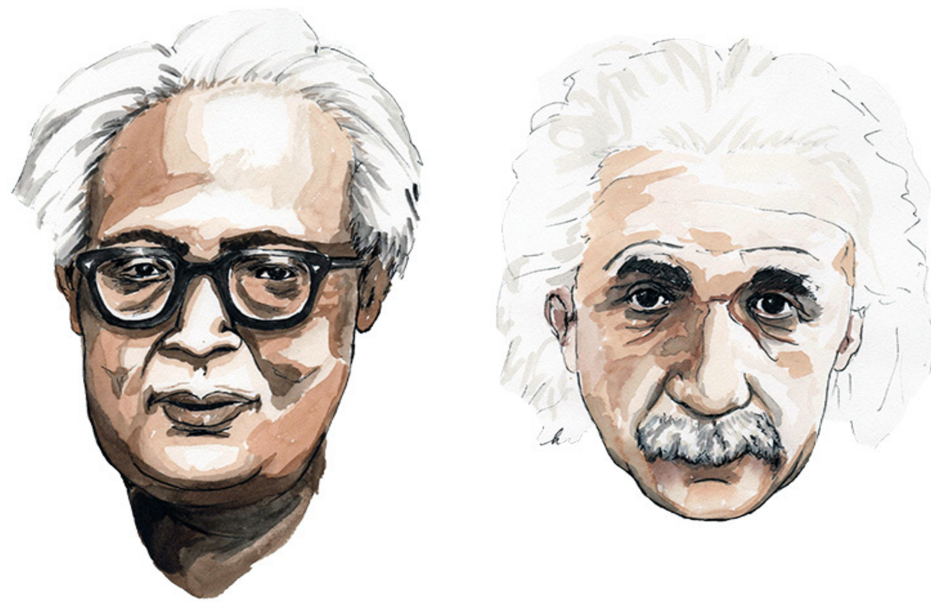
A hybrid code for solving the Gross-Pitaevskii equation



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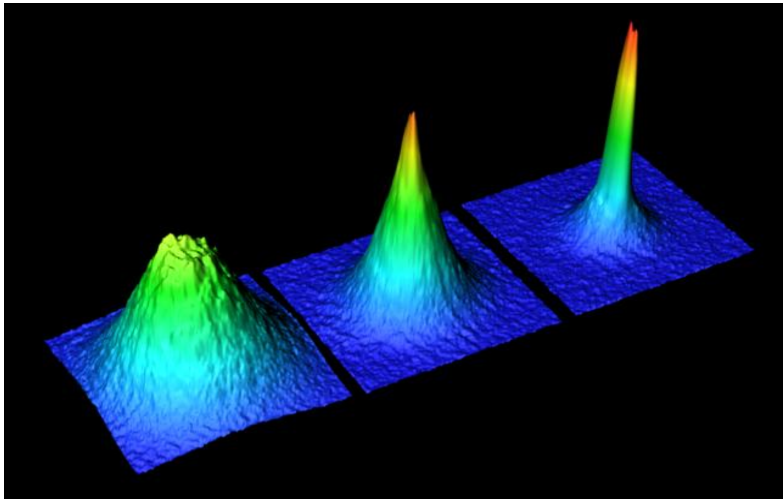
Plan

- Physical context and model
- Numerical methods
- HPC
- Benchmarks
- Conclusions

Bose–Einstein condensate



Prediction:

- ✓ **1924: Bose and Einstein**

Detection:

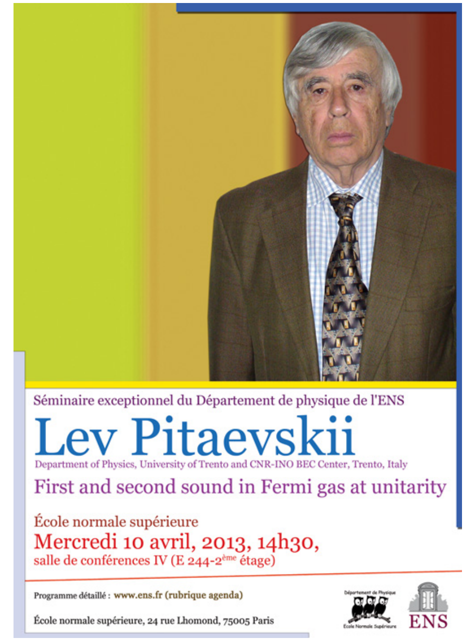
- ✓ **1937: Superfluid Hélium,** *Kapitsa (Nobel, 1978) /= atomic gases*

Strike:

- ✓ **1995: Condensation of atomic gases, 1***995 Cornell et Wieman (Rubidium), following Ketterle (Sodium), (Nobel-2001)*

Gross-Pitaevskii equation

EUGENE P. GROSS
1926–1991

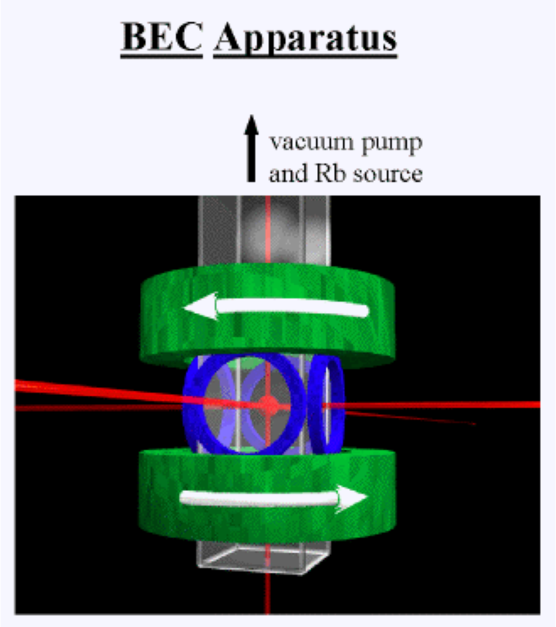


Hypothesis :

- ✓ **No temperature;**
- ✓ **Low density gas;**
- ✓ **Interaction model macroscopic way (mean field theory);**
- ✓ **All particles in same quantic state.**

Gross-Pitaevskii equation

$$\imath\frac{\partial}{\partial t}\psi(\mathbf{x},t) = (-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta|\psi(\mathbf{x},t)|^2 - \Omega L_z)\psi(\mathbf{x},t)$$



- ✓ <0 , attractive
- ✓ = 0, no interaction
- ✓ > 0, repulsive
- ✓ | | >> 1, strong interaction, if > 10 Thomas-Fermi (Ground State).

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Stationary state: Normalized gradient flow

$$\frac{\partial}{\partial t}\phi(\mathbf{x},t) = \left(\frac{1}{2}\nabla^2 + \Omega L_z - V(\mathbf{x}) - \beta|\phi(\mathbf{x},t)|^2\right)\phi(\mathbf{x},t) \quad x \in \mathcal{D},\ t \in (t_n, t_{n+1}),$$

$$\phi(\mathbf{x}, t_{n+1}^{+}) = \frac{\phi(\mathbf{x}, t_{n+1}^{-})}{||\phi(\cdot, t_{n+1}^{-})||}$$

1°) *Semi-implicit Backward Euler :*

2°) *Full non-linear method with Crank-Nicolson :*

3°) *Explicit Euler with Sobolev preconditioner* :

Time evolution :

$$\imath\frac{\partial}{\partial t}\psi(\mathbf{x},t) = (-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta|\psi(\mathbf{x},t)|^2 - \Omega L_z)\psi(\mathbf{x},t)$$

1. *ADI-Time splitting method (Lie order 1, Strang order 2)*
2. *Crank-Nicolson*
3. *Relaxation, based on Crank-Nicolson*

Two-components:
Stationary state: Normalized gradient flow

$$\frac{\partial\phi_1}{\partial t} = \left[\frac{1}{2d_1}\nabla^2 - V_{t1}(\mathbf{x},t) - \beta_{11}|\phi_1|^2 - \beta_{12}|\phi_2|^2\right]\phi_1,$$

$$\frac{\partial\phi_2}{\partial t} = \left[\frac{1}{2d_2}\nabla^2 - V_{t2}(\mathbf{x},t) - \beta_{21}|\phi_1|^2 - \beta_{22}|\phi_2|^2\right]\phi_2.$$

1°) *Semi-implicit Backward Euler*

$$\phi_i(\mathbf{x},t_{n+1}) = \frac{\phi_i^*(\mathbf{x},t_{n+1})}{\|\phi_i^*(\mathbf{x},t_{n+1})\|}.$$

2°) *Full non-linear method with Crank-Nicolson :*

Time evolution :

$$\frac{\partial\psi}{\partial t} = (A+B)\psi \Longrightarrow \psi(x,t+\delta t) = e^{(A+B)\delta t}\psi(x,t)$$

$$\approx e^{A\delta t}e^{B\delta t}\psi(x,t) \quad \text{(Lie, 1st order)}$$

$$\approx e^{A\delta t/2}e^{B\delta t}e^{A\delta t/2}\psi(x,t) \quad \text{(Strang, 2nd order)}$$

$$A_1 = i\frac{1}{2d_1}\nabla^2, \quad B_1 = -i\left[V_{t1}(\mathbf{x},t) + \beta_{11}|u_1|^2 + \beta_{12}|u_2|^2\right],$$

$$A_2 = i\frac{1}{2d_2}\nabla^2, \quad B_2 = -i\left[V_{t2}(\mathbf{x},t) + \beta_{21}|u_1|^2 + \beta_{22}|u_2|^2\right].$$

1. *ADI-Time splitting method (Lie order 1, Strang order 2)*
2. *Crank-Nicolson*
3. *Relaxation, based on Crank-Nicolson*

Stationary state

Initial conditions

- **Low interaction** *:* $\phi_0(\mathbf{x}) = \dfrac{(1-\Omega)\phi_{h0}(\mathbf{x}) + \Omega\phi_{h0}^{v}(\mathbf{x})}{\|(1-\Omega)\phi_{h0}(\mathbf{x}) + \Omega\phi_{h0}^{v}(\mathbf{x})\|}$

$$\phi_{h0}(\mathbf{x}) = \frac{1}{\pi^{d/4}}\begin{cases}(\gamma_x\gamma_y)^{0.25}e^{-\frac{\gamma_x x^2+\gamma_y y^2}{2}} \\ (\gamma_x\gamma_y\gamma_z)^{0.25}e^{-\frac{\gamma_x x^2+\gamma_y y^2 \gamma_z z^2}{2}}\end{cases},\ \phi_{h0}^{v}(\mathbf{x}) = \frac{1}{\pi^{d/4}}\begin{cases}(\gamma_x\gamma_y)^{0.25}(\gamma_x x + \imath\gamma_y y)e^{-\frac{\gamma_x x^2+\gamma_y y^2}{2}} & d=2 \\ (\gamma_x\gamma_y\gamma_z)^{0.25}(\gamma_x x + \imath\gamma_y y)e^{-\frac{\gamma_x x^2+\gamma_y y^2 \gamma_z z^2}{2}} & d=3\end{cases}$$

- **Strong interaction (Thomas Fermi), Ground state** *:*

$$\phi_0^{TF}(\mathbf{x}) = \begin{cases}\sqrt{\mu_0^{TF} - V(\mathbf{x})/\beta}, & V(\mathbf{x}) < \mu_0^{TF} \\ 0, & \text{otherwise}\end{cases},\ \mu_0^{TF} = \frac{1}{2}\begin{cases}(4\beta\gamma_x\gamma_y/\pi)^{1/2}, & \mathrm{d}=2 \\ (15\beta\gamma_x\gamma_y\gamma_z/4\pi)^{2/5}, & \mathrm{d}=3\end{cases}$$

