Development of multi-scale simulation method via pseudo-particle method

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Contents

Introduction and motivation

- Multi-scale simulation method is useful when kinetic effects work like singular perturbation in a local area. MHD-PIC simulation is a typical example of multi-scale method in which a kinetic PIC simulation region is surrounded by a large MHD simulation region.

- A key issue of the multi-scale simulation algorithm is to find a macroscopic coarse-grained description of phenomena. This process naively corresponds with renormalization.

- The most microscopic description is the one via charged particles.

$$L = \sum \left(\frac{m}{2}\frac{d\boldsymbol{x}_i}{dt}^2 + e\boldsymbol{A}(\boldsymbol{x}_i,t)\cdot\frac{d\boldsymbol{x}_i}{dt} - e\phi(\boldsymbol{x}_i,t)\right) + \int dx^3 \left[\frac{\epsilon_0}{2}(-\nabla\phi - \frac{\partial \boldsymbol{A}}{\partial t})^2 - \frac{\mu_0}{2}(\nabla\times\boldsymbol{A})^2\right]$$

- Macroscopic description is formulated from the view-point of pseudo-particles (fluid-element or wave quanta).

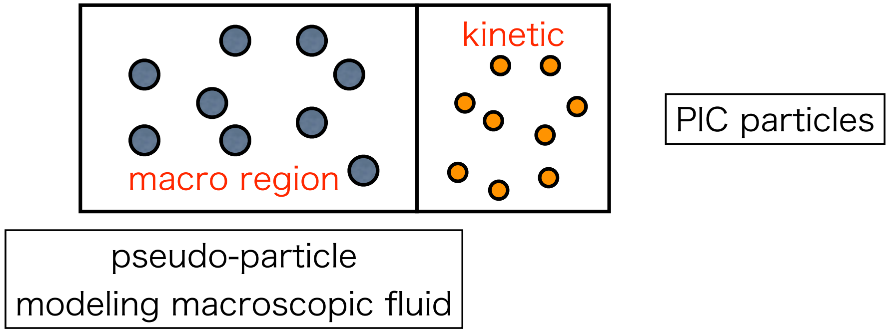
- Formulation on the basis of particle-like picture may be useful for tackling the multi-scale phenomena.

In this study, we developed a multi-scale simulation method in which both macroscopic fluid and microscopic kinetic model can be simulated by particle method. (**Analogy with the field theory**)

Basic concepts of multi-scale simulation by pseudo-particle method

・A plasma (matter) is understood as a collection of pseudo-particles. (PIC particles and macroscopic pseudo-particles)

・The character of pseudo-particles may change according to the state of the system in which particles are embedded.



Macroscopic flow is expressed in terms of pseudo-particles which model fluid plasma.

When kinetic effects are important in some region, the system is expressed via PIC particles in the region.

Advantage of this method

The governing equations for macro-scale and micro-scale are eqs. of motion of particles and field equations (Maxwell's equations). Accordingly, a change of model is easily performed in a single numerical code.

Especially, in this study we developed a multi-scale pseudo-particle method where a pseudo-particle method for fluid plasma is switched to PIC method for kinetic when it is needed.

Pseudo-particle method which models fluid

- Smoothed Particle Hydrodynamics is a pseudo-particle method, which is popular in modeling self-gravitating neutral fluids.

Reviews of Basic SPH

- The heart of SPH is an interpolation method which allows a field variables to be expressed in terms of its values at a set of disordered points - the particles.

$$
\begin{aligned}
A(\boldsymbol{r}) &= \int A(\boldsymbol{r}')W(\boldsymbol{r}-\boldsymbol{r}',h)d\boldsymbol{r}' \\
&= \int [mn(\boldsymbol{r}')d\boldsymbol{r}'] \frac{A(\boldsymbol{r}')}{mn(\boldsymbol{r}')} W(\boldsymbol{r}-\boldsymbol{r}',h) \\
&\simeq \sum_b m_b \frac{A(\boldsymbol{x}_b)}{mn(\boldsymbol{x}_b)} W(\boldsymbol{r}-\boldsymbol{x}_b,h) \quad (m_b = mn(\boldsymbol{x}_b)\Delta r)
\end{aligned}
$$

W(x) is some analytic function such as Gaussian profile. .

W approaches asymptotically the δ-function in the limit of h→0.

