Kinetic Simulations of Turbulent Fusion Plasmas

Y.Idomura, T.H.Watanabe, H.Sugama, Comptes Rendus Physique 7, 650 (2006)

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Acknowledgements to **H. Sugama and T.H. Watanabe**

1st ITER Summer School, Aix-en-Province, France, July 16-20, 2007

Outline

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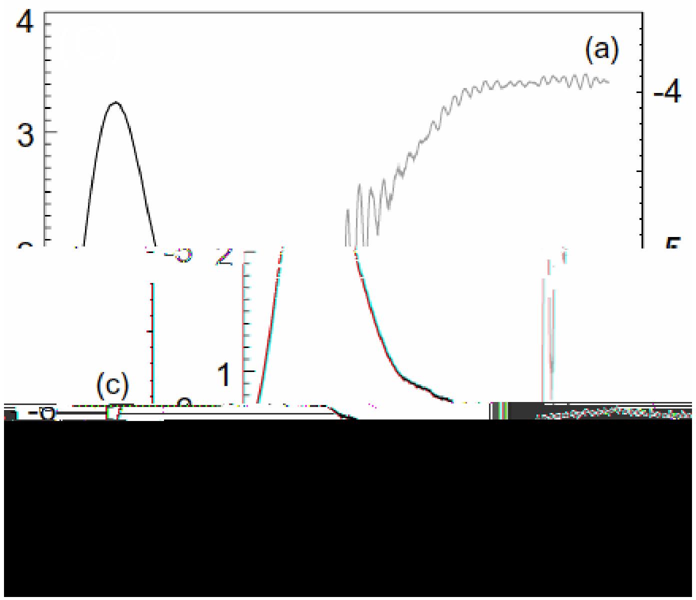
2. Gyrokinetic model
3. Various approaches in gyrokinetic simulations
4. Particle/Lagrangian approach
5. Mesh/Eulerian approach
6. Collisionless gyrokinetic simulation

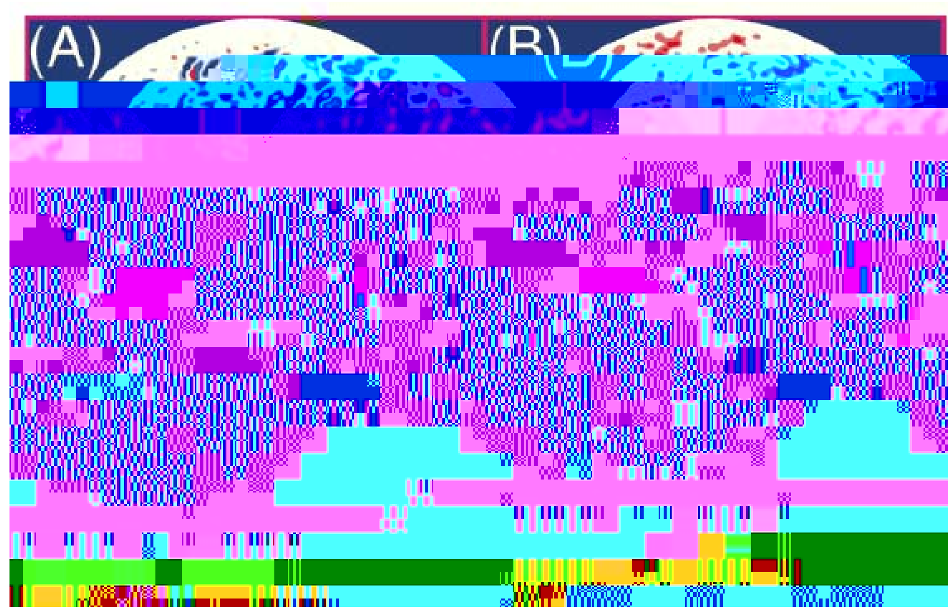
1. Introduction

Micro-instabilities in tokamak plasmas

Toroidal ITG turbulence simulation with and without zonal flows

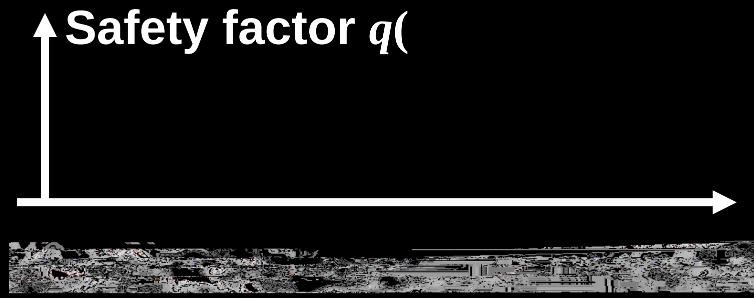
(Lin,Science98, Diamond,NF01)





- Various zonal flow instabilities
  (Diamond,IAEA98, Chen,POP00, Rogers,PRL00)
- Nonlinear upshift of effective critical ITG by zonal flows
  (Dimits,POP00)
- Linear damping mechanism of zonal flows
  (Rosenbluth-Hinton,PRL98)

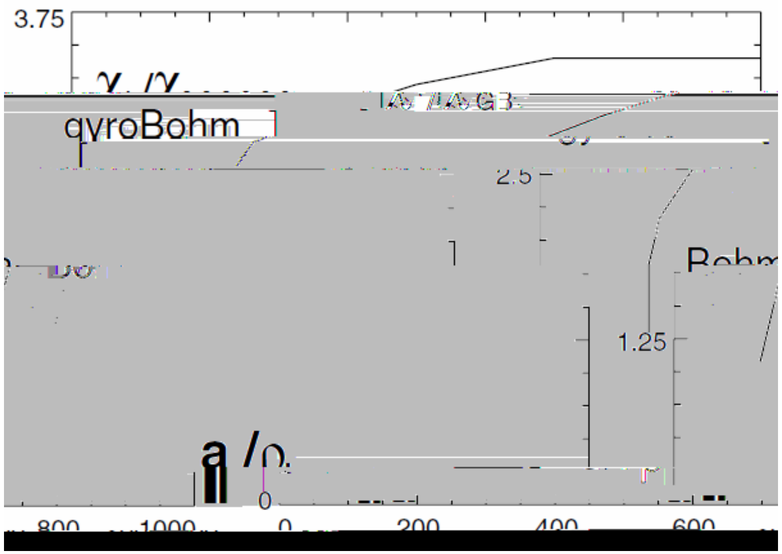
Structure formations in microscopic ETG turbulence