Time evolution

- **Stationary state solution enough converged.**

Potentials :

1. *Harmonic*

$$V(\mathbf{x}) = \begin{cases} \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2), \\ \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2). \end{cases}$$

2. *Harmonic-Plus-Quartic-Cylindric*

$$V(\mathbf{x}) = \begin{cases} \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) + \frac{\kappa}{4}(\gamma_x^2 x^2 + \gamma_y^2 y^2)^2, \\ \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2) + \frac{\kappa}{4}(\gamma_x^2 x^2 + \gamma_y^2 y^2)^2. \end{cases}$$

3. *Harmonic-Plus-Quartic-Spheric*

$$V(\mathbf{x}) = \begin{cases} \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) + \frac{\kappa}{4}(\gamma_x^2 x^2 + \gamma_y^2 y^2)^2, \\ \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2) + \frac{\kappa}{4}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2)^2. \end{cases}$$

4. *Harmonic-Plus-Sin* (optical)

$$V(\mathbf{x}) = \begin{cases} \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) + \frac{a_1}{2} sin(\frac{\pi x}{d_1})^2 + \frac{a_2}{2} sin(\frac{\pi y}{d_2})^2, \\ \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2) + \frac{a_1}{2} sin(\frac{\pi x}{d_1})^2 + \frac{a_2}{2} sin(\frac{\pi y}{d_2})^2 \frac{a_3}{2} sin(\frac{\pi z}{d_3})^2. \end{cases}$$

5. *Harmonic-Plus-Double-Well*

$$V(\mathbf{x}) = \begin{cases} \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) + V_0 e^{\frac{-x^2}{2d^2}}, \\ \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2) + V_0 e^{\frac{-x^2}{2d^2}}. \end{cases}$$

6. *Harmonic-Plus-1D-Optical-Lattice*

$$V(\mathbf{x}) = \frac{(1-\alpha)}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2) + V_0 sin(\pi z/d)^2.$$

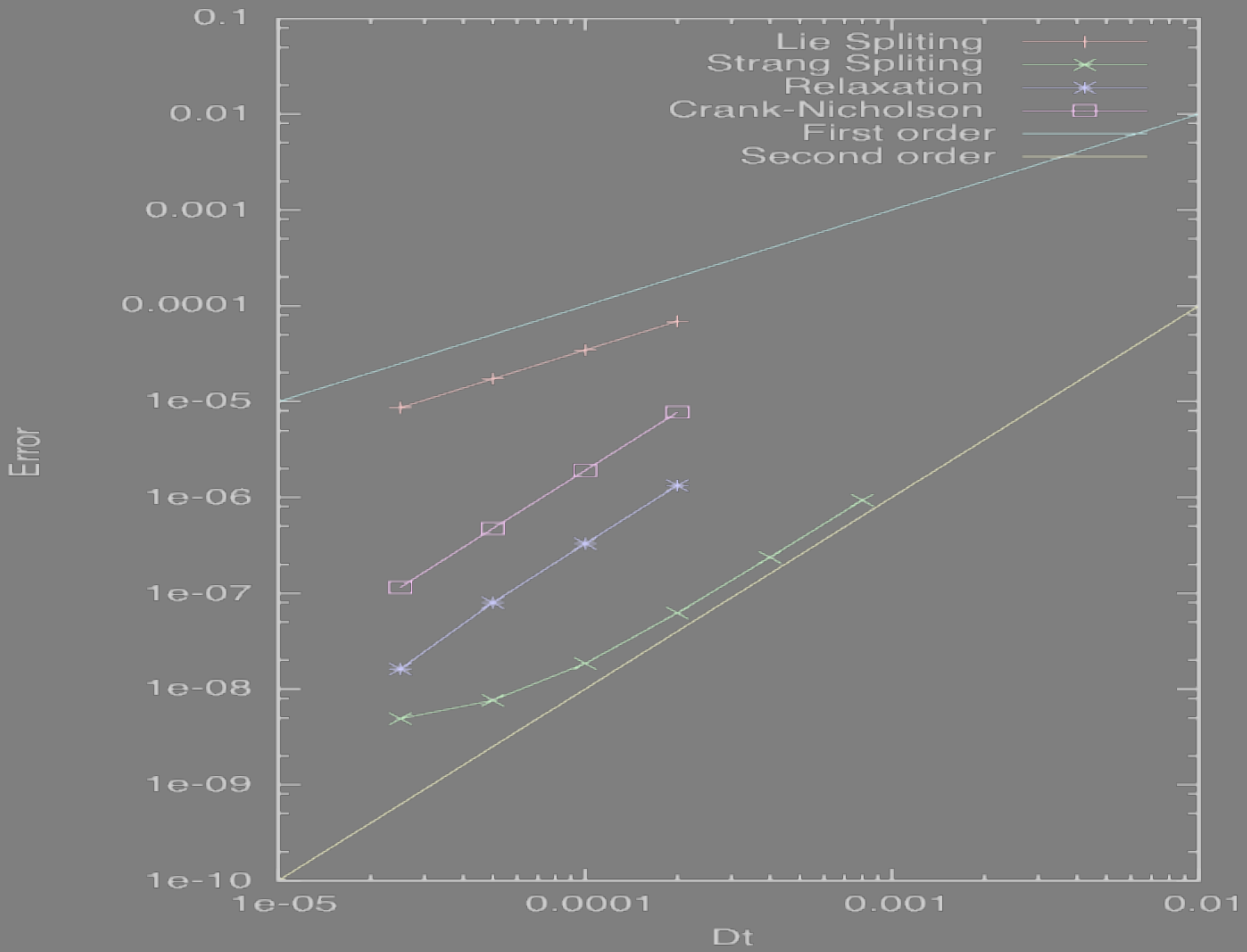
Discretization, boundary condition …

Pseudo spectral approximation:
FFT (FFTW-1D) or Compact schemes.

Boundaries conditions :
Periodic, Dirichlet.

Linear solvers :
BiCGStab , GCR, Newton-Raphson

Only One external library: Easier to install and to compile !



Lie Spliting
Strang Spliting
Relaxation
Crank-Nicholson
First order
Second order
Error
Dt
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
1e-09
1e-10
1e-05
0.0001
0.001
0.01

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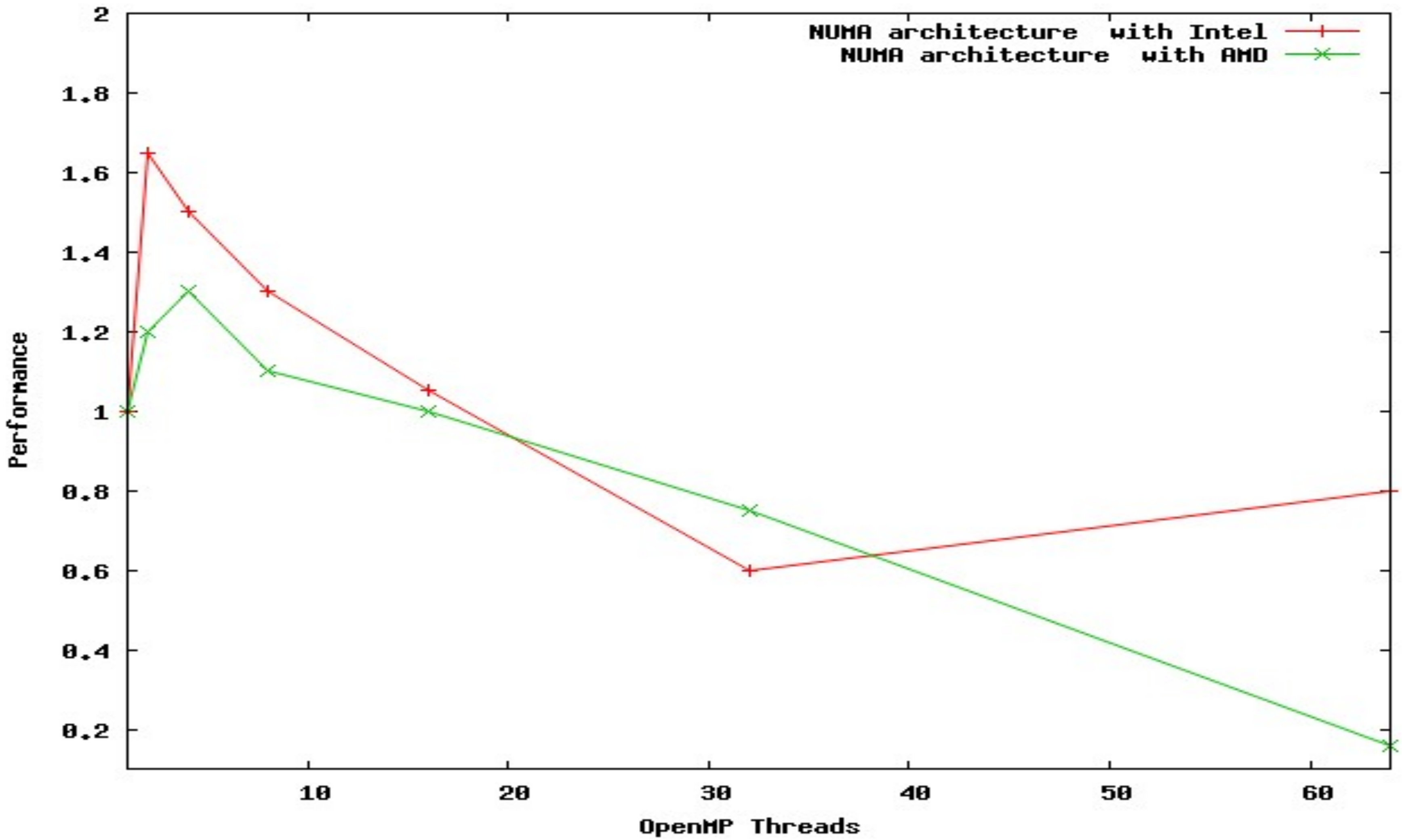
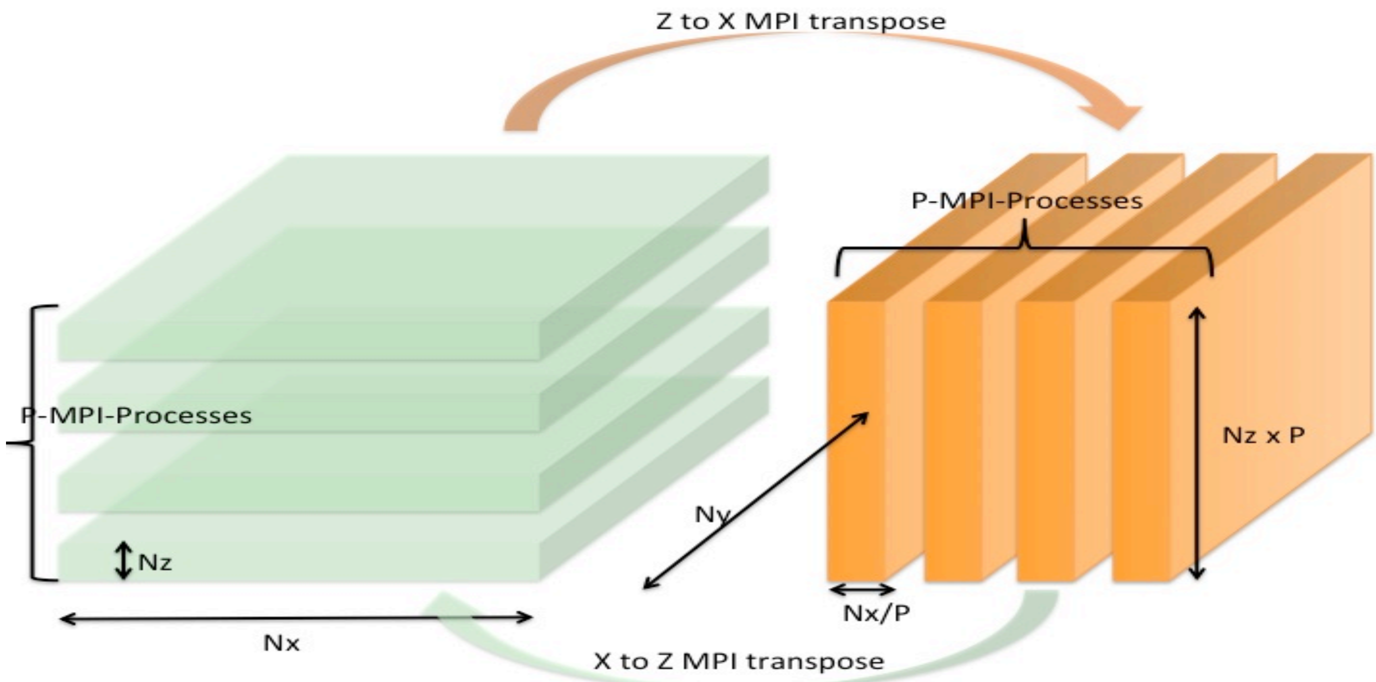
OpenMP scalability, Case 2D (512x512),

