

“Japan-Russia Workshop on Supercomputer Modelling, Instability and Turbulence  
in Fluid Dynamics (JR SMIT2015)” March 2015, Moscow

# *Clustering and Entropy Growth of Quasi-geostrophic Point Vortices under Periodic Boundary Conditions*

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# Outline

## Background

The relevance of vortices in Geophysical flows

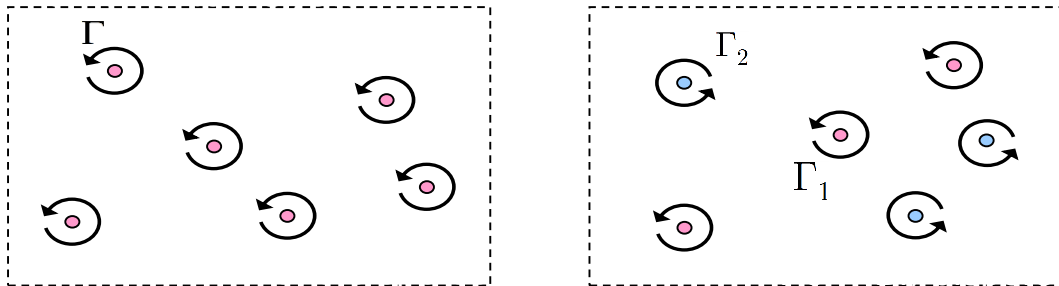
## Quasi-geostrophic Approximation

Hierarchy of vortex based models of geostrophic turbulence

## Statistical Mechanics of QG Point Vortices

Mono-disperse system in an infinite domain (briefly)

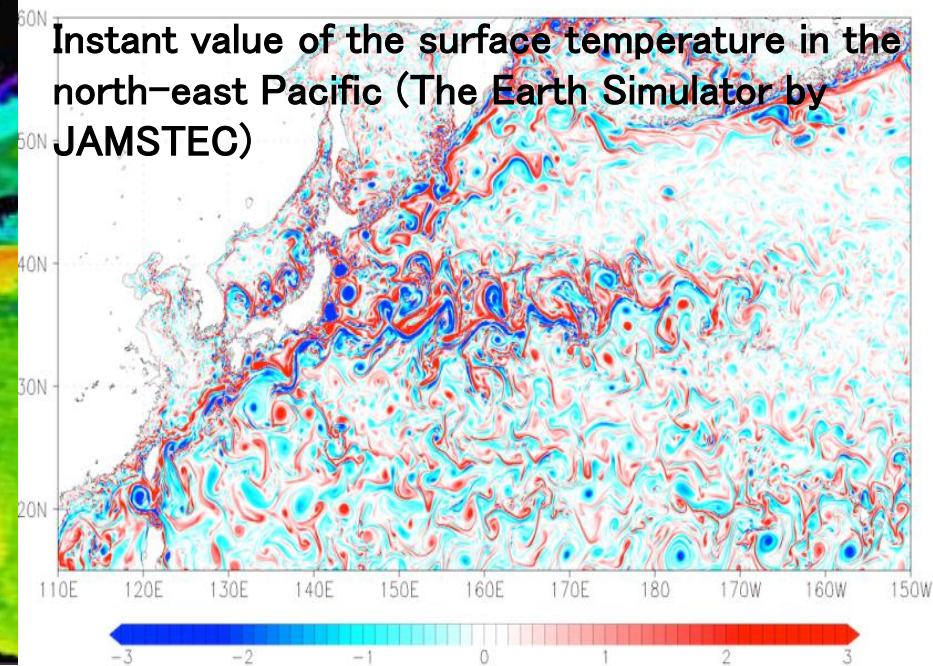
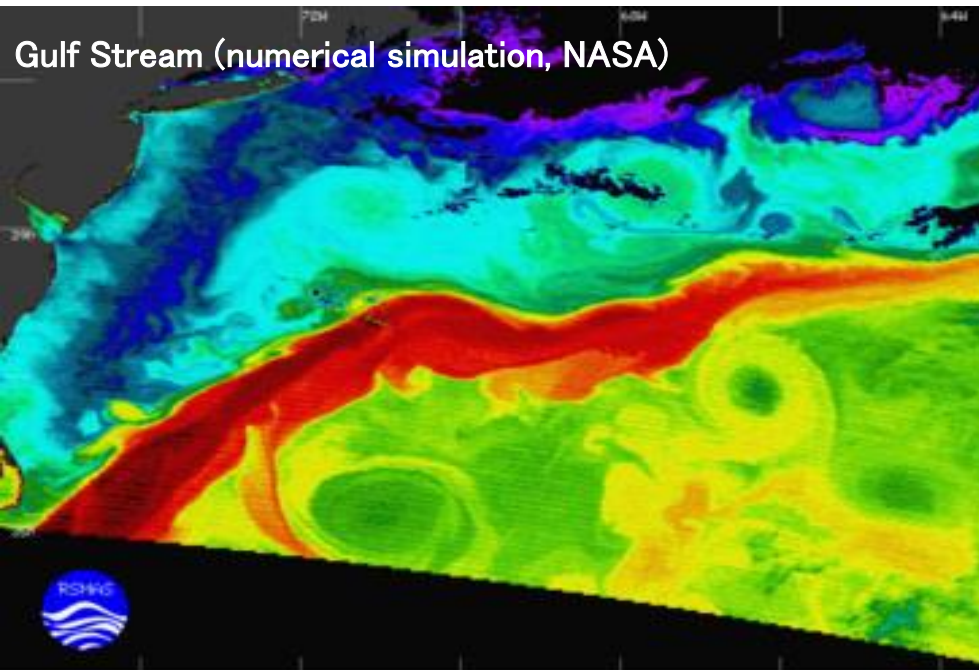
Bi-disperse system of mixed sign under periodic conditions



- Simulation results  $\longrightarrow$  Transient behavior and Equilibrium state
- Comparison with the Maximum entropy theory
- Stability of the equilibrium state



# Background-1



Geophysical flows ...

**Vertical motion is suppressed due to the Coriolis force and stable stratification.**

In a rotating stratified fluid, the interactions of isolated coherent vortices dominate the turbulence dynamics.

# Background-2: Theoretical Approach

## Two-dimensional point vortex systems

lowest order approximation of geophysical flows

### ■ Many statistical studies

have been made on purely 2D flows.

## Statistical mechanics

- ☑ L. Onsager (1949),  
negative temperature
- ☑ D. Montgomery and G. Joyce (1974),  
canonical ensemble
- ☑ Y. B. Pointin and T. S. Lundgren (1976),  
micro canonical ensemble
- ☑ Yatsuyanagi *et al.* (2005),  
very large numerical simulation ( $N = 6724$ )

**J. C. McWilliams *et al.* (1994)**  
**Coherent vortex structures  
in QG turbulence**

2-layer QG point vortex system (2001)  
by Mark T. DiBattista and Andrew J. Majda

The actual geophysical flows are 3D.

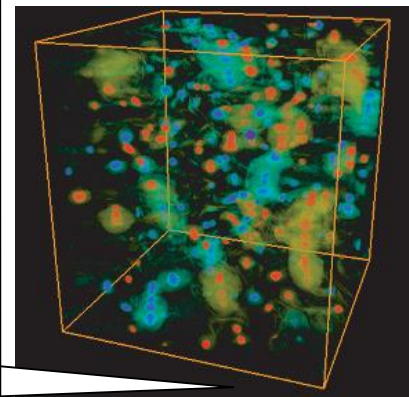
■ The fluid motions are almost confined within a horizontal plane.

■ Different motions are allowed on different horizontal planes.

## ‘Quasi-geostrophic approximation’

(next order approximation)

⇒ The QG-approximation confines the motion in different horizontal planes.



## Vortex models

Point vortex

$N$  degrees of freedom

Spheroidal vortex

$2N$  degrees of freedom

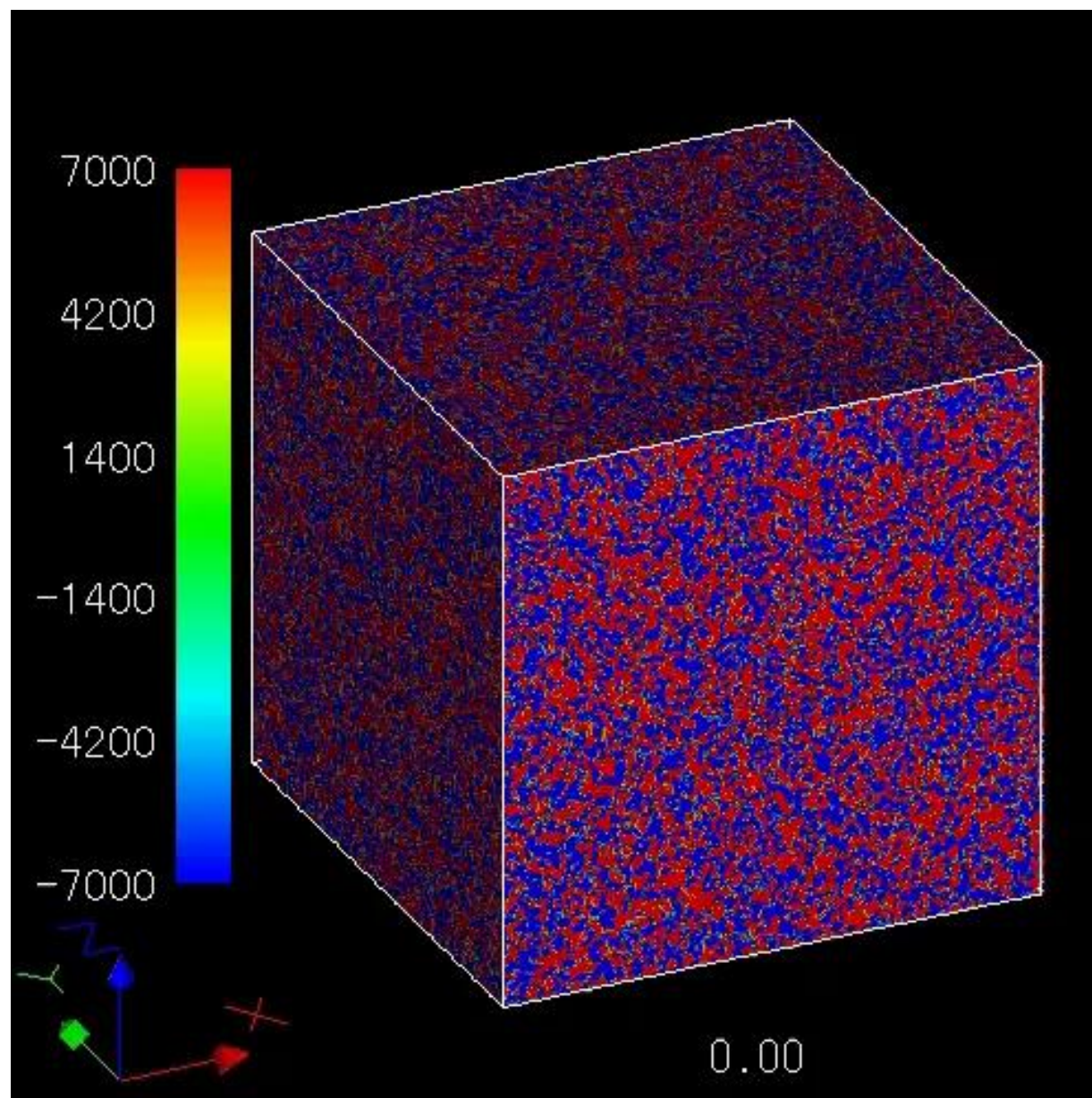
Miyazaki *et al.* (2005)

Ellipsoidal vortex

$3N$  degrees of freedom

Li *et al.* (2006)





# Objective

## Statistical Mechanics of QG Point Vortices

Numerical Computations using

Special Purpose Computers

Theoretical Studies based on

Maximum Entropy Theory

Quick review of

Mono-disperse System in an Infinite Domain

Mainly

Bi-disperse System in a Periodic Box

# Quasi-geostrophic Approximation

2D Fluid motion ( $\Psi$  : stream function)

$$u = \frac{\partial \Psi}{\partial y}, \quad v = -\frac{\partial \Psi}{\partial x}, \quad w = O\left(\frac{f_0}{N}\right)$$

$$N \doteq 1.16 \times 10^{-2} \text{ s}^{-1}, \quad f_0 \sim 1/(24[\text{h}])$$

$N$  : Brunt-Vaisala frequency

$f_0$  : Coriolis parameter ( $f_0 = 2\Omega \sin \theta$  by at latitude  $\theta$ )

Time-evolution under the quasi-geostrophic approximation

$$\left( \frac{\partial}{\partial t} + \frac{\partial \Psi}{\partial y} \frac{\partial}{\partial x} - \frac{\partial \Psi}{\partial x} \frac{\partial}{\partial y} \right) q = 0$$

Potential vorticity

$$q = -\Delta \Psi = -\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi$$

Point vortex systems  $\hat{\Gamma}_i$  : strength,  $\mathbf{R}_i$  : location

$$q = \sum_{i=1}^N \hat{\Gamma}_i \delta(\mathbf{r} - \mathbf{R}_i), \quad \mathbf{r} = (x, y, z)$$

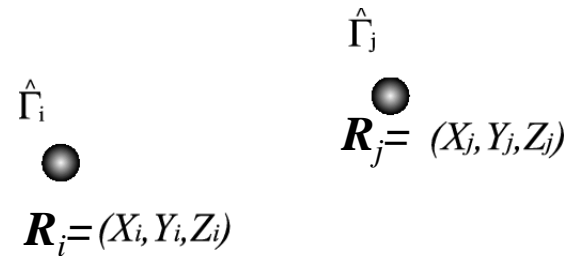
Assuming  $\delta$ -function like concentration at  $N$  points, each vortex is advected by the flow field induced by other vortices.

# Equations of Motion for Quasi-geostrophic Point Vortices

**Canonical Variables : X, Y**

**Hamiltonian of QG  $N$  point vortex system (invariant)**

$$H = \sum_{(i,j)}^N H_{mij}, \quad H_{mij} = \frac{\hat{\Gamma}_i \hat{\Gamma}_j}{4\pi |\mathbf{R}_i - \mathbf{R}_j|} \quad \text{interaction energy}$$



**Canonical equations of motion for the  $i$ -th vortex**

$$\frac{dX_i}{dt} = \frac{1}{\hat{\Gamma}_i} \frac{\partial H}{\partial Y_i}, \quad \frac{dY_i}{dt} = -\frac{1}{\hat{\Gamma}_i} \frac{\partial H}{\partial X_i}$$

Computation on Special Purpose Computers: **MDGRAPE-3, -DR, GRAPE9**  
Time Integration with **LSODE** (6 significant digits)

$t$  : dimensionless time (in units of the inverse potential vorticity)

▣ **MDGRAPE-3, MDGRAPE-DR, GRAPE9**



© <http://mdgrape.gsc.riken.jp>



## Specifications

Number of MFGRAPE-3 Chip : 2  
Performance : 330 Gflops (peak)  
Host Interface : PCI-X 64bit/100MHz  
Power Consumption : 40 W



# Maximum Entropy Theory for Mono-disperse System

Conserved quantities

*Vertical distribution*

$$P(z) = \iint F(\mathbf{r}) dx dy \quad \left( \int_{z_1}^{z_2} P(z) dz = 1 \right)$$

*Angular momentum*

$$\hat{I} = \iiint (x^2 + y^2) F(\mathbf{r}) d^3 \mathbf{r} = 1$$

*Energy*

$$\frac{8\pi H}{\hat{N}^2} = \iiint \iiint \frac{F(\mathbf{r}) F(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r} d^3 \mathbf{r}'$$

"0-inverse-temperature"

$$F^{zit}(r, z) = \frac{P(z)}{\pi} e^{-r^2}$$

Shannon entropy

$$\log \hat{Z} = -\hat{N} \iiint F(\mathbf{r}) \log F(\mathbf{r}) d^3 \mathbf{r}$$

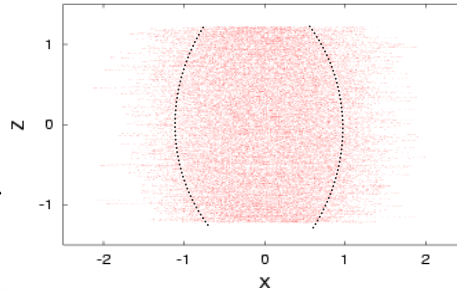
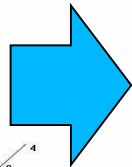
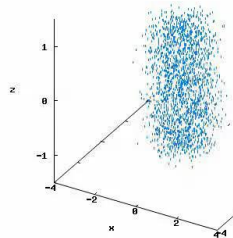
Lagrange's undetermined multipliers

Numerical iteration

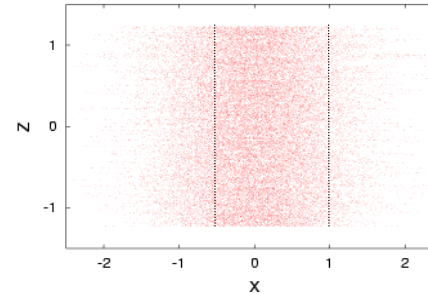
$$\log F(\mathbf{r}) + 1 + \alpha(z) + \beta(x^2 + y^2) + \frac{\gamma}{4\pi} \iiint \frac{F(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}' = 0$$

$\gamma = 0$

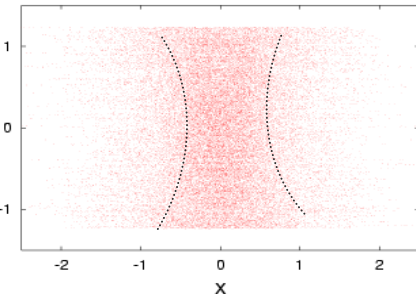
# Equilibrium States in an Infinite Domain