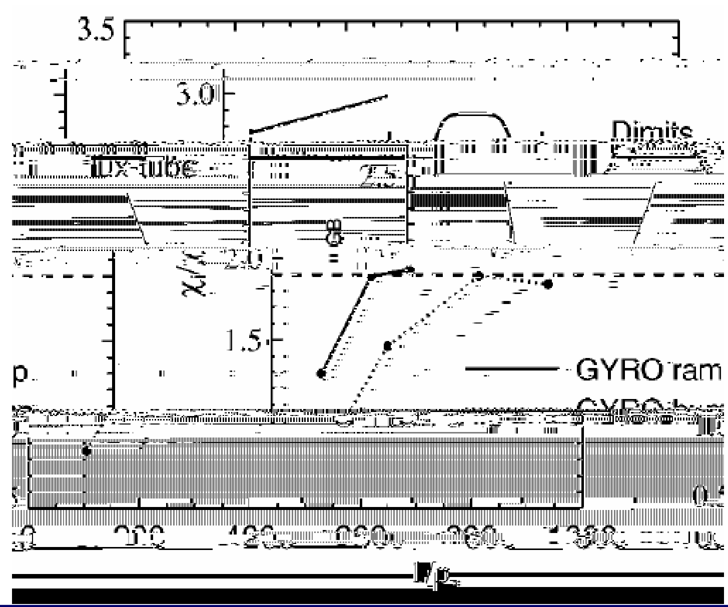


Plasma size scaling of ITG turbulence

Transition of plasma size scaling from Bohm to gyro-Bohm

(Lin,PRL02, Candy,POP04)





- Linear ballooning theory with equilibrium profile shear effects
  (Connor,PRL93, Romanelli,PFB93, Kim,PRL94)
- Shearing effects of equilibrium x flows on size scaling
  (Garbet,POP96, Waltz,POP02)
- Turbulence spreading into less unstable or stable regions
  (Lin,POP04, Hahm,PPCF04, Waltz,POP05)

Simulation for multi-scale tokamak micro-turbulence

Ion scale turbulence

~5mm,~1μs

2. Gyrokinetic model

Primitive kinetic model of weakly coupled plasma

- Vlasov-Poisson system in canonical coordinates **Z** =(;**q**,**p**)

$$\frac{}{} \equiv \frac{\partial}{\partial} + \{ \quad , \quad \} = \frac{\partial}{\partial} + \frac{\partial}{\partial \mathbf{p}} \cdot \frac{\partial}{\partial \mathbf{q}} - \frac{\partial}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}} = 0 \qquad \text{Vlasov Eq.}$$

$$\{ \;,\; \} = \frac{\partial}{\partial}\frac{\partial}{\partial} - \frac{\partial}{\partial}\frac{\partial}{\partial} \qquad \text{Poisson bracket}$$

$$(\mathbf{q}\;\mathbf{p}) = \frac{1}{2}\left|\mathbf{p} - -\mathbf{A}\right|^2 + \phi(\mathbf{q}) \qquad \text{Hamiltonian}$$

$$-\nabla^2\phi = 4\pi\sum \quad , \quad = {}_0\int \quad \mathbf{p} \qquad \text{Poisson Eq.}$$

  - Continuity equation of transported by Hamiltonian flows in 6D phase space
  - Spatio-temporal scales are given by $\sim\lambda$ and $\sim\omega$

Very expensive model for studying tokamak micro-turbulence

Particle motion in guiding-centre coordinates

- Lagrangian in canonical coordinates **Z** =(;**q**,**p**)

$$\gamma \quad = \mathbf{p} \cdot \quad \mathbf{q} - \qquad , \qquad = \frac{1}{2} \left| \mathbf{p} - - \mathbf{A} \right|^2 + \quad \phi(\mathbf{q})$$

- Guiding-centre coordinates **Z**

$$\mathbf{R} \quad = \mathbf{q} - \boldsymbol{\rho}, \qquad {}_{//} \quad = \mathbf{b} \cdot \mathbf{v}$$

$$= \frac{\left| \mathbf{v}_\perp \right|^2}{2}, \qquad = \tan^{-1} \frac{\mathbf{v} \cdot \mathbf{e}_1}{\mathbf{v} \cdot \mathbf{e}_2}$$

- Lagrangian in **Z** =(;**R** , $_{//}$,μ ,α)

(Littlejohn, J. Math. Phys.79, PF81, J. Plasma Phys.83)

$$\gamma \quad = \quad - \mathbf{A} + \quad {}_{//} \quad \mathbf{b} \quad \cdot \quad \mathbf{R} \quad + \text{—} \mu \quad \alpha \quad -$$

$$(\mathbf{R} \quad , \quad {}_{//} \quad , \mu \quad , \alpha \quad) = \frac{1}{2} \quad {}_{//}^{2} \quad + \mu \qquad + \quad \phi(\mathbf{R} \quad , \mu \quad , \alpha \quad)$$

– Fast α-dependence in (μ is approximate invariant)

Reduction of problem to 5D phase space

- Find gyro-centre coordinates **Z** using near identity transformations

(Cary-Littlejohn,Ann. Phys.83, Brizard-Hahm,Rev. Mod. Phys.06)

Gyrokinetic equation

- Gyrokinetic equation

$$\frac{}{} \qquad \frac{\partial}{\partial} + \{\ ,\ \} = \frac{\partial}{\partial} + \quad \cdot\nabla \quad + \ {}_{//}\frac{\partial}{\partial\ {}_{//}} = 0$$