- By using the above interpolation, neutral fluid equations can be discretized as

$$
\rho(\boldsymbol{x}_a) = \sum_b m_b W(\boldsymbol{x}_a - \boldsymbol{x}_b), \quad \text{or} \quad \rho_a = \sum_b m_b W_{ab}
$$

$$
\frac{d\boldsymbol{v}_a}{dt} = -\sum m_b \left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2}\right)\nabla_a W_{ab},
$$

$$
\frac{d\boldsymbol{x}_a}{dt} = \boldsymbol{v}_a,
$$

$$
P_a = f(\rho_a) \quad \text{if we employed the barotoropic condition}
$$

・The pressure force is modeled as interaction with neighboring particles.
・A particle carries physical variables, which characterize a fluid element, such as position, velocity, pressure, mass.
・Equation of motion can be derived from the variational principle.
・A trajectory of the particle is considered as a characteristics of the original fluid equations.

Development of Electromagnetic SPH (EMSPH)

We succeeded to extend the original SPH to electromagnetic two-fluid plasma model by coupling with EM fields.

Fluid quantities are defined on particles (Lagrange grid) and EM fields are defined on Eulergian grid. In the previous EMSPH, Lagrange grids are used.

This method can be categorized as a hybrid method between SPH and PIC.

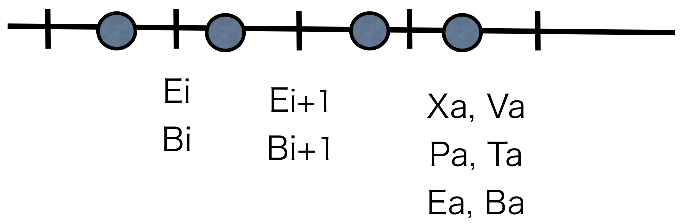


Fig. Relation between grids and physical variables

Formulations of EMSPH

Basic equations of two-fluid theory are as follows;

$$\frac{\partial n_s}{dt} + \nabla \cdot (n_s \boldsymbol{v}_s) = 0,$$
$$\frac{d\boldsymbol{v}_s}{dt} = \frac{q_s}{m_s}(\boldsymbol{E} + \boldsymbol{v}_s \times \boldsymbol{B}) - \frac{1}{m_s n_s}\nabla P_s,$$
$$P_s = f(n_s),$$
$$\frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}, \quad , \nabla \cdot \boldsymbol{E} = \frac{1}{\epsilon_0}\sum q_s n_s,$$
$$\nabla \times \boldsymbol{B} = \mu_0 \sum q_s n_s \boldsymbol{v}_s + \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{dt}$$

Following the same procedure in SPH, the above equations can be discretized as

$$n(\boldsymbol{x}) = \sum_b n_b W(\boldsymbol{x} - \boldsymbol{x}_b), \quad P_a = f(n_a)$$
$$\frac{d\boldsymbol{v}_a}{dt} = \frac{q_s}{m_s}(\boldsymbol{E}_a + \boldsymbol{v}_a \times \boldsymbol{B}_a) - \sum_b m_b\left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right)\nabla_a W_{ab},$$
$$\boldsymbol{E}_a = \sum_l \nabla S_{al}\phi_l \Delta x, \quad S_{al} = S(\boldsymbol{x}_a - \boldsymbol{x}_l),$$
$$\boldsymbol{B}_a = \sum_l \nabla_a S_{al} \times \boldsymbol{A}(\boldsymbol{x}_l)\Delta x$$

a, b: label for particles
l: label for eulerian grids

・W is a kind of Green's function for particles.
・S is an shape factor for grids.
・EMSPH particles exhibit the mutual interaction force modeling the pressure gradient, while PIC particles obey EM force only.
・These equations can be obtained by a variational principle shown in the next slide.

Variational Principle of EMSPH

An important feature of SPH is that the eq. of motion can be derived on the basis of variational principle. Here we show that the eq. of motion for EMSPH can be also derived from variational principle.