sequentiel: 1 week for converge results
, OpenMP: 1 day at worst !



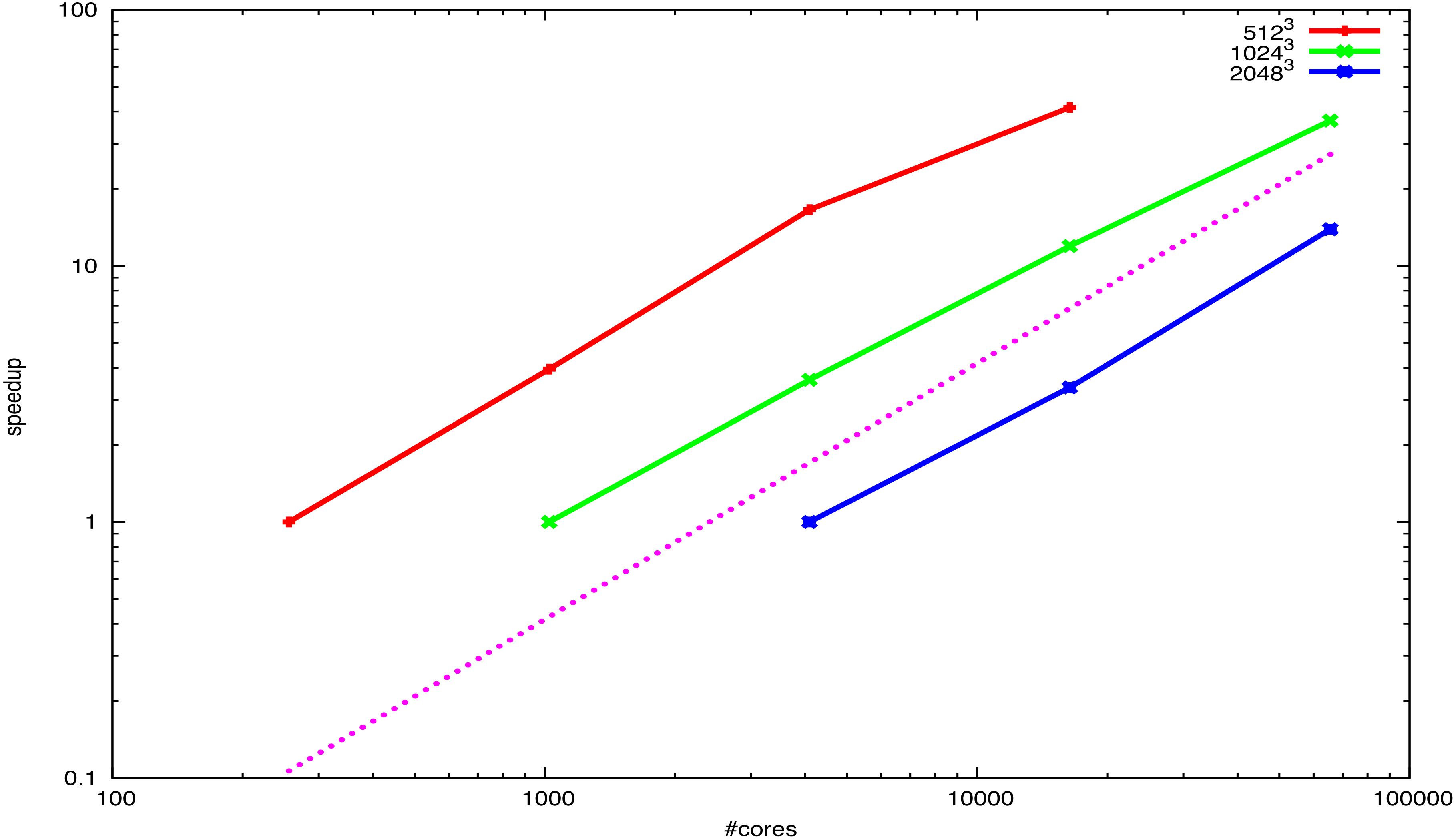
Hybrid MPI-OpenMP parallelization

"Slab decomposition"

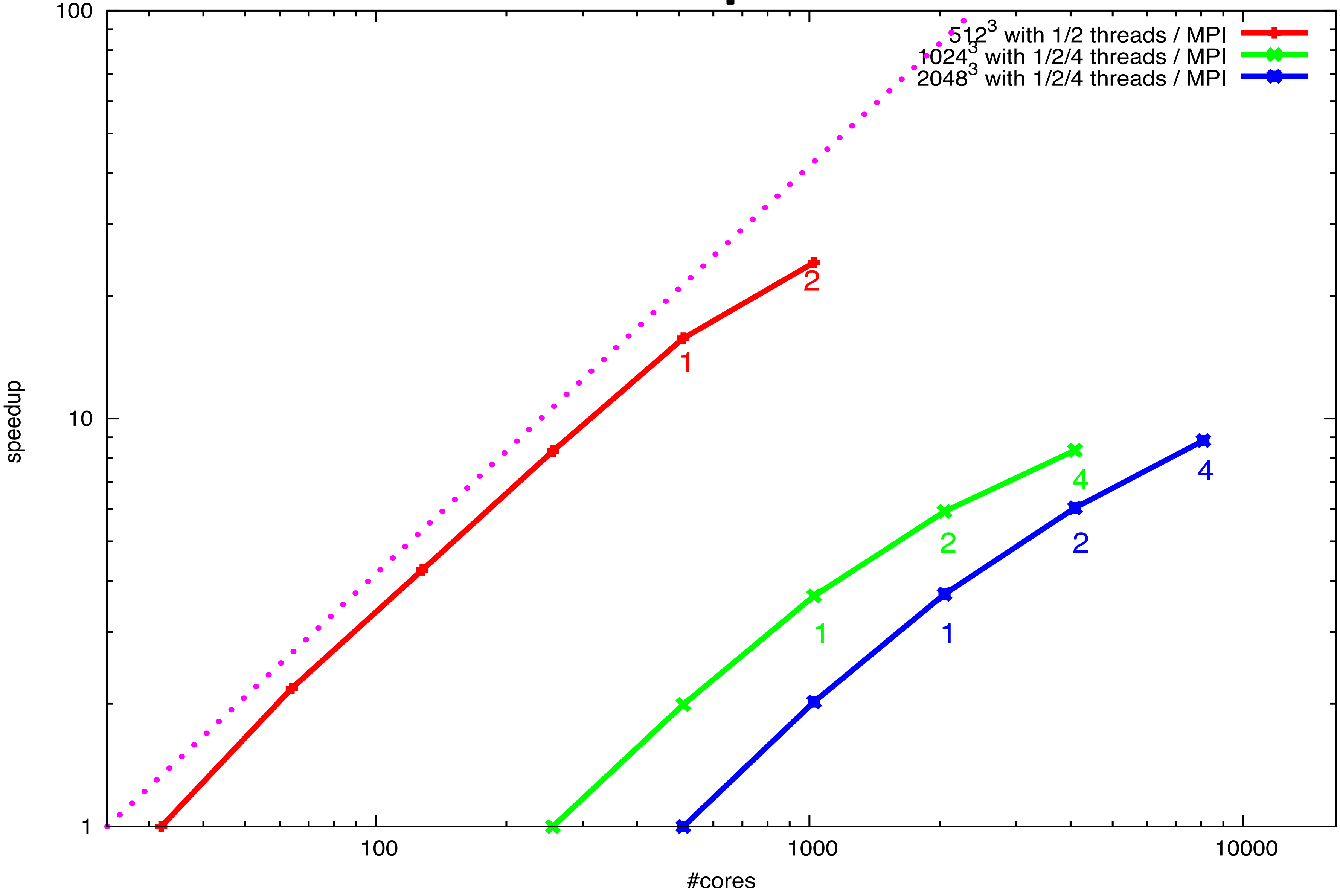


Non-blocking collective communication implemented (LibNBC/MPI-3).