**Positive**

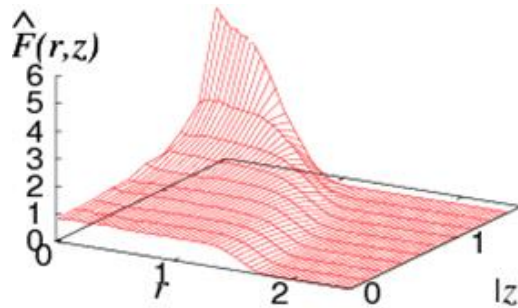


**Zero inverse temperature**

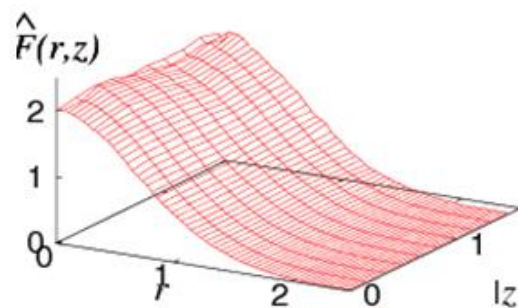


**Negative**

Potential vorticity

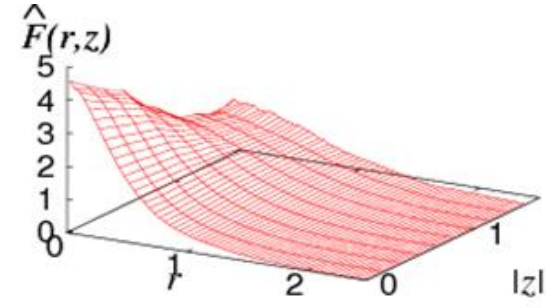


**Positive**



**Zero inverse**

**Maximum entropy states**



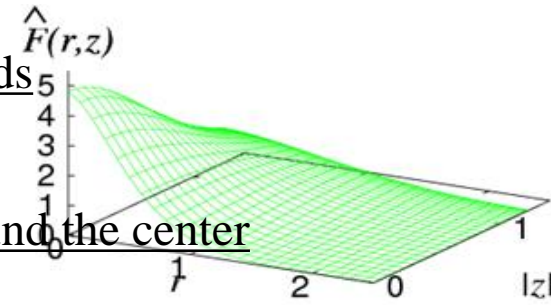
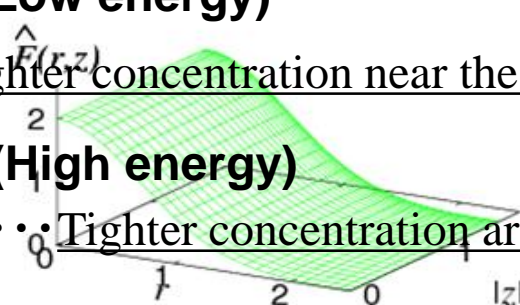
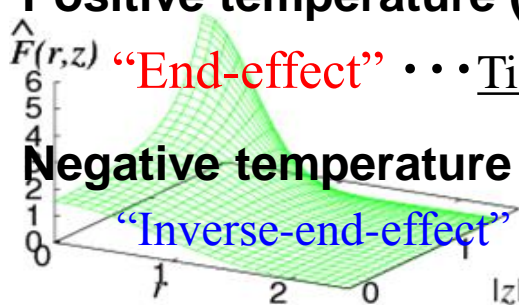
**Negative**

**Positive temperature (Low energy)**

**“End-effect”** . . . Tighter concentration near the lids

**Negative temperature (High energy)**

**“Inverse-end-effect”** . . . Tighter concentration around the center



# Mono-disperse System in an Infinite Domain

## Quick summary

- Mono-disperse system of same sign:  
the radial distribution changes with the **energy level**:  
**Positive, zero-inverse and negative temperature states**
- Numerical results are **consistent** with the theoretical results  
of the **Maximum entropy theory**
- It takes **quite long** to obtain a well developed numerical equilibrium

### References ;

- S. Hoshi and T. Miyazaki: Fluid Dynamics Research (2008)
- T. Miyazaki, T. Sato, H. Kimura and N. Takahashi:  
Geophysical and Astrophysical Fluid Dynamics (2011)
- T. Miyazaki, T. Sato and N. Takahashi: Phys. Fluids (2012)

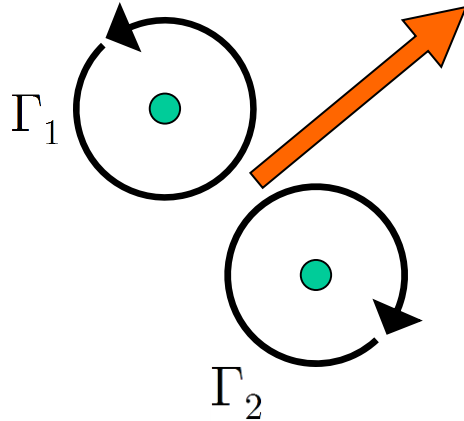
↳ **Bi-disperse system of mixed sign:**  $\Gamma_1 = -\Gamma_2$



# QG Bi-disperse Point Vortices: $\Gamma_1 = -\Gamma_2$ $N = N_+ = N_-$

■ Geophysical flows ··· Poly-disperse, Mixed sign, ···

translational motion



Counter-rotating:  $\Gamma_1 = -\Gamma_2$

We have to calculate under  
periodic boundary conditions



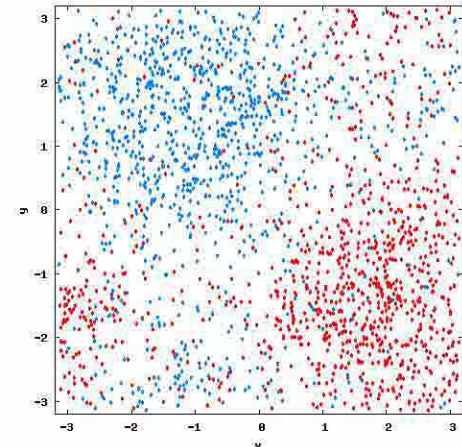
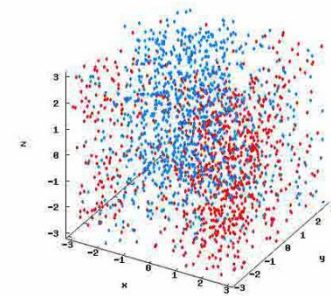
“Ewald sum”, as frequently used in Molecular Dynamics

Replacement of real-space summation with equivalent  
summation in Fourier space under the periodic boundary  
conditions

## Problem

Because the vortices diffuse towards infinity,  
They drift outside the secure calculation area  
of the MDGRAPE-3, GRAPE-DR and GRAPE9.

Red : plus sign  
Blue : minus sign

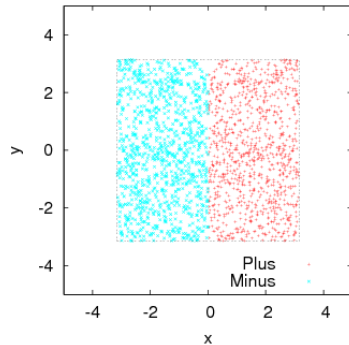


# Numerical Results: Small System ( $N=1000$ )

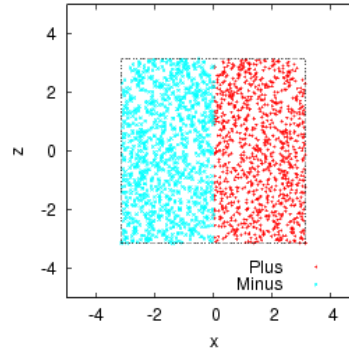
□ Initial structure : Two-dimensional

$$E=6.413 \times 10^{-3}$$

X-Y



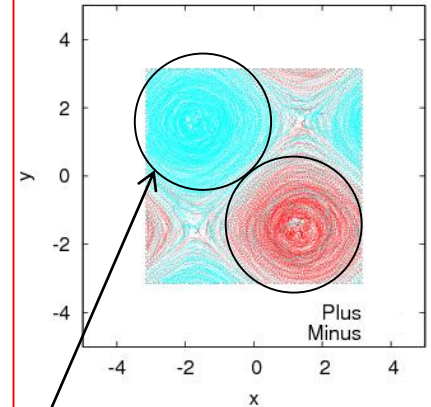
X-Z



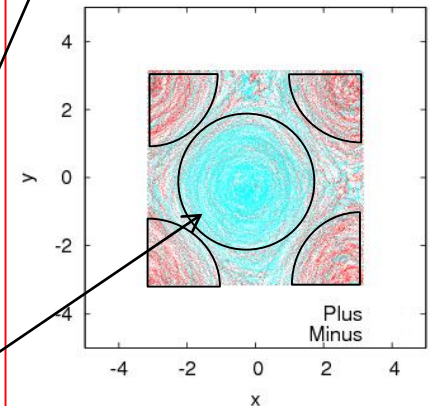
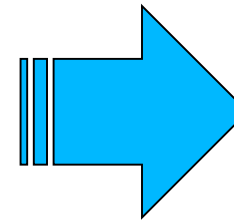
Plus  
 $N_{\pm} = 1000$   
Minus

Equilibrium

X-Y



Time-evolution



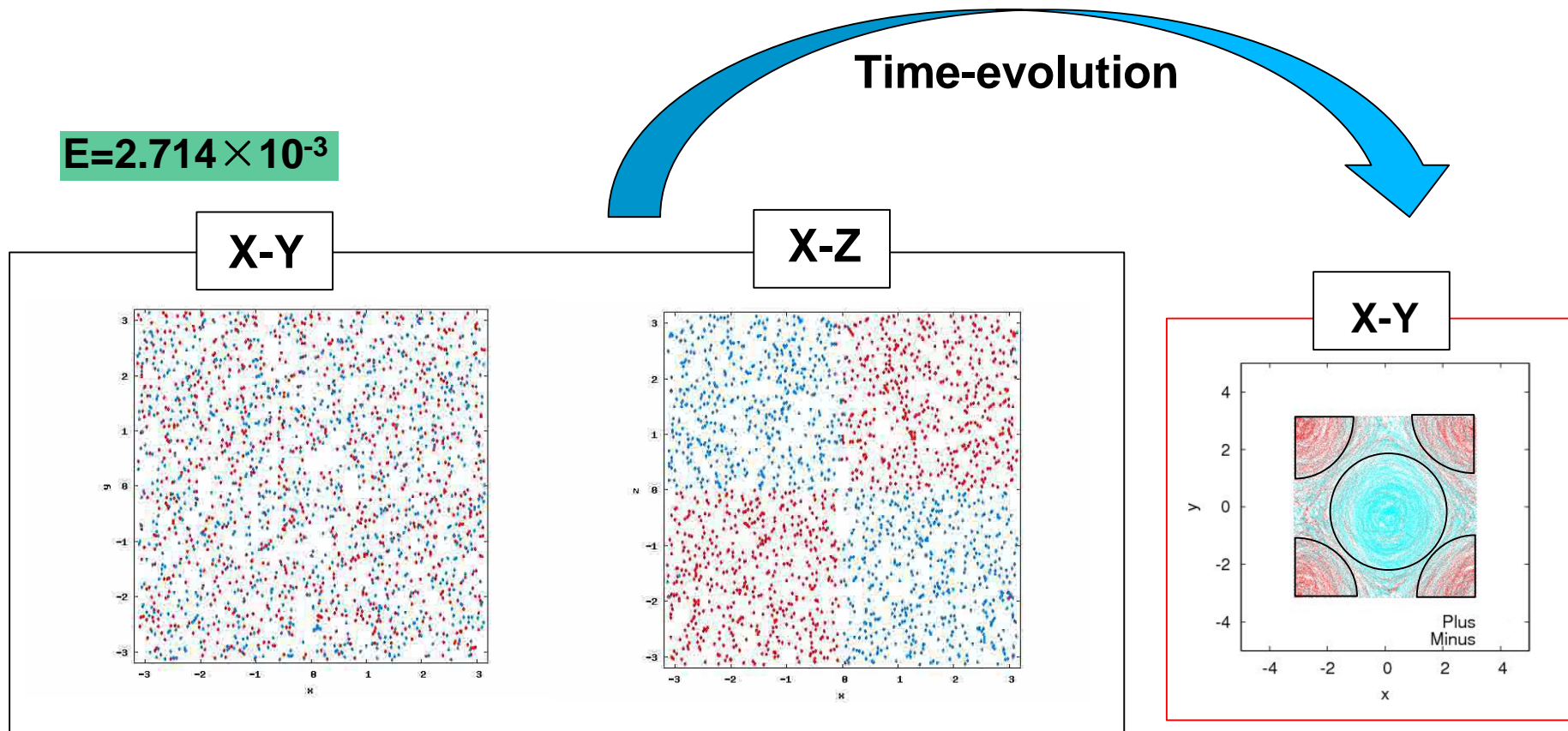
Clustering

$$P_{\pm}(z) = 1/2\pi$$

- Does the energy determine the equilibrium state uniquely ?
- Are all equilibrium states two-dimensional ?

# Numerical Results: Small System ( $N=1000$ )

## Three-dimensional Initial Distribution



- Transition from three-dimensional to two-dimensional structure !
- Is there a unique equilibrium state at a specified energy level ?
- How does the system approach the equilibrium state ?



# Transient Behavior: Larger Systems

$$L_x:L_y:L_z = 2\pi:2\pi:2\pi$$

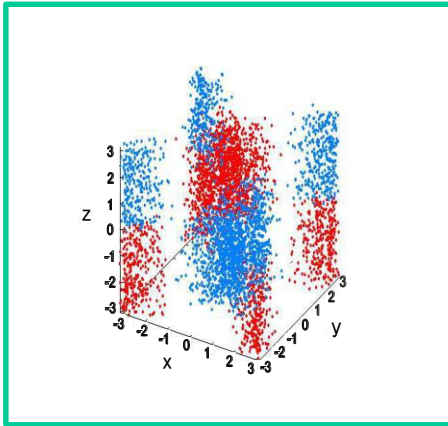
Case A: **3D dipole**

$$E = 10.01 \times 10^{-3}$$

$$N_+ = 4000$$

$$N_- = 4000$$

$$\hat{\Gamma}_{\pm} = 0.062$$



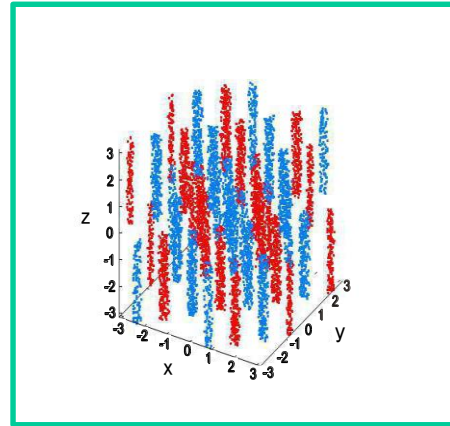
Case B: **Checkerboard**

$$E = 4.428 \times 10^{-3}$$

$$N_+ = 4000$$

$$N_- = 4000$$

$$\hat{\Gamma}_{\pm} = 0.062$$



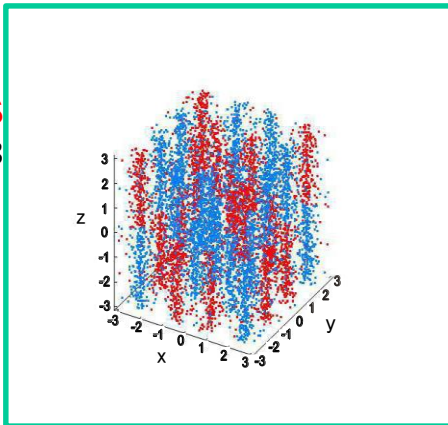
Case C: **16 pillars**

$$E = 2.426 \times 10^{-3}$$

$$N_+ = 4000$$

$$N_- = 4000$$

$$\hat{\Gamma}_{\pm} = 0.062$$



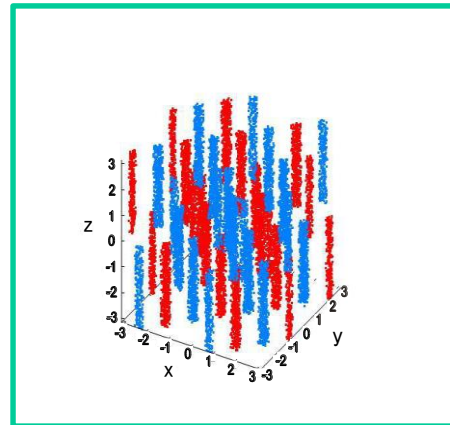
Case D: **Checkerboard**

$$E = 4.536 \times 10^{-3}$$

$$N_+ = 8000$$

$$N_- = 8000$$

$$\hat{\Gamma}_{\pm} = 0.031$$



# End States of Larger Computations

$$L_{x,y,z} = 2\pi$$

$$N = 4000$$

**Plus**  $N_+ = 4000$

**Minus**  $N_- = 4000$

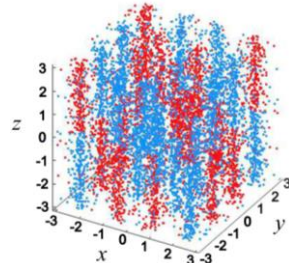
**Strength**

$$\hat{I}_{\pm} = \pm 0.062$$

**Dipole Pair Moves**

**Not in Equilibrium**

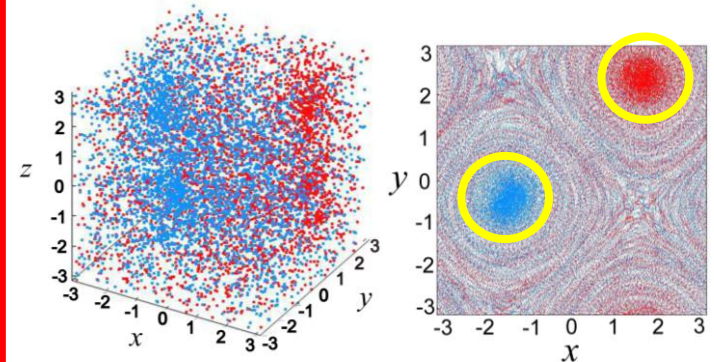
**Initial  
Case C**



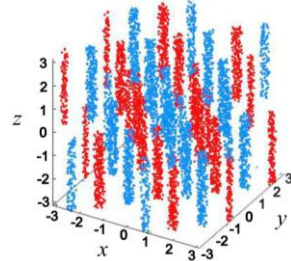
$$E = 2.426 \times 10^{-3}$$

$t = 150$

**End States: sn-sn dipole ?**

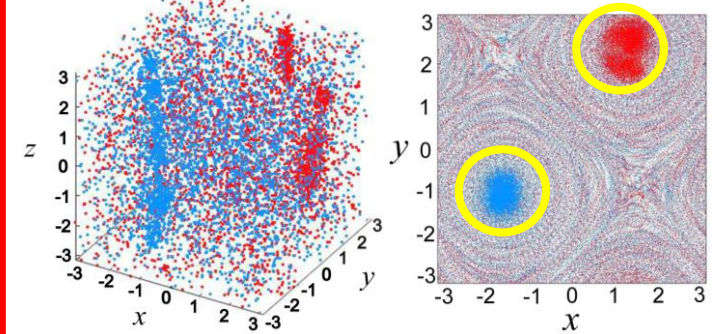


**Case B**

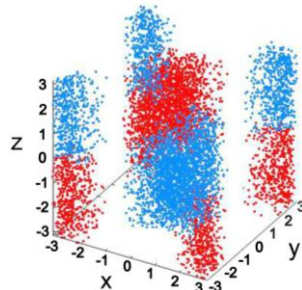


$$E = 4.428 \times 10^{-3}$$

$t = 158$

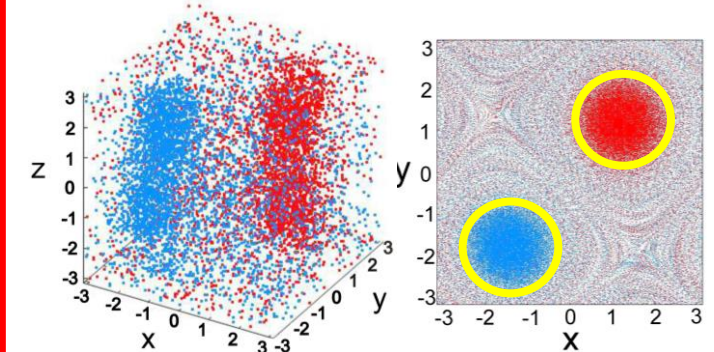


**Case A**



$$E = 10.01 \times 10^{-3}$$

$t = 180$

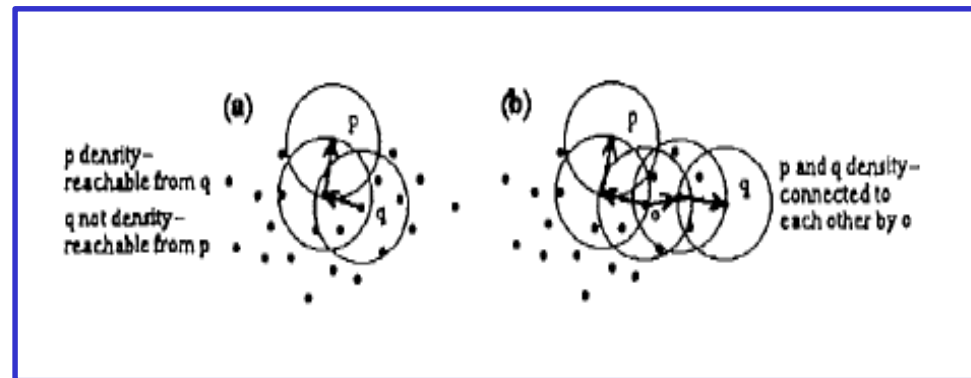


# Density based Clustering Analysis

Quantitative analysis of  
transient process:

**DBSCAN method**

(Ester *et al.* 1996)



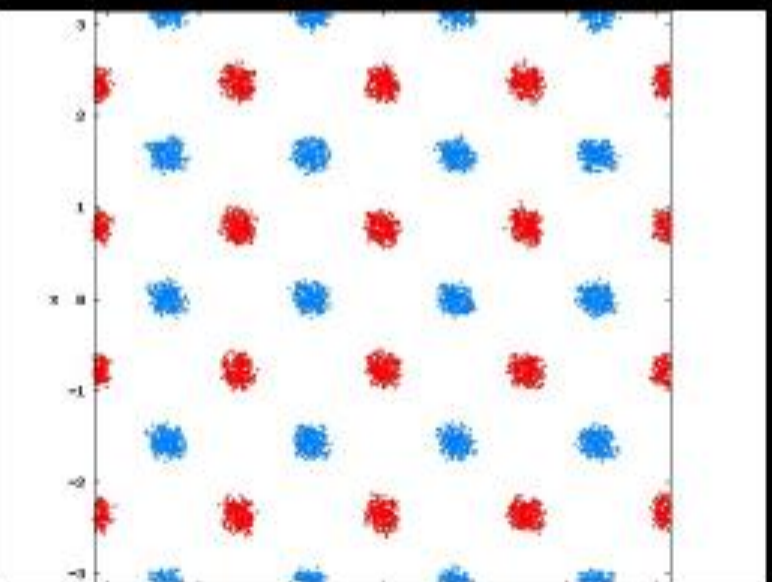
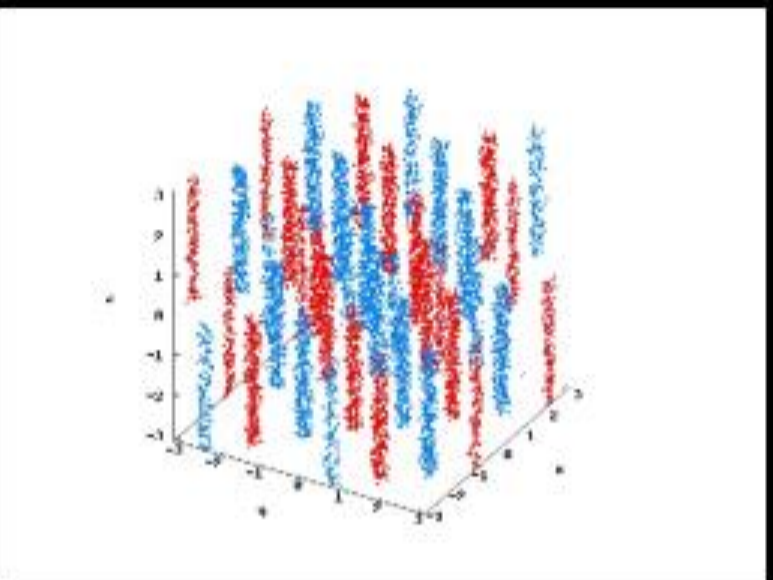
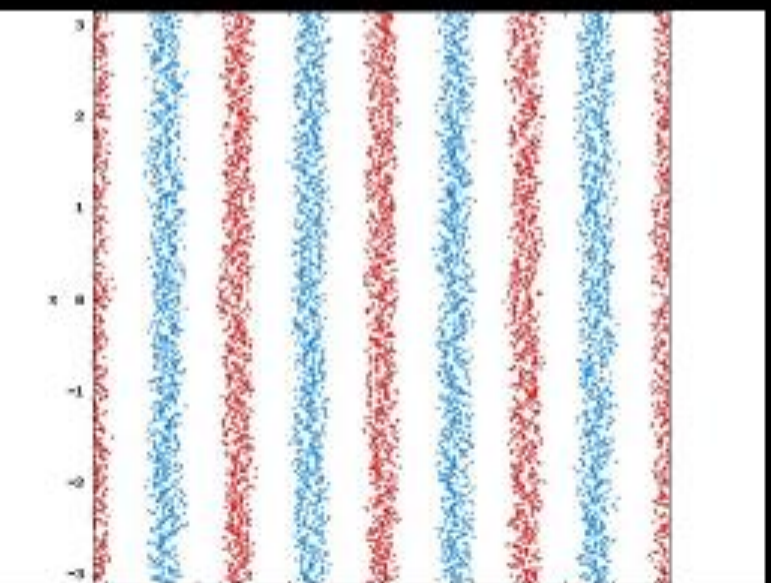
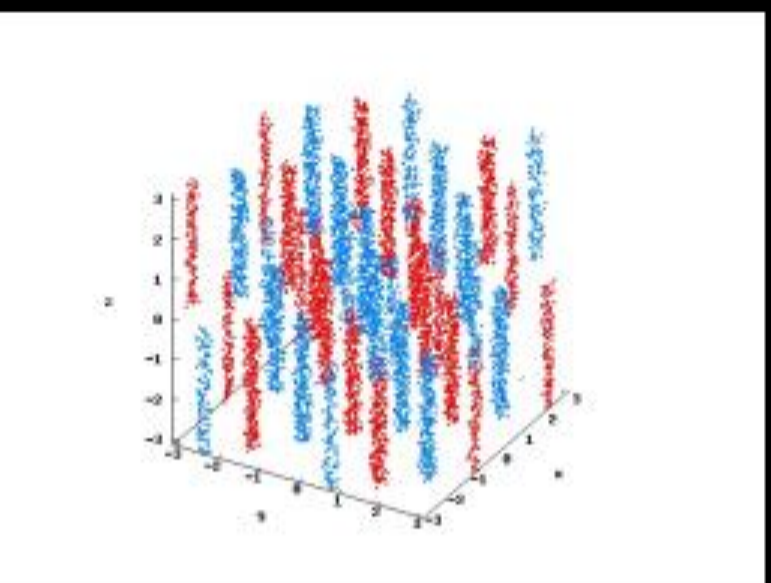
↑ Density based algorithm (Ester *et al.*)

A group of vortices is identified as a cluster, if its size is greater than the minimum radius:  $r$  and the number of vortices inside exceeds the minimum number:  $N_c$

Case	$r$	$N_c$
A	0.4	25
B	0.4	25
C	0.4	25
D	0.3	22

↑ Used parameters





# Number of Clusters

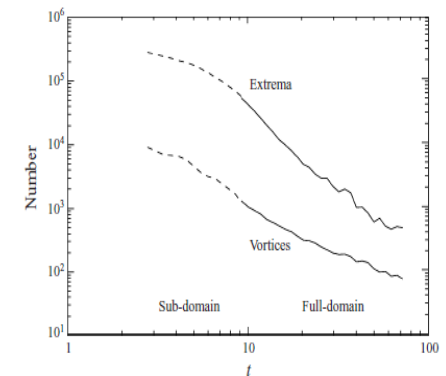
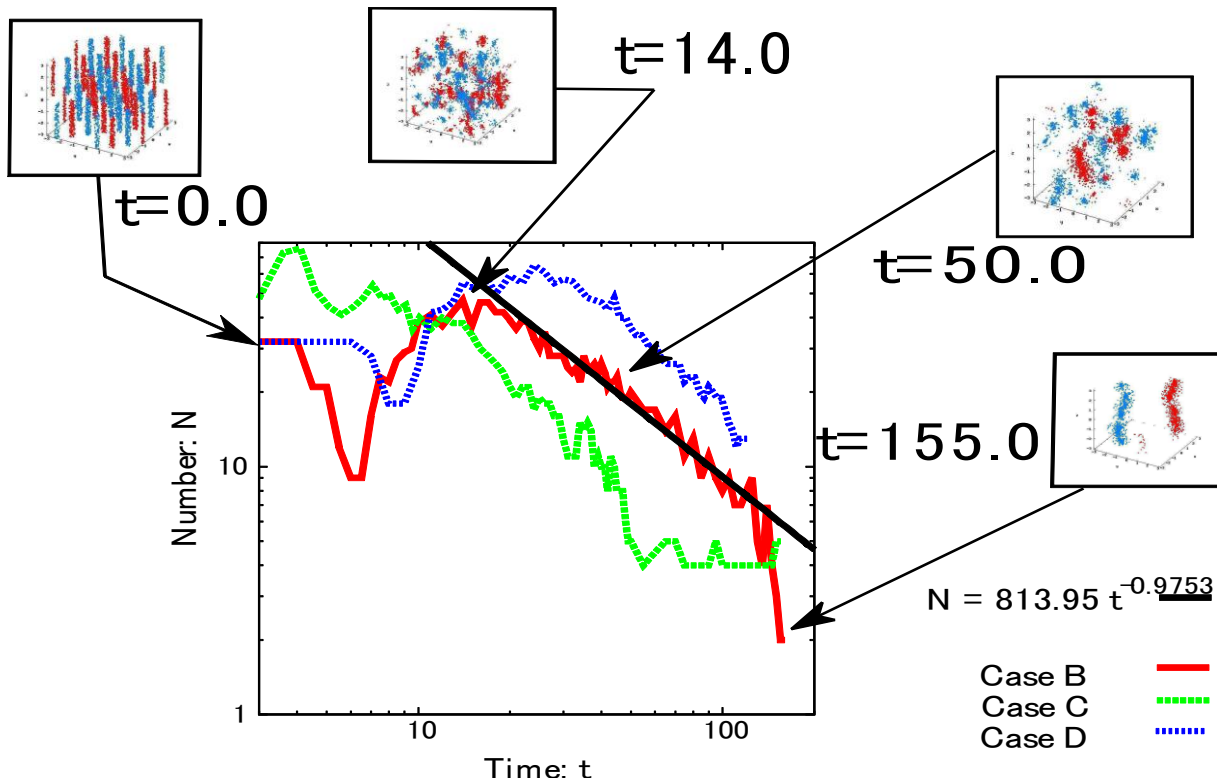


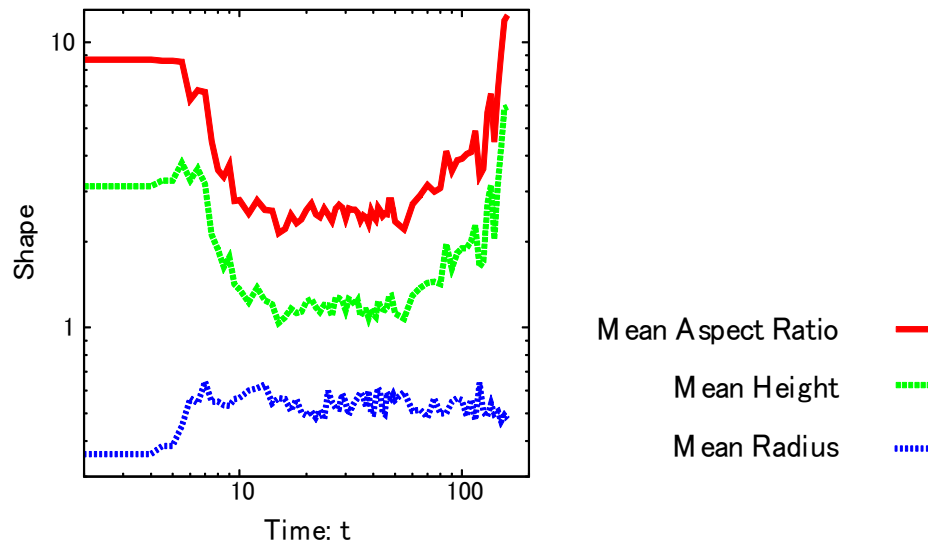
FIGURE 4. The number of extrema and compound vortices,  $n_e(t)$  and  $n_{cv}(t)$ , from the vortex census.

McWilliams *et al.* 1999  
Spectral Computation

Cluster number decays like  $t^{-1}$ , which is **slower** than in **McWilliams'** numerical simulations ( $t^{-1.25}$ ).

McWilliams J C, Weiss J B and Yavneh I: *J.Fluid Mech.* **401** 1-16, 1999

# Cluster Shape



*J. C. McWilliams, J. B. Weiss and I. Yavneh*

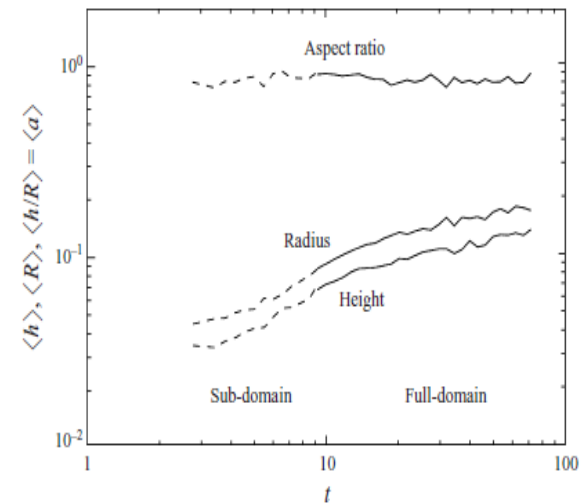


FIGURE 8. The population-mean vortex-element radius,  $\langle R \rangle(t)$ , half-height,  $\langle h \rangle(t)$ , and aspect ratio,  $\langle a \rangle(t)$ , from the vortex census.

- Mean aspect ratio  $a = \frac{h}{r}$  of clusters increases with time ( $2 \rightarrow 10$ ).
- Mean radius  $r$  remains **constant**.
- Mean height  $h$  increases.

Clusters align vertically  
but never merge.

- Mean aspect ratio  $a = \frac{h}{r}$  of clusters remains **constant** (about 1.6).
- Mean radius  $r$  increases.
- Mean height  $h$  increases.

Clusters merge and align.



# Maximum Entropy Theory for QG Vortices of Mixed Sign

## Conserved quantities

Probability density function: PDF

### Vertical vortex distributions

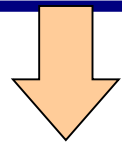
$$P_+(z) = \iint F_+(x, y, z) dx dy, \quad P_-(z) = \iint F_-(x, y, z) dx dy$$

### Energy

$$E = \frac{1}{2} \iiint \iiint G(\mathbf{r}, \mathbf{r}') [F_+(\mathbf{r})F_+(\mathbf{r}') + F_-(\mathbf{r})F_-(\mathbf{r}') - 2F_+(\mathbf{r})F_-(\mathbf{r}')] d^3\mathbf{r} d^3\mathbf{r}'$$

### Shannon entropy

$$\log \hat{Z} = \frac{1}{N} \log Z = - \iiint [F_+(\mathbf{r}) \log F_+(\mathbf{r}) + F_-(\mathbf{r}) \log F_-(\mathbf{r})] d^3\mathbf{r}$$



Lagrange's method of undetermined multipliers

### Variational equations

$$\delta F_+ : -1 - \log F_+ - \alpha_+(z) - \beta \iiint G(\mathbf{r}, \mathbf{r}') [F_+(\mathbf{r}') - F_-(\mathbf{r}')] d^3\mathbf{r}' = 0$$

$$\delta F_- : -1 - \log F_- - \alpha_-(z) - \beta \iiint G(\mathbf{r}, \mathbf{r}') [F_-(\mathbf{r}') - F_+(\mathbf{r}')] d^3\mathbf{r}' = 0$$

$$\alpha_{\pm}(z) \Rightarrow P_{\pm}(z)$$

$$\beta \Rightarrow E$$

Turkington .B & Whitaker .N : SIAMJ. Sci. Comput. (1996)

Funakoshi, S. & Miyazaki, T.,: Fluid Dyn. Res. 44 (2012)

# Mean Field Equation for QG Point Vortices

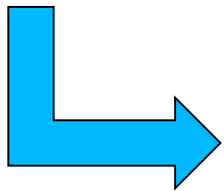
□ For Quasi-geostrophic point vortices

$$\left[ \begin{array}{lcl} \text{Potential vorticity : } q(\mathbf{r}) & \equiv & F_+(\mathbf{r}) - F_-(\mathbf{r}) \\ \text{Stream function : } \psi(\mathbf{r}) & \equiv & \iiint G(\mathbf{r}, \mathbf{r}') [F_+(\mathbf{r}') - F_-(\mathbf{r}')] d^3 \mathbf{r}' \end{array} \right.$$

- Symmetric case:  $\alpha_+(z) = \alpha_-(z) = \alpha(z)$
- The maximum entropy state satisfies the following equation:

$$q(\mathbf{r}) = -2e^{-\alpha(z)-1} \sinh \beta \psi(\mathbf{r})$$

Potential vorticity:  $q(\mathbf{r}) = -\Delta \psi(\mathbf{r})$



Mean field equation

$$\Delta \bar{\psi}(\mathbf{r}) + \lambda^2(z) \sinh \bar{\psi}(\mathbf{r}) = 0$$

$$* \bar{\psi}(\mathbf{r}) = \beta \psi(\mathbf{r}), \quad \lambda^2(z) = -2\beta e^{-\alpha(z)-1}$$

□ It reduces to the **Sinh-Poisson equation** for 2D point vortices

$$\Delta \psi(\mathbf{r}) + \lambda^2 \sinh \psi(\mathbf{r}) = 0$$

Joyce & Montgomery : J. Plasma Phys. (1973)

# Dual Problem of the Maximum Entropy Theory

## Dual problem

$$\alpha_+^{k+1}(z)P_+(z) + \alpha_-^{k+1}(z)P_-(z) + \beta^{k+1}(E^k + E_0) \\ + \iiint \exp[-1 - \alpha_+^{k+1}(z) - \beta^{k+1}\psi^k(\mathbf{r})]d^3\mathbf{r} + \iiint \exp[-1 - \alpha_-^{k+1}(z) + \beta^{k+1}\psi^k(\mathbf{r})]d^3\mathbf{r}$$

 **Minimum**

## Conserved quantities

$$\left\{ \begin{array}{l} P_+(z) = \iint \exp[-1 - \alpha_+^{k+1}(z) - \beta^{k+1}\psi^k(\mathbf{r})]dxdy = \iint F_+^{k+1}(\mathbf{r})dxdy \\ P_-(z) = \iint \exp[-1 - \alpha_-^{k+1}(z) + \beta^{k+1}\psi^k(\mathbf{r})]dxdy = \iint F_-^{k+1}(\mathbf{r})dxdy \\ E^k + E_0 = \iiint \psi^k \{F_+^{k+1}(\mathbf{r}) - F_-^{k+1}(\mathbf{r})\}d^3\mathbf{r} \end{array} \right.$$

Where,  $\Delta\psi^k(\mathbf{r}) = -F_+^k(\mathbf{r}) + F_-^k(\mathbf{r})$

- Assuming  $F_+^k, F_-^k, \alpha_+^k(z), \alpha_-^k(z), \beta^k$  are given,
- determine  $\alpha_+^{k+1}(z), \alpha_-^{k+1}(z), \beta^{k+1}$  by an iteration method.