- Conservative form of gyrokinetic equation

$$\frac{{}^{2}\quad {}^{*}_{//}}{} \equiv \frac{\partial\ {}^{2}\quad {}^{*}_{//}}{\partial} + \nabla\cdot\left({}^{2}\quad {}^{*}_{//}\dot{\mathbf{R}}\right) + \frac{\partial\ {}^{2}\quad {}^{*}_{//}\dot{}_{//}}{\partial\ {}_{//}} = 0$$

- Phase space conservation

$$\nabla\cdot\left({}^{2}\quad {}^{*}_{//}\dot{\mathbf{R}}\right) + \frac{\partial}{\partial\ {}_{//}}\left({}^{2}\quad {}^{*}_{//}\dot{}_{//}\right) = 0$$

$${}^{2}\quad {}^{*}_{//}\dot{\mathbf{R}} = \quad \mathbf{B}^{*}\frac{\partial}{\partial\ {}_{//}} + \frac{{}^{2}}{}\mathbf{b}\times\nabla \quad , \qquad {}^{2}\quad {}^{*}_{//}\dot{}_{//} = - \quad \mathbf{B}^{*}\cdot\nabla$$

$${}^{2}\quad {}^{*}_{//} : \text{Jacobian of gyro-centre coordinates } \mathbf{Z}$$

Continuity equation of   transported by incompressible Hamiltonian flows in 5D phase space (4D:**R**, $_{//}$ + 1D parameter:μ)

GK Poisson equation for self-consistent fields

- obtained by pull-back transform
- Poisson equation in **Z**
  - 2nd

First principles in gyrokinetic equations

- Conservation of phase space volume

$$\nabla\cdot\left(\ ^{2}\ {}^{*}_{//}\dot{\mathbf{R}}\right)+\frac{\partial}{\partial\ _{//}}\left(\ ^{2}\ {}^{*}_{//}\dot{}_{//}\right)=0$$

- Conservation of Casimir invariants ( ) in Liouville equation

$$\frac{\quad(\ )}{\quad}\equiv\frac{\partial\ (\ )}{\partial}+\{\ (\ ),\ \}=0$$

  – particle number , kinetic entropy $\log(\ )$, ^{2}, etc…

- Energy conservation

$$\sum\int\ \frac{\partial}{\partial}\ ^{2}\ {}^{*}_{//}\ \mathbf{Z}=\frac{\quad}{\quad}+\frac{\quad}{\quad}\ =0$$

$$=\sum\int\frac{1}{2}\ {}^{2}_{//}+\mu\ \ ^{2}\ {}^{*}_{//}\ \mathbf{Z}$$

$$=\frac{1}{8\pi}\int\left|\nabla\phi\right|^{2}\ \mathbf{x}+\frac{1}{8\pi}\sum\sum_{\mathbf{k}}\frac{1}{\lambda^{2}}\left[1-\ _{0}\left(\ {}^{2}_{\perp}\rho^{2}\right)\exp\left(-\ {}^{2}_{\perp}\rho^{2}\right)\right]\left|\phi_{\mathbf{k}}\right|^{2}$$

Summary of modern gyrokinetic theory

- Gyrokinetic Vlasov-Poisson system

$$\frac{\partial}{\partial} + \{ \quad , \quad \} = 0$$

$$-\nabla^2 \quad + \sum \frac{1}{\;^2}\left(\phi \langle \bar{\;} \rangle_\alpha \right)_\lambda = 4 \sum \quad _0 \int \delta[(\mathbf{R}+\boldsymbol{\rho})-\mathbf{q}] \quad ^2 \quad ^*_{//} \; \mathbf{Z}$$

  – Spatio-temporal scales are given as $\sim\rho$ and $\omega << \Omega$
  – Problem is reduced to 5D (4D hyperbolic PDE + 1D parameter)
  – Keeps important kinetic effects (FLR, Landau resonance, etc…)
  – Keeps all the first principles which the original system has
    - Phase space conservation
    - Conservation of particle number, kinetic entropy, etc…
    - Total energy conservation

Important for avoiding spurious phenomena

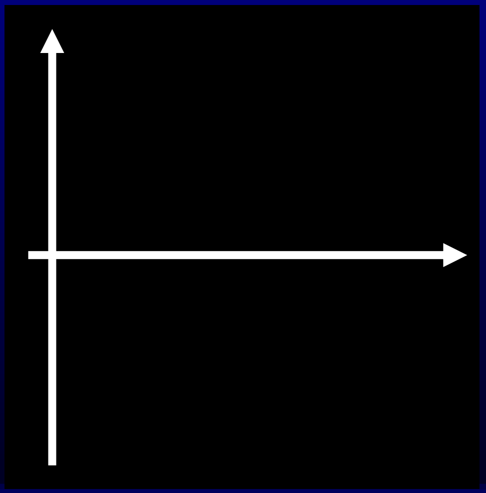
Useful for checking the quality of numerical simulations