Scalability MPI alone: Slab decomposition

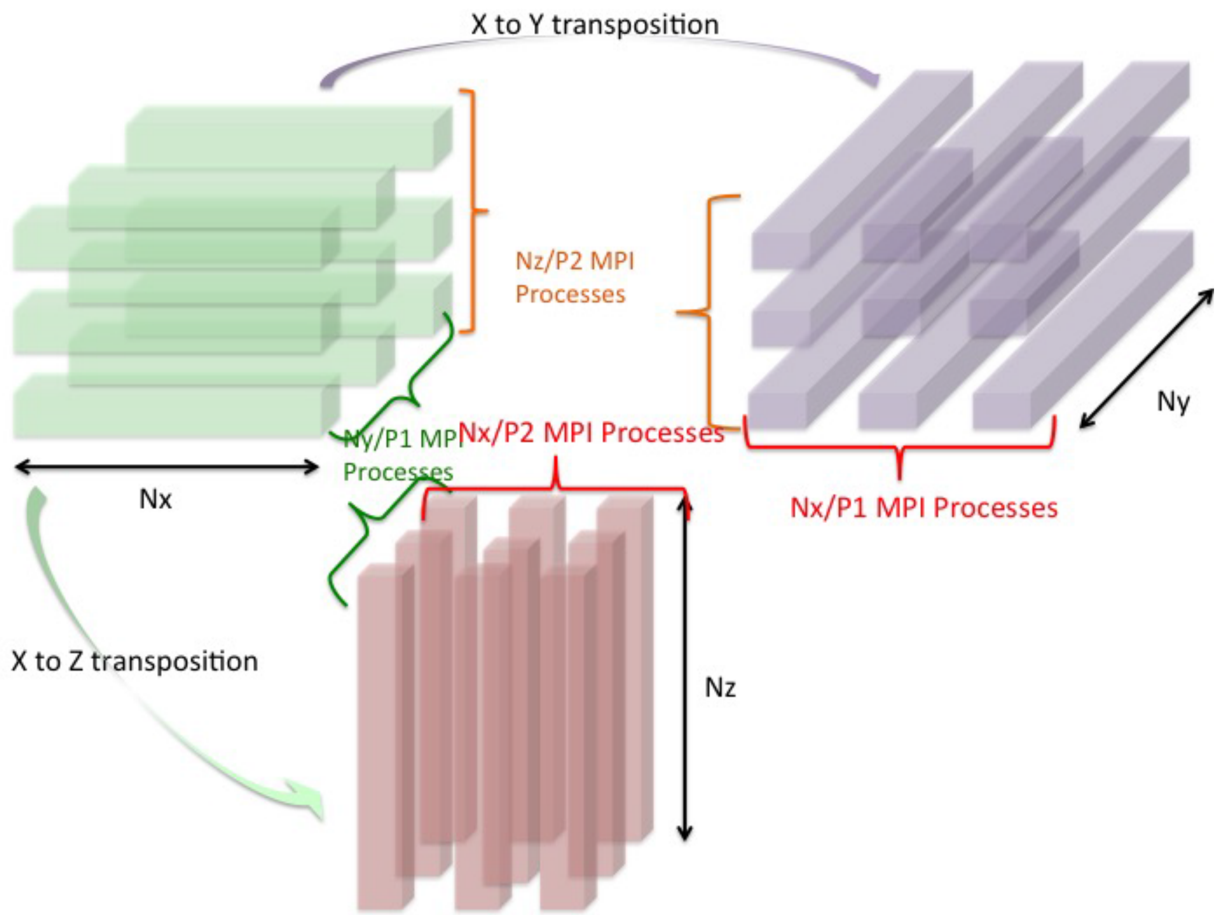


Scalability MPI+OpenMP: Slab decomposition

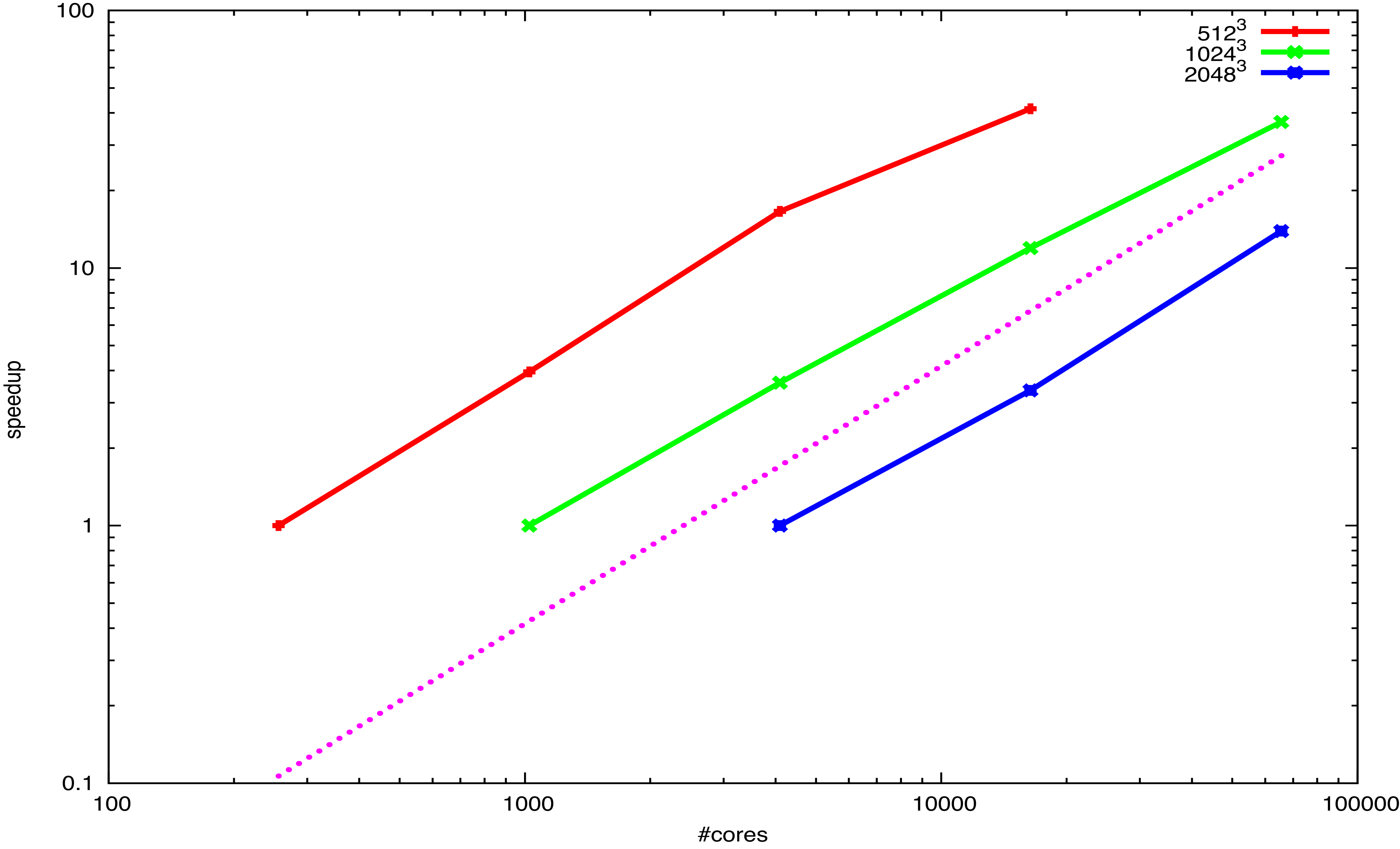


Hybrid MPI-OpenMP parallelization

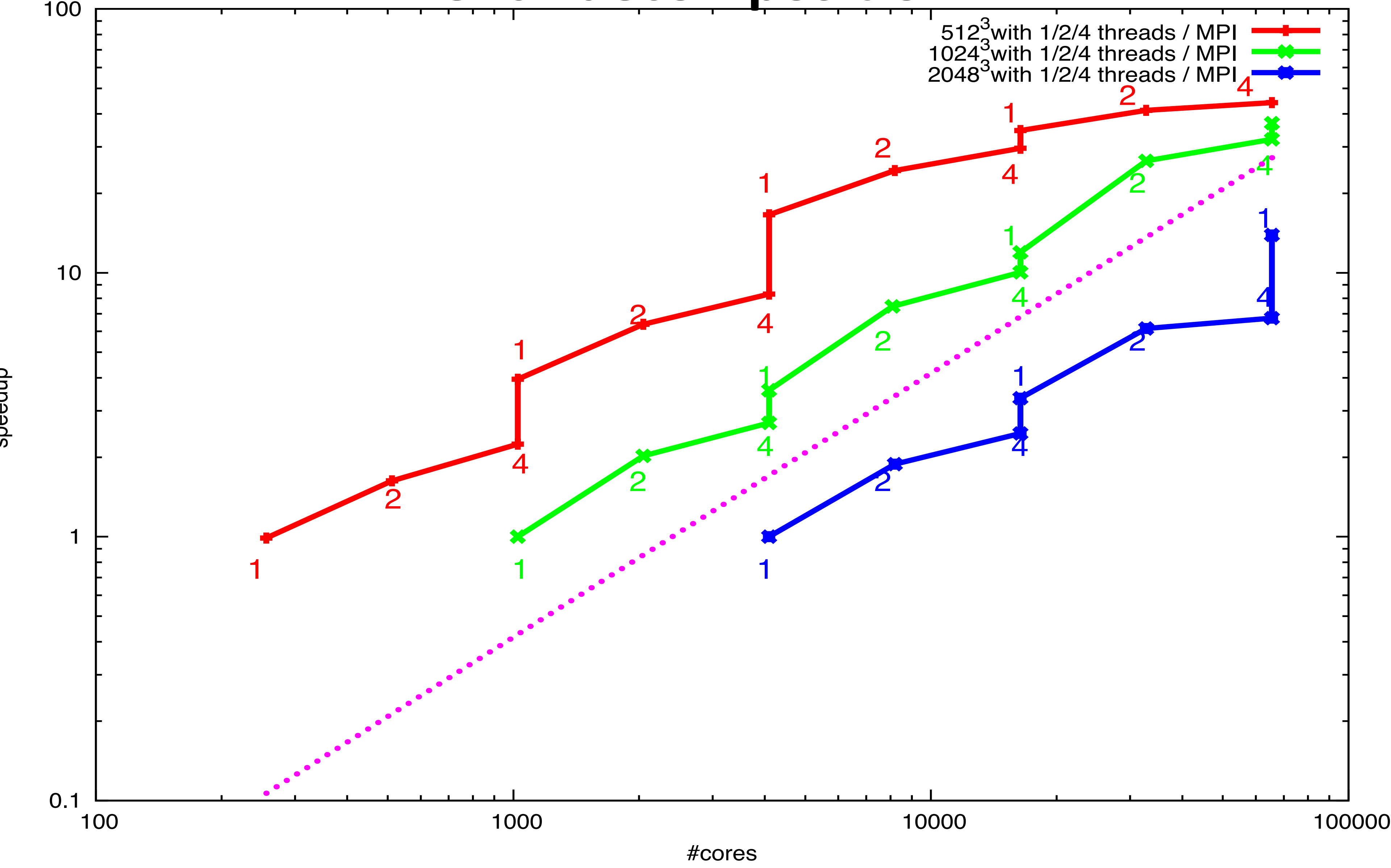
“Pencil decomposition”



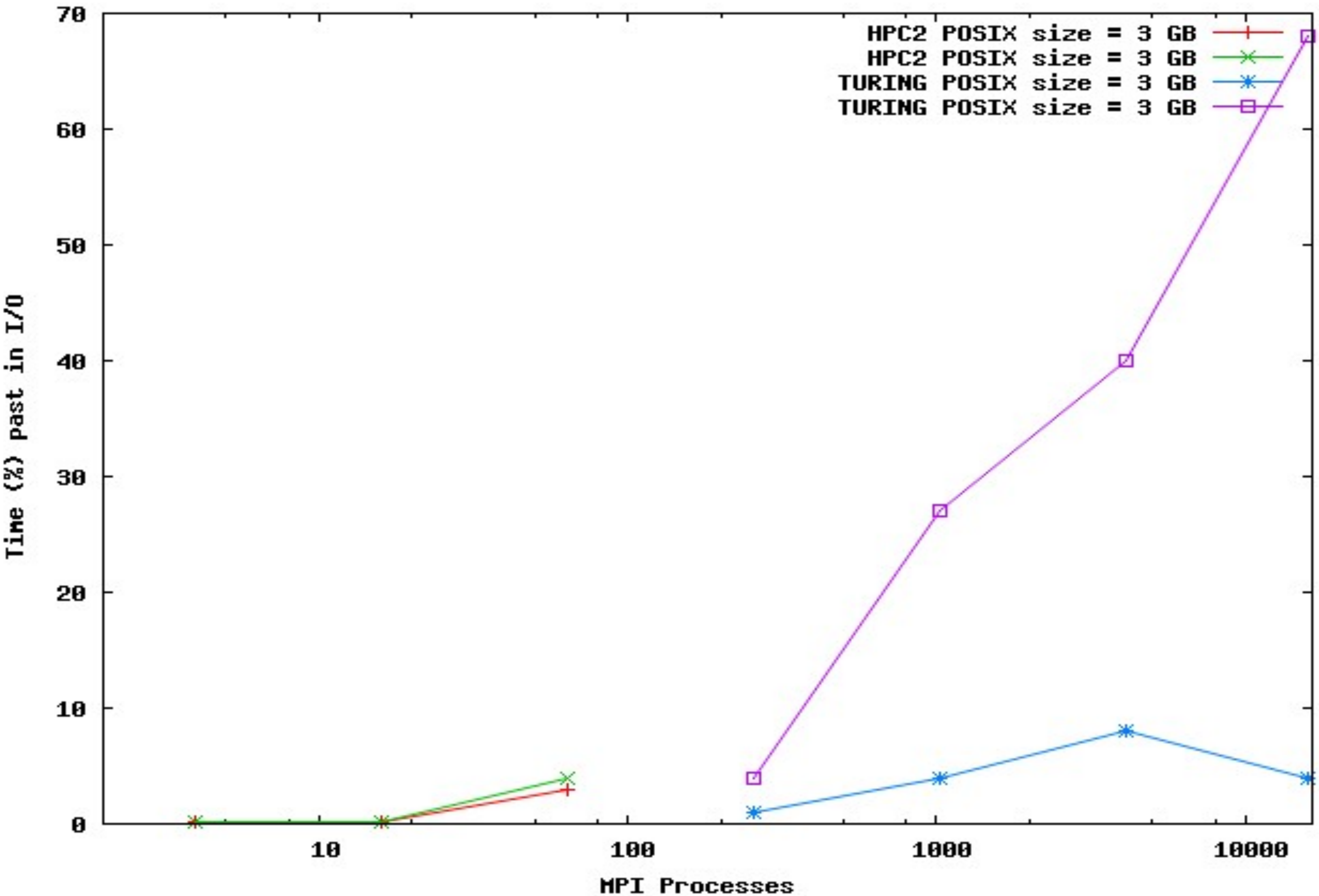
Scalability MPI alone: Pencil decomposition