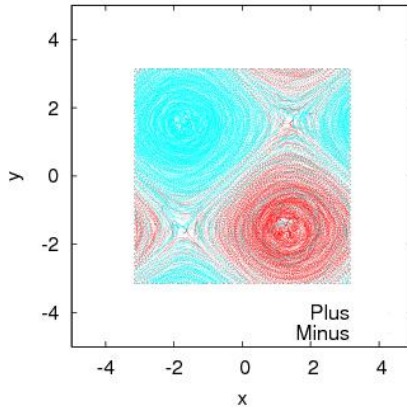
Accuracy:  $EPS = \sum_{i=1}^n [|\alpha_+^{k+1}(z(i)) - \alpha_+^k(z(i))|^2 + |\alpha_-^{k+1}(z(i)) - \alpha_-^k(z(i))|^2 + |\beta^{k+1} - \beta^k|^2] \leq 10^{-8}$



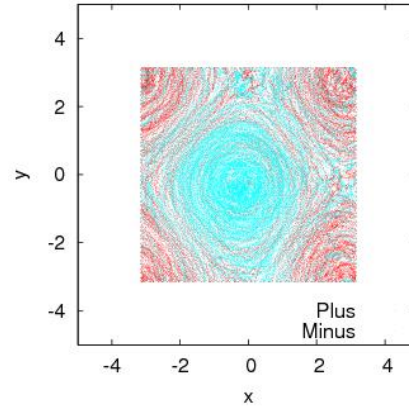
# Comparison between Numerical and Theoretical Results

◆ Numerical results by point vortex simulation

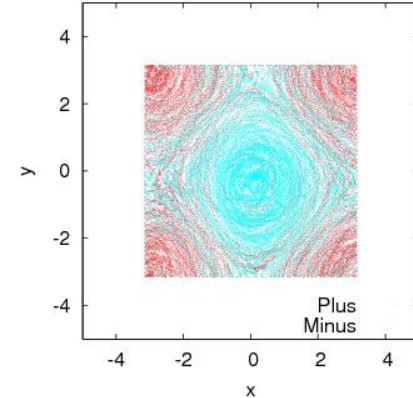
**caseA**  $E=6.413 \times 10^{-3}$



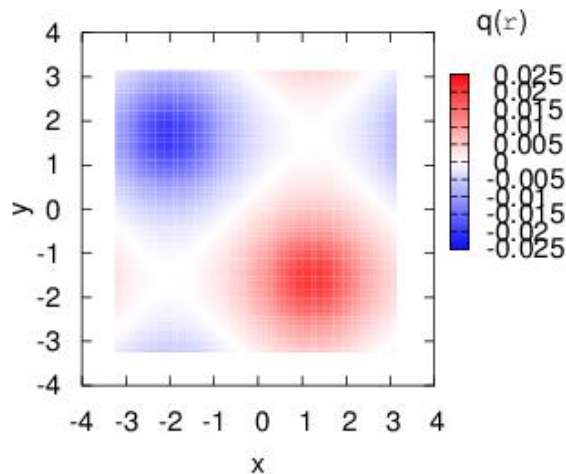
**caseB**  $E=2.424 \times 10^{-3}$



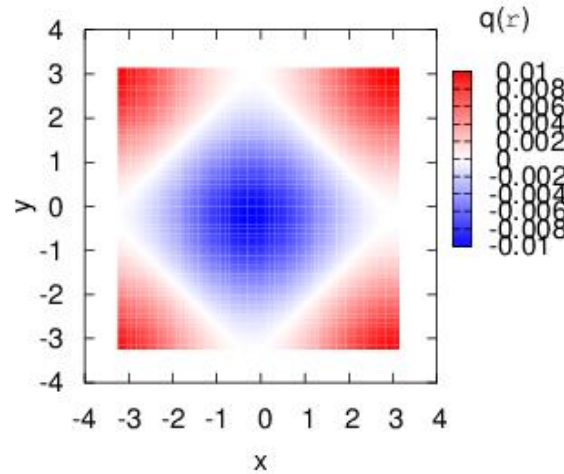
**caseC**  $E=2.714 \times 10^{-3}$



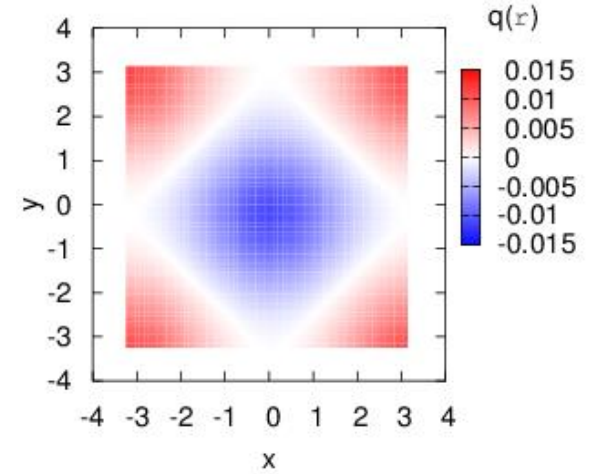
◆ Theoretical results : initial potential vorticity → numerical results



$E=6.413 \times 10^{-3}$



$E=2.424 \times 10^{-3}$

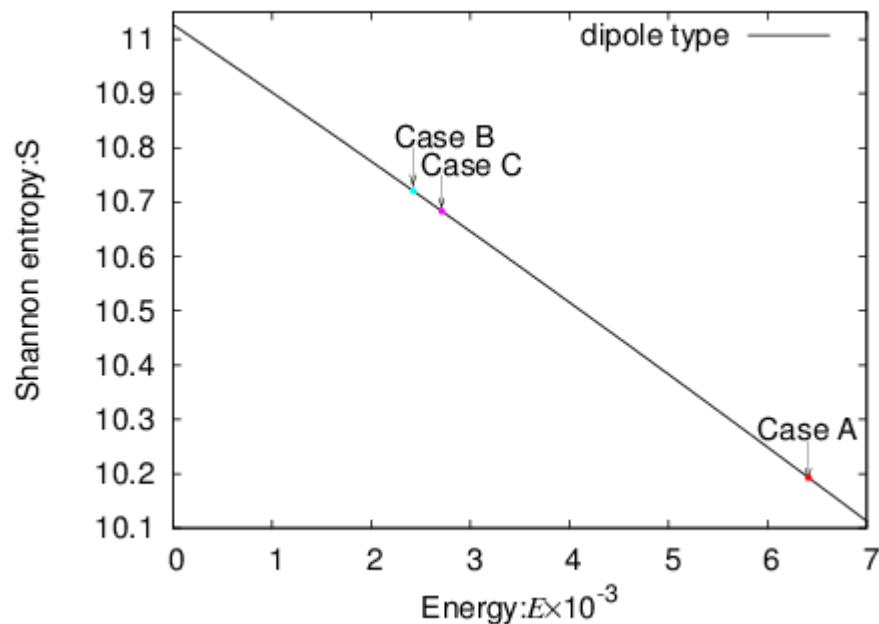


$E=2.714 \times 10^{-3}$

✓ Numerical equilibria are Maximum entropy states !

# 2D Exact Solutions

- Diagram in  $E$ - $S$  plane: Cases A~C

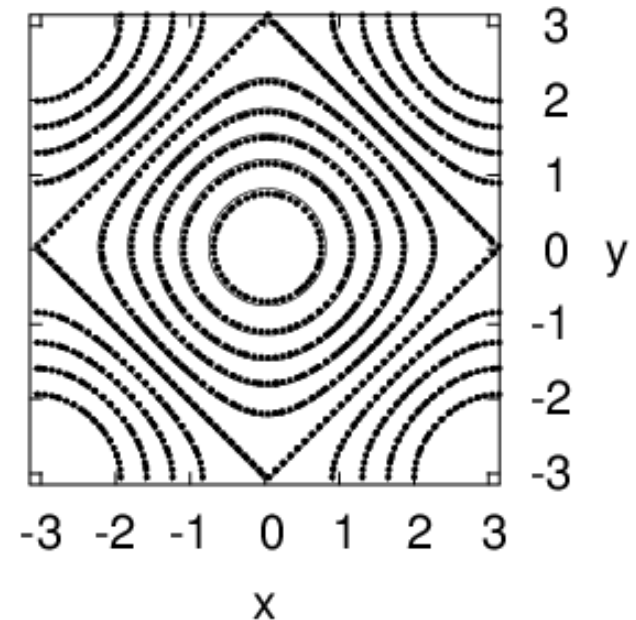


Cases A~C are on the same branch.

“Sinh-Poisson Eq.” has **Soliton solutions**.

- Stream function

Case B :  $\lambda^2(z) = 0.8852$ ,  $k = 0.02074$



Cases A~C are two-dimensional  
“sn-sn dipole”-type solutions.

$$\Psi = 4 \tanh^{-1} \left[ \frac{\sqrt{k} \operatorname{sn}(rx, k) - \sqrt{k_1} \operatorname{sn}(sy, k_1)}{1 + \sqrt{k k_1} \operatorname{sn}(rx, k) \operatorname{sn}(sy, k_1)} \right]$$

$$s^2(1 - k_1)^2 = \lambda^2 + 4r^2 k, \quad s(1 + k_1) = r(1 + k)$$

**Gurarie & Chow : Phys. Fluids. (2004)**

$2\pi$ -Cubic box

$$s = r = 2K(k)/\pi$$

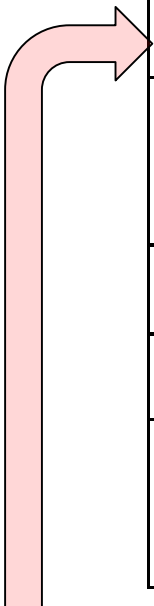
$$k = k_1$$

Elliptic integral:  $K(k)$

Elliptic function:  $\operatorname{sn}(u, k)$

# Other Maximum Entropy States ?

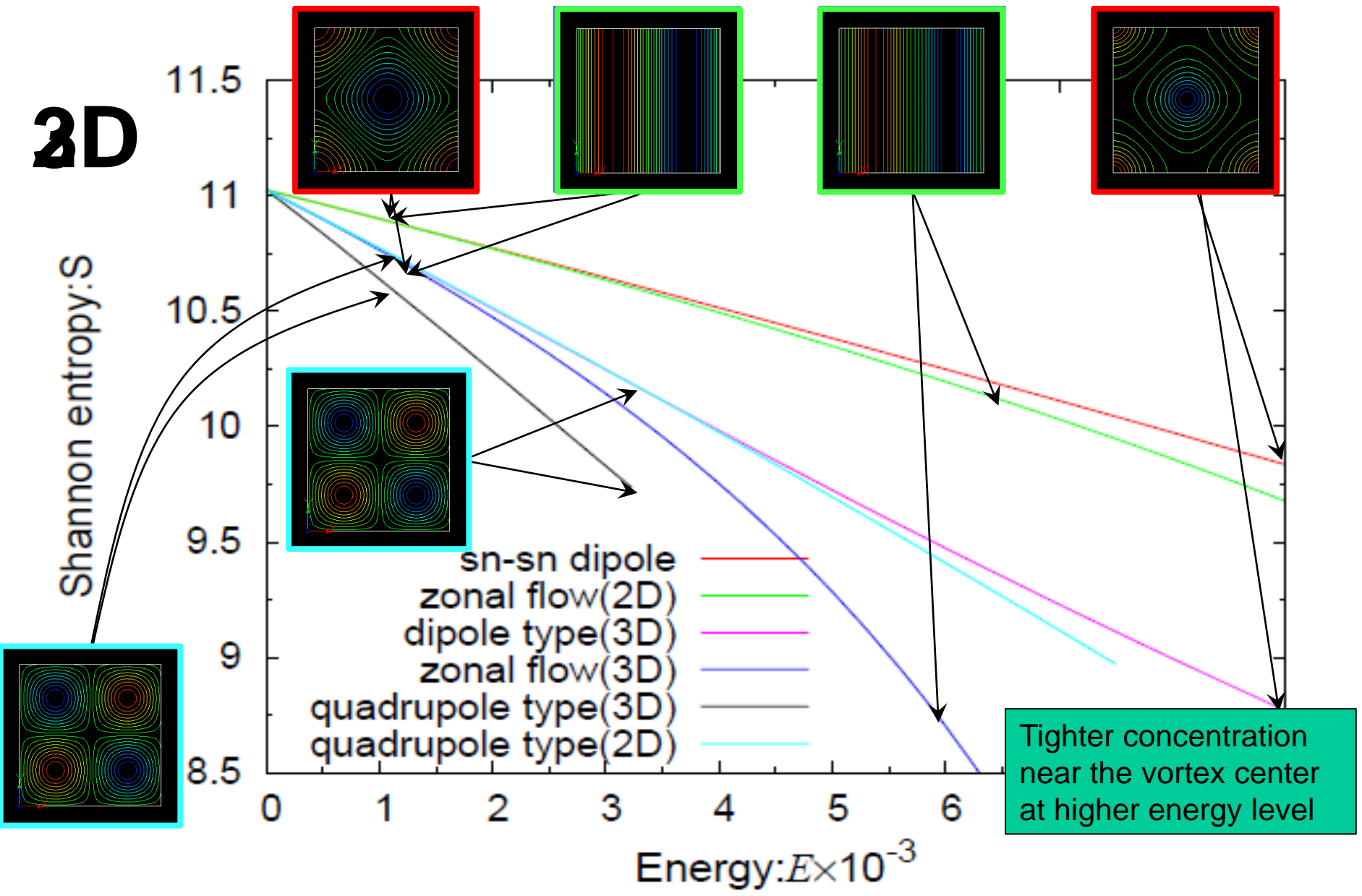
Initial vorticity guess	Vortex type	Vertical distribution: $P(z)$
$A \sin x$	zonal flow (2D)	$1/(2\pi)$
$A (\cos x + \cos y)$	dipole (2D)	$1/(2\pi)$
$A \sin x \sin y$	quadrupole (2D)	$1/(2\pi)$
$A \sin x \sin z$	zonal flow (3D)	$1/(2\pi)$
$A (\cos x + \cos y) \sin z$	dipole (3D)	$1/(2\pi)$
$A \sin x \sin y \sin z$	quadrupole (3D)	$1/(2\pi)$