Lagrangian of two-fluid plasma except for the EM field part

$$L_{fl} = \int (mndx^3)[\frac{1}{2}\boldsymbol{v}^2 - u(\rho, s) + \frac{q}{m}\boldsymbol{v}\cdot\boldsymbol{A} - \frac{q}{m}\phi],$$

$$\simeq \sum_b m_b[\frac{1}{2}v_b^2 - u_b(\rho_b, s_b)] + \sum_b \frac{q}{m_s} m_b \boldsymbol{v}_b \cdot \boldsymbol{A}_b - \sum_b \frac{q}{m_s} m_b \phi_b,$$

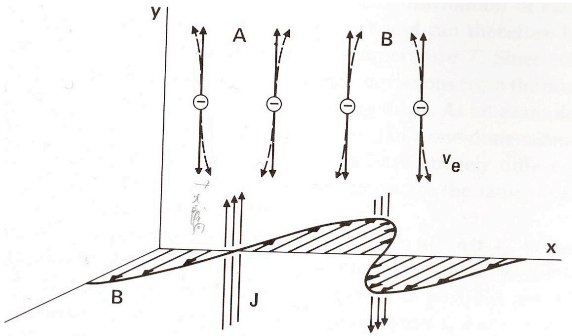
$$= \sum_b \frac{m_b}{2} v_b^2 - \sum m_b u(\rho_b, s_b) + \sum_b \frac{q}{m_s} m_b \boldsymbol{v}_b \cdot \sum_l \boldsymbol{A}_l S_{bl} \Delta V - \sum_b \frac{q}{m} m_b \sum_l S_{bl} \phi_l \Delta V$$

Taking a variation about the position of a particle X, the eq. of motion of the particle X is derived.

Therefore, EMSPH is a physically natural pseudo-particle method which models plasma fluid.

Weibel instability as an example of multi-scale phenomena

- Weibel instability is the well-known kinetic instability. The schematic view is shown in the figure. When counter streams of electrons are perturbed, the perturbation grows by a resulting current.



F. F. Chen, Introduction to plasma physics

- Initial behavior of the Weibel instability(especially, current filamentaion instabiliy) can be described via two-fluid theory by regarding the plasma such that it is composed of two-fluids streaming in the counter direction with each other. Not Usual electron fluid!

- When the perturbation grows, small scale structures are created and the structure in the phase space is strongly disturbed. Then, kinetic effects must be important and the instability moves into the kinetic regime.

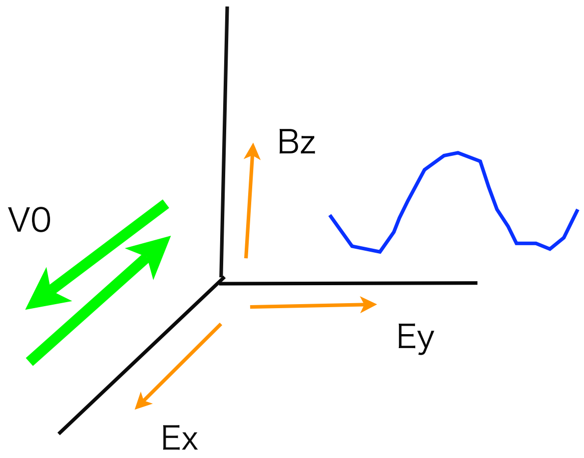
- Accordingly, Weibel instability can be understood as a multi-scale phenomenon which exhibits a switch of model from the macroscopic two-fluid theory to the microscopic kinetic theory during the time evolution.

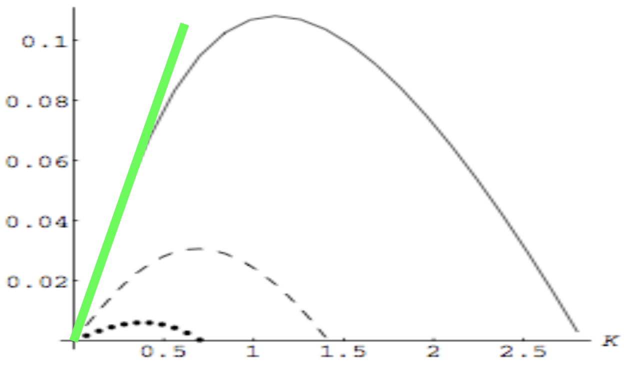
This kind of instability is a suitable example treated by the multi-scale pseudo-particle method

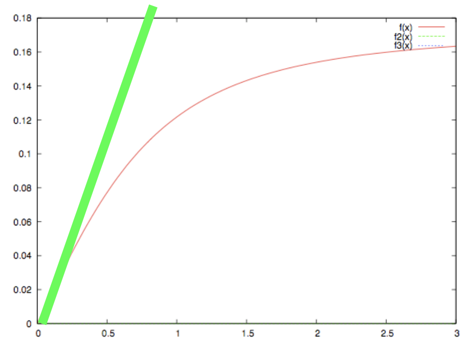
Comparison between fluid simulation and kinetic simulation

- Here we will consider how difference between fluid simulation and kinetic simulation in the nonlinear regime appears. Clarification of the difference is important to implement the multi-scale pseudo-particle method, because we need to clarify the parameter regime where EMSPH is valid.
- Weibel instability is a mechanism of magnetic field (helicity) generation. A saturation level of magnetic field is the important measure of the instability. Therefore, we mainly investigate the difference in saturation level of magnetic field.
- In both simulations, particles are moving in the system. We investigate how the difference can be understood in the view point of the particle's property.