3 –

Coordinate system in tokamak configuration

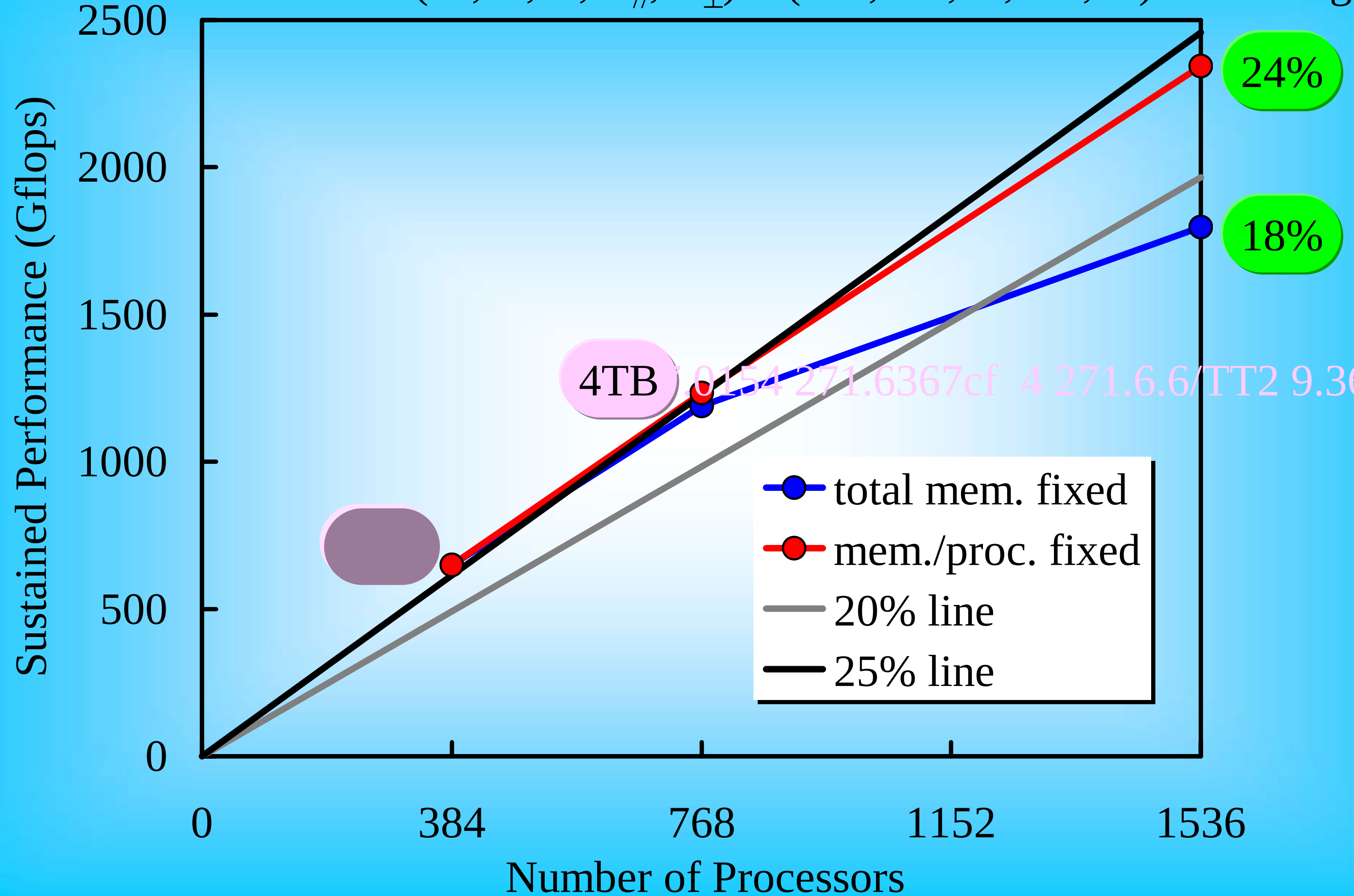
- Tokamak configuration written using poloidal flux function ψ
- Field aligned flute perturbation with $_{//}$~0 (gyrokinetic ordering)
  - Components far from ~ suffer from Landau damping
- Quasi 2D representation of flute perturbation
  - Field-line-following coordinates

    $(\psi,$



Parallel performance of mesh code on Altix3700Bx2

Problem size with 8TB (, , , //, ⊥) = (512,512,64,100,98) ~ 0.164Tgrids



From Klimontovich Eq. to Vlasov Eq.

- Introduce statistical average < > for Klimontovich distribution

$$\langle \;(\qquad)\rangle = {}_0\,{}_1(\qquad)$$

$$\langle \;(\qquad)\;(\;'\;\;'\;)\rangle = {}^{2}_{0}\,{}_2(\qquad\;'\;\;'\;) - \delta(\;-\;')\delta(\;-\;')\,{}_0\,{}_1(\qquad)$$

M

- Statistical average of Klimontovich equation

$$\frac{\partial\;_1}{\partial} + \;\frac{\partial\;_1}{\partial} - \frac{^2}{_0}\left\langle \int \frac{\partial}{\partial}\frac{(\;'\;\;'\;)}{|\;-\;'|}\frac{\partial\;(\qquad)}{\partial}\quad ,\;\; , \right\rangle = 0$$

- Lowest order equation in BBGKY hierarchy

$$(\qquad)\qquad\frac{(\qquad)}{|\qquad|}$$

$$(\qquad\qquad)\quad(\qquad)\;(\qquad)\quad(\qquad\qquad)$$

– $_2$ is ~ (ε) effect in discreteness parameter $\varepsilon = 1/({}_0\lambda^{3}) << 1$

Vlasov limit and super particles

- Lowest order equation in BBGKY hierarchy

- Rosenbluth chopping with

Reduce enhanced collisions with finite size particles

- Newton-Poisson system for PIC simulation

$$\& = \qquad \& = - — \frac{\partial}{\partial}\phi(\qquad)$$

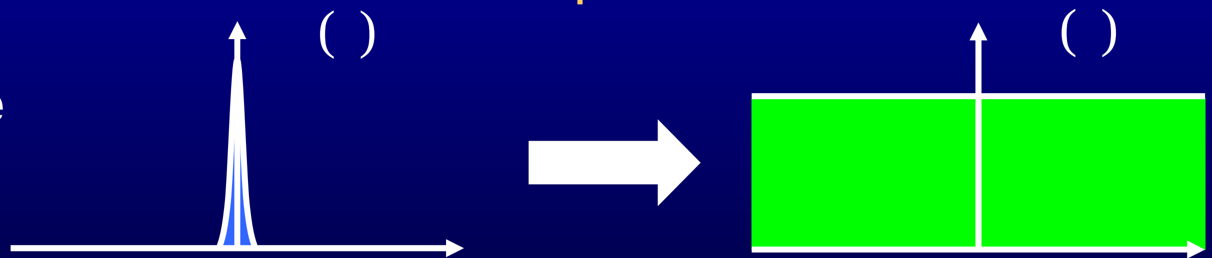
$$(\qquad) = \sum_{j=1} (\ - \ (\ ))\delta(\ - \ (\ ))$$

