EOS, etc…
- Interaction with cluster targets can produce warm dense matter with exceptional parameters
- Adaptive mesh refinement can give an essential profit in runtime and work memory used
- For 2D and 3D simulation of PHELIX experiments we develop hydro-electro code with AMR and in parallel
- Multidimensional calculations with AMR and in parallel are in sight