Simulation Settings



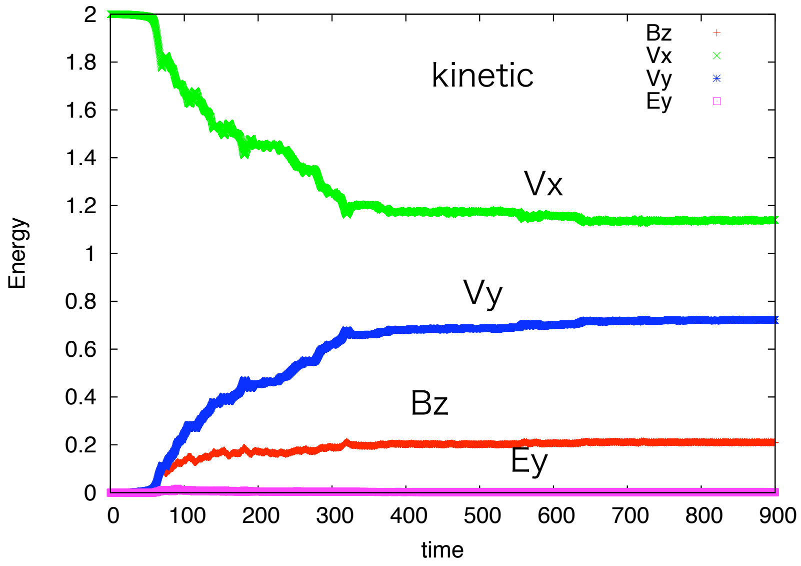


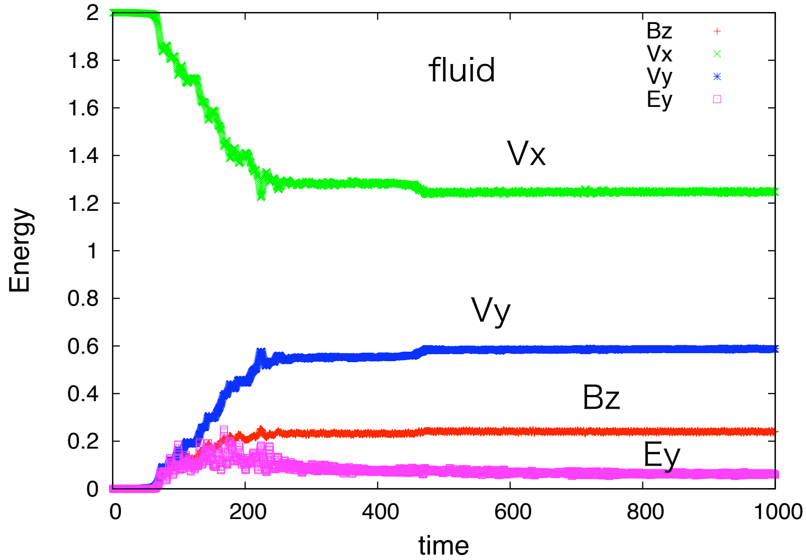


- Ions are assumed to be immobile. We consider electrons' motion only.
- There are counter streaming electrons in the x-direction.
- In fluid simulation, electrons are divided into two kinds of electron fluids (one flowing in the positive direction and the other flowing in the opposite direction)
- The particles are distributed along the y-direction in both fluid and kinetic simulation.
- When the wavelength is long enough, the growth rate of the instability by two-fluid theory is same as one by kinetic theory. Accordingly, at the such wavelength, the difference of time evolution is clearly observed.