$$-\frac{\partial^2\phi}{\partial^{\ 2}} = 4\pi M \int \quad (\qquad)$$

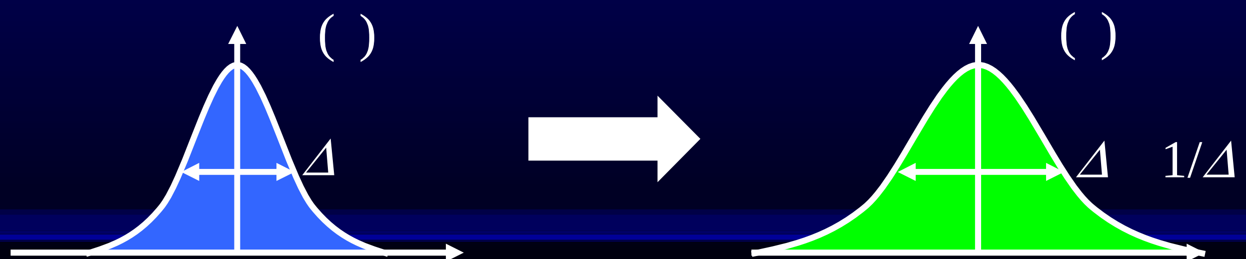
– Shape factor works as low-pass Fourier filter

Point charge

$(\ ) = \delta(\ )$



Finite size particle



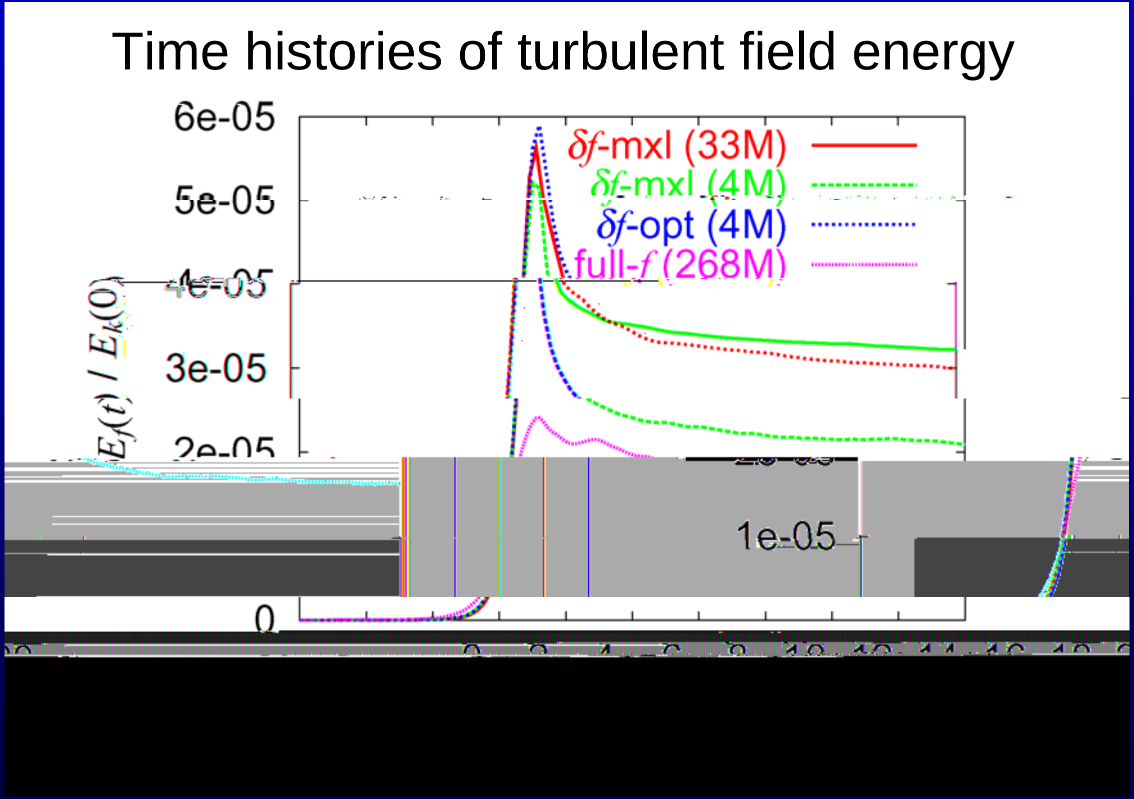
Reduce particle weight with δf PIC method

- Equation system of δ PIC simulation

Comparisons of PIC and δf PIC simulations

- Gyrokinetic simulations of ion temperature gradient driven turbulence

G3D code (Idomura,POP00), = =16ρ , =8000ρ , / =0, / =0.42



- δ-mxl(33M)
  δ-PIC, Maxwellian
  ~9.9x10^3 particles/cell-mode
- δ-mxl(4M)
  δ-PIC, Maxwellian
  ~1.2x10^3 particles/cell-mode
- δ-opt(4M)
  δ-PIC, Optimised
  ~1.2x10^3 particles/cell-mode
- full- (268M)
  PIC, Maxwellian
  ~8x10^4 particles/cell-mode

– δ PIC converges significantly faster than conventional PIC

– Optimization of sampling points accelerates convergence

Summary of Particle/Lagrangian approach

- PIC simulation model
  - Many body system with heavier particles enhance collisions
  - Enhanced collisions are reduced by finite size particle model
- δ PIC simulation model
  - Monte-Carlo sampling of δ using marker particles
  - Particle weight and collisions reduced by δ / $_0$~0.01
  -