Scalability MPI-OpenMP: Pencil decomposition



Remark : (I/O)/Elapsed time



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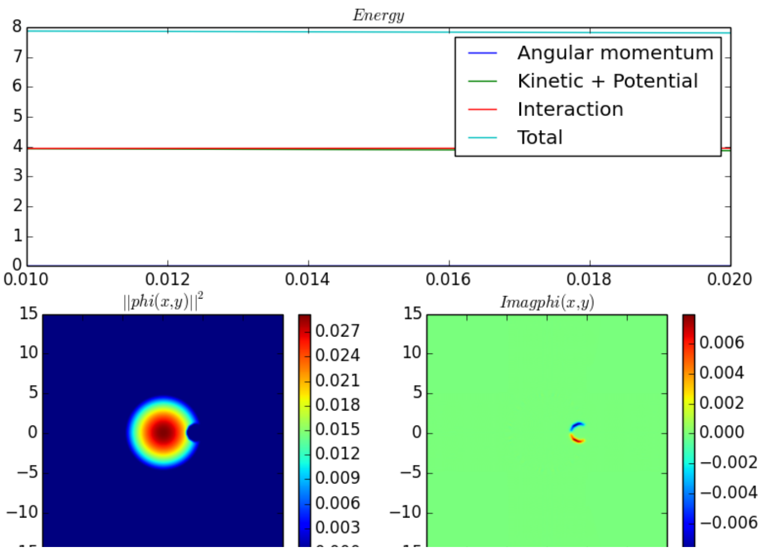
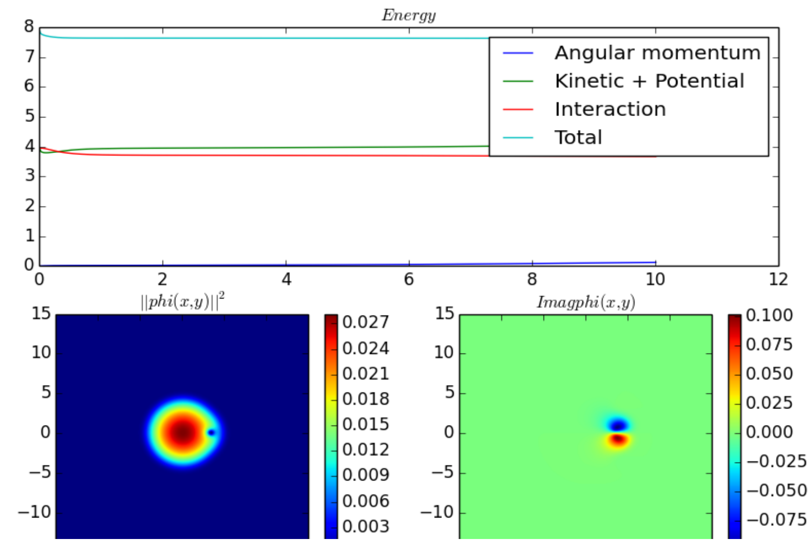
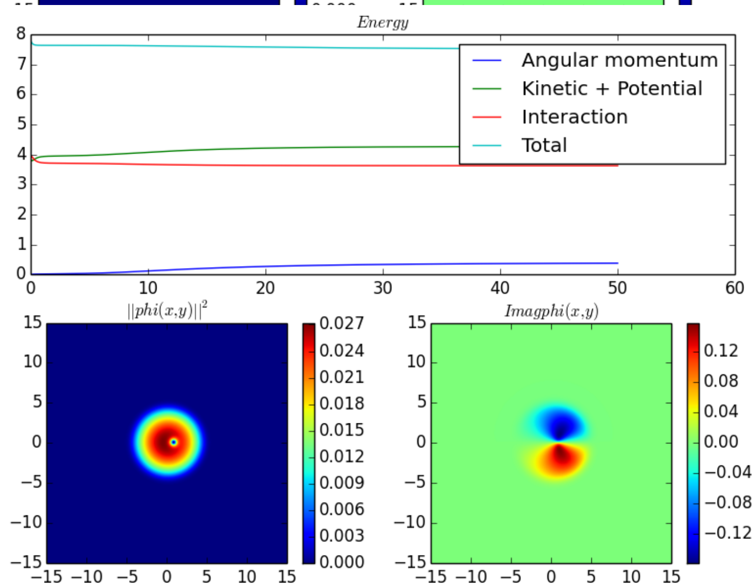
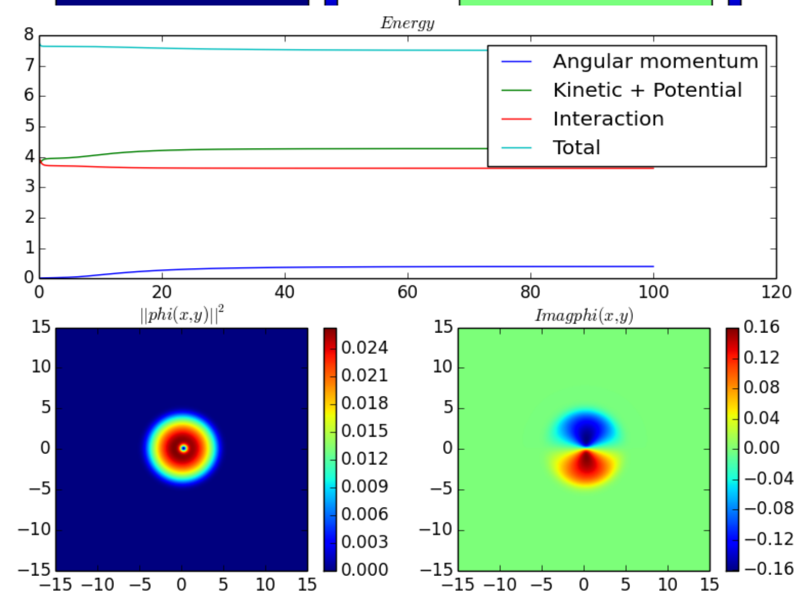
Benchmark-2D: Off-center vortex case





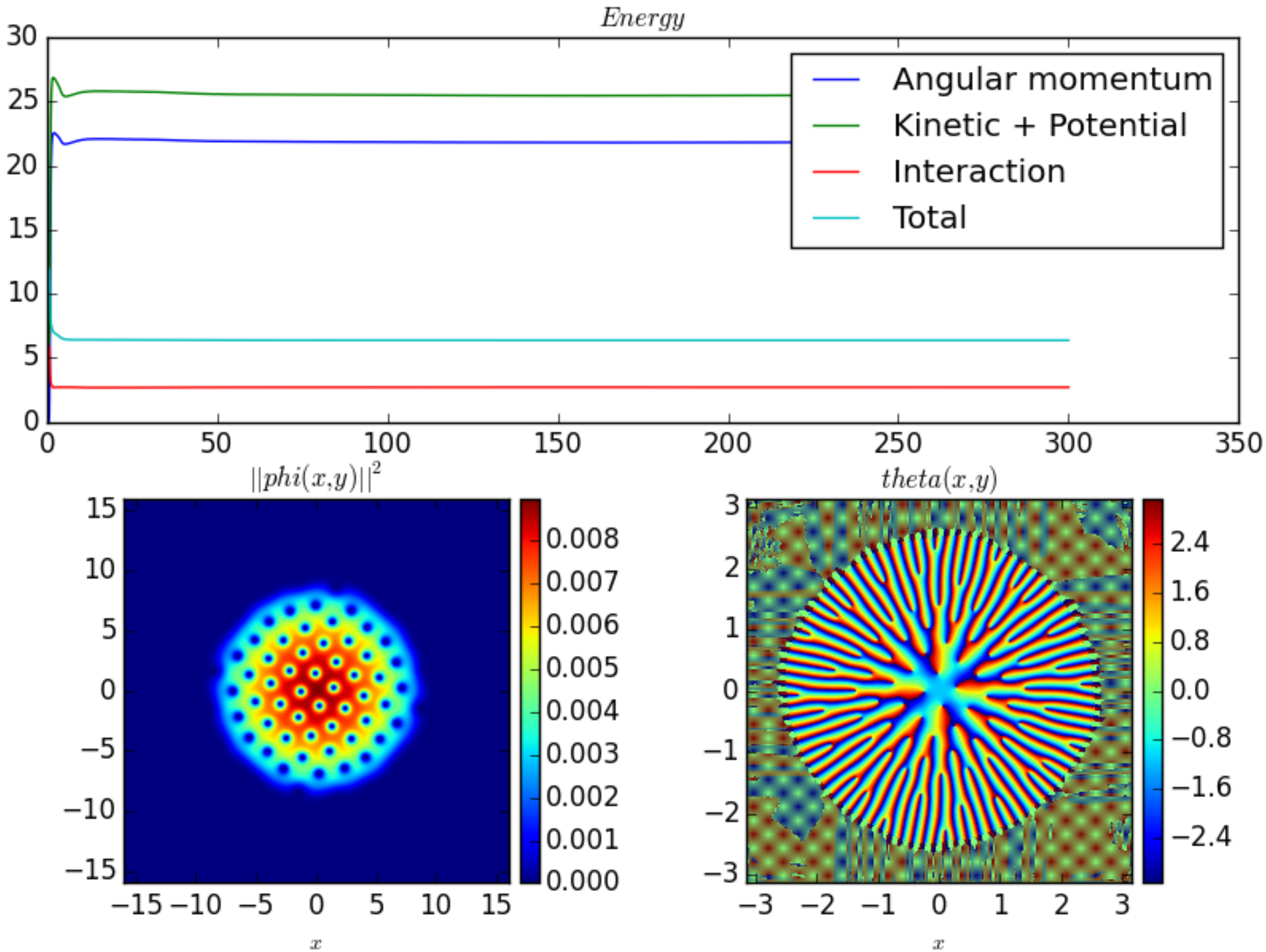




Benchmark-2D: Vortex array cases

(Lx,Ly)=(32,32)/(Nx,Ny)=(512,512)