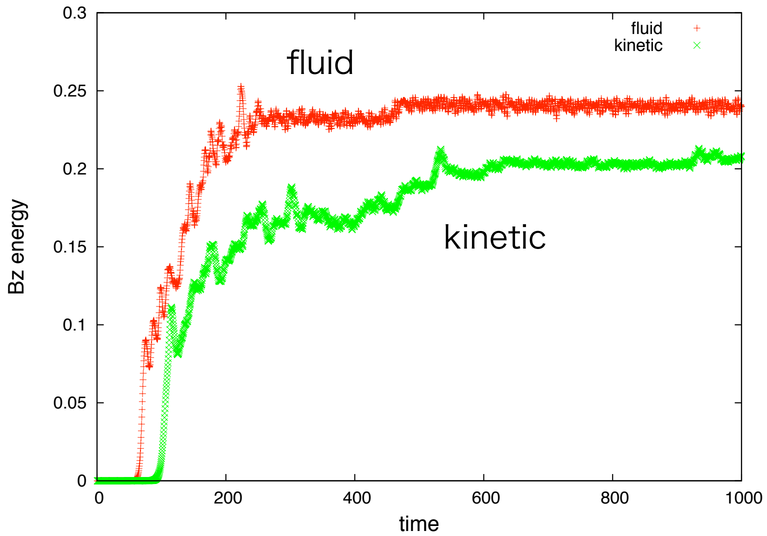
Simulation results

Time evolution of energy



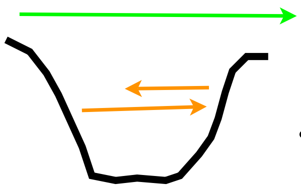


Comparison of magnetic energy



- A difference in saturation level of energy is observed.
- In the fluid simulation, the longitudinal electric field energy has a finite level due to the absence of Landau damping.
- The growth rate in the initial phase is same in both kinetic and fluid simulations.
- The difference in the time to be saturated is observed.
- The saturation level of the magnetic energy in fluid simulation is higher than that in kinetic simulation.

Consideration about the saturation level (magnetic trapping)

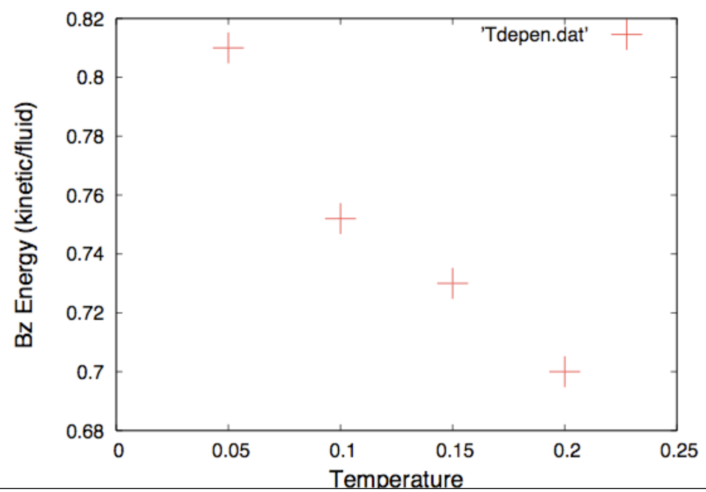


- Morse clarified the saturation mechanism that particles are trapped in magnetic well in the nonlinear stage. In the mechanism, conservation laws resulting from 1D geometry are important.

- Seeing from the equation below, the conservation law is broken by mutual interaction between particles (pressure) in the fluid simulation. This means that the effect of magnetic trapping becomes weak. The difference in the saturation level can be easily understood by using the pseudo-particle method.

$$\frac{d\boldsymbol{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right)\nabla_a W_{ab} + \frac{q_s}{m_s}(\boldsymbol{E}_a + \boldsymbol{v}_a \times \boldsymbol{B}_a)$$

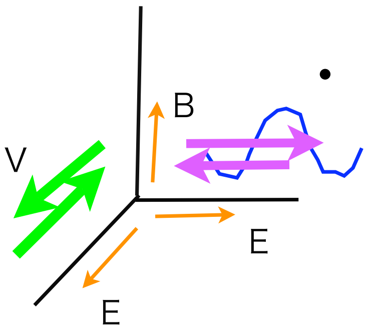
Temperature dependence of the ratio of magnetic field energy in EMSPH to the one in PIC



The ratio of the magnetic field energy in EMSPH to the one in PIC decreases when the temperature becomes high.
→When the pressure interaction, which breaks the conservation law, becomes stronger, the difference in saturation becomes larger.

