Statistical measure correction for discretized geophysical fluids

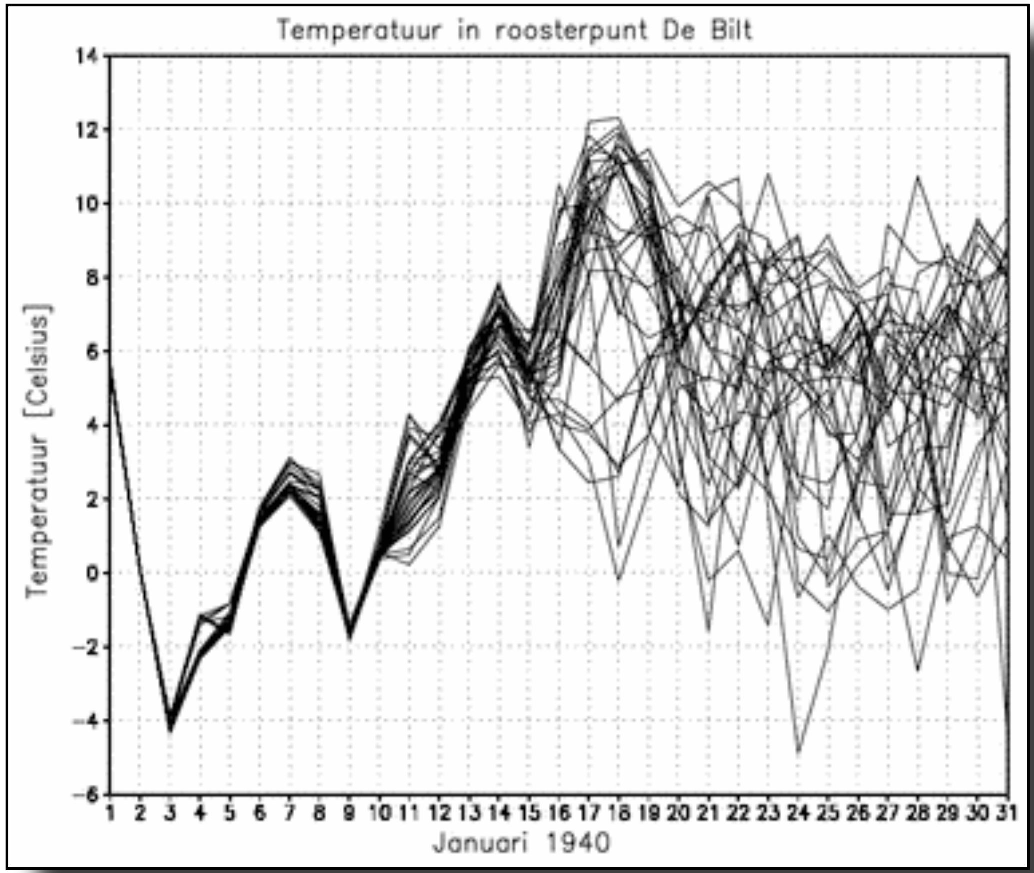
Jason Frank, CWI Amsterdam

with: Svetlana Dubinkina (Louvain), Ben Leimkuhler (Edinburgh)

SciCADE 2011 - Toronto - 11 July

Climate simulations (KNMI)

- Dutch Challenge Project (2004) to assess climate change impact: frequency of precipitation, drought, storms, etc.
- Global climate model (atmos., ocean, ice, land, insolation, chemistry)
- Simulation time 140 yrs., IC Jan. 1, 1940
- Ensemble simulations: 64 independent runs. Uniform random scaling of atmospheric temp in [0.999, 1.001]
- Numerical errors in the first hour exceed this perturbation.
- Numerical errors overwhelm the computation in the first month.