Numerical Results

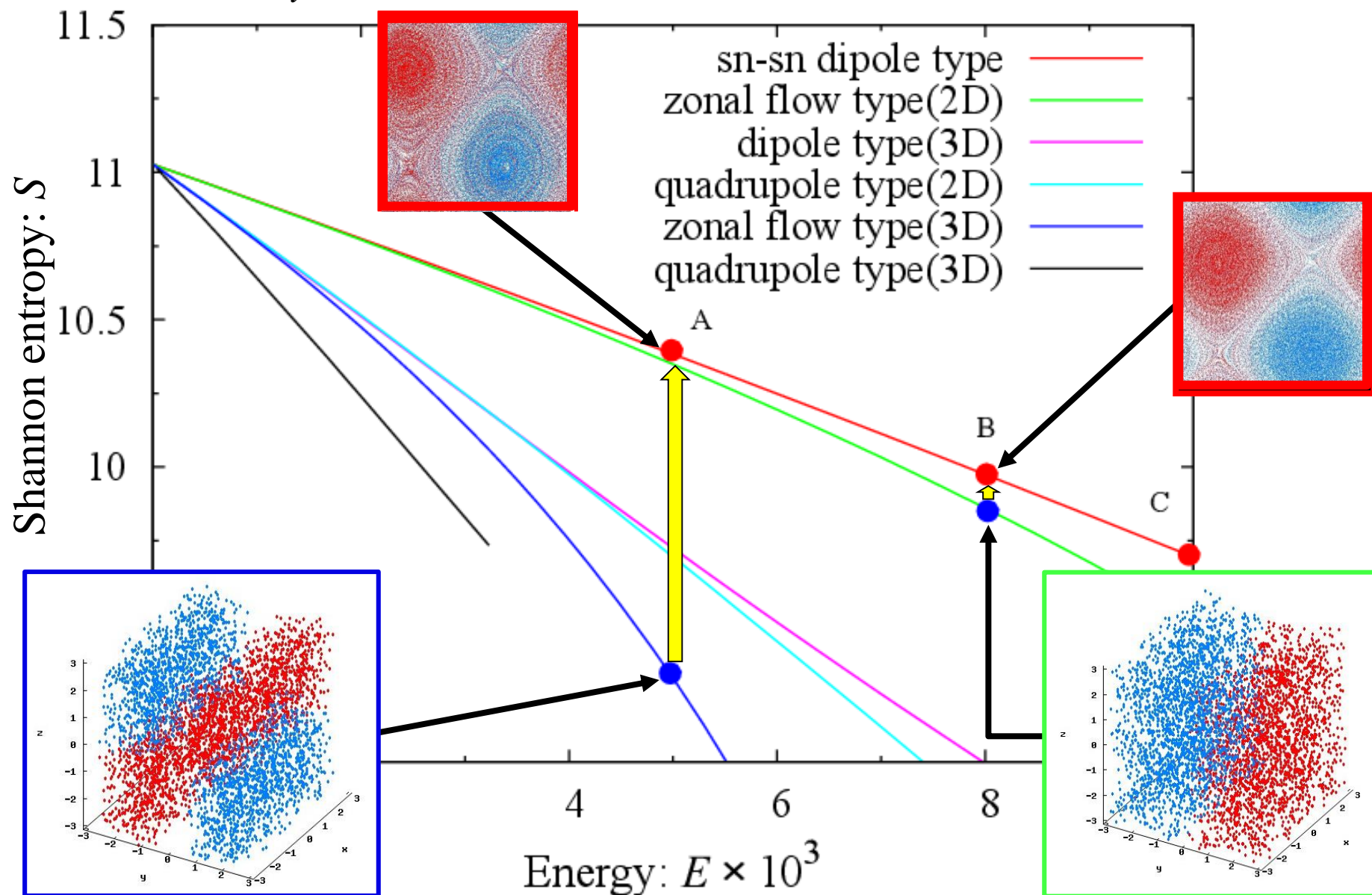


# Bifurcation Diagram in the $E$ - $S$ plane: 2D and 3D Maximum Entropy States



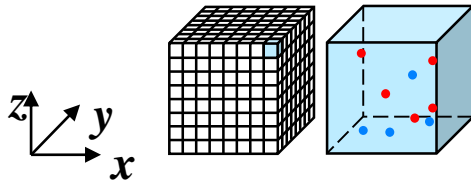
# Transition to Maximum Entropy State

Box size:  $L_x : L_y : L_z = 2\pi : 2\pi : 2\pi$



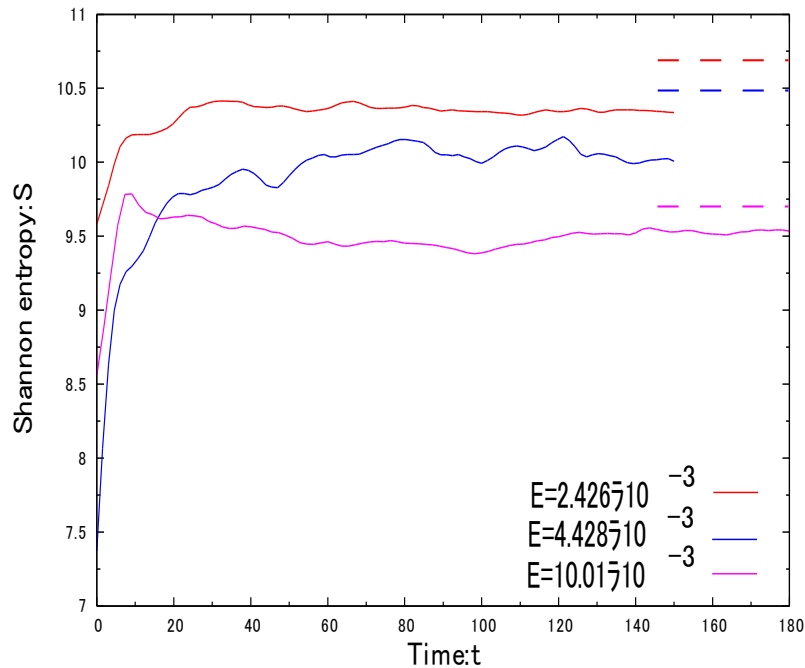
# Entropy Growth

## \* Entropy Evaluation



$$\nabla V = \frac{(2\pi)^3}{N} \quad F_{\pm}(\mathbf{r}) = \frac{n_{\pm}}{N\Delta V} = \frac{n_{\pm}}{(2\pi)^3}$$

$$S = - \iiint [F_+(\mathbf{r}) \log F_+(\mathbf{r}) + F_-(\mathbf{r}) \log F_-(\mathbf{r})] d^3\mathbf{r}$$



Shannon entropy grows with time and seems to approach the equilibrium value from below.



# Stability Analysis by Arnold's Method

## Conserved Quantities

$$H = \frac{1}{2} \iiint q \psi dx dy dz, \quad C = \iiint F(q, z) dx dy dz$$

$\psi \leftarrow \underbrace{\psi_0}_{\text{Equilibrium}} + \underbrace{\delta\psi}_{\text{Disturbance}}$  **variations of**  $H_C = H + C$

$$-F(q_0, z) = q_0 \sinh^{-1} \left( \frac{q_0}{\lambda^2(z)} \right) - \sqrt{\lambda^4(z) + q_0^2} \quad \text{to have the Mean Field Equation}$$

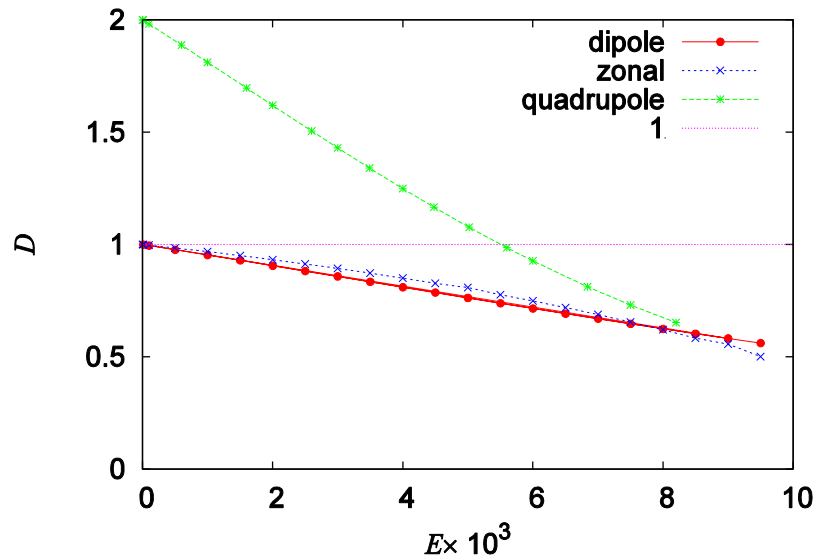
**First variation:**  $\delta H_C = \iiint \left[ q_0 - \Delta \left( \frac{\partial F}{\partial q_0} \right) \right] \delta\psi dx dy dz = 0$

**Second variation:**  $\delta^2 H_C = \frac{1}{2} \iiint \left[ |\text{grad} \delta\psi|^2 - \frac{(\Delta(\delta\psi))^2}{\sqrt{\lambda^4(z) + q_0^2}} \right] dx dy dz \quad ? \quad 0$

**Stability cannot be proved in general**

# Results of Stability Analysis

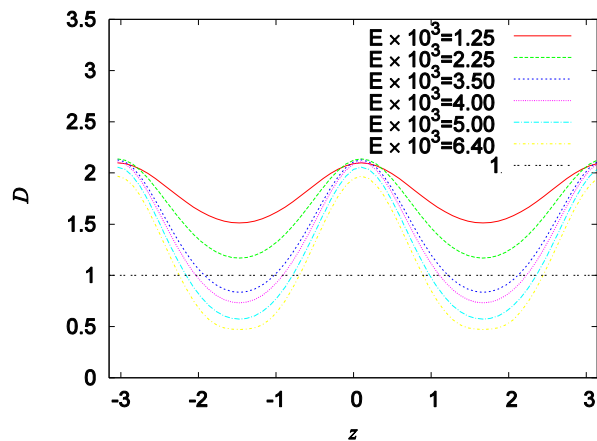
## 2D



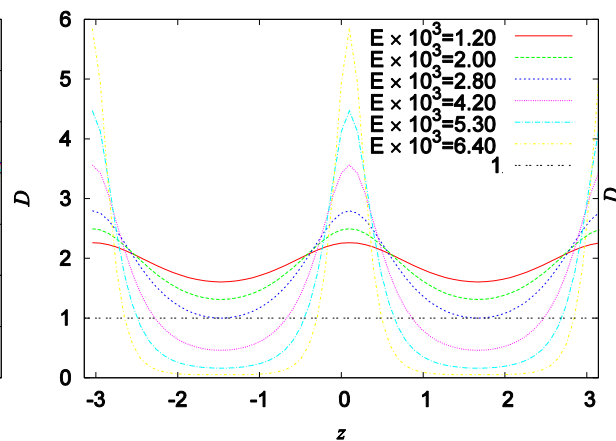
Less than 1 for 2D-dipole  
and 2D-zonal: “Stable”  
More than 1 for 2D-quadrupole:  
“Possibly Unstable”

## 3D

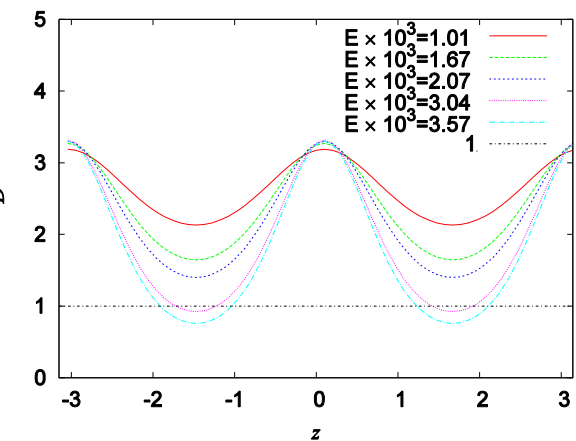
### 3D-dipole



### 3D-zonal



### 3D-quadrupole



More than 1 for any case : “Possibly Unstable”

# Direct Numerical Simulations of QG equation

## Continuous QG equation

$$\left( \frac{\partial}{\partial t} + \frac{\partial \psi(\mathbf{r}, t)}{\partial y} \frac{\partial}{\partial x} - \frac{\partial \psi(\mathbf{r}, t)}{\partial x} \frac{\partial}{\partial y} \right) q(\mathbf{r}, t) = \underbrace{(-1)^{p+1} \nu \Delta^p q(\mathbf{r}, t)}_{\text{Dissipation term}}$$

$\nu$  : Viscosity

$p$  : Order of dissipation

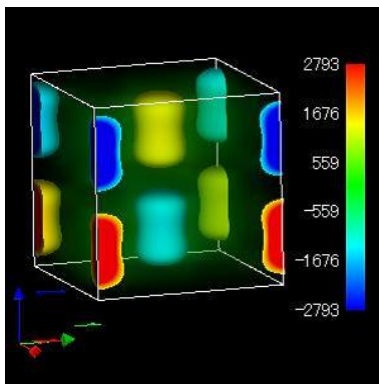
## Fourier Modes (Quasi-Spectral Method)

$$\hat{q}(k_x, k_y, k_z, t) = (k_x^2 + k_y^2 + k_z^2) \hat{\psi}(k_x, k_y, k_z, t)$$

Wave number vector:  $\mathbf{k} = (k_x, k_y, k_z)$

## Initial Equilibrium States

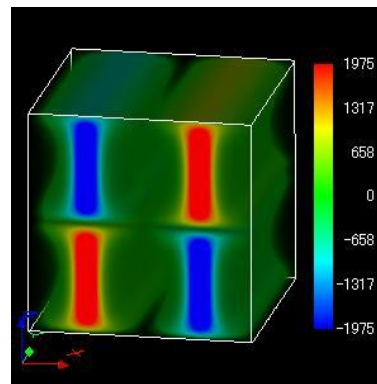
①



3D-dipole

$$E = 6.40 \times 10^{-3}$$

②

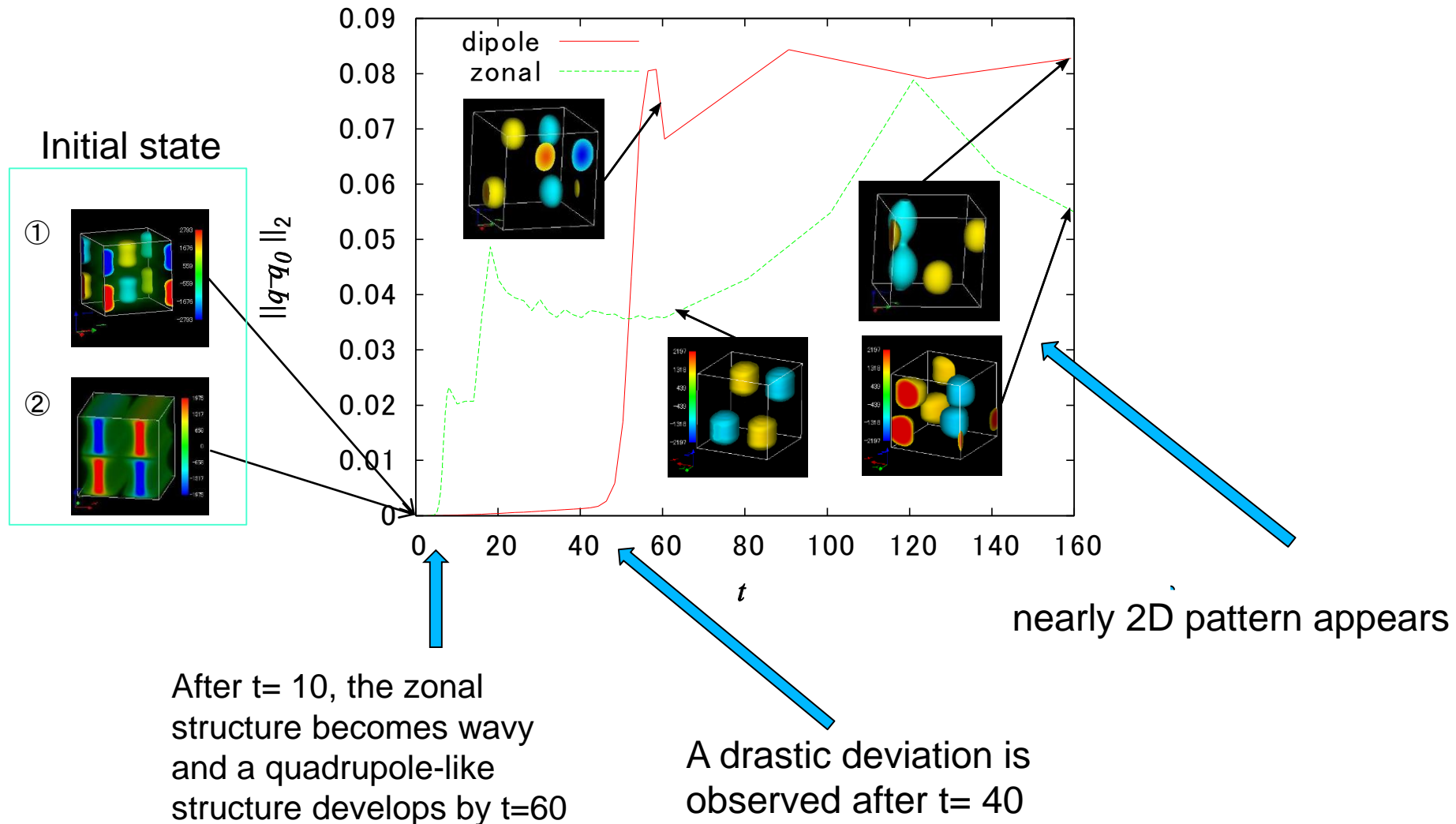


3D-zonal

$$E = 6.40 \times 10^{-3}$$

Adding small disturbances  
4<sup>th</sup> order RK time marching  
De-aliasing by 2/3 rule

# Results of Direct Numerical Simulations of QG equation





# Summary

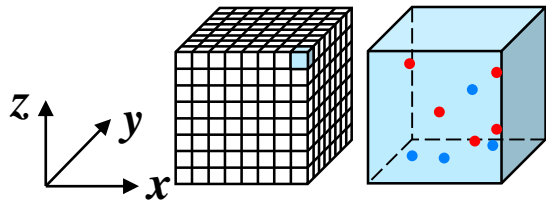
- We investigate the statistical mechanics of bi-disperse quasi-geostrophic point vortices numerically and theoretically.

1. Clustering of vortices of like sign occurs (negative temperature state), and the equilibrium has two-dimensional dipole structure.
2. Shannon entropy increases and the number of cluster decreases like  $t^{-1}$ .
3. The maximum entropy states are determined theoretically by solving the mean field equation. They coincide with the numerical end states.
4. Two- and three-dimensional maximum entropy states are found.
5. The two-dimensional  $sn$ - $sn$  dipole solution has the largest entropy, which is the reason only this branch is found numerically.
6. The two-dimensional  $sn$ - $sn$  dipole and zonal flow solutions are found to be stable.

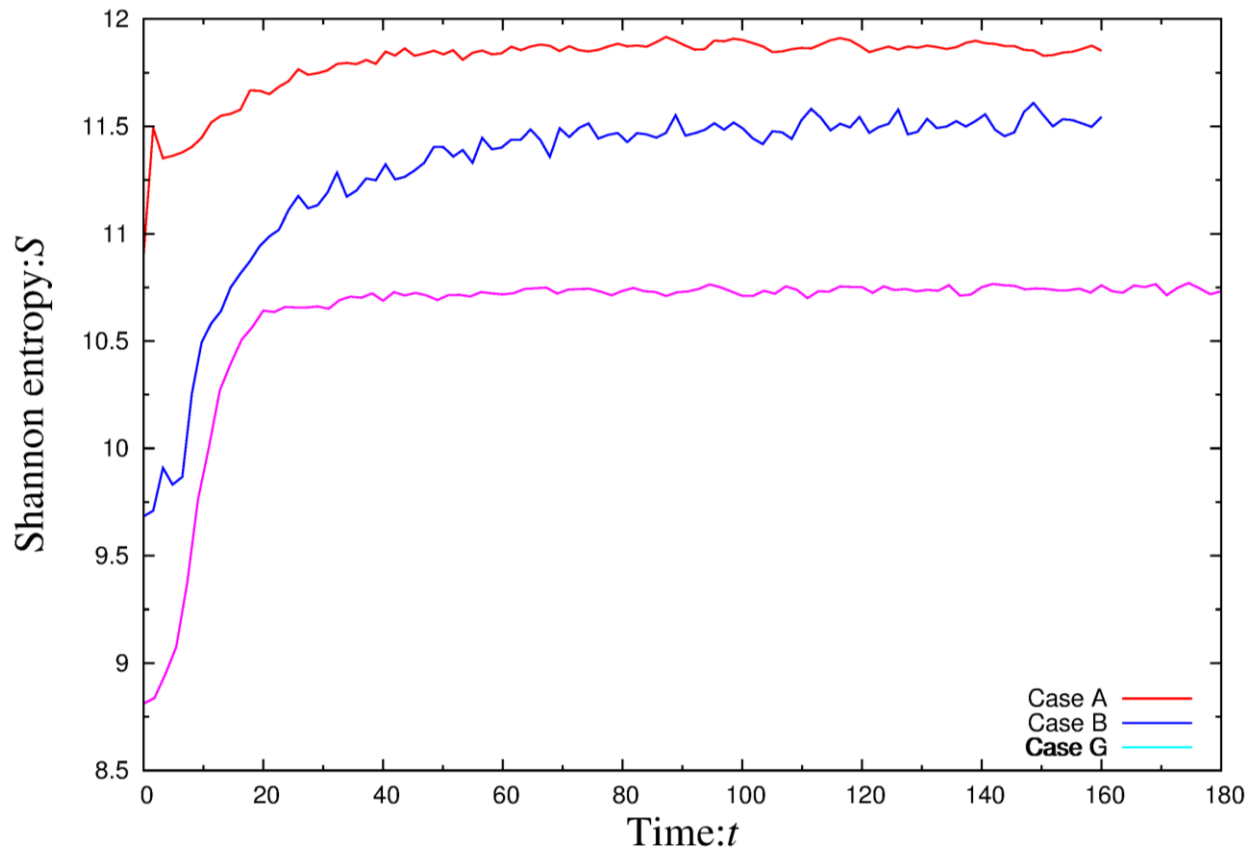
Thank you for your attention

# Entropy Growth in Numerical Simulations

## Shannon Entropy



$$\nabla V = \frac{(2\pi)^3}{N} \quad F_{\pm}(\mathbf{r}) = \frac{N_{\pm}}{N \nabla V} = \frac{N_{\pm}}{(2\pi)^3}$$
$$S = - \iiint [F_+(\mathbf{r}) \log F_+(\mathbf{r}) + F_-(\mathbf{r}) \log F_-(\mathbf{r})] d^3 \mathbf{r}$$