5. Mesh/Eulerian approach

Vlasov simulation based on mesh approaches

- Vlasov-Poisson system for electrostatic one component plasma
  - All the dynamics determined by $_1$ and ϕ_1
- Semi-Lagrangian approach: mapping of using / =0
  - Splitting method, Semi-Lagrangian method, CIP method, etc (Cheng,JCP76, Sonnendrucker,JCP99, Nakamura,JCP99)
-

Splitting scheme (Cheng-Knorr,JCP76)

- Vlasov equation is given by separable Hamiltonian

$$(\;,\;) = \frac{1}{2} \quad ^{2} + \phi(\;) = (\;) + (\;)$$

$$\& = \frac{\partial}{\partial} = \frac{\partial \;(\;)}{\partial}, \quad \& = -\frac{\partial}{\partial} = \frac{\partial \;(\;)}{\partial}$$

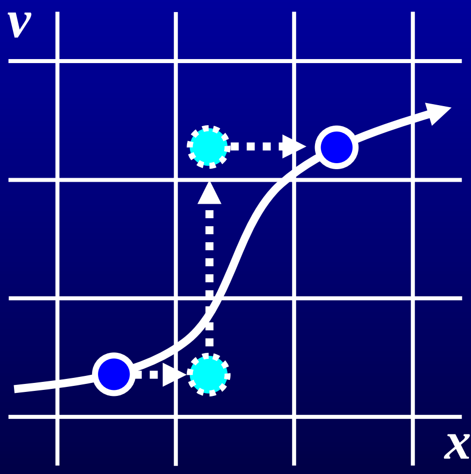
  – Hamilton’s Eq. consists of free motions in and

- Mapping is splitted into three free motions

$$^{*}(\;,\;) = \; (\; - \&\Delta /2, \;)$$

$$^{**}(\;,\;) = \; ^{*}(\;,\; - \&\Delta \;)$$

$$^{+1}(\;,\;) = \; ^{**}(\; - \&\Delta /2, \;)$$



  – Each free motions are canonical transform
  – 2nd order symplectic integrator
  – Semi-Lagrangian method for non-separable Hamiltonian (Brunetti,CPC04, Grandgirard,JCP06)

- Phase mixing leading to fine scale structures in turbulent flows

- Aliasing errors in resolving fine scales with finite grid widths

  - Aliasing errors are inevitable in finite difference approach
  -

Dissipative finite difference operator

- Finite difference approximation for 1D advection problem

$$\frac{\partial}{\partial} + \frac{\partial}{\partial} = 0, \qquad > 0$$

$$\frac{\partial}{\partial}\Big|_{,} = \frac{{}_{+1} - {}_{-1}}{2} = {}' + \frac{{}^{2}}{6}{}''' + \left({}^{4}\right) \qquad \text{Centred finite difference}$$

$$\frac{\partial}{\partial}\Big|_{,} = \frac{- {}_{-1}}{} = {}' + \frac{}{4}{}'' + \left({}^{3}\right) \qquad \text{Upwind finite difference}$$

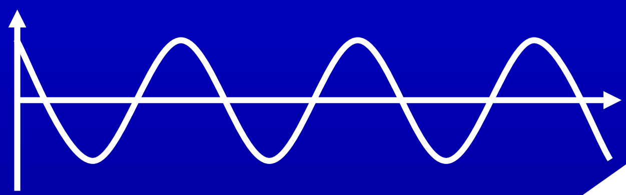
$${}_{\pm 1} = \pm {}' + \frac{{}^{2}}{2}{}'' \pm \frac{{}^{3}}{6}{}''' + \ldots$$

- – Centered finite difference is non-dissipative, but its dispersive errors do not suppress numerical oscillations
- – Dissipative error in upwind finite difference smear out not only numerical oscillations but also solution itself
- – Various less dissipative higher order schemes are available

(Candy,JCP03, Watanabe,NF06, Xu,IAEA06)

Non-dissipative finite difference operator

- Finite difference method for Poisson bracket operator
  (Arakawa,JCP66, Morinishi,JCP97)
  – Suppress numerical oscillations by conserving and ^{2}



- Finite difference operat… …wa and Morinishi

$$\frac{\partial}{\partial} + \{\ ,\ \} = \frac{\partial}{\partial} + \frac{\partial}{\ } \cdots \frac{\ }{\partial\ _{\mu}} \cdots \frac{\ }{\partial\ _{\mu}} = 0$$