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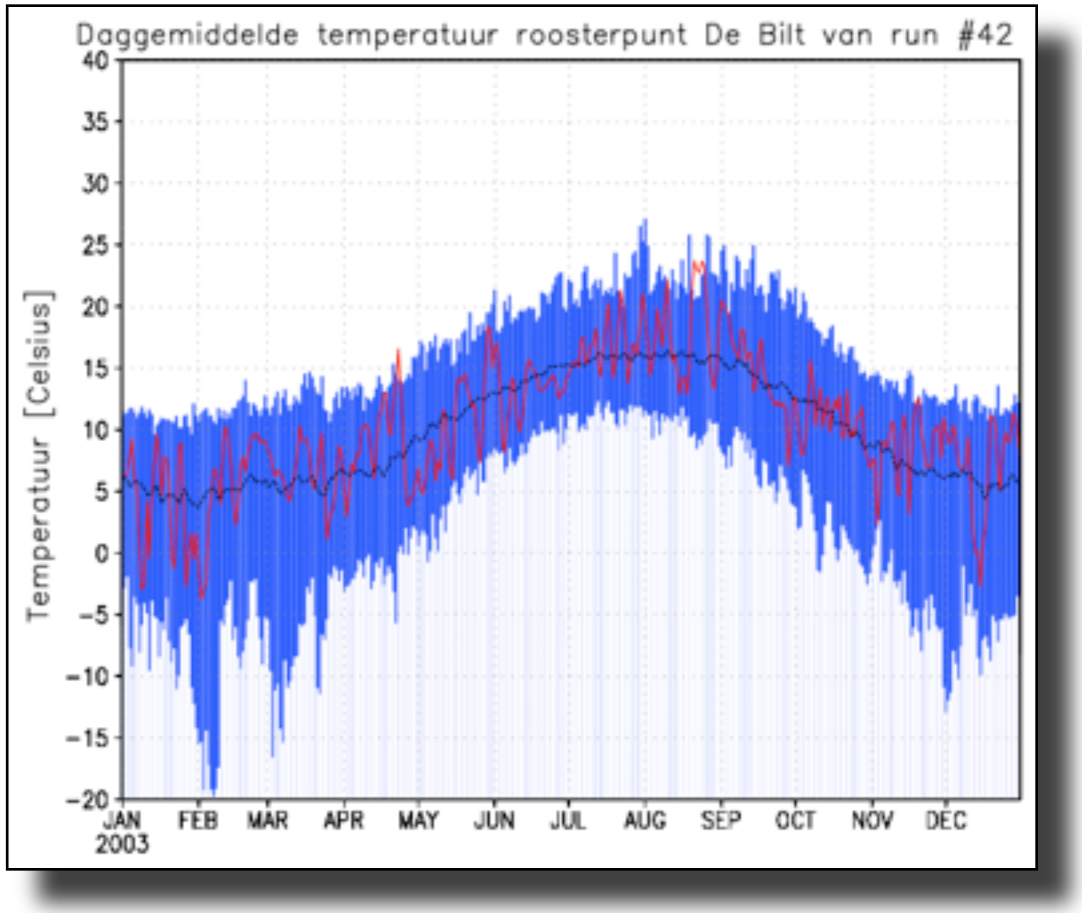
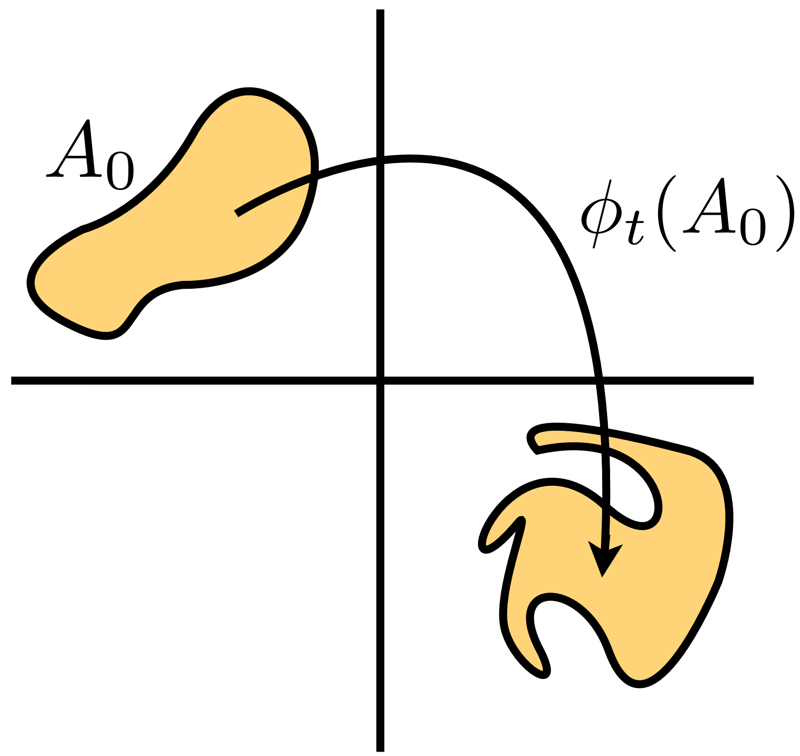