# Ewald Sum : Energy under periodic boundary conditions

## ■ Energy (Hamiltonian)

$$H = \underbrace{H^{(1)}}_{\text{Real space}} + \underbrace{H^{(2)}}_{\text{Wavenumber space}} + \underbrace{H^{(3)}}_{\text{Constant term}}$$

**Assume:**  $F(r) = \Gamma \left( \frac{\alpha}{\pi} \right)^{\frac{3}{2}} \exp(-\alpha^2 r^2)$ : **Gaussian**  
 (  $\alpha[\text{L}^{-1}]$  : **scaling parameter** )

[ for cubic cell  $L^3$  ]  $L = \pi - (-\pi) = 2\pi$

## ■ Real space

$$H^{(1)} = \frac{1}{2} \sum_{\mathbf{n}} \sum_i \sum_j' \frac{\hat{\Gamma}_i \hat{\Gamma}_j}{4\pi} \frac{\text{erfc}(\alpha |\mathbf{R}_i - \mathbf{R}_j + L\mathbf{n}|)}{|\mathbf{R}_i - \mathbf{R}_j + L\mathbf{n}|}$$

## ■ Wavenumber space

$$H^{(2)} = \frac{2\pi}{L^3} \sum_{\mathbf{G} \neq 0} \frac{\exp(-|\mathbf{G}|^2 / 4\alpha^2)}{|\mathbf{G}|} \sum_i \sum_j \frac{\hat{\Gamma}_i \hat{\Gamma}_j}{4\pi} \cos\{\mathbf{G} \cdot (\mathbf{R}_i - \mathbf{R}_j)\}$$

## ■ Self energy (Constant term)

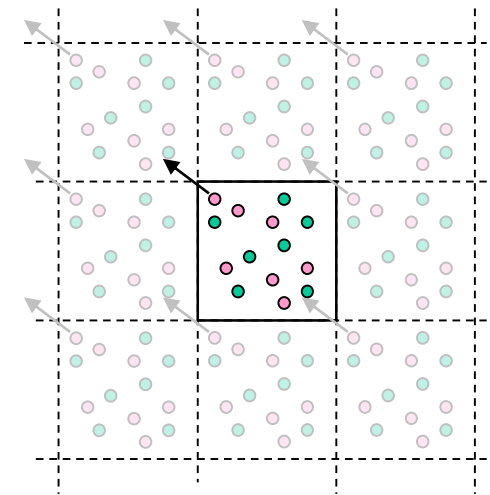
$$H^{(3)} = - \sum_i \frac{\hat{\Gamma}_i^2}{4\pi} \frac{\alpha}{\sqrt{\pi}}$$

$$\mathbf{G} = \frac{2\pi}{L} \mathbf{h}: \text{ wavenumber vector ( } \mathbf{h}: \text{ integer vector ) }$$

Canonical equations of motion  
for the  $i$ -th vortex

$$\frac{dX_i}{dt} = \frac{1}{\hat{\Gamma}_i} \frac{\partial H}{\partial Y_i}, \quad \frac{dY_i}{dt} = -\frac{1}{\hat{\Gamma}_i} \frac{\partial H}{\partial X_i}$$

$$E = H / (\sum_{i=1}^N |\hat{\Gamma}_i|)^2$$



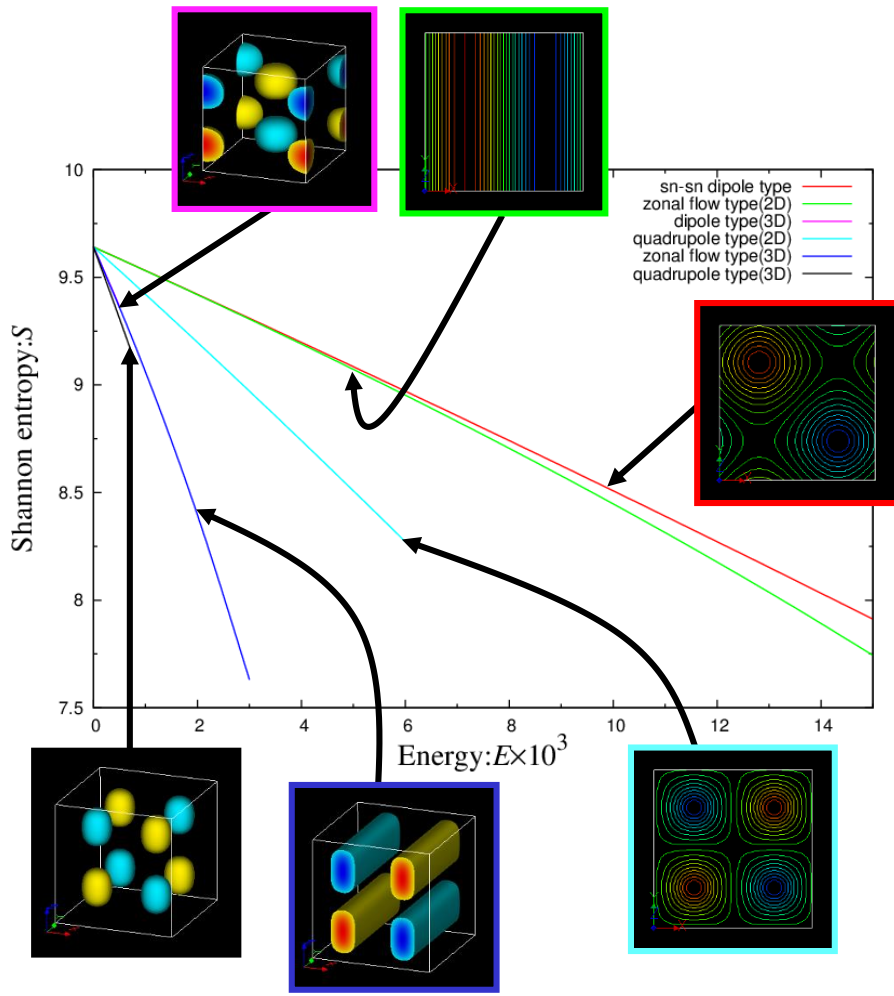
Real space and image cells

# Influence of Aspect ratio: $L_z / L_x = 0.5$ and $4.0$

Box size:

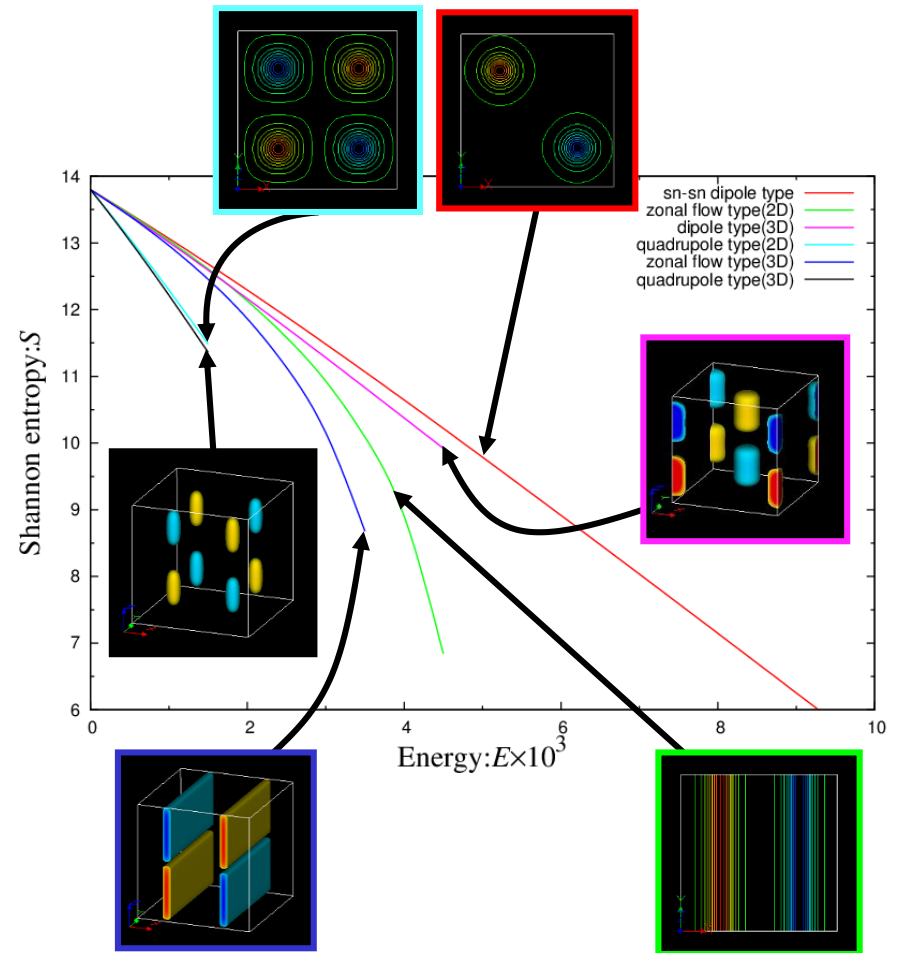
$$L_x : L_y : L_z = 2\pi : 2\pi : \pi$$

Entropy decrease of 3D solutions



$$L_x : L_y : L_z = 2\pi : 2\pi : 8\pi$$

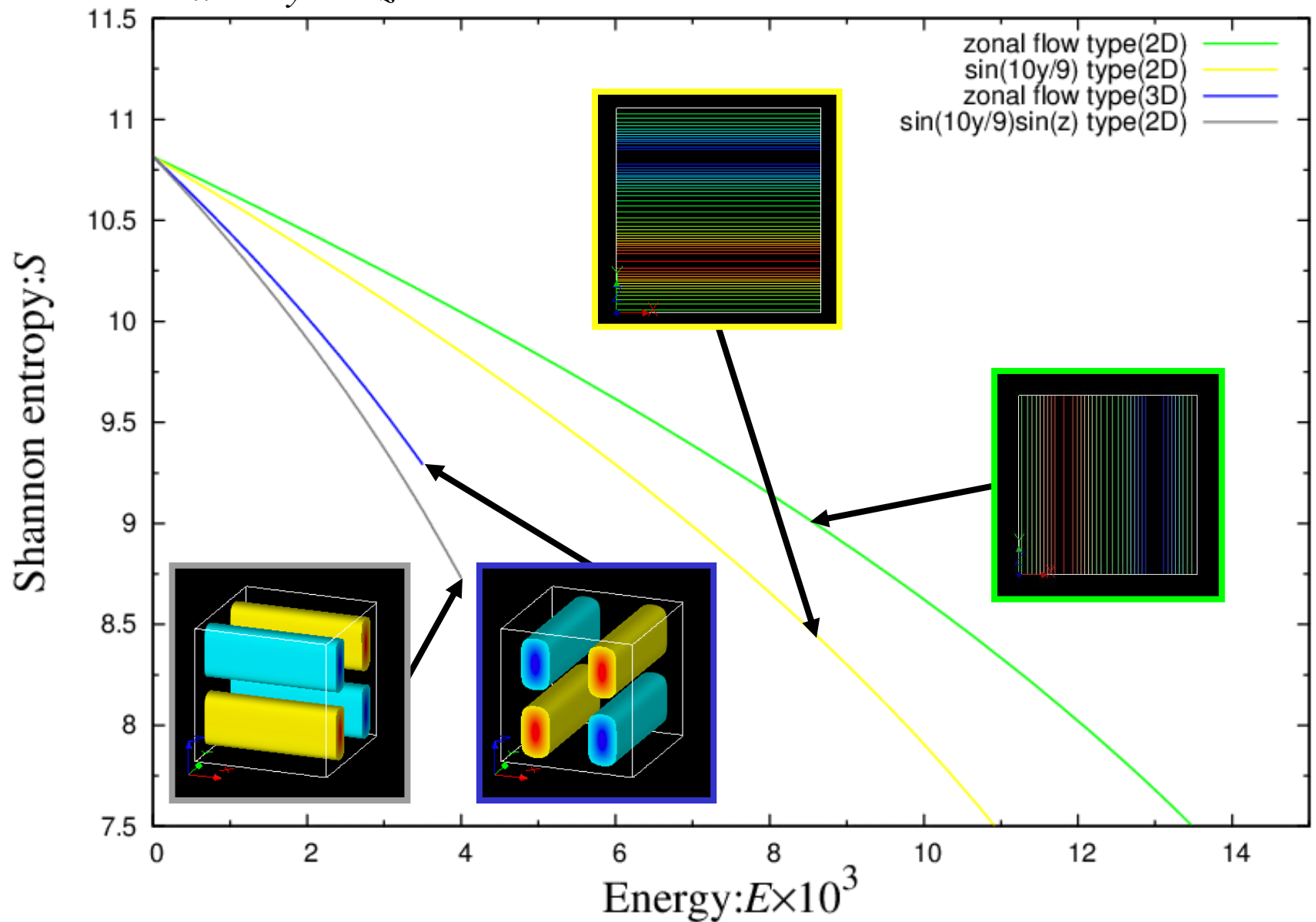
Entropy increase of 3D solutions





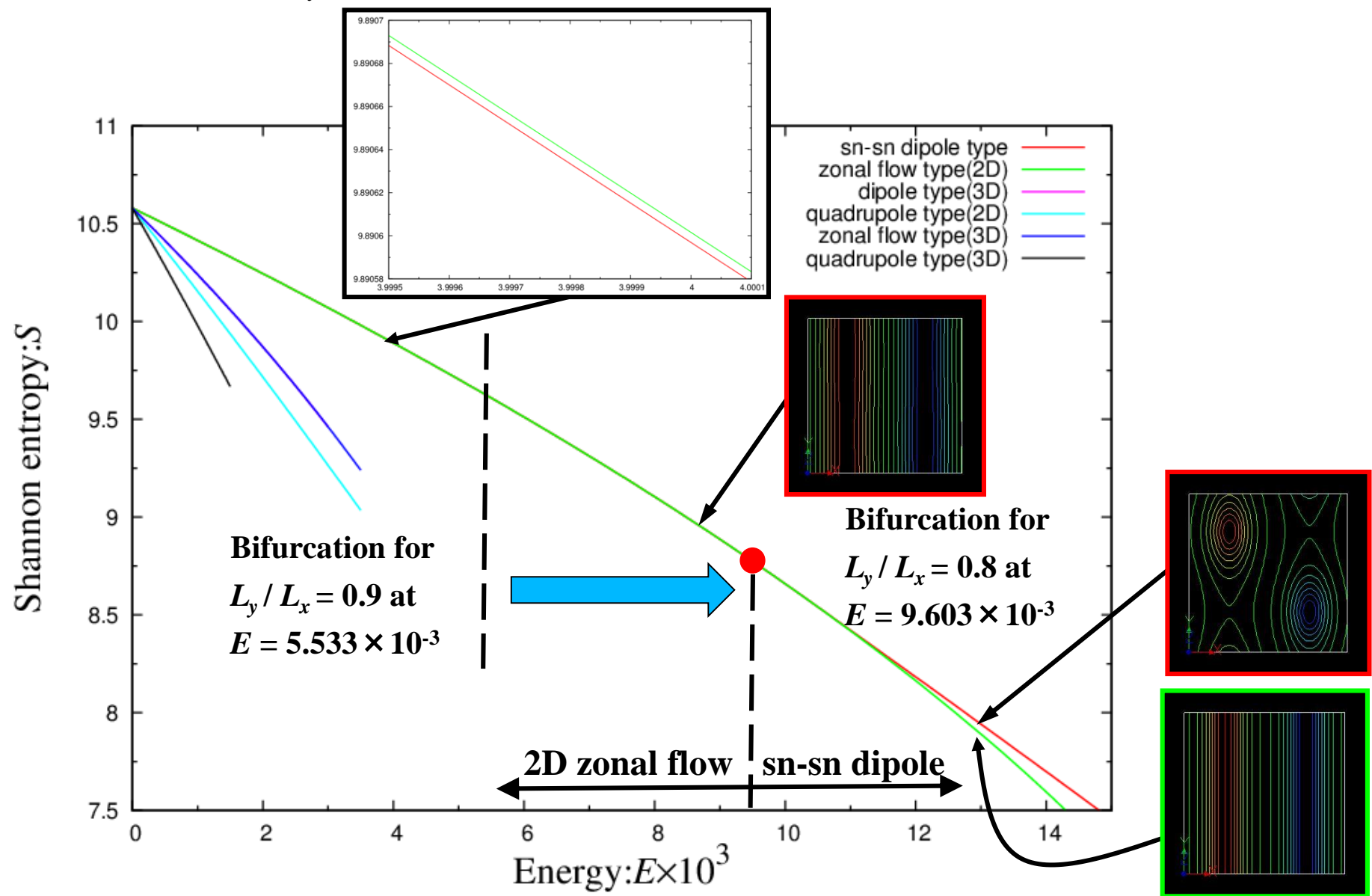
# Two types of Zonal Flow for $L_y / L_x = 0.9$