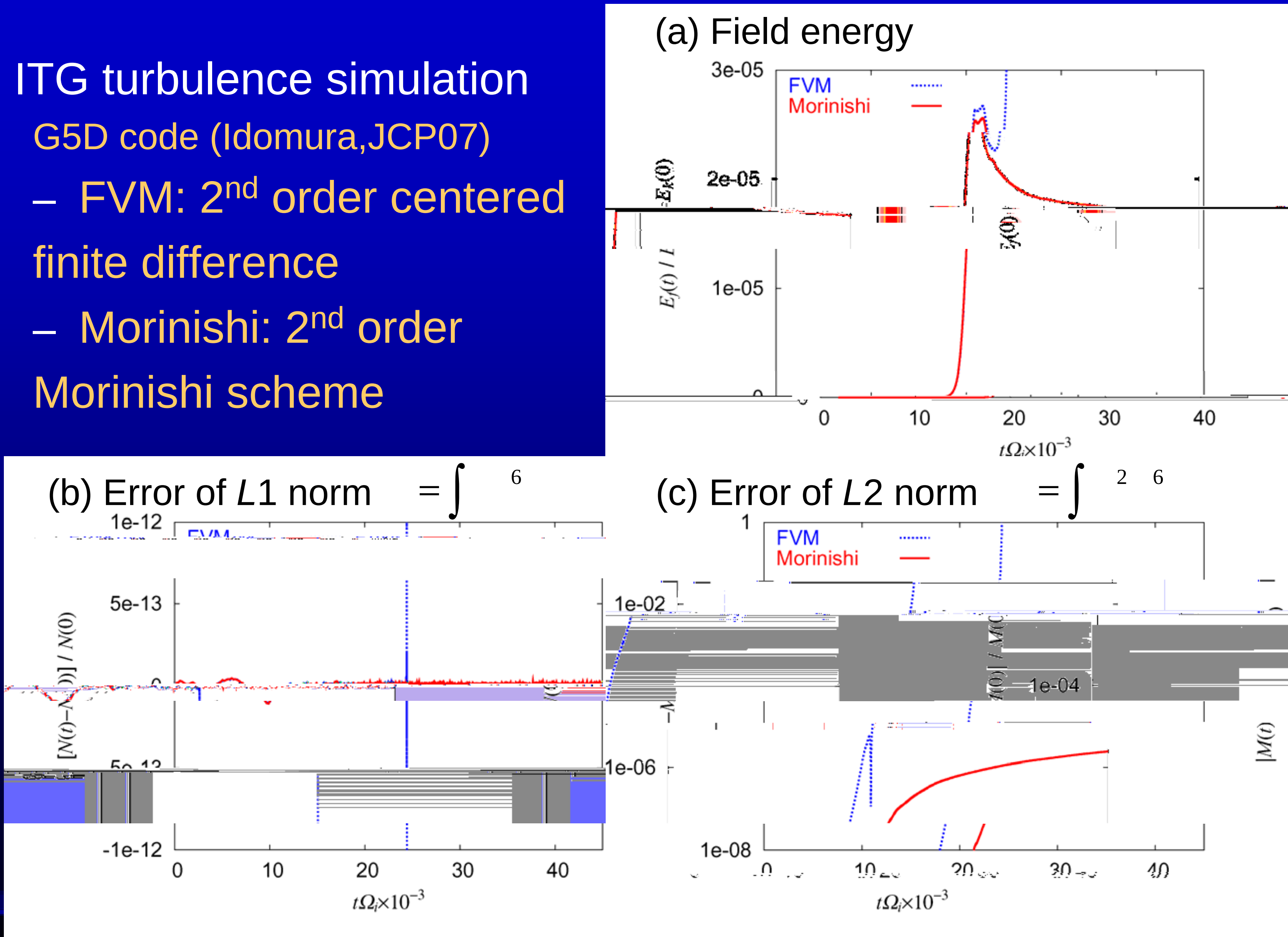
$$[\{\ ,\ \}] = {}_{1}\ {}_{,}(\ ,\ ) + {}_{2}\ {}^{+\times}_{,}(\ ,\ ) + {}_{3}\ {}^{\times +}_{,}(\ ,\ )$$ 2D Arakawa scheme

$$\frac{\partial\ _{\mu}}{\partial\ _{\mu}} = \frac{1}{2}\frac{\partial\ _{\mu}}{\partial\ _{\mu}} + \frac{1}{2}\ _{\mu}\frac{\partial}{\partial\ _{\mu}}$$ Morinishi scheme

  – Both operators are conservative for { , } and { , }
  – Morinishi scheme can be extended to higher dimension
  (Idomura,JCP07)

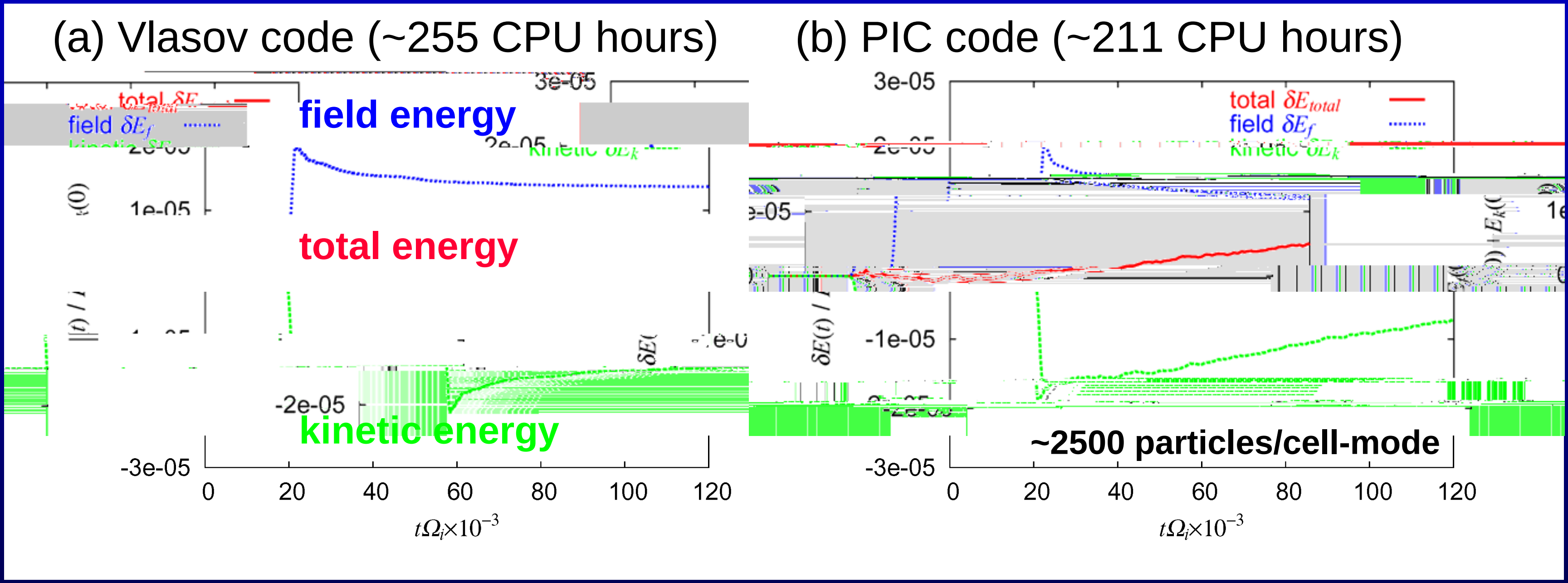
Non-dissipative gyrokinetic simulation

- ITG turbulence simulation
  G5D code (Idomura,JCP07)
  – FVM: 2nd order centered finite difference
  – Morinishi: 2nd order Morinishi scheme