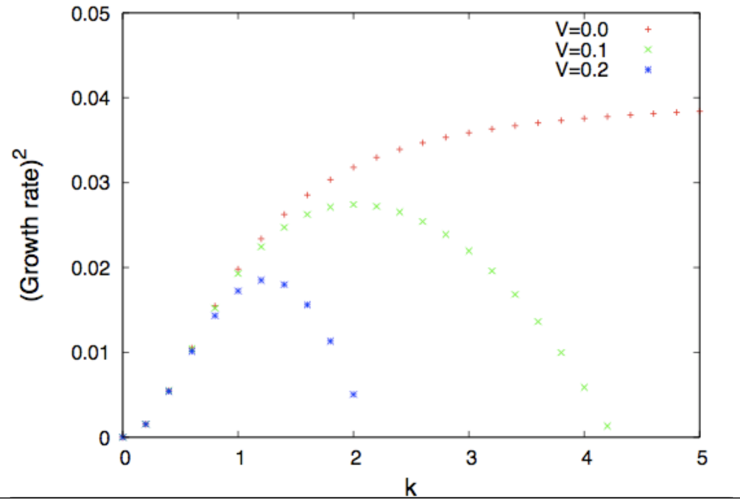
Consideration about the saturation level 2

- Actually, the numbers of particles passing through the magnetic well increases when the temperature becomes high. Then, here we investigate whether those particles enhance the instability



- particles passing through the potential have large velocity along the direction of propagation. Therefore, we investigate a linear stability of Weibel instability for counter-streaming electrons which have 0-th order velocity.

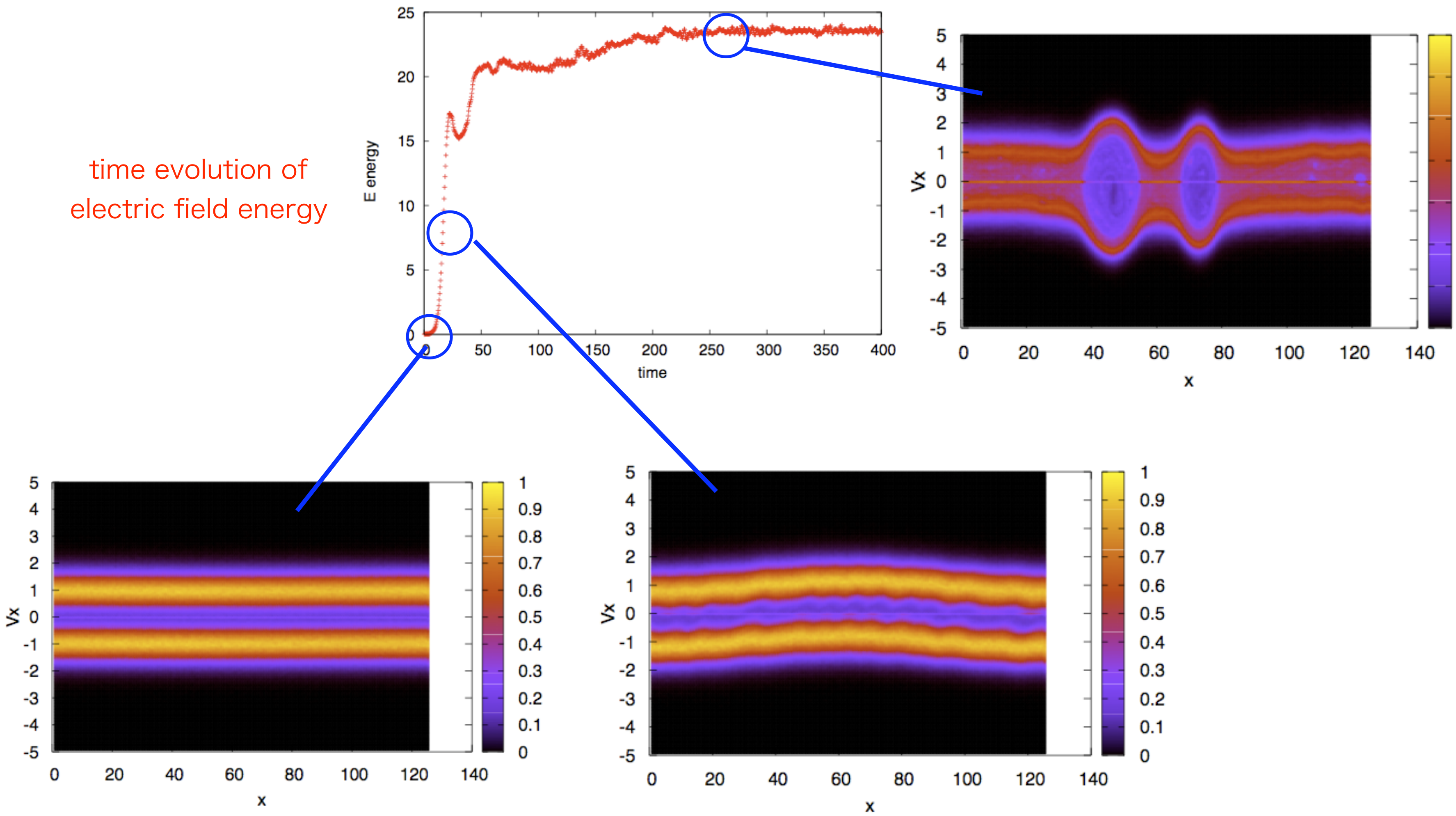
Growth rate of weibel instability
with 0-th order flow