**Box size:**  $L_x : L_y : L_z = 2\pi : 1.8\pi : 2\pi$



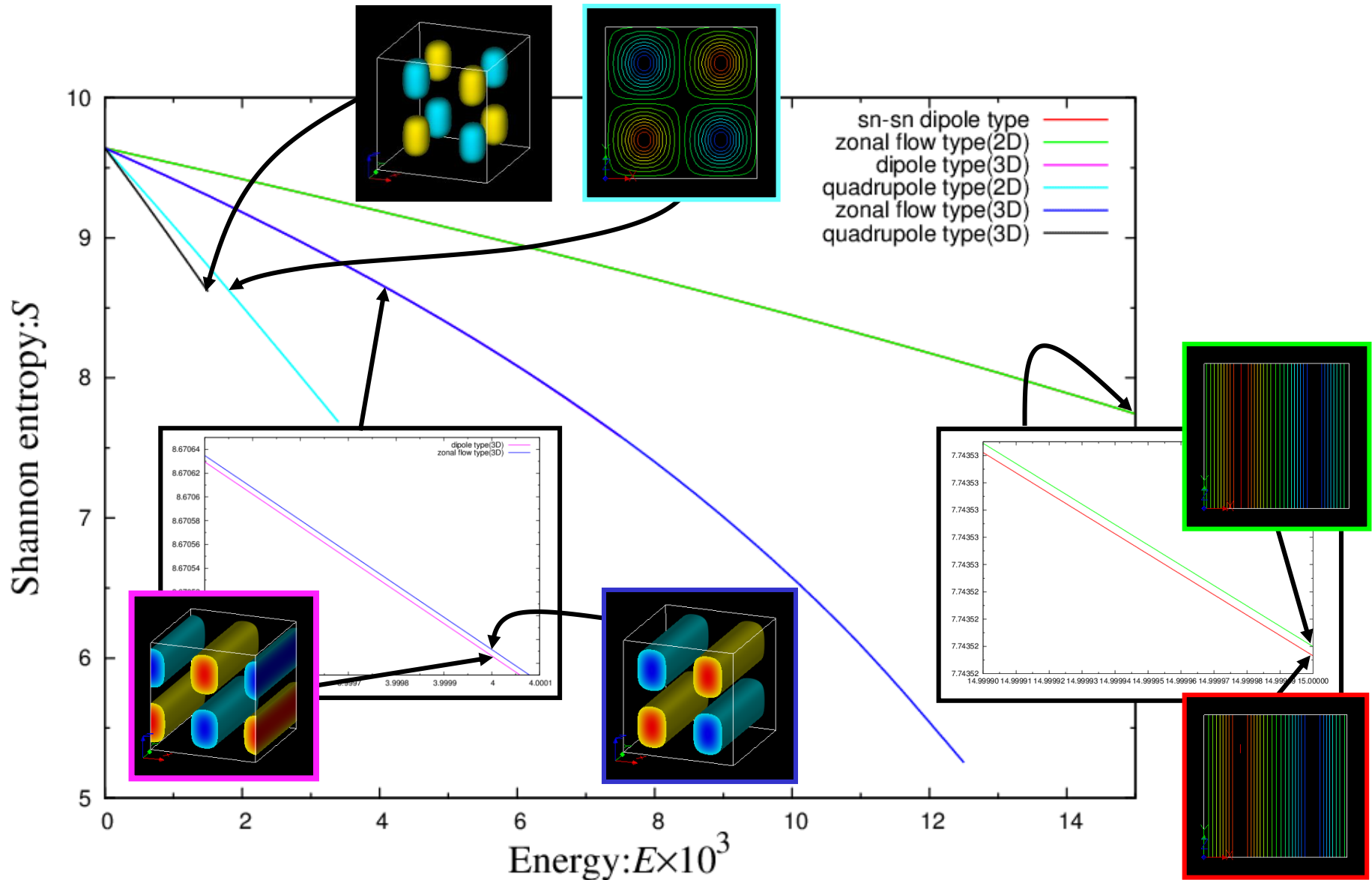
# Influence of Aspect ratio: $L_y / L_x = 0.8$

Box size:  $L_x : L_y : L_z = 2\pi : 1.6\pi : 2\pi$



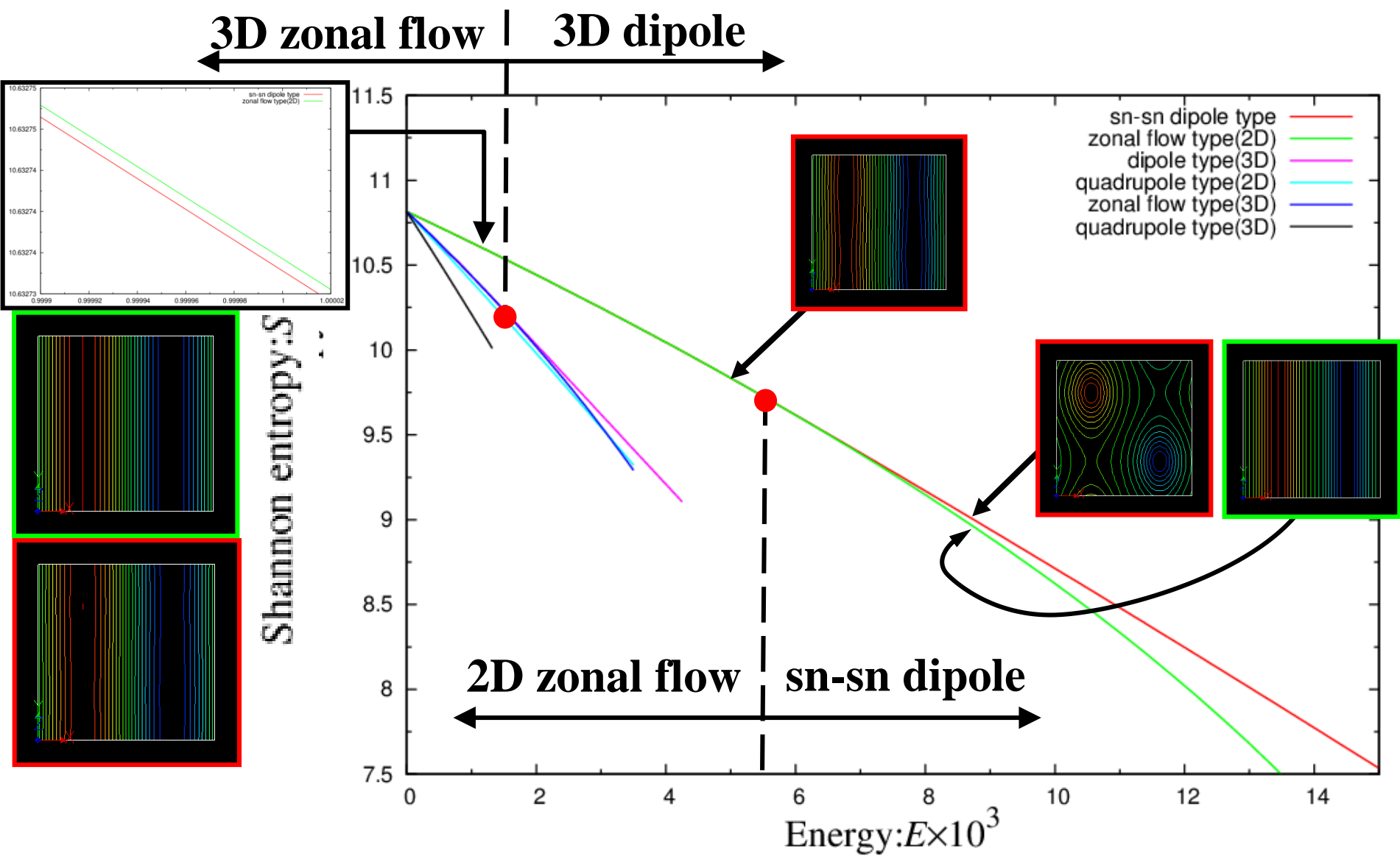
# Influence of Aspect ratio: $L_y / L_x = 0.5$

Box size:  $L_x : L_y : L_z = 2\pi : \pi : 2\pi$



# Influence of Aspect ratio: $L_y / L_x = 0.9$

Box size:  $L_x : L_y : L_z = 2\pi : 1.8\pi : 2\pi$

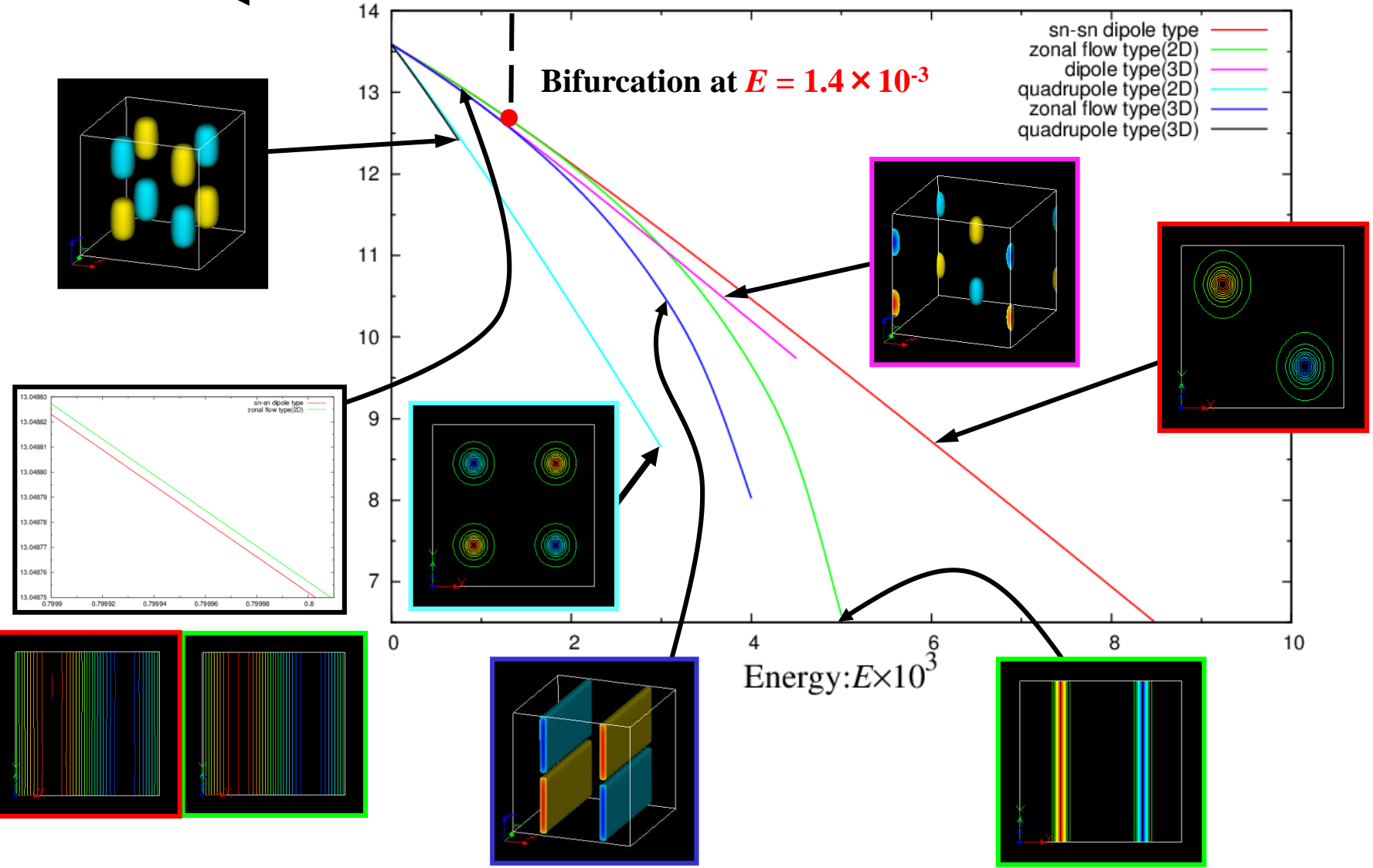




# Influence of Aspect ratio: $L_y / L_x = 0.9, L_z / L_x = 4.0$

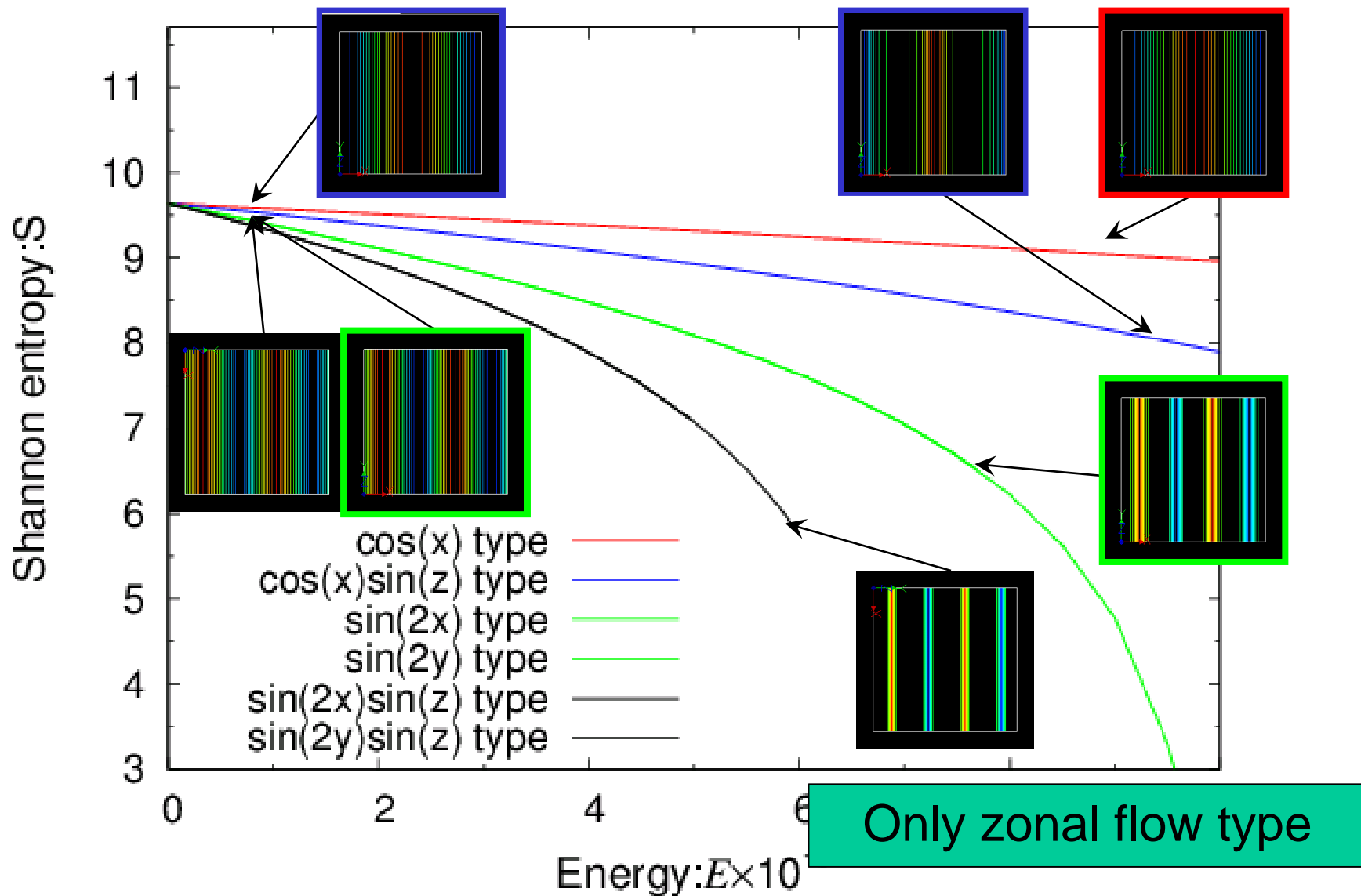
Box size:  $L_x : L_y : L_z = 2\pi : 1.8\pi : 8\pi$

← 2D zonal flow | sn-sn dipole →



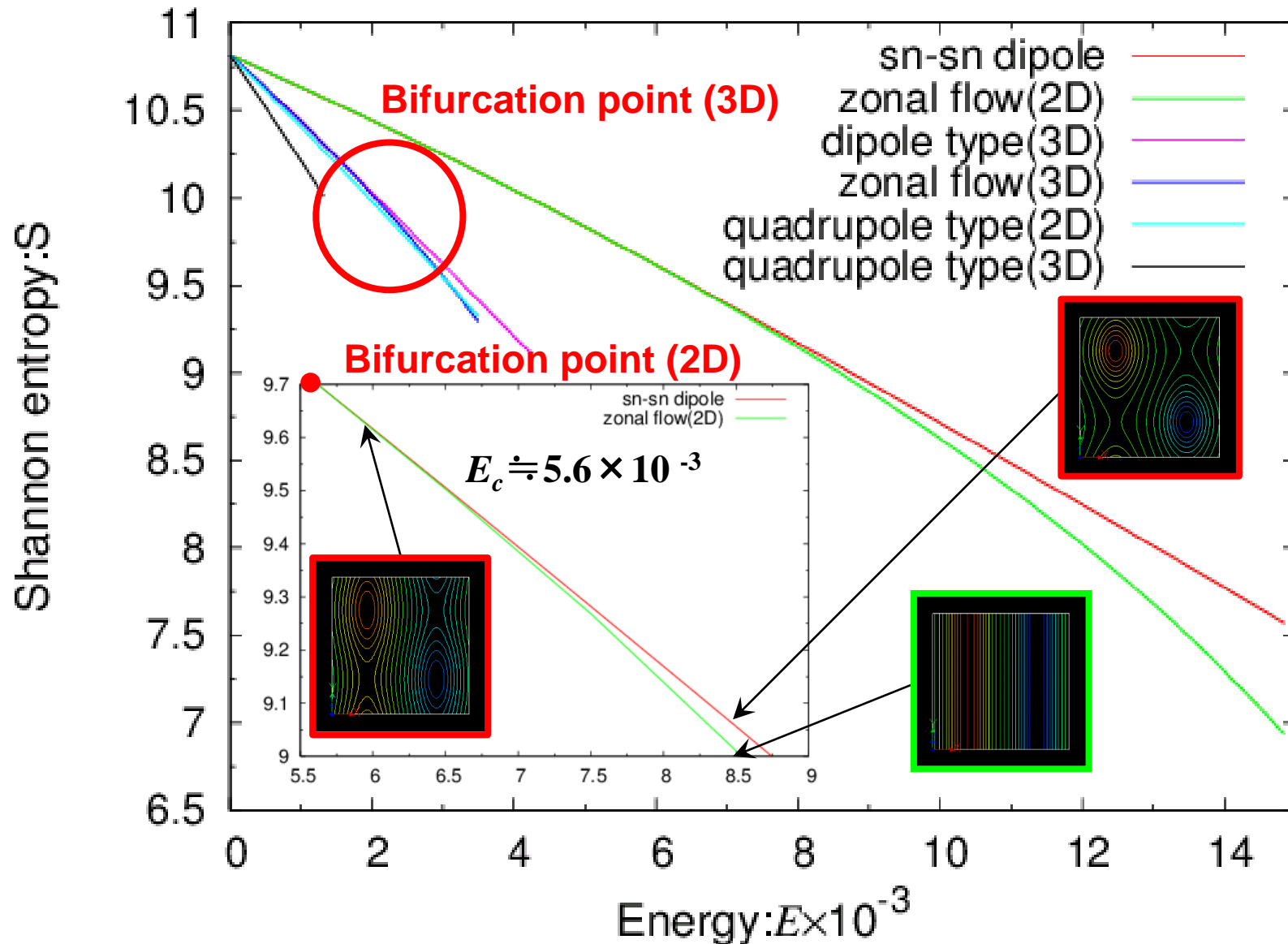
# Influence of the Aspect Ratio (1)