Liouville equation, invariant measure, and sampling



ODE $\dfrac{dX}{dt} = f(X)$

phase flow operator $X(t) = \phi_t(X_0)$

Probability density $\rho(X,t)$
on (a set A(t)) in phase space

Liouville equation governs
transport of probability:

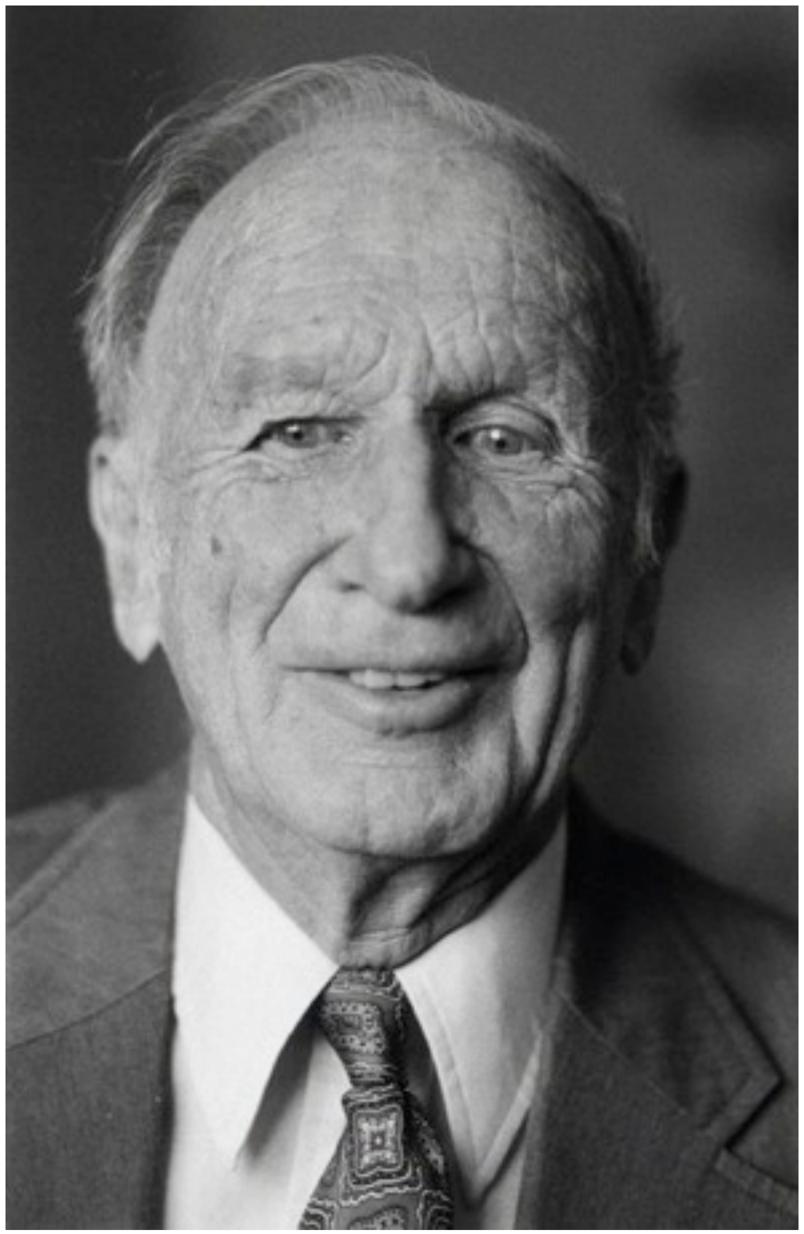
$$\partial_t \rho = \mathcal{L}\rho \equiv -\nabla_X \cdot \rho f$$

Ergodicity implies a unique
invariant measure:

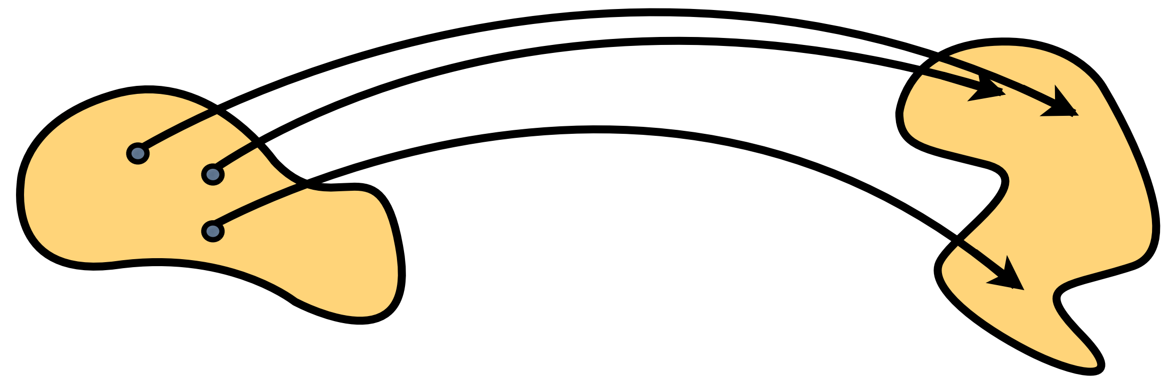
$$\mathcal{L}\tilde{\rho} = 0$$

Almost every solution
samples this measure: $X(t) \sim \tilde{\rho}$

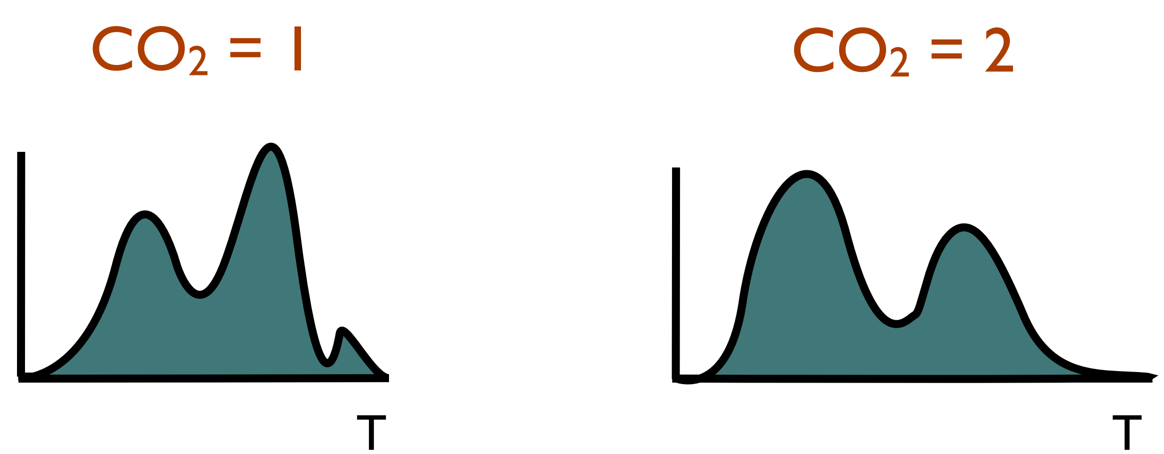
Prediction types (Lorenz)



- Prediction of the first kind: out-of-equilibrium transport of a probability ensemble



- Prediction of the second kind: parameter study using equilibrium sampling



Climate Feedback
the climate change blog

« No more to top? Go for the opposite | Main | Shaping the Kyoto successor »

CURRENT CONTENT

FOR HIGHLIGHTS OF THE LATEST RESEARCH ON CLIMATE CHANGE, VISIT THE

Predictions of climate

Bookmark in Connotea

Posted by Oliver Morton on behalf of Kevin E. Trenberth

Nature Climate Feedback Blog Entry (June 4, 2007)

Kevin Trenberth
Climate Analysis Section
National Center of Atmospheric Research, USA,

Lead Author, IPCC Reports
1995, 2001, 2007.

IPCC currently uses 2nd-kind Projections:

"… the projections are based on model results that provide differences of the future climate relative to that today …

The current projection method works to the extent it does because it utilizes differences from one time to another and the main model bias and systematic errors are thereby subtracted out. This assumes linearity …"

used by IPCC are initialized to the observed state and none of the climate states in the models correspond even remotely to the current observed climate. In particular, the state of the oceans, sea ice, and soil moisture has no relationship to the observed state at any recent time in any of the IPCC models. There is neither an El Niño sequence nor any Pacific Decadal Oscillation that replicates the recent past; yet these are critical modes of variability that affect Pacific rim countries and beyond. The Atlantic Multidecadal Oscillation, that may depend on the thermohaline circulation and thus ocean currents in

IPCC wants to go to 1st-kind Predictions, but one important obstacle is *overcoming numerical bias*:

"… the science is not done because we do not have reliable or regional predictions of climate. But we need