Weibel instability is stabilized by 0-th order flow along the direction of propagation.
Since small scale structure are created in the nonlinear stage, energy transfer to magnetic energy becomes weak.

Multiscale pseudo-particle method (two-stream instability)

- Two-stream instability can also be understood as a multiscale phenomenon.



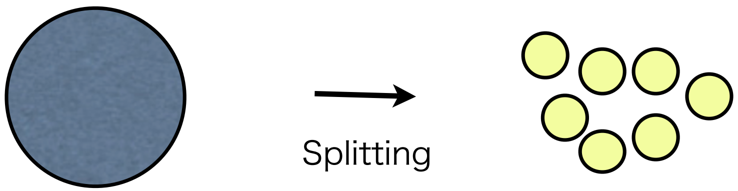
Procedure of switching from fluid simulation (EMSPH) to kinetic(PIC)

As shown in the previous slide, the initial stage of the instability can be analyzed by two-fluid theory.

Here, we accomplish the following simulation.

Initial phase fluid simulation EMSPH	→	nonlinear phase kinetic simulation PIC

schematic view



an EMSPH pseudo-particle x, v, n, T	PIC particles (x, v)

Equation of motion

$$\frac{d\boldsymbol{v}_a}{dt} = \frac{q_s}{m_s}\boldsymbol{E}_a - \sum_b m_b\left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right)\nabla_a W_{ab} \longrightarrow \frac{d\boldsymbol{v}_i}{dt} = \frac{q_s}{m_s}\boldsymbol{E}_i$$

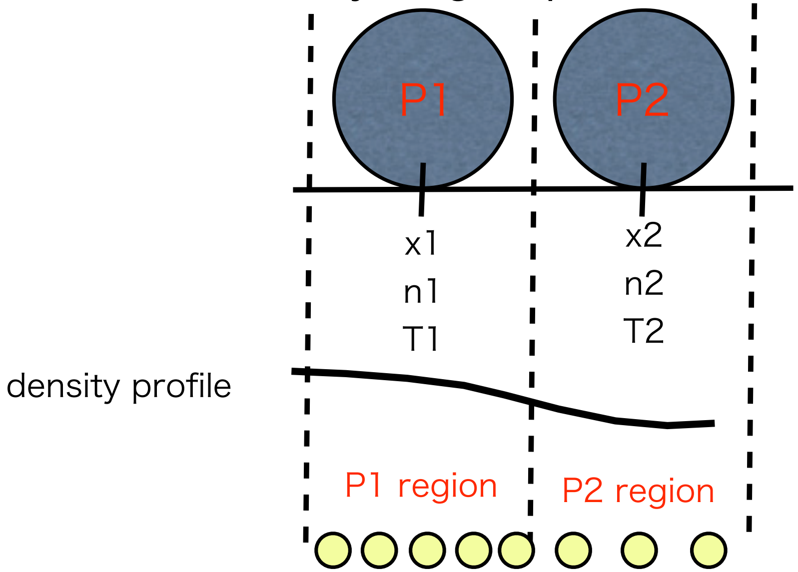
dropping pressure term

Switching from fluid simulation to kinetic simulation can be easily performed in the viewpoint of pseudo-particle method.

However, it is not trivial whether the time evolution is not affected by the switching.

Concrete method of implementation of splitting

・When an EMSPH particle is split into many PIC particles, it is necessary to give position and velocity to PIC particles.



The numerical domain is divided into N domains in which a EMSPH particle exists.
We call the region in which a Nth particle exists as Pn region.