Aspect ratio of the periodic domain:  $x : y : z = 2\pi : \pi : 2\pi$

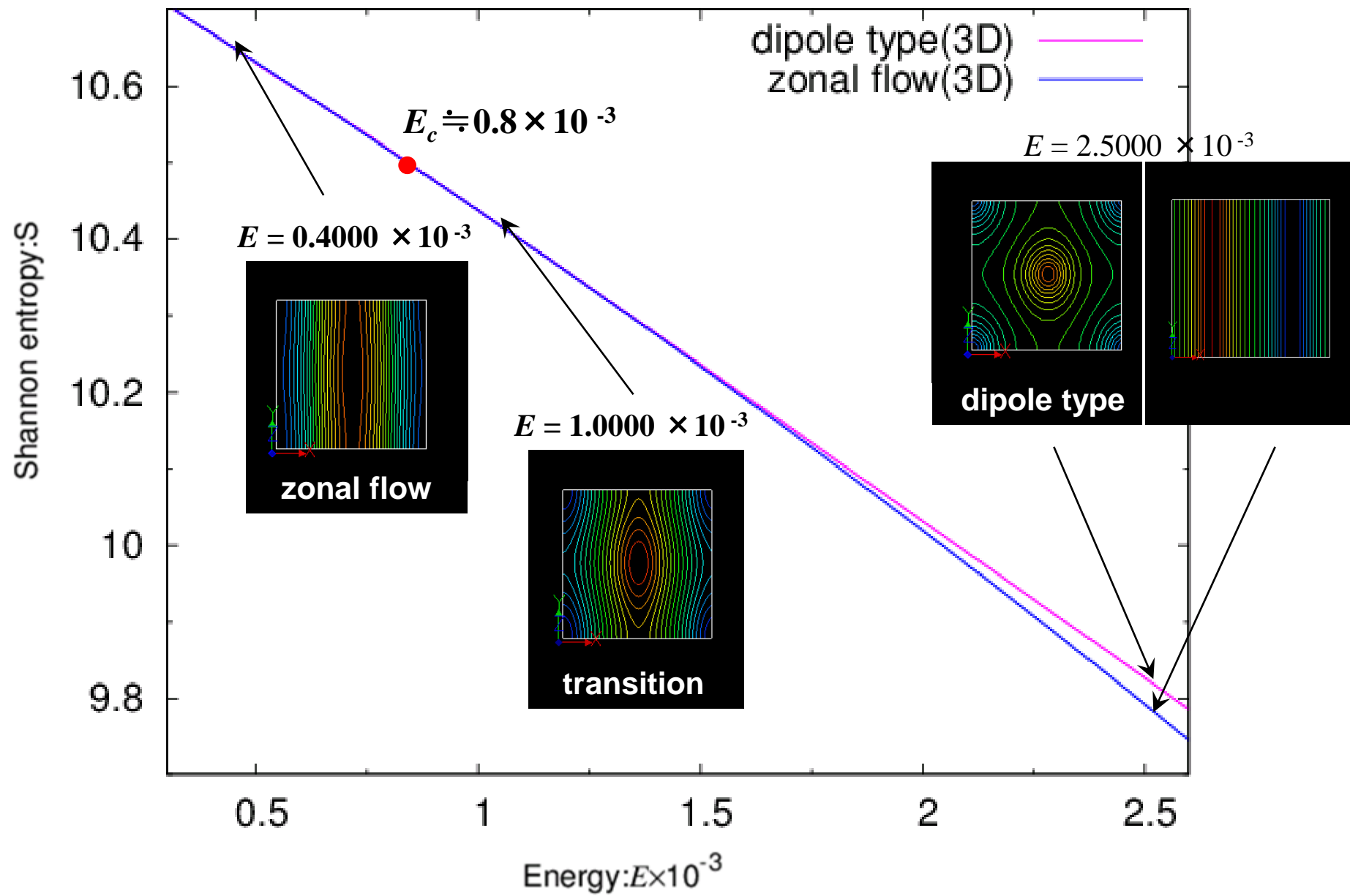


# Influence of the Aspect Ratio (2)

Aspect ratio of the periodic domain:  $x : y : z = 2\pi : 1.8\pi : 2\pi$

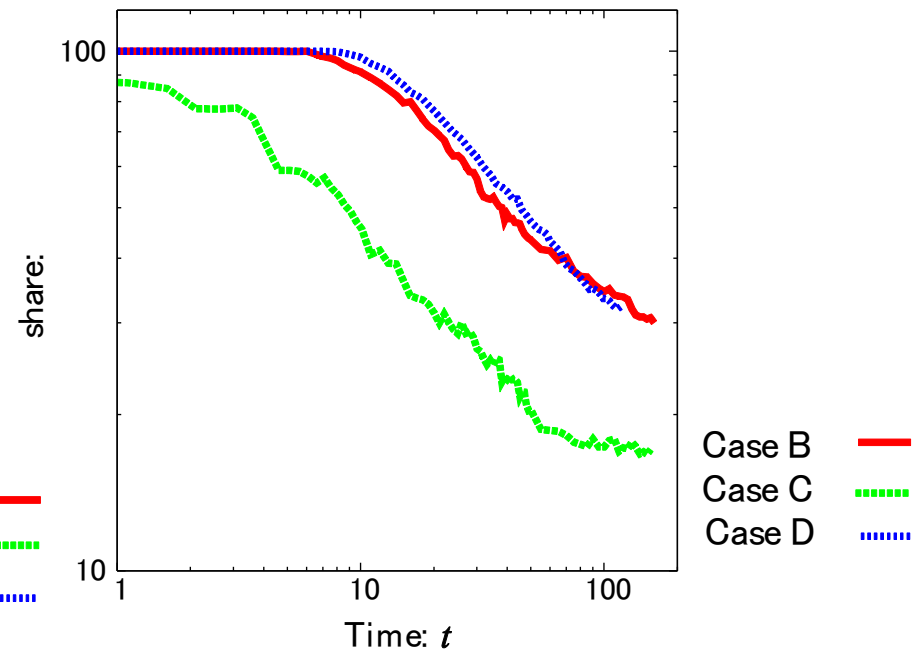
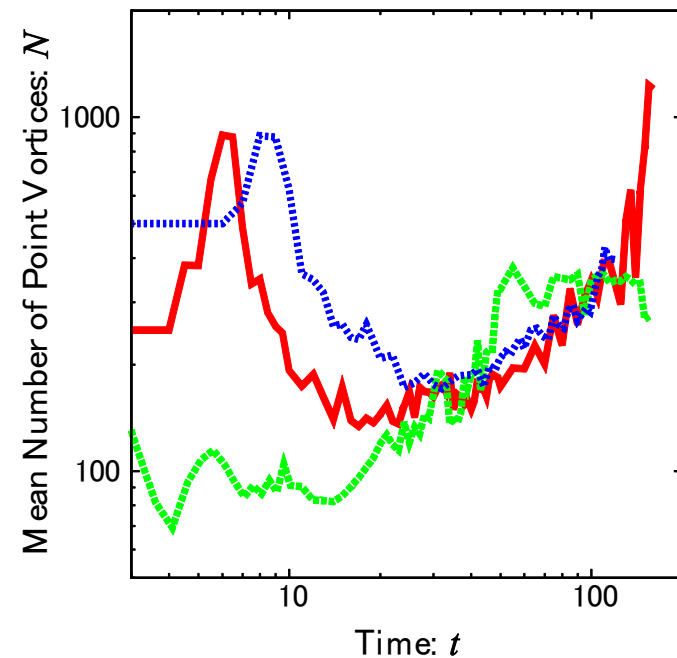


# Transition from 3D zonal to 3D dipole type

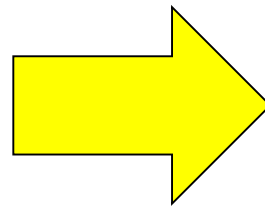




# Cluster Strength



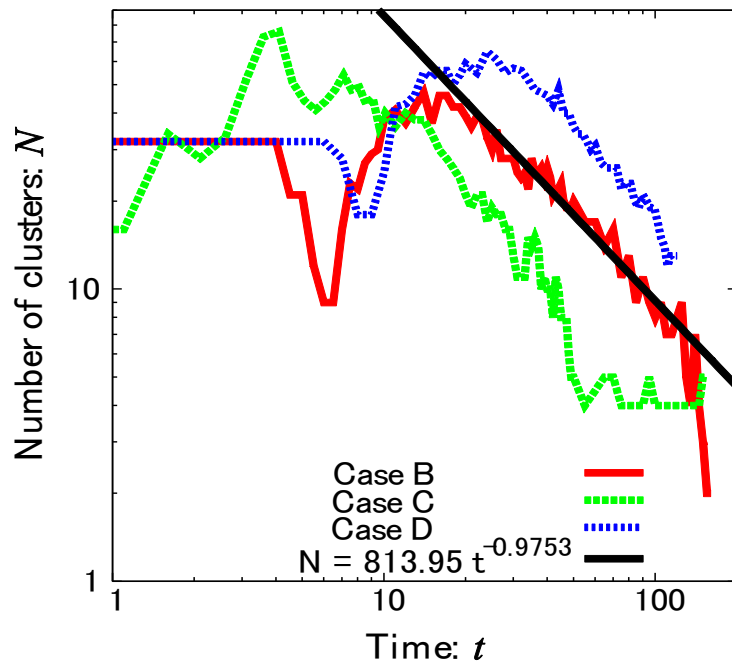
- Number of point vortices in a cluster increases.
- Share of point vortices inside clusters decreases.



- Cluster size grows due to vertical alignment.
- Some of point vortices are emitted from clusters.

# スペクトル法による数値計算結果との比較

## 本研究における 解析結果



$\sim t^{-1.00}$ にしたがってク  
ラスター数が減少

## McWilliams *et al.* [2]によるス ペクトル法の数値シミュレーシ ョン結果

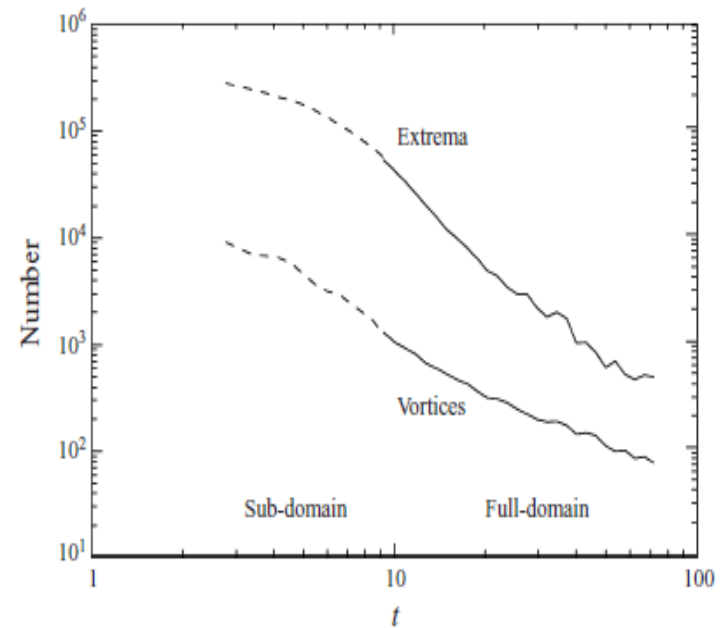
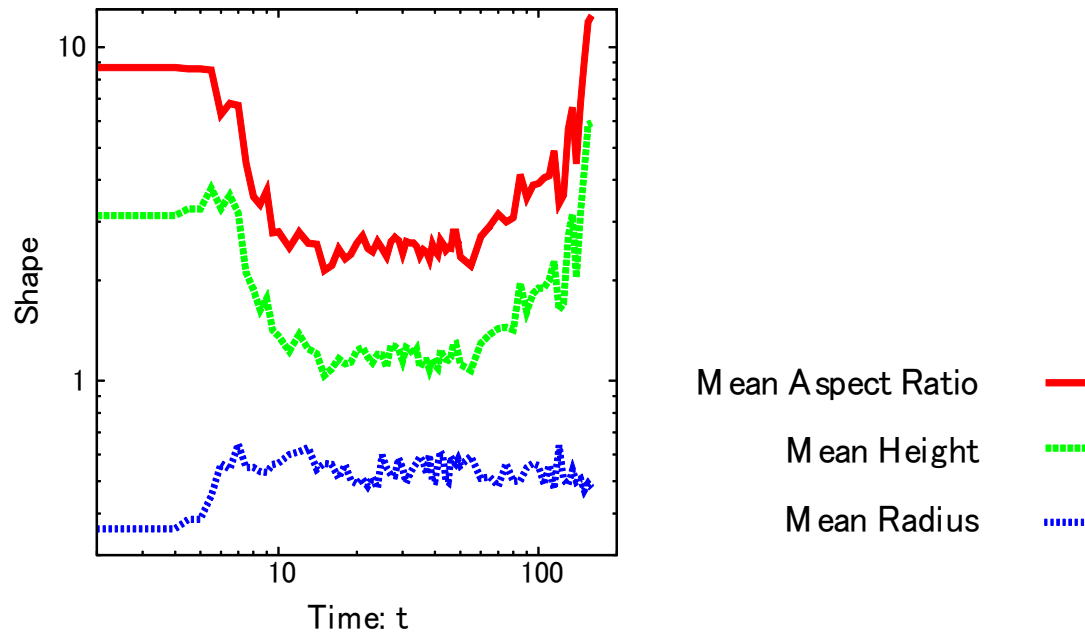


FIGURE 4. The number of extrema and compound vortices,  $n_e(t)$  and  $n_{cv}(t)$ , from the vortex census.

$\sim t^{-1.25}$ にしたがって渦  
数が減少

# スペクトル法による数値計算結果との比較

## 本研究における解析結果 (Case B)



- ・平均半径がほとんど変化しない
- ・アスペクト比と高さが同程度のスピードで増加

## McWilliams *et al.* [2]によるスペクトル法の数値シミュレーション結果

*J. C. McWilliams, J. B. Weiss and I. Yavneh*

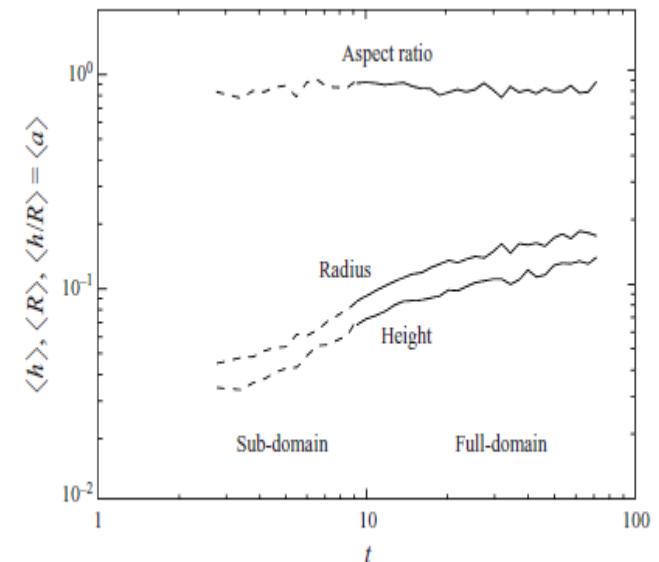
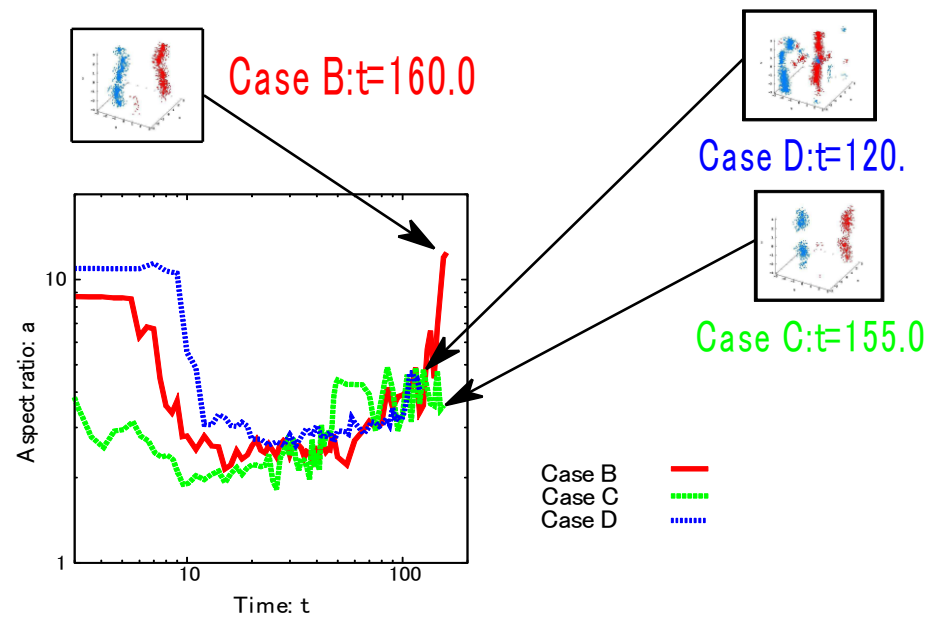


FIGURE 8. The population-mean vortex-element radius,  $\langle R \rangle(t)$ , half-height,  $\langle h \rangle(t)$ , and aspect ratio,  $\langle a \rangle(t)$ , from the vortex census.

- ・平均半径と平均高さが同程度のスピードで増加
- ・アスペクト比の変化がほとんどない



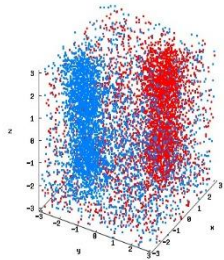


# End States

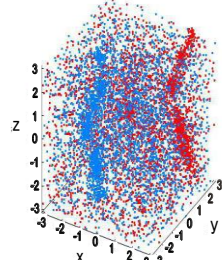
$$L_x:L_y:L_z = 2\pi:2\pi:2\pi$$

## 3D view

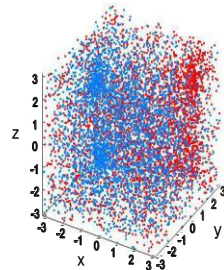
Case A: **3D dipole**



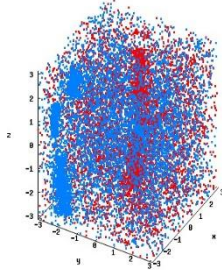
Case B: **Checkerboard**



Case C: **16 pillars**

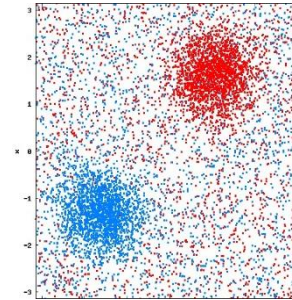


Case D: **Checkerboard**

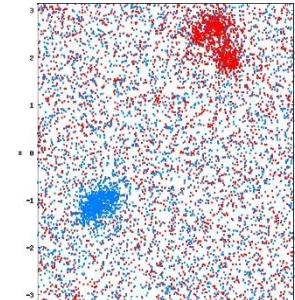


## Top view

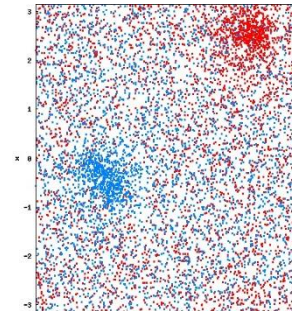
Case A: **3D dipole**



Case B: **Checkerboard**



Case C: **16 pillars**



Case D: **Checkerboard**