Comparison between Vlasov and PIC simulations

- Gyrokinetic simulations of slab ion temperature gradient turbulence
  G3D/G5D (Idomura,POP00,JCP07), =2 =32ρ , =8000ρ , / =0, / =0.86



– Results show quantitative agreement up to saturation phase
– PIC simulation show spurious heating due to numerical noise
– Secular accumulation of error is not observed in Vlasov simulation (Memory usage was ~5 times larger in Vlasov simulation)

Summary of Mesh/Eulerian approach

- Semi-Lagrangian approach
  - Vlasov simulation was initiated by splitting method
  - Splitting method works as symplectic integrator for Vlasov Eq.
  - Semi-Lagrangian method is used for Gyrokinetic Eq.
- Dissipative upwind finite difference approach
  - Suppress numerical oscillations by numerical dissipation
  - Less dissipative higher order schemes are available
- Non-dissipative finite difference approach
  - Suppress numerical oscillations by conserving and

6. Collisionless gyrokinetic simulation

Collisionless gyrokinetic simulation?

- Collisionless gyrokinetic equation

$$\frac{\quad}{\partial} + \{ \quad , \quad \} = 0$$

  - Similar to Euler equation which describes ideal fluids (=∞)
  - Where does turbulent field energy go?
- One possible scenario in micro-turbulence simulations

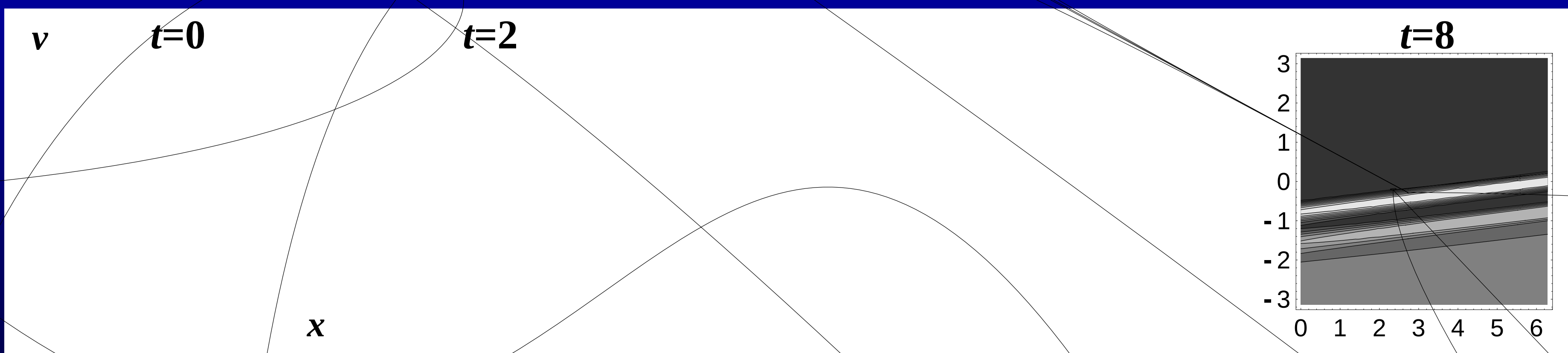
Phase mixing due to parallel streaming motion

- Free streaming starting from (0) $(2\pi)^{-1/2}\exp(\ {}^2/2)\cos(\ )$

$$\frac{\partial}{\partial} + \frac{\partial}{\partial} = 0$$

$$(\ ,\ ,\ ) = (\ -\ ,\ ,0) = (2\pi)^{-1/2}\exp\left(-\ {}^2/2\right)\cos(\ [\ -\ ])$$

$$(\ ,\ ) = \int (\ ,\ ,\ ) = \exp\left(-\ {}^2\ {}^2/2\right)\cos(\ )$$



– damps away with conserving

– Fine scale structures are continuously produced

– In reality, weak collisions, , smear out fine structures

Entropy balance relation in gyrokientic equation

- Slab gyrokinetic equation (drop (ρ)), local limit)

- Balance relation of fluctuation entropy δ

(Lee,PF88, Krommes,POP94, Sugama,POP96)

$$\frac{}{} + \frac{}{} = +$$

$$\equiv \int \frac{}{} \qquad \mathbf{Z} = \int [\quad - \quad] \quad \mathbf{Z} + O(\quad)$$

$$= -\frac{}{} \sum_{\mathbf{k}} [- \ (\ \perp \ ) \ (- \ \perp \ )] \left| \frac{\mathbf{k}}{} \right| + \frac{}{} \sum_{\neq} \left| \frac{\mathbf{k}}{} \right|$$

$$= -\frac{}{} \int \frac{}{} \mathbf{b} \times \nabla \langle \ \rangle \quad \mathbf{R} \ \cdot \nabla \qquad = \int (\ ) \frac{}{} \quad \mathbf{Z}$$

Asymptotic behavior of *Q* in weak collisional limit

- Relevant steady state determined by + =0
  - Is determined by forcing (gradients) or dissipation?
- Collisionality ν dependence of diffusivity χ in weak collisional limit
  - Collisionless simulation is possible with finite but small enough numerical or physical dissipation
  - Convergence study for numerical dissipation is important
  - (Wa imabe-Sugama,POP04)nough 2 1 0.8 1 0.8 1 scn /C2_0 1

Summary of entropy balance relation

- Phase mixing in velocity space
  - Parallel streaming continuously produce fine scale structures
  - damps away with conserving (phase mixing damping)
  - Discrete system shows spurious recurrence effect
  - To avoid recurrence numerical/physical dissipation is needed
- Collisionless limit in gyrokinetic simulations
  - Steady solution of entropy balance is given by $+ \;=0$
  - χ approaches to collisionless limit asymptotically with $\nu \to 0$
  - Forcing determines heat flux at weakly collisional regime
  - Collisionless simulation is possible with finite but small enough numerical or physical dissipation