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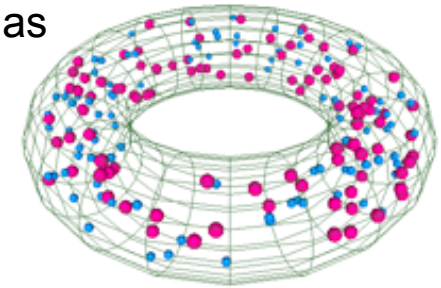

# Global MHD simulation by the gyrokinetic PIC code

Hiroshi Naitou,

Masatoshi Yagi[1,2], Shinji Tokuda[3]

Graduate School of Science and Engineering, Yamaguchi University, Japan

[1]Research Institute for Applied Mechanics, Kyushu University, Japan

[2]Aomori Research and Development Center, Japan Atomic Energy Agency, Japan

[3]International Fusion Energy Research Center, Japan

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# Outline

1. Motivation
2. Overview of the Gpic-MHD code

   + proposal of advanced algorithm
3. Parallelization performance of Gpic-MHD with 2d domain decomposition
4. Summary

Gpic-MHD: Gyrokinetic PIC code for MHD simulation

# 1. Motivation

## Do Kinetic MHD simulation by the gyrokinetic PIC code !!

Gyrokinetic PIC Code: gyr3d

H. Naitou et al., Phys. Plasmas 2, 4257 (1995)
H. Naitou et al., Plasma and Fusion Res. 72, 259 (1996)

moment equation ↓

same formulation

Gyrokinetic Fluid Code: GRM

H. Naitou et al, J. Plasma and Fusion Res. SERIES 2, 259 (1999)
H. Naitou et al. J. Plasma and Fusion Res. 76, 778 (2000)

technique ↓

New Gyrokinetic PIC Code: Gpic-MHD

Still difficult to access high beta and large scale tokamak parameter regime

2D: single helicity  3D: multi-helicities

H. Naitou et al., J. Plasma and Fusion Res. SERIES 8, 1158 (2009)

Proposal of a new algorithm !!

+ HPC

H. Naitou et al. DPS-APP 2009
H. Naitou et al., Plasma Science and Technology, Issue 5, October 2011

# Parallelization of 3d version of Gpic-MHD

- Gpic-MHD follows huge number of gyrokinetic particles.
- To resolve collisionless electron skin depth
  huge number of spatial meshes is required.

Needs huge computer resources.

The number of cores are increasing. $N_{\mathrm{core}} > 10^3 - 10^6$

1. Particle decomposition.
   Use replicas of field quantities.
   Useful for small system.

2. Domain decomposition.
   Necessary for large system.
   1d decomposition in z
   2d decomposition in r and z

3. Domain decomposition + particle decomposition : Domain cloning
   number of cores > number of decomposed domains

Parallelization performance on SR16000 8192 logical cores

H. Naitou et al., Plasma and Fusin Res. 6, 2401084 (2011)
H. Naitou et al, Progress in Nuclear Science and Technology (accepted)

# 2. Overview of the Gpic-MHD code

----- simulation of kinetic internal kink mode -----

# + proposal of advanced algorithm

Based on gyrokinetic theory.

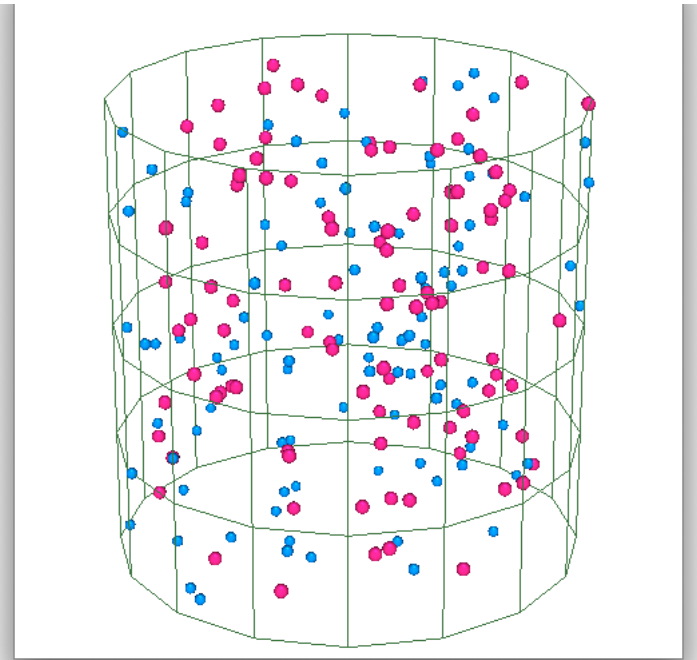
Gyrokinetic PIC code with $\delta$f - scheme.

Follows huge number of gyrokinetic particles.

Cylindrical geometry: $(r, \theta, z)$

Nonuniform mesh in the radial direction.

Fourier mode expansions in $\theta$ and $z$.



# gyrokinetic Vlasov equation

$$p_z = v_z + \frac{q_s}{m_s} A_z$$

Field Quantities: $\phi, \quad A_z$

$v_z$ - version

$$\frac{df_s}{dt} = \frac{\partial f_s}{\partial t} + \frac{d\mathbf{x}_s}{dt} \cdot \frac{\partial f_s}{\partial \mathbf{x}} + \frac{dv_{zs}}{dt} \frac{\partial f_s}{\partial v_z} = 0$$

$p_z$ - version

$$\frac{df_s}{dt} = \frac{\partial f_s}{\partial t} + \frac{d\mathbf{x}_s}{dt} \cdot \frac{\partial f_s}{\partial \mathbf{x}} + \frac{dp_{zs}}{dt} \frac{\partial f_s}{\partial p_z} = 0$$

where

$$\frac{d\mathbf{x}_s}{dt} = -\frac{\nabla\phi \times \mathbf{b}}{B_0} + v_z \mathbf{b}^*$$

$$\frac{dv_{zs}}{dt} = -\frac{q_s}{m_s}\left(\mathbf{b}^* \cdot \nabla\phi + \frac{\partial A_z}{\partial t}\right)$$

$$\frac{dp_{zs}}{dt} = -\frac{q_s}{m_s}\left(\mathbf{b} \cdot \nabla\phi - v_z \mathbf{b} \cdot \nabla A_z\right)$$

and

$$\mathbf{b}^* = \mathbf{b} + \frac{\nabla A_z \times \mathbf{b}}{B_0}$$

# standard version of Gpic-MHD

$p_z - \text{version}$

gyrokinetic Poisson's equation :

$$\frac{\omega_{pi}^2}{\omega_{ci}^2}\nabla_\perp^2\phi = \frac{e}{\varepsilon_0}\int f_e dv_z - \frac{e}{\varepsilon_0}\int f_i dv_z$$

Ampere's law :

$$\nabla_\perp^2 A_z = \mu_0 e\int v_z f_e dv_z - \mu_0 e\int v_z f_i dv_z$$

$$p_z = v_z + \frac{q_s}{m_s}A_z$$

“cancellation problem”
extention of the split-weight-scheme for $p_z$-version

# advanced version of Gpic-MHD

$$\frac{\partial}{\partial t}\nabla_\perp^2\phi = -v_A^2\mathbf{b}^*\cdot\nabla\left(\nabla_\perp^2 A_z\right) - \frac{\mathbf{b}\times\nabla\phi}{B_0}\cdot\nabla\left(\nabla_\perp^2\phi\right)$$

: vorticity equation

$$\frac{\partial}{\partial t}\nabla_\perp^2 A_z = \mu_0 e^2\left(\frac{n_e}{m_e}+\frac{n_i}{m_i}\right)\left(\frac{\partial A_z}{\partial t}+\mathbf{b}^*\cdot\nabla\phi\right) - \frac{\mathbf{b}\times\nabla\phi}{B_0}\cdot\nabla\left(\nabla_\perp^2 A_z\right)$$
$$-\mu_0 e\mathbf{b}^*\cdot\nabla\int v_z^2 f_e\, dv_z + \mu_0 e\mathbf{b}^*\cdot\nabla\int v_z^2 f_i\, dv_z$$