In each Pn region,

particle position→using cumulative density function for linearly approximated density profile .

particle velocity→Vn(mean flow) +Maxwell distribution corresponding to Tn. 10^5 particles are necessary to reproduce the Maxwell distribution with sufficient accuracy.

Simulation Results

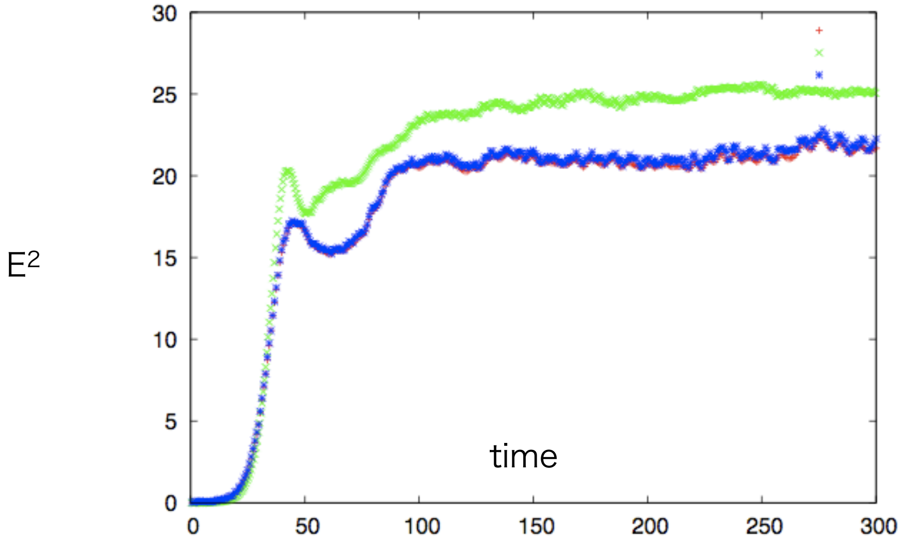
Comparing three simulation results

Case 1; pure PIC simulation ($N=2\times10^7$)

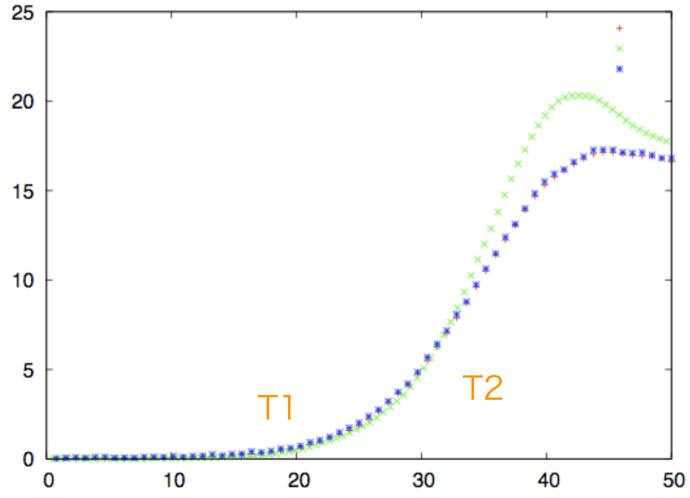
Case 2; multiscale simulation from fluid to kinetic (T1 = 20) (N = 500 to $N=5*10^7$)

Case 3; multiscale simulation from fluid to kinetic (T2 = 35) (N=500 to $N=5*10^7$)

time evolution of E^2 for 3 cases



enlarged view of the left figure



・The result of Case 1(Red line) and Case 2 (Blue line) is almost same. Especially, any discontinuity is not observed around T1, that is, switching of scheme from fluid to kinetic was successful.

・The result of Case 3 (Green line) is different compared with other two cases. This discrepancy is the result of large T2. The switching when the perturbed electric field energy becomes 5% of the free energy was late in this simulation.

・Multiscale pseudo-particle method is efficient if the scheme is switched before the instability grows to a certain level.

Summary

- In this study, we proposed a multi-scale simulation method using pseudo-particles. As the first step, we developed a numerical scheme in which the EMSPH fluid simulation is switched to the PIC kinetic simulation.

- We formulated pseudo-particle method for fluid plasma (EMSPH). For weibel instability, we performed fluid simulation via EMSPH and we clarified how the difference with kinetic simulation appeares.

- The difference in saturation mechanism is easily understood in the view point of the particle's property.

- For two-stream instability, we implemented multi-scale pseudo-particle method. The scheme worked well when the switching is performed before the instability grows. Optimization of the time of switching and construction of theoretical estimation are future works.