Beta=1000 Omega=0.9 / T-F / Harmonic-+-Quartic / FFT



Benchmark-2D: Harmonic-sym or asym trap

(Lx,Ly)=(32,32)/(Nx,Ny)=(512,512)

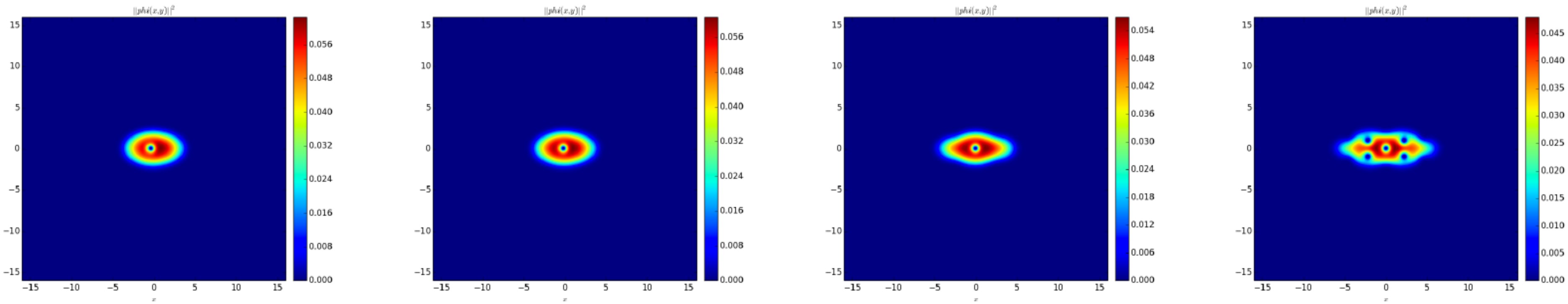


Figure 3: Computation of harmonic asymetric trap with $\beta = 100$, $\Omega = [0.6, 0.7, 0.8, 0.95]$

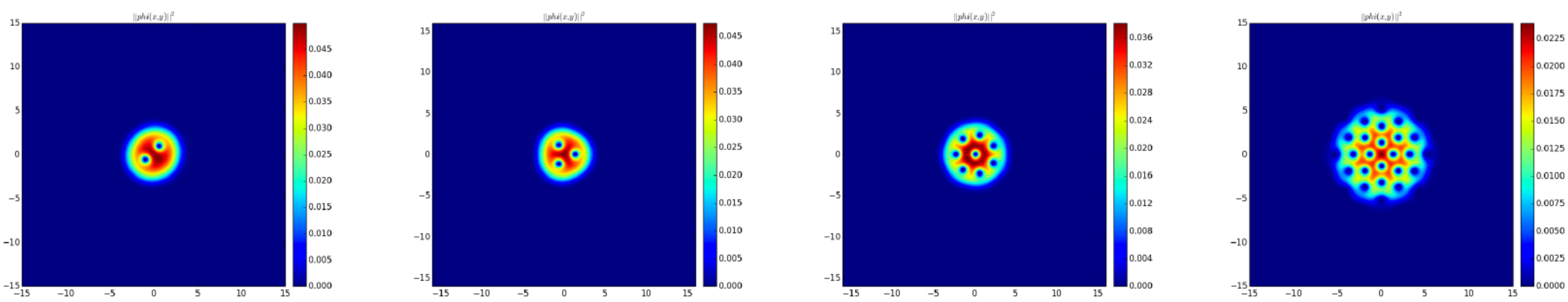
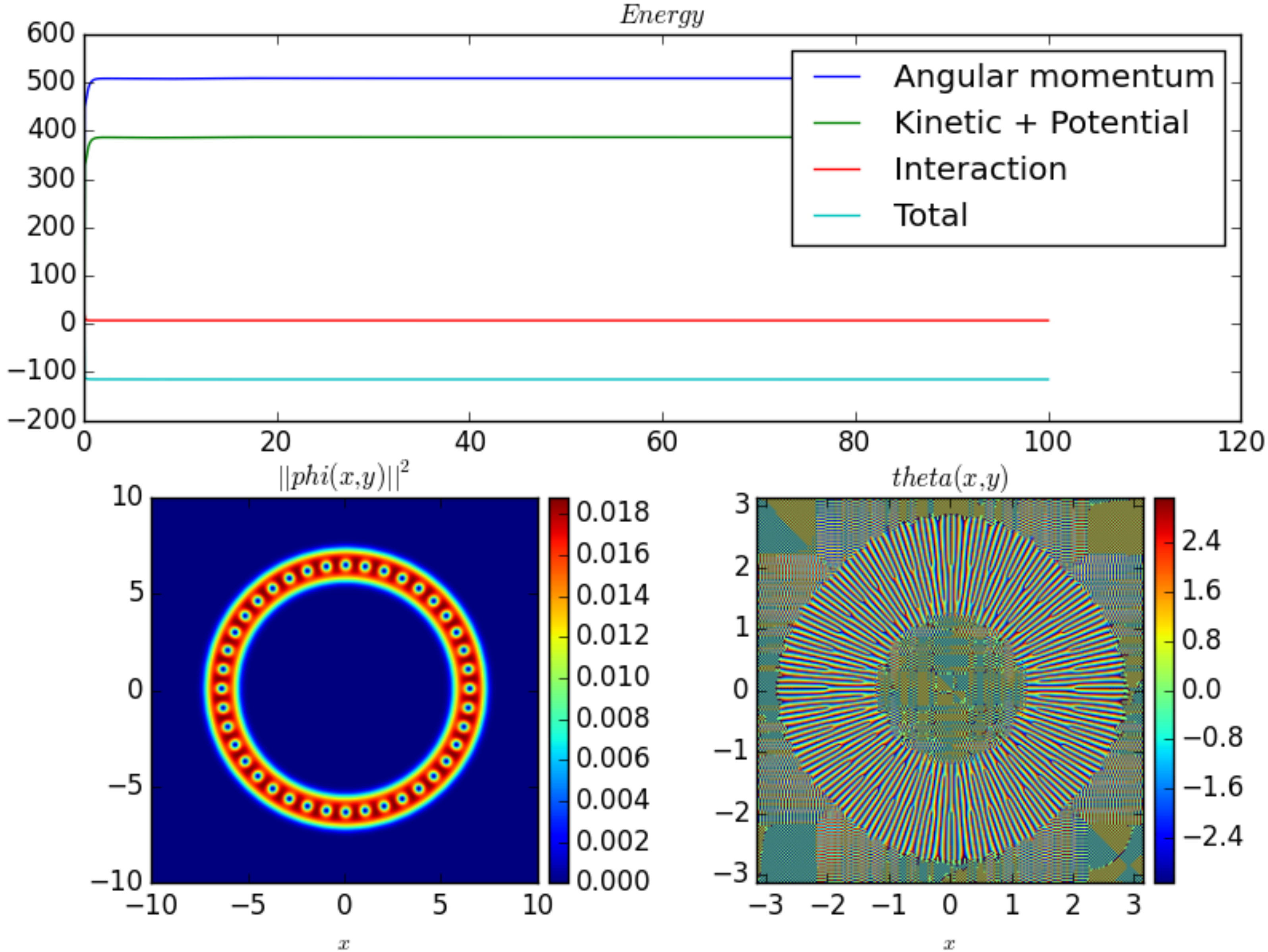


Figure 4: Computation of harmonic symetric trap with $\beta = 100$, $\Omega = [0.6, 0.7, 0.8, 0.95]$

Benchmark-2D: Giant vortex FFT versus CS

(Lx,Ly)=(20,20)/(Nx,Ny)=(256,256)

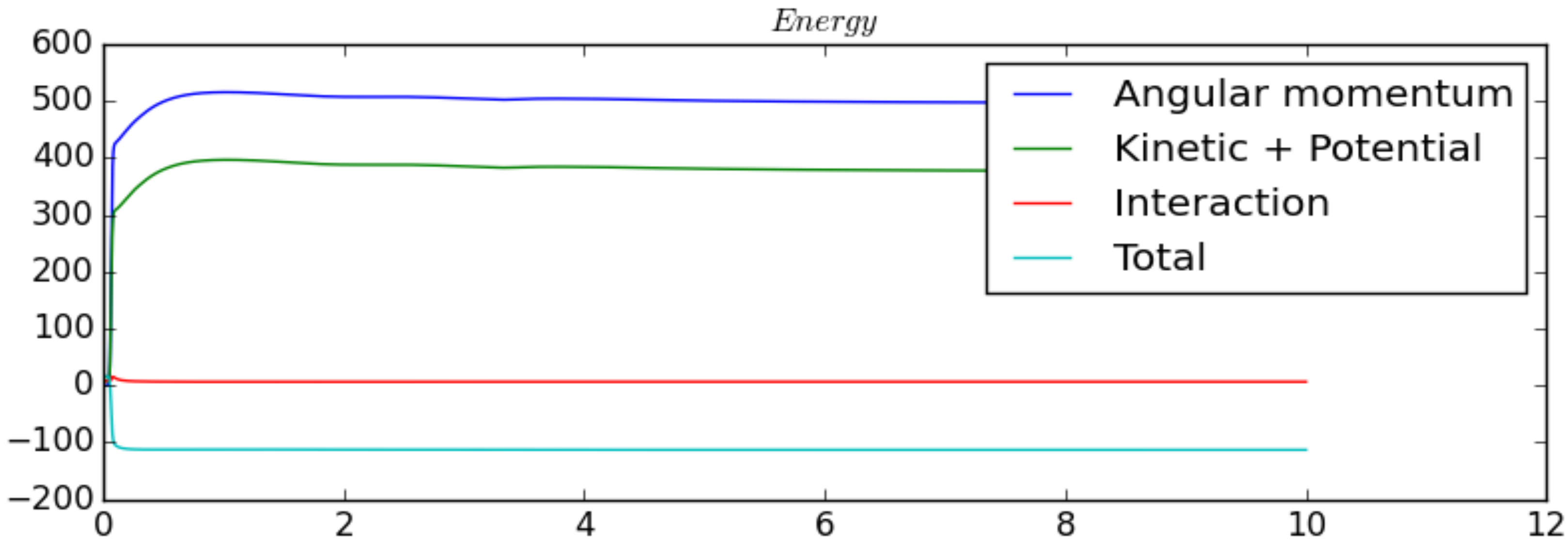
Beta=1000 Omega=3.5 / T-F / Harmonic-+-Quartic /FFT

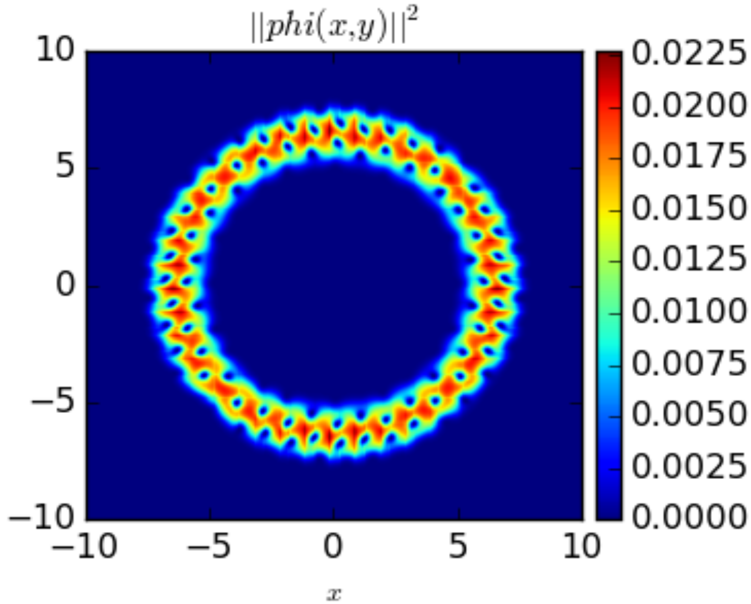


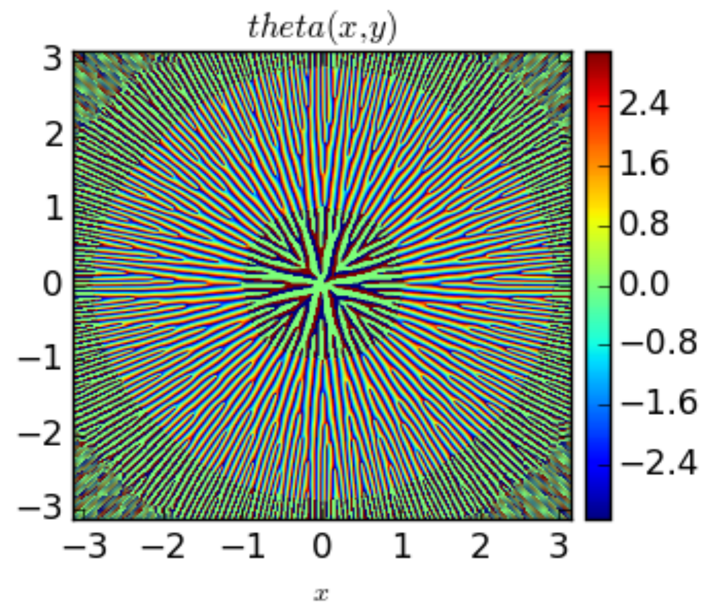
Benchmark-2D: Giant vortex FFT versus CS

(Lx,Ly)=(20,20)/(Nx,Ny)=(256,256)

Beta=1000 Omega=3.5 / T-F / Harmonic-+-Quartic / CS



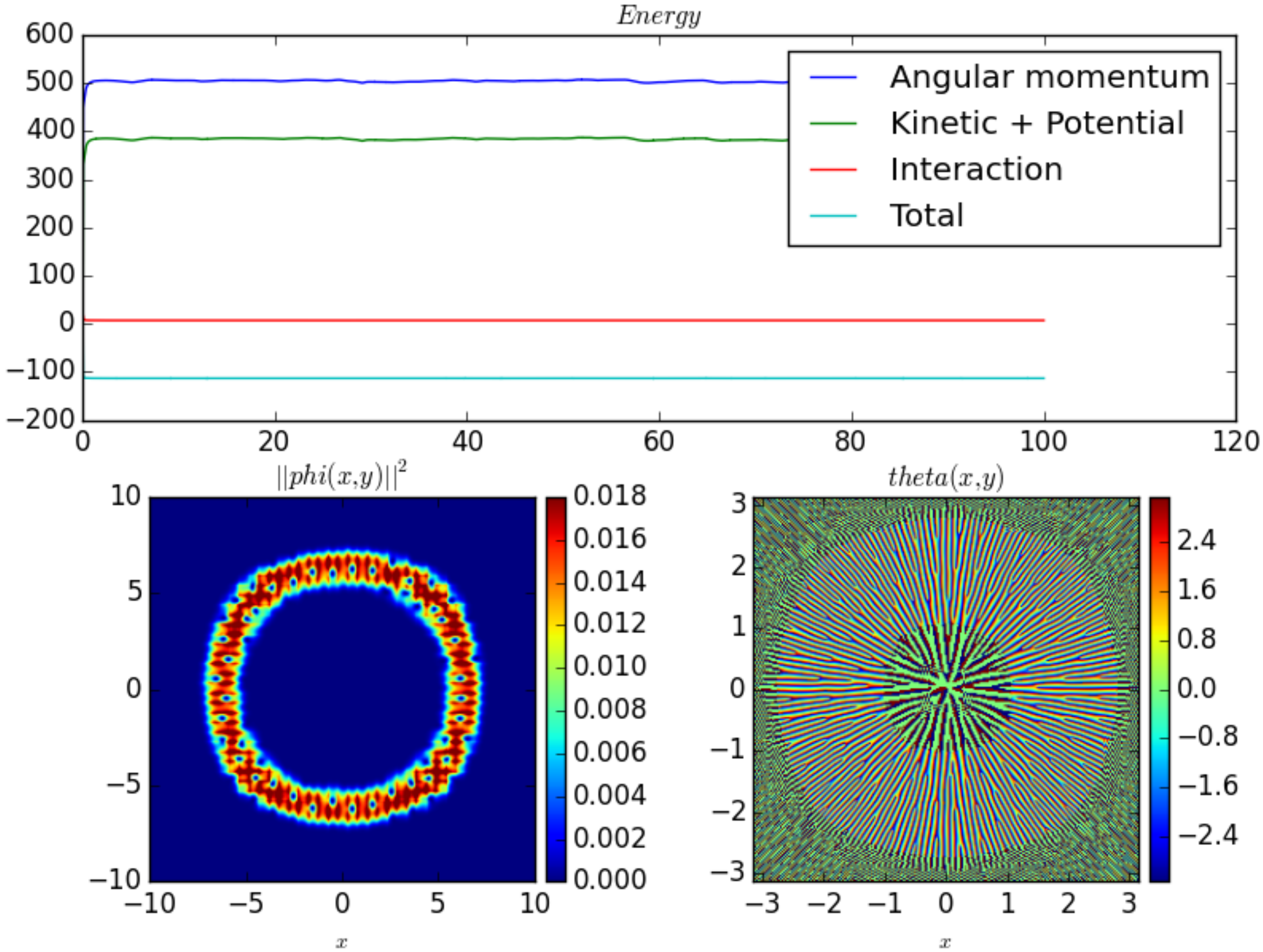




Benchmark-2D: Giant vortex FFT versus CS

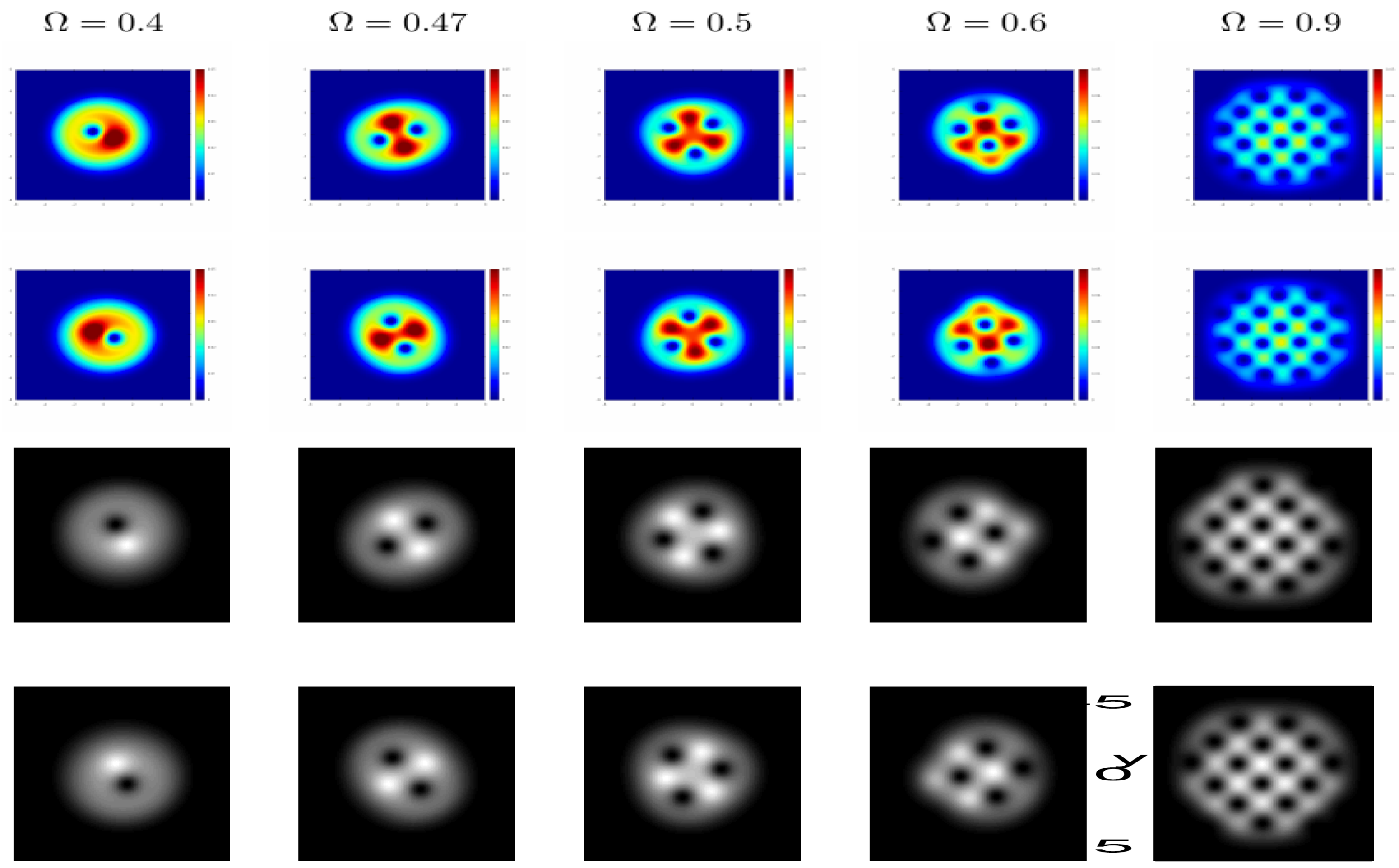
(Lx,Ly)=(20,20)/(Nx,Ny)=(512,512)

Beta=1000 Omega=3.5 / T-F / Harmonic-+-Quartic /CS



Benchmark-2D: 2components

(Lx,Ly)=(12,12)/(Nx,Ny)=(128,128)
(Beta11,Beta12,Beta21,Beta22)=(100,70,70,100)
Low interaction/ Harmonic potential



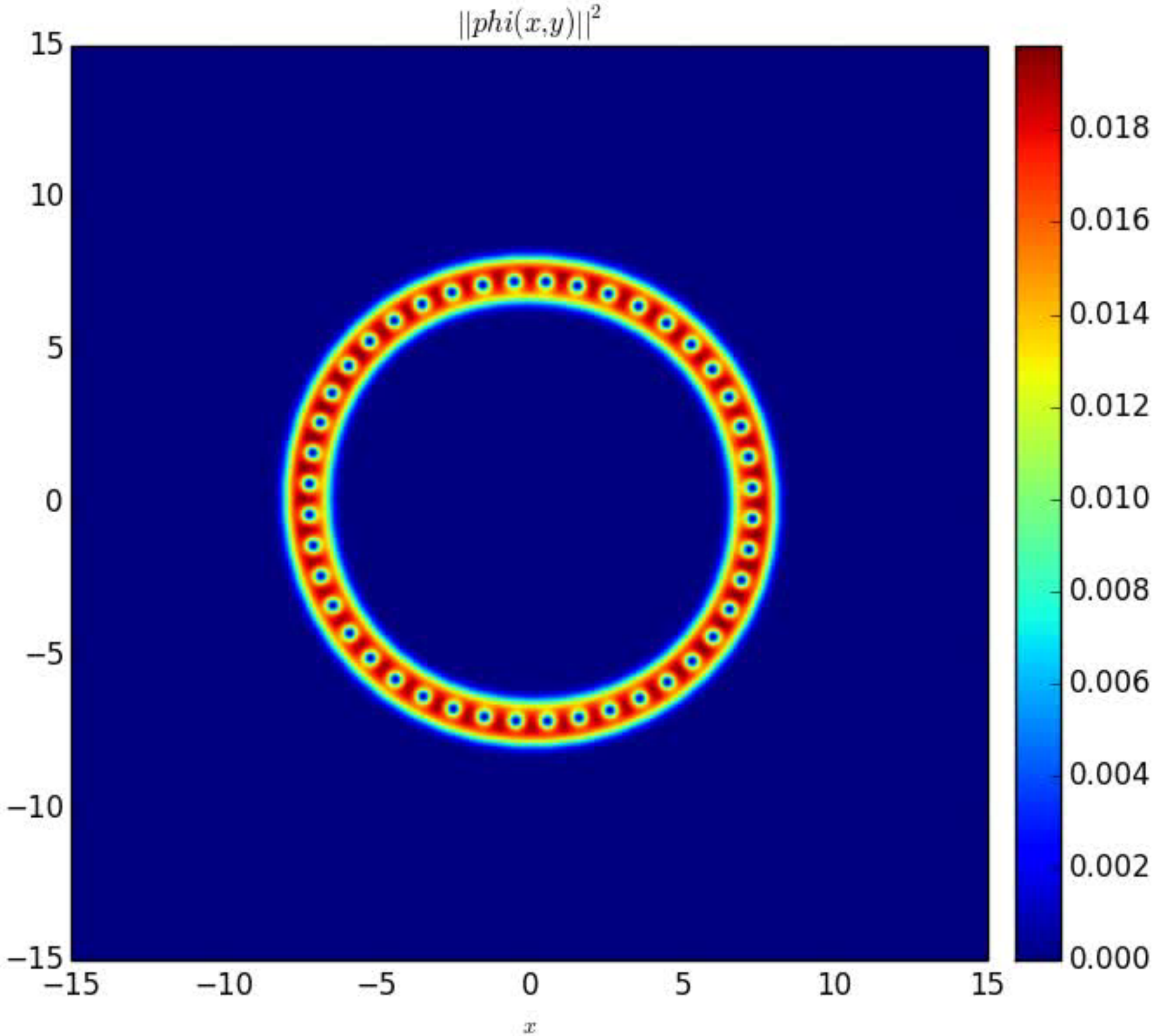
G.P.S

Wang's thesis

Benchmark-2D: Giant vortex dynamic

(Lx,Ly)=(20,20)/(Nx,Ny)=(256,256)

Omega=[1, 2, 3, 4]/ Fermi

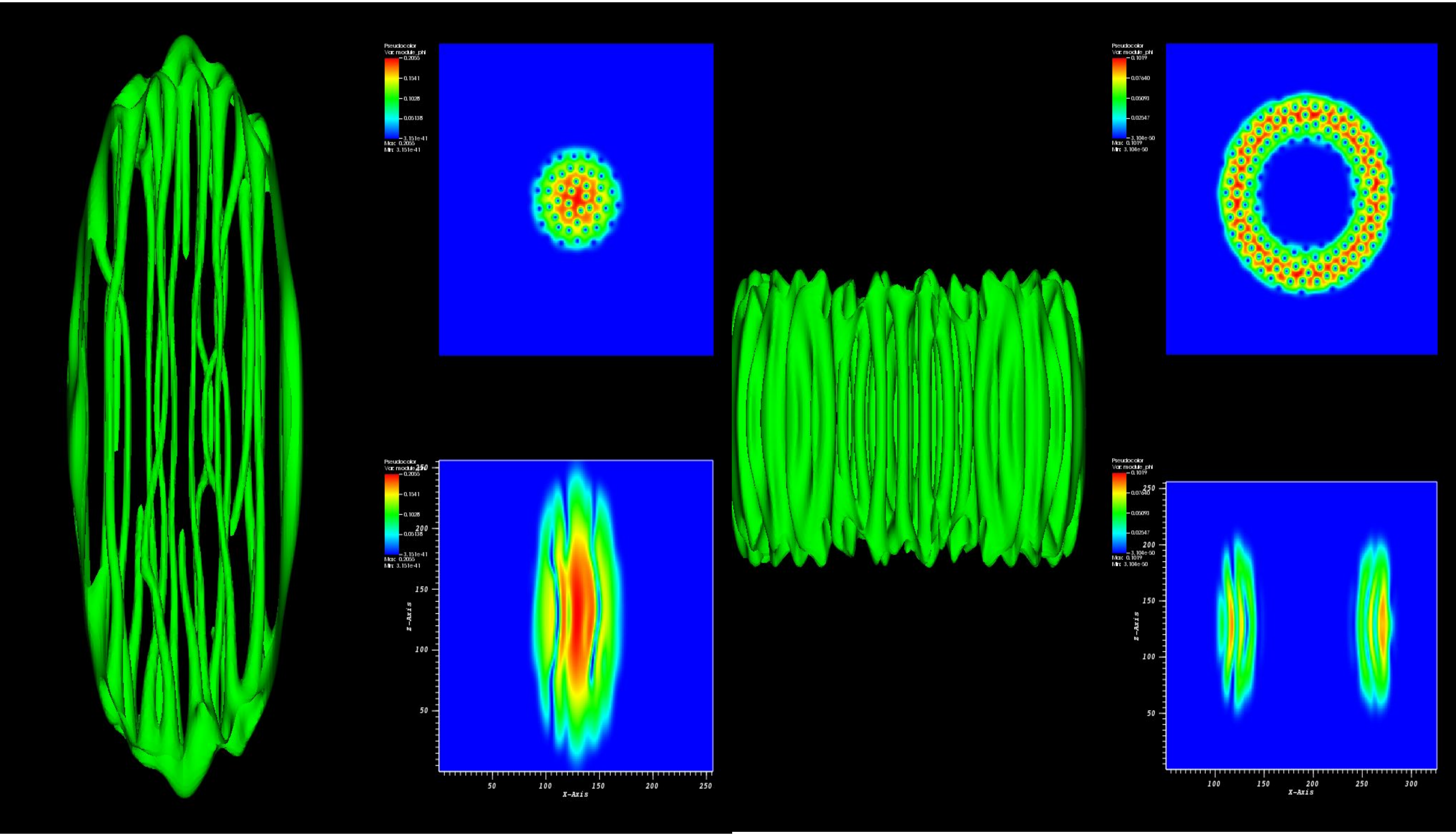


Benchmark 3D: Abrikosov lattice and Giant Vortex

(Lx,Ly,Lz)=(30,30,100)/(Nx,Ny,Nz)=(384,384,256)

(Beta)=(16715)

Omega=[0.80,0.96]/ T-F / Harmonic + quartic cylindric potential

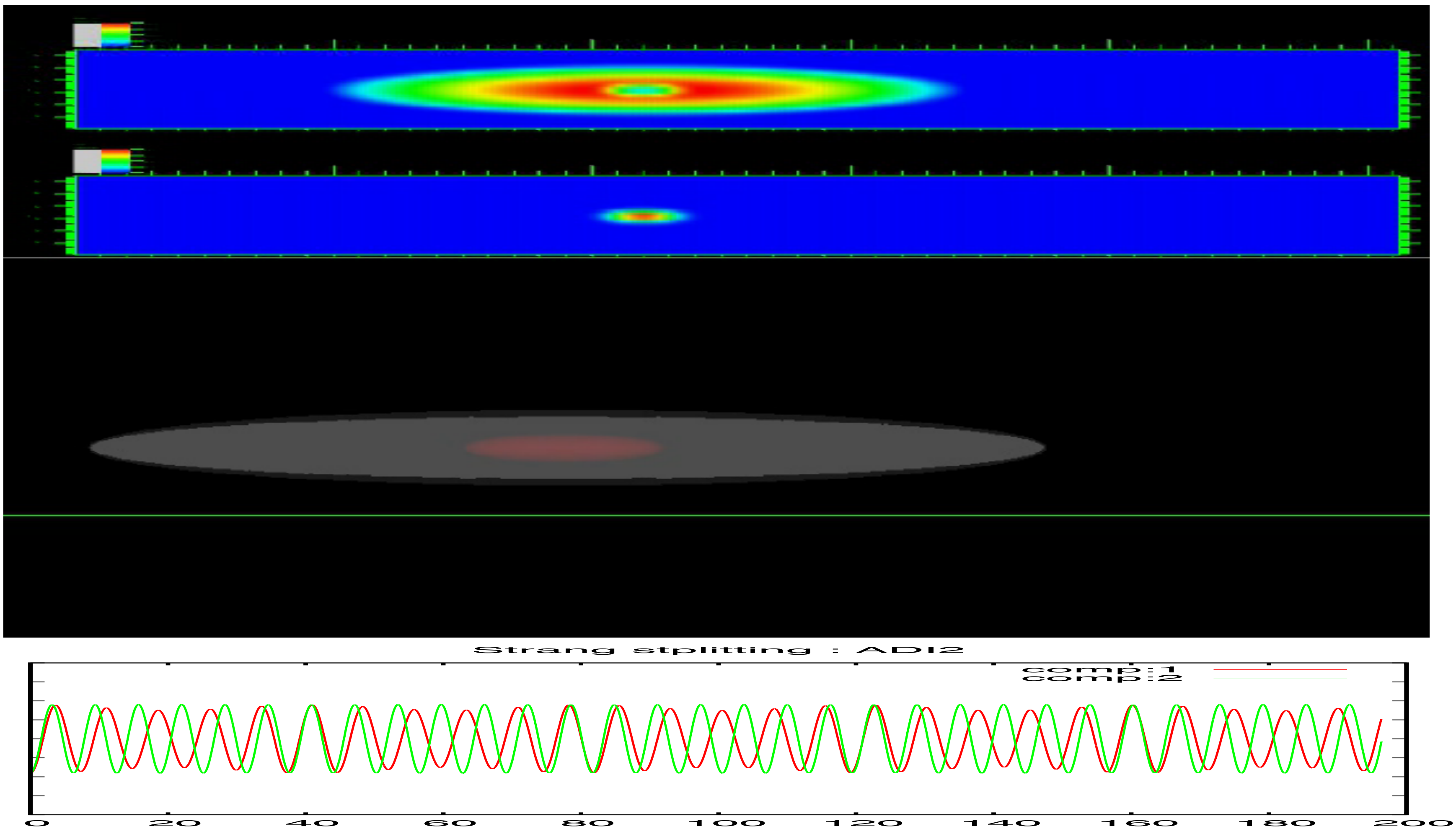


Benchmark-3D : 2components (hardcore, close to phase separation)

(Lx,Ly,Lz)=(8,8,64)/(Nx,Ny,Nz)=(128,128,1024)

(Beta11, Beta12,Beta21,Beta22)=(60, 6000, 200,20000)

Dt= 5.10-3



- **Performance & Accuracy**
- **Scalability & Efficiency**
- **G.P.S could solve others problems: dynamic cases, quantic turbulence**
- **G.P.S will be accessible on internet in few months**