: generalized Ohm's law along the magnetic field

- Use above equations to advance $\phi$ and $A_z$ in time.

$$\frac{\partial\phi}{\partial t} = F(\phi, A_z), \quad \frac{\partial A_z}{\partial t} = G(\phi, A_z, \delta n_e, \delta n_i, \delta P_e, \delta P_i)$$

$v_z$ – version

# Generalized Ohm's law along the magnetic field

$$\left[\nabla_\perp^2 - \mu_0 e^2\left(\frac{n_{e0}}{m_e}+\frac{n_{i0}}{m_i}\right)\right]\frac{\partial A_z}{\partial t} = \mu_0 e^2\left(\frac{\boxed{\delta n_e}}{m_e}+\frac{\boxed{\delta n_i}}{m_i}\right)\frac{\partial A_z}{\partial t}$$

$$+\mu_0 e^2\left(\frac{\boxed{n_e}}{m_e}+\frac{\boxed{n_i}}{m_i}\right)\boldsymbol{b}^*\cdot\nabla\phi - \frac{\boldsymbol{b}\times\nabla\phi}{B_0}\cdot\nabla\left(\nabla_\perp^2 A_z\right)$$

$$-\boxed{\mu_0 e\boldsymbol{b}^*\cdot\nabla\int v_z^2 f_e\, dv_z} + \boxed{\mu_0 e\boldsymbol{b}^*\cdot\nabla\int v_z^2 f_i\, dv_z},$$

Above equation is solved iteratively.

Particle information is used to estimate $\delta n_e$, $\delta n_e$ and the perturbed parts of the electron and ion second moments ($\delta P_e$ and $\delta P_i$).

The dominat term is $\delta P_e$.

This term is the order of $\rho_s^2 / a^2$ smaller than other term.

"Particle closure" or "Complete closure" or "Kinetic closure"

# GRM Model Including Ion Landau Damping

Gyro-Reduced-MHD

$$\frac{\partial}{\partial t}\nabla_\perp^2\phi = -\frac{\boldsymbol{b}\times\nabla\phi}{B_0}\bullet\nabla(\nabla_\perp^2\phi) - v_A^2\boldsymbol{b}^*\bullet\nabla(\nabla_\perp^2 A_z)$$

$$\frac{\partial}{\partial t}A_z = -\boldsymbol{b}^*\bullet\nabla\phi + d_e^2\frac{d}{dt}(\nabla_\perp^2 A_z) + \frac{T_{e0}}{n_{e0}e}\boldsymbol{b}^*\bullet\nabla n_e$$

$$\frac{\partial}{\partial t}n_e = -\frac{\boldsymbol{b}\times\nabla\phi}{B_0}\bullet\nabla n_e - \frac{1}{e\mu_0}\boldsymbol{b}^*\bullet\nabla(\nabla_\perp^2 A_z) - \underline{\boldsymbol{b}^*\bullet\nabla\Gamma_i}$$

3-Field Model

$$\Gamma_i = 0$$

$$\frac{\partial}{\partial t}\Gamma_i = -\frac{\boldsymbol{b}\times\nabla\phi}{B_0}\bullet\nabla\Gamma_i - \left(\frac{T_{e0}}{m_i} + \frac{T_{i0}}{m_i}\right)\boldsymbol{b}^*\bullet\nabla n_e$$

$$+\frac{\varepsilon_0 T_{i0}\omega_{pi}^2}{m_i\omega_{ci}^2}\boldsymbol{b}^*\bullet\nabla\left(\nabla_\perp^2\phi\right) - \underline{\frac{n_{i0}}{m_i}\boldsymbol{b}^*\bullet\nabla\tilde{T}_i}$$

added

$$\frac{\partial}{\partial t}\tilde{T}_i = -\frac{\boldsymbol{b}\times\nabla\phi}{B_0}\bullet\nabla\tilde{T}_i - T_{i0}\boldsymbol{b}^*\bullet\nabla V_i - \underline{\frac{2^{3/2}}{\sqrt{\pi}}|k_{11}|v_{Ti}\tilde{T}_i}$$

ion Landau damping

$\tilde{T}_i$ : perturbed ion temperature

# simulation of kinetic internal kink mode

Cylindrical geometry

Nonuniform mesh in the radial direction

Single helicity (2D-code)

Gyrokinetic PIC code with $\delta$f scheme

Parallelization by particle decomposition

Benchmark run (standard version):

$d_e / a = 0.06, \quad \rho_s / a = 0.06, \quad T_i / T_e = 1.0$

$N_r = 129, \; N_\theta = 128$

$m \leq 20$

10000 steps

$$q(r) = q_0 \left[ 1 - 4\,(1 - q_0) \left( \frac{r}{a} \right)^2 \right]^{-1}$$

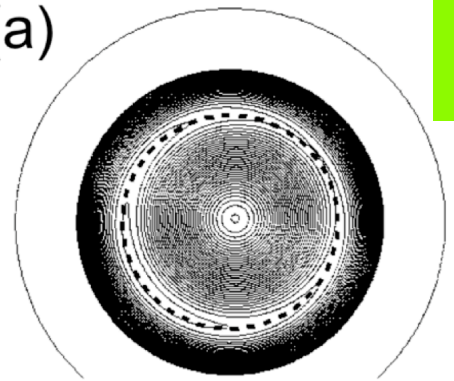
$q_0 = 0.85, q(0.5a) = 1.0, q_a = 2.125$

(0.5 million electrons + 0.5 million ions) × number of cores

Standard version of Gpic-MHD
$p_z$-version
512 processes

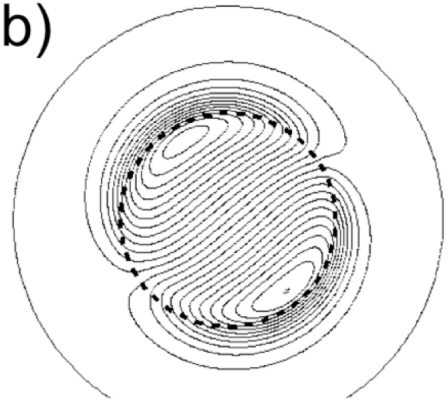
(a)

magnetic field structure



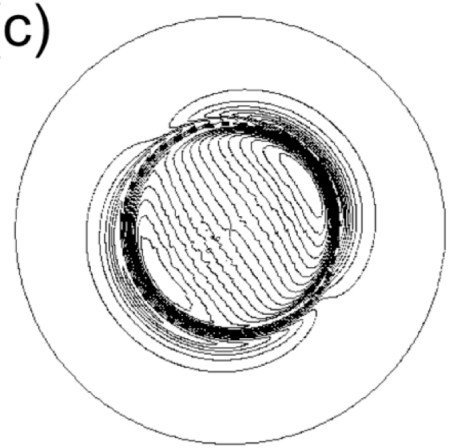
(b)

electrostatic potential profile

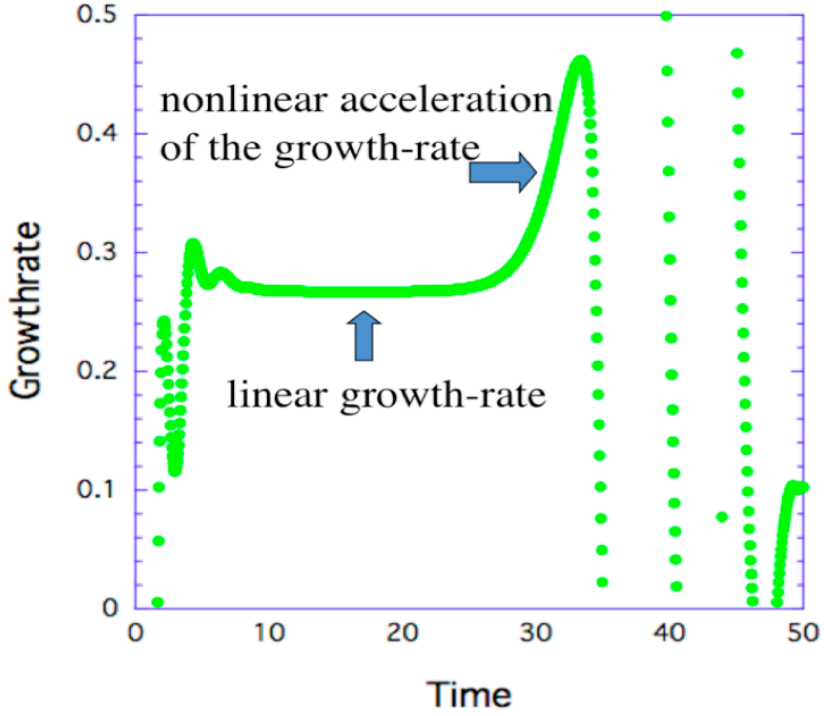


(c)

current density profile



$$d_e/a = 0.06, \quad \rho_s/a = 0.06$$

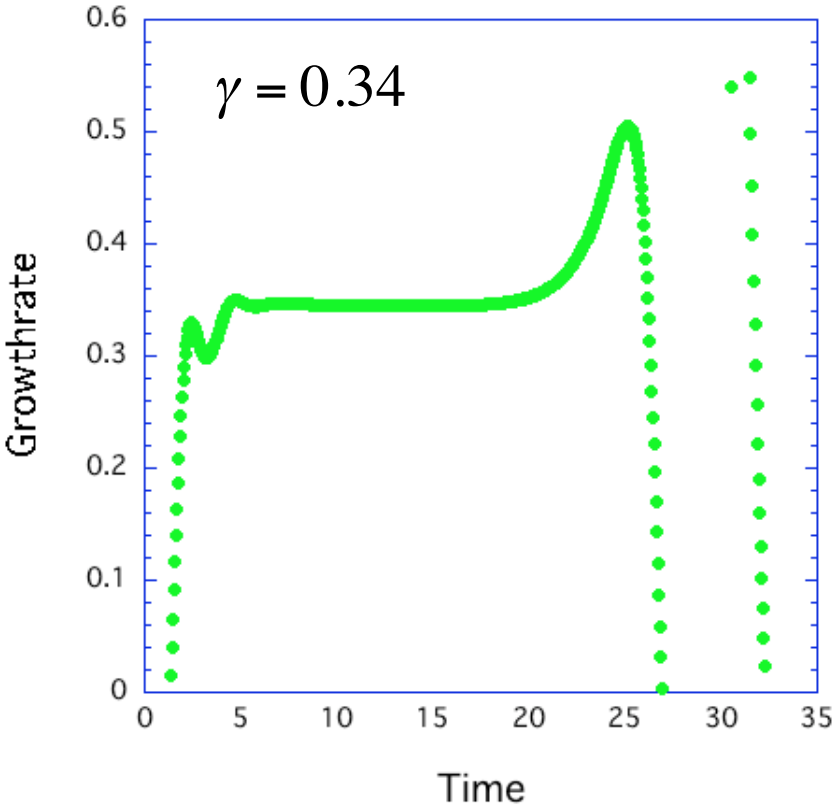


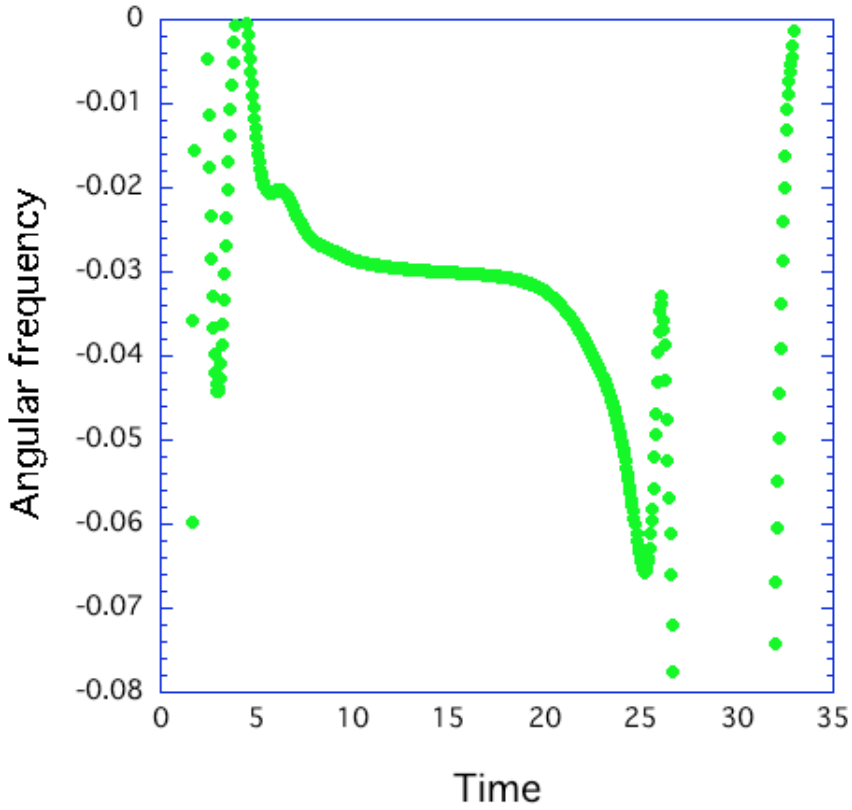

It is difficult to reduce $d_e/a$ and to increase $\rho_s/a$.
To simulate larger scale and higher beta tokamaks,
we propose a brand-new algorithm.

Advanced version of Gpic-MHD

# Temporal evolution of γ and $\omega_r$ 64 processes

$$d_e = 0.06, \quad \rho_s = 0.06, \quad N_r = 129, \quad N_\theta = 64$$




$\mathrm{CF}: \gamma = 0.32(\mathrm{GRM})$

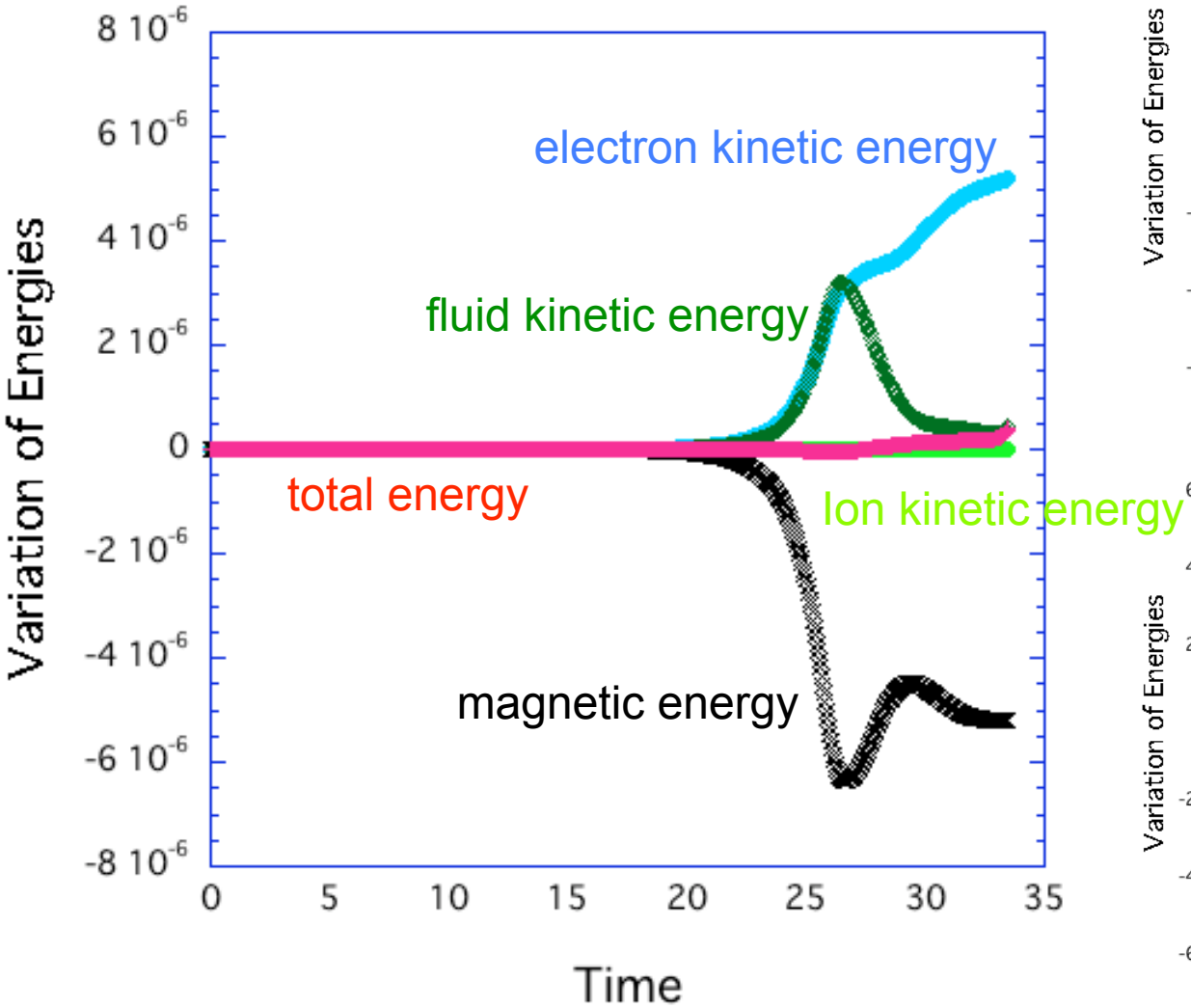
$\gamma = 0.27(\text{standard Gpic-MHD})$

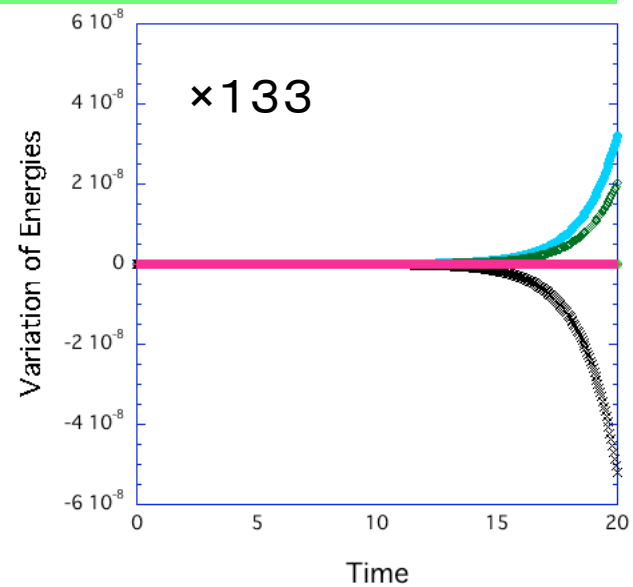
$\mathrm{CF}: \omega_r = 0.0\ (\mathrm{GRM})$

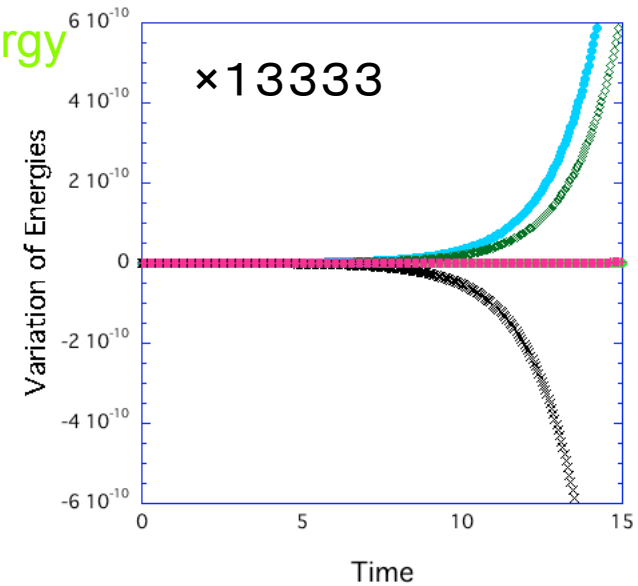
Advanced version of Gpic-MHD

# Energy Conservation 64 processes

$$d_e = 0.06, \quad \rho_s = 0.06, \quad N_r = 129, \quad N_\theta = 64$$



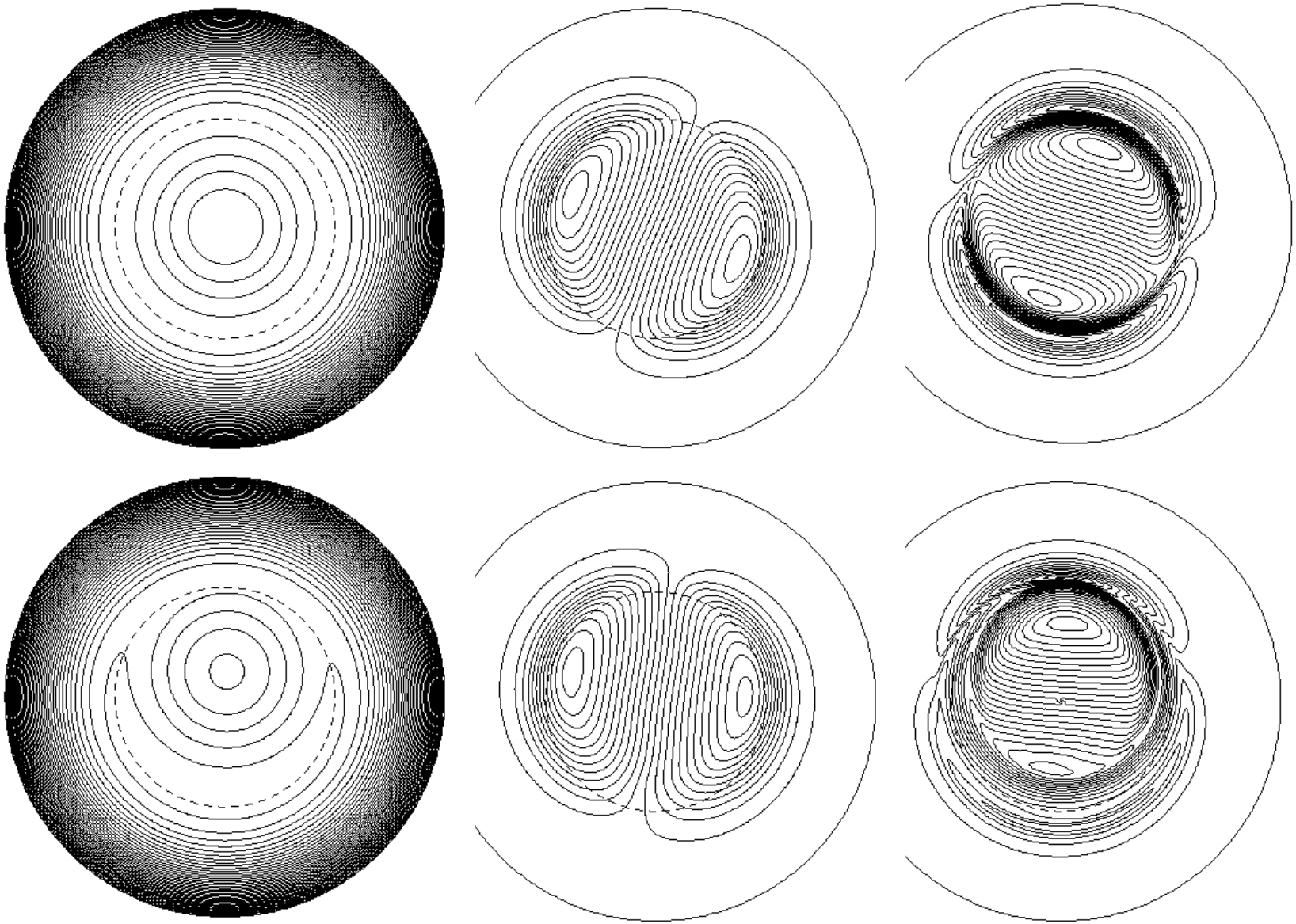



# Mode profiles

upper figures
t = 15

lower figures
T = 22.5

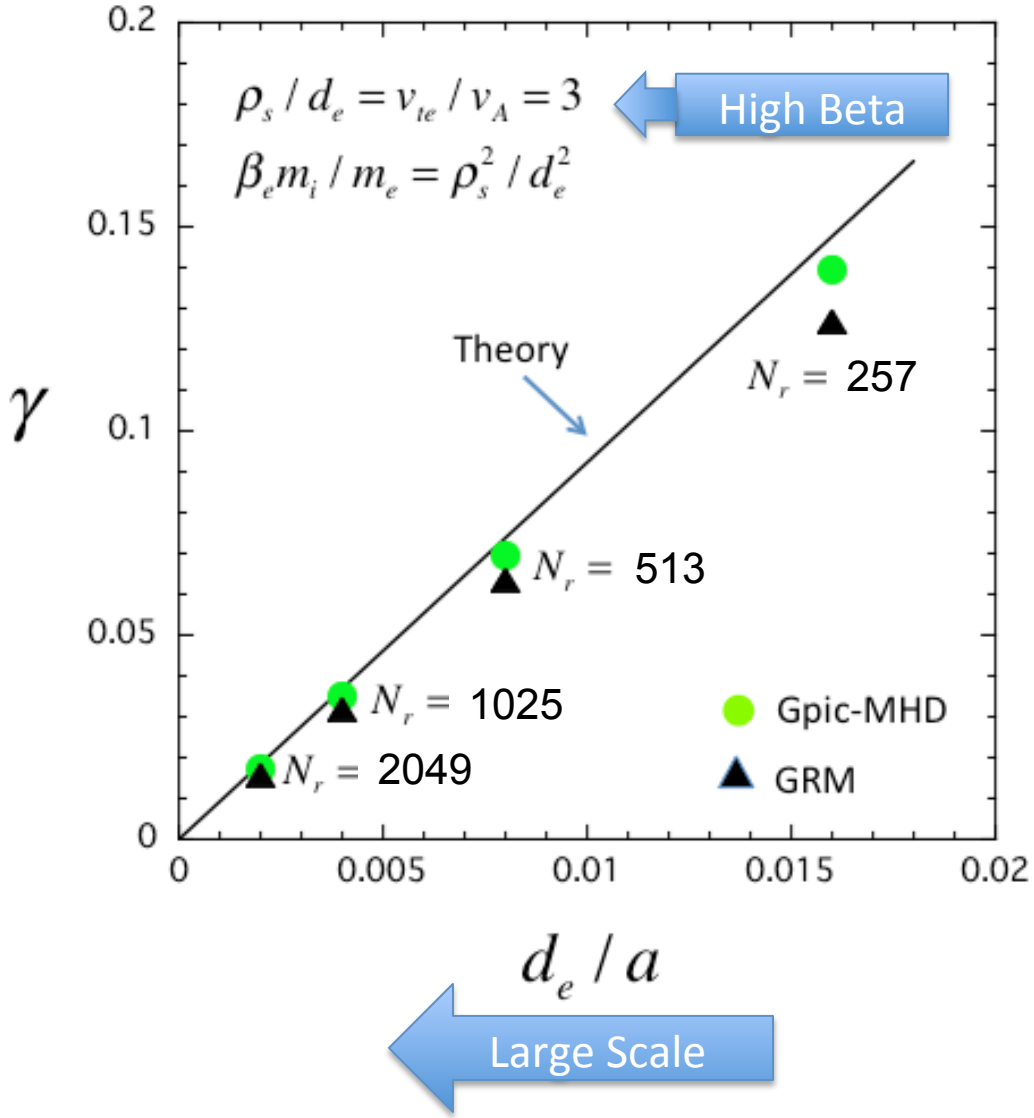


Magnetic structure  electrostatic potential  perturbed current density

# Growthrate versus collisionless electron skin depth

SR16000: “plasma simulator” at NIFS
scalar SMP cluster system, 128 nodes × 64 logical cores

advanced version of Gpic-MHD




$$A / a = 18$$

$$N_\theta = 64$$

256 – 512 processes

16 threads: SMP=16

1000000 - 4000000 particles/process

# Question?

- Numerically the following equations are not assured especially in the long time scale.

gyrokinetic Poisson's equation:

$$\frac{\omega_{pi}^2}{\omega_{ci}^2}\nabla_\perp^2\phi = \frac{e}{\varepsilon_0}\int f_e\, dv_z - \frac{e}{\varepsilon_0}\int f_i\, dv_z$$

Ampere's law:

$$\nabla_\perp^2 A_z = \mu_0 e\int v_z f_e\, dv_z - \mu_0 e\int v_z f_i\, dv_z$$

LHS: Calculated by time integration

RHS: determined by particle dynamics

# Some references

- Total characteristic method

  Y. Todo and Atsushi ITO, Plasma and Fusion Research: Regular Articles 2, 020 (2007)

- Fluid-kinetic hybrid electron model

  I. Holod, W. L. Zhang, Y. Xiao, Z. Lin, Physics of Plasmas 16, 122307 (2009)

- Fluid electrons with kinetic closure

  Y. Chen, Scott E. Parker, Physics of Plasmas 18, 055703 (2011)

# 3. Parallelization performance of Gpic-MHD with 2d domain decomposition

## 3d Gpic-MHD, standard version

1025x128x128 mesh → future: 10000x128x128
1000 time steps
domain decomposition in r and z
+ particle decomposition (replicas)
SMP=2 (auto-parallelization)

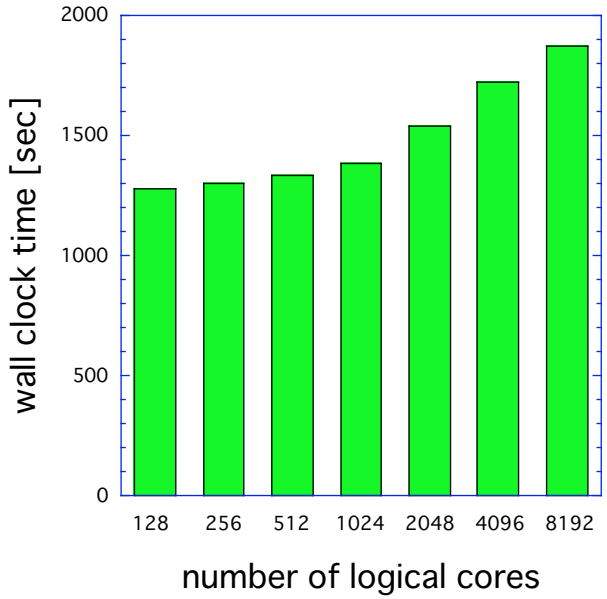
z direction is uniformly decomposed.

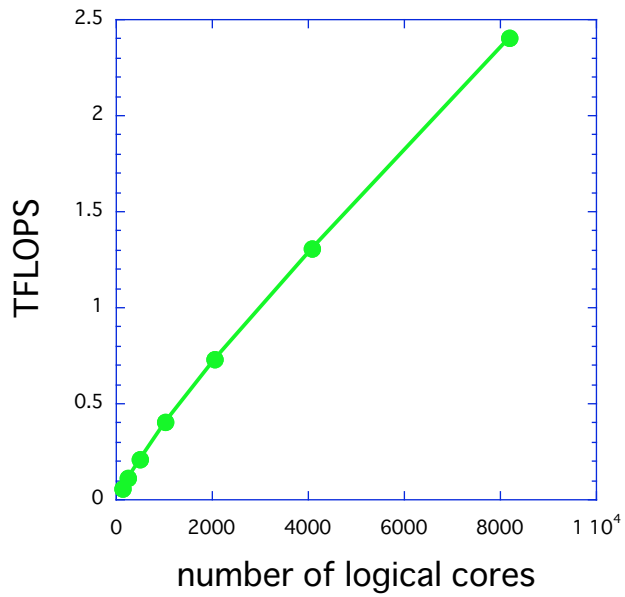
r direction is nonuniformly decomposed.

Each domain include approximately same number of particles.
Some load imbalance remains for field calculation.

For Poisson solver, the global data distributed over the radial direction is gathered to the local domains. Tentative (present version)

# 1d domain cloning




$129 \times 128 \times 128$ mesh

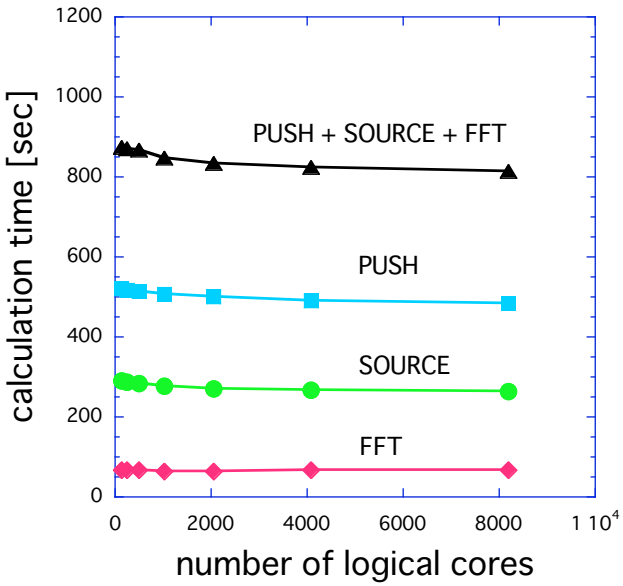
million particles / logical core

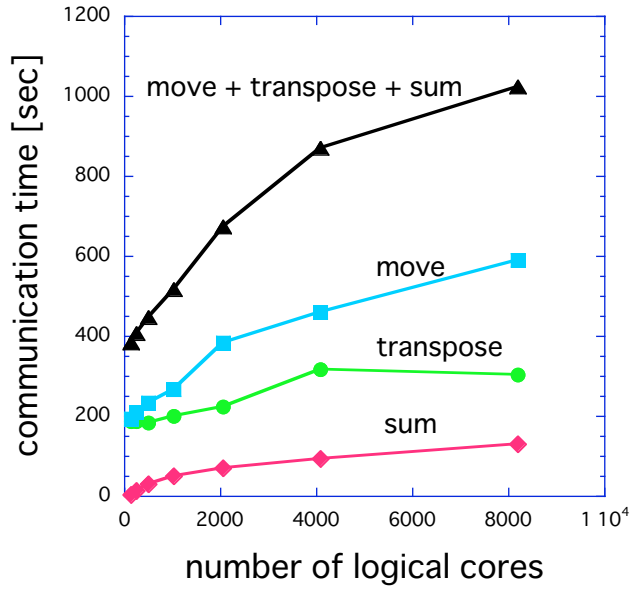
$N_{thread} = 2 \quad (\mathrm{SMP} = 2)$

$N_{process} = N_{DD-z} \times N_{RP}$

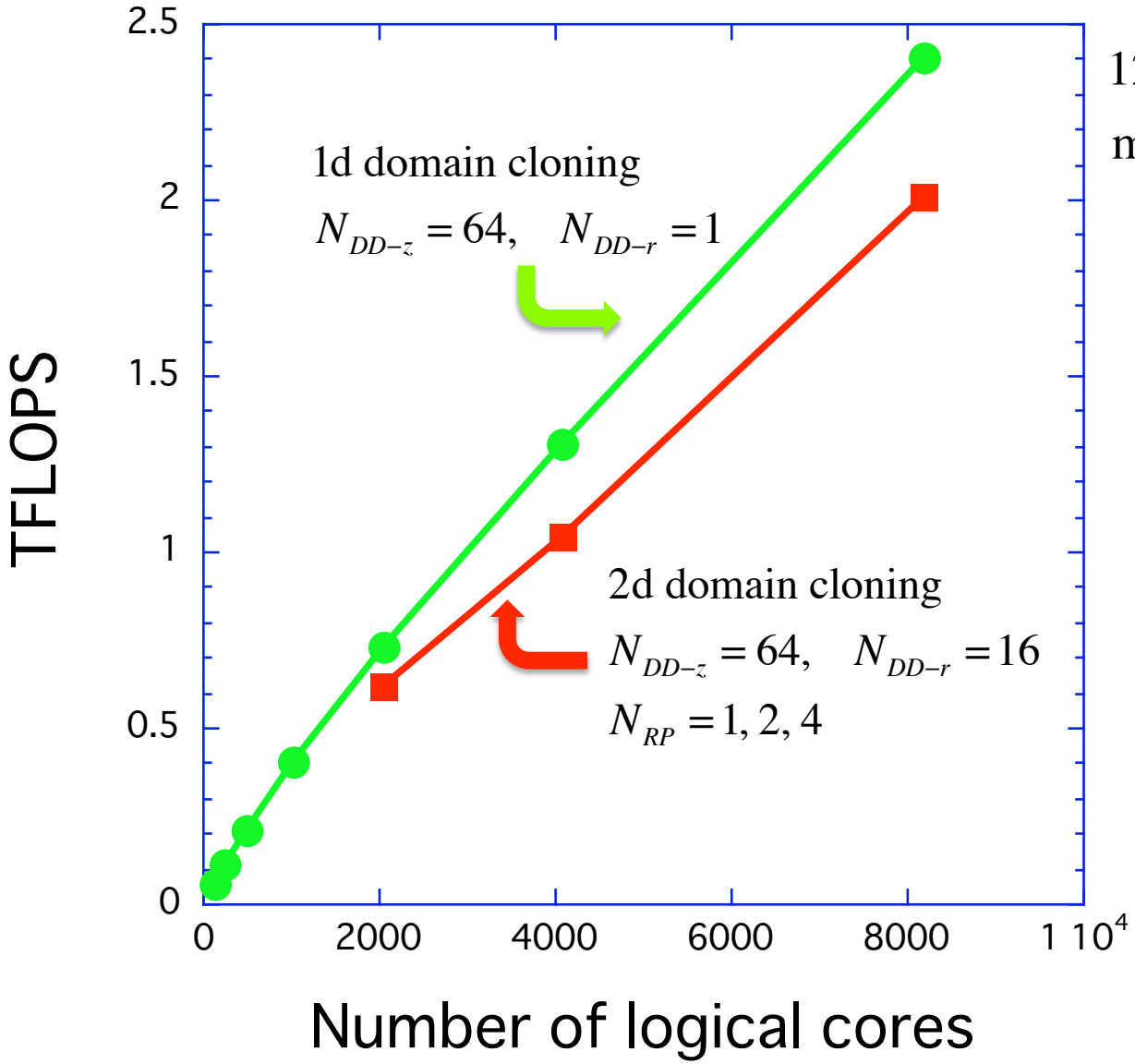
$N_{DD-z} = 64$

$N_{RP} = 1, 2, 4, 8, 16, 32, 64$



# 1d versus 2d domain cloning




$129 \times 128 \times 128$ mesh

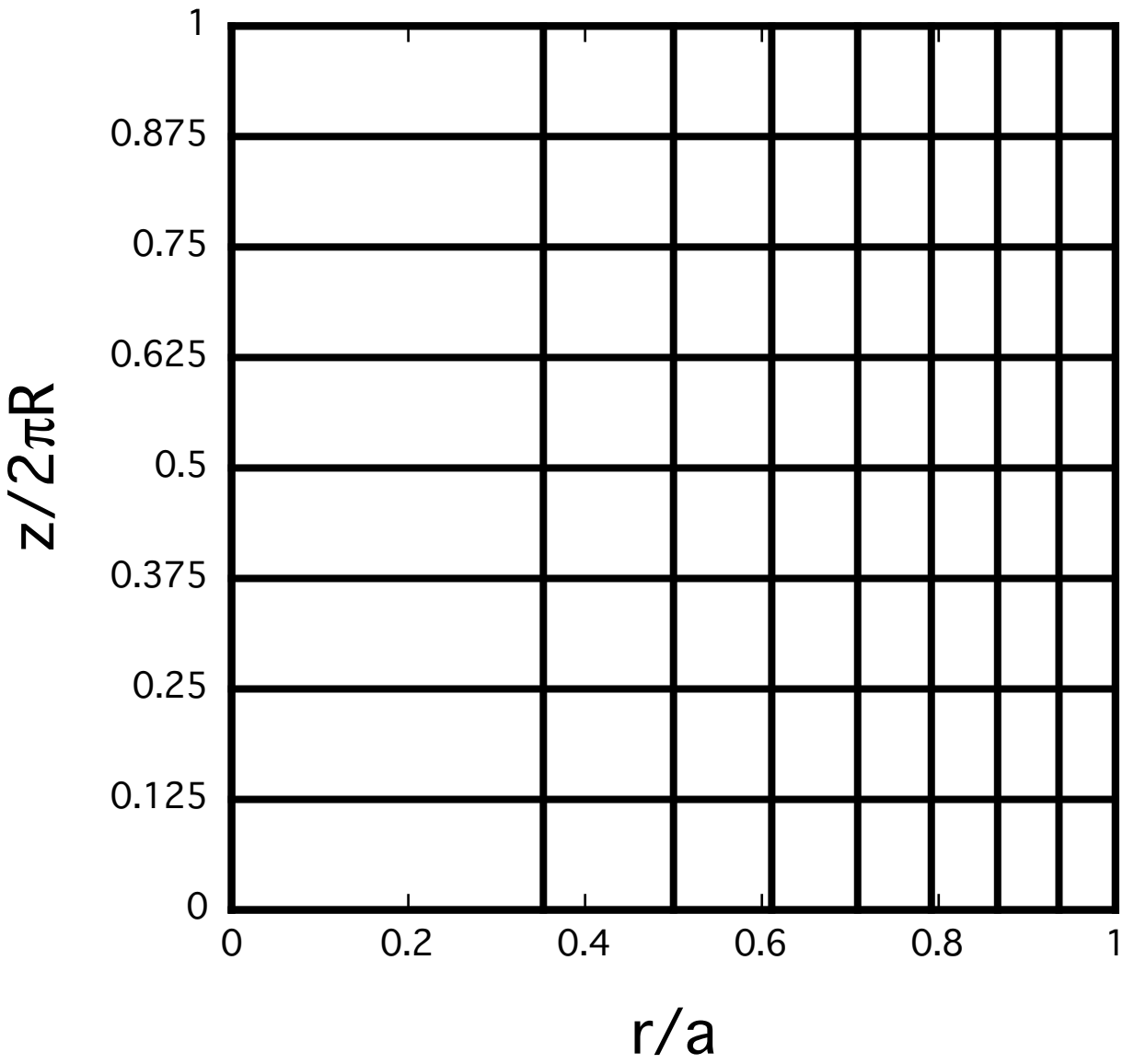
million particles / logical core

Small mesh size
129 x 128 x 128

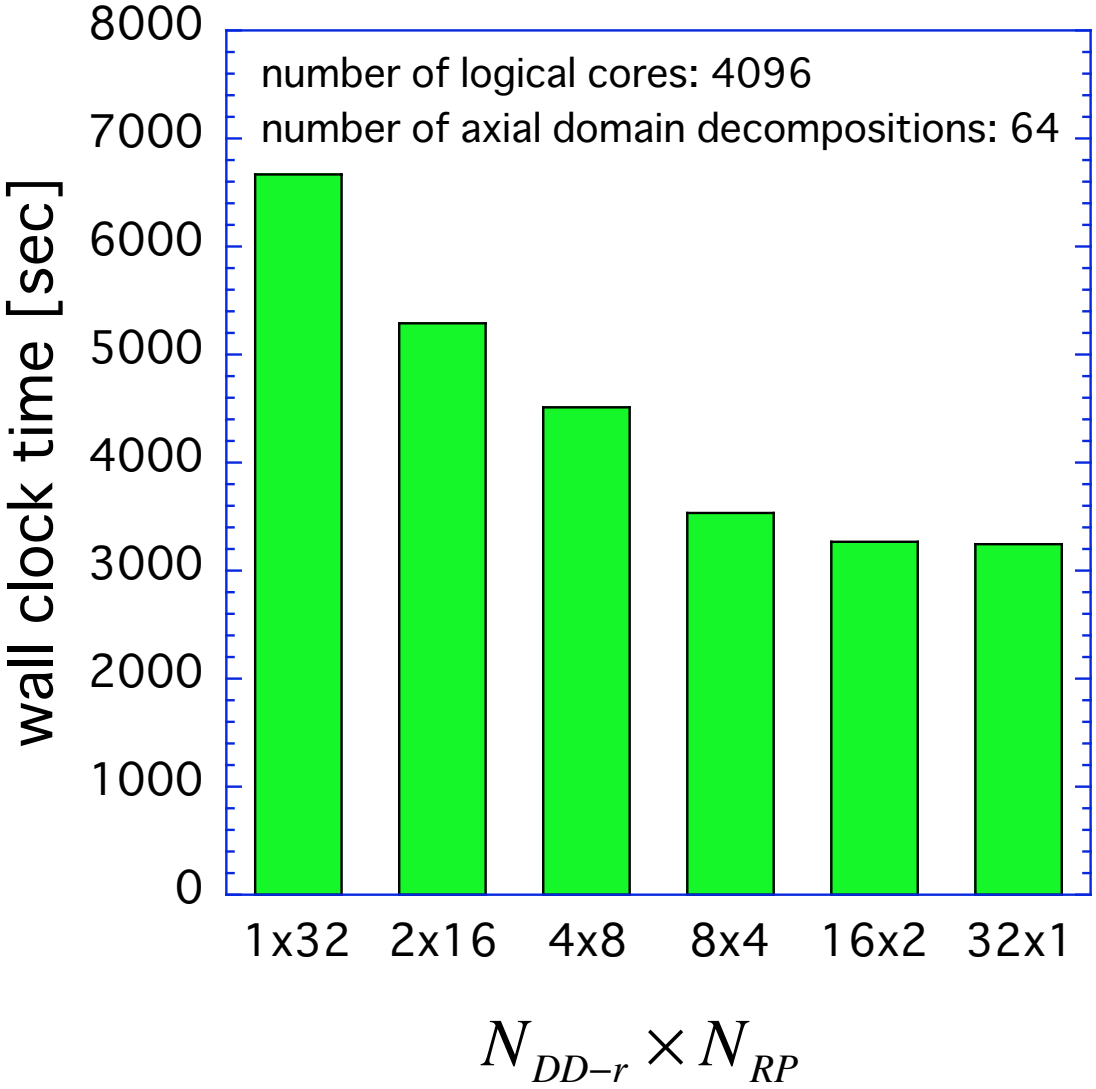
Medium mesh size
1025 x 128 x 128

Large mesh size (future)
10000 x 128 x 128

# 2d domain decomposition in z and r



# Wall clock time versus various decompositions

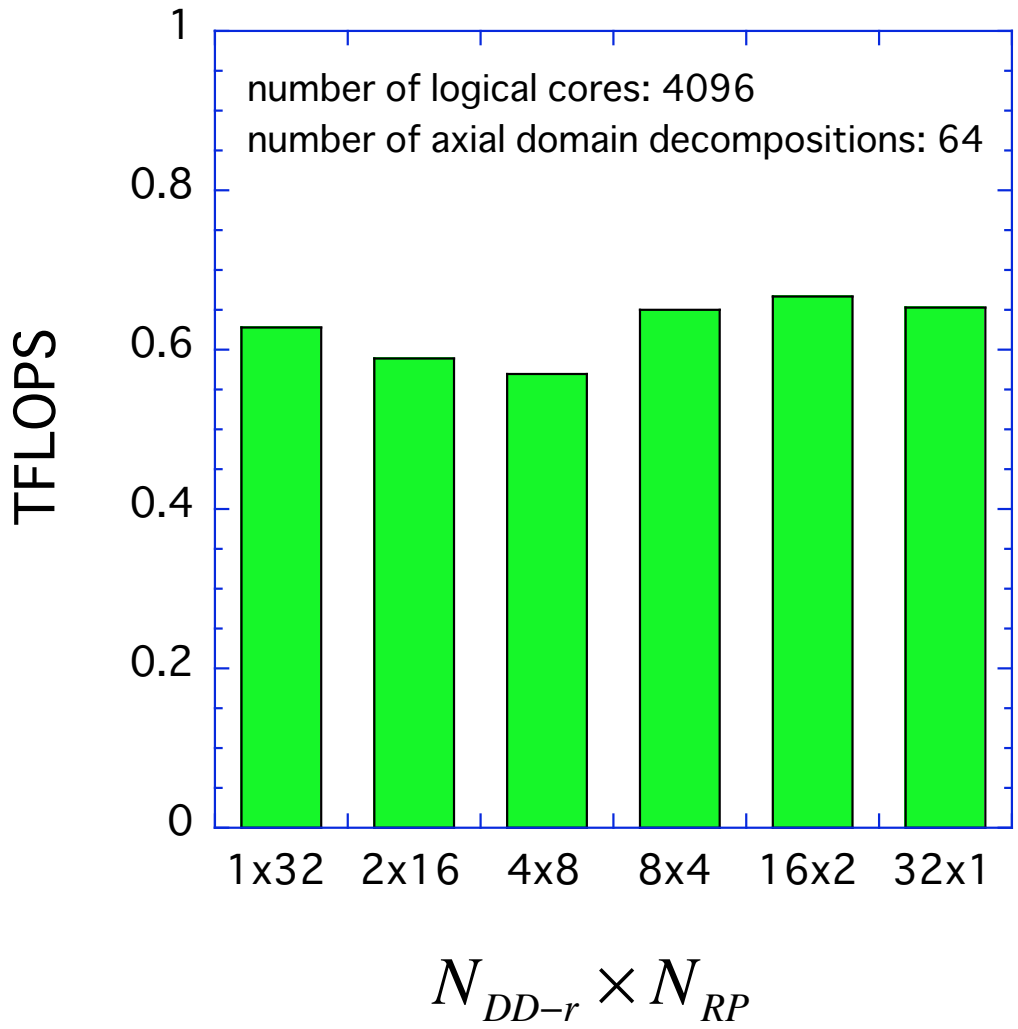



1025x128x128 meshes
4 billion particles

$$N_{thread} = 2 \quad (\mathrm{SMP} = 2)$$
$$N_{process} = N_{DD-r} \times N_{DD-z} \times N_{RP}$$
$$N_{DD-z} = 64$$
$$N_{DD-r} \times N_{RP} = 32$$

Radial domain decomposition is useful for good performance.

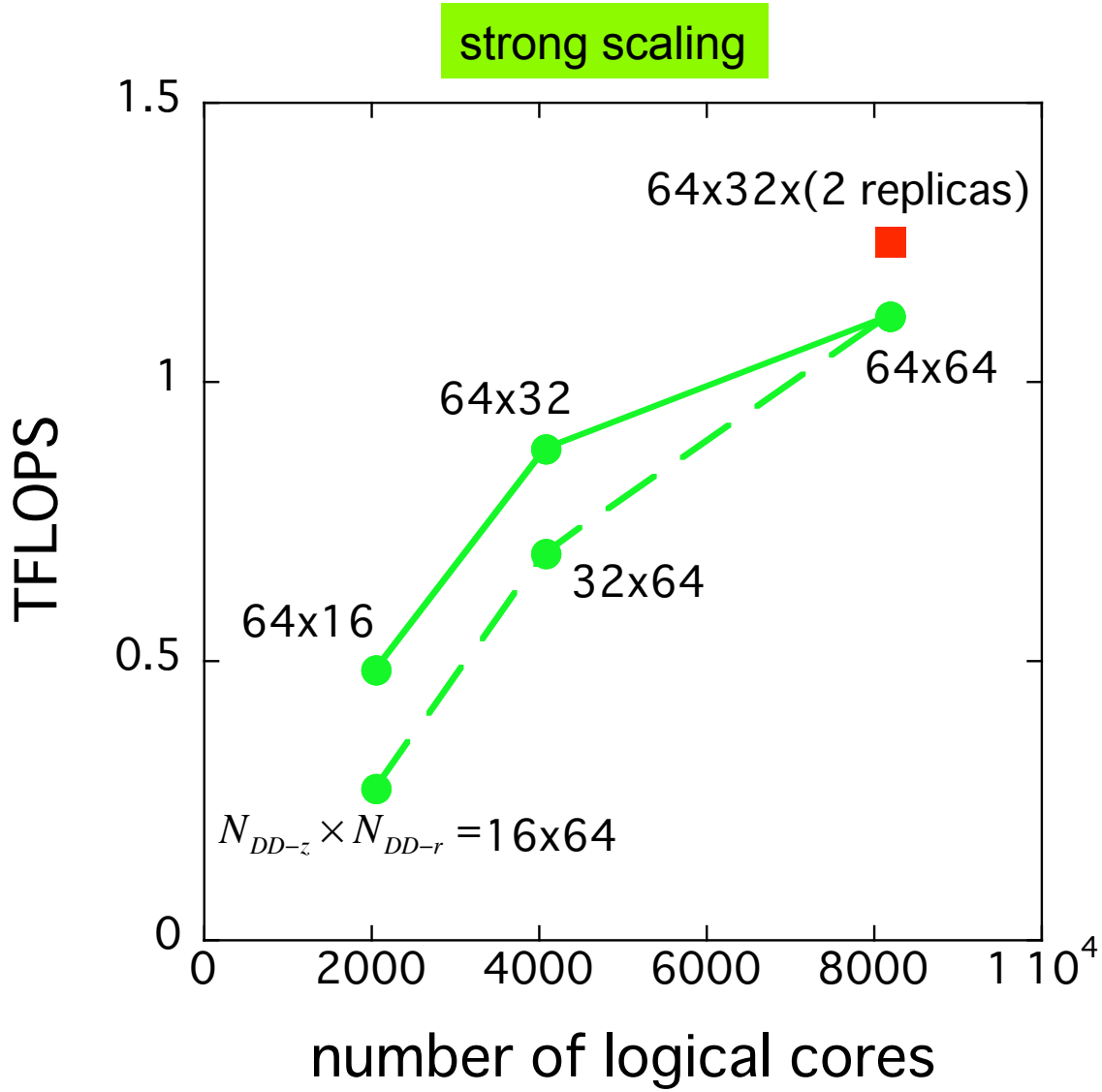
# Flops versus various decompositions




1025x128x128 meshes
4 billion particles

$$N_{thread} = 2 \quad (\mathrm{SMP} = 2)$$
$$N_{process} = N_{DD-r} \times N_{DD-z} \times N_{RP}$$
$$N_{DD-z} = 64$$
$$N_{DD-r} \times N_{RP} = 32$$

# Flops versus number of logical cores




1025x128x128
meshes
8 billion particles

$N_{thread} = 2 \quad (\mathrm{SMP} = 2)$

$N_{process} = N_{DD-r} \times N_{DD-z} \times N_{RP}$

$N_{RP} = 1$ [or 2 (one case)]

# 4. Summary (1)

1. We proposed a new algorithm for the advanced version of Gpic-MHD.
2. The advanced version of Gpic-MHD successfully simulated the kinetic internal kink mode.
3. Extension to the higher beta and larger scale simulation is promissing.
4. Energy conservation is quite well.
5. Noise due to particle discreteness is very low.
6. Particle information is mainly used to estimate second-order moment.

→ "particle closure" "complete closure"

7. Question for a very long time scale run.

# 4. Summary (2)

- The parallelization performance of 3d Gpic-MHD on SR16000 is studied.
- Gpic-MHD with 2d domain cloning shows good parallelization performance up to 8192 logical cores.
- Gpic-MHD with 2d domain cloning will be preferable for larger system with larger number of cores.
- How to obtain good parallelization performance?
  - (1) use maximum number of axially decomposed domains.
  - (2) use optimum number of radially decomposed domains.
  - (3) use replicas if the maximum number of logical cores is larger than the number of decomposed domains.
  - (4) increase $N_{thread}$ (?)
- Development of Poisson solver in Fourier space for radially distributed data is important. (Present version tentatively uses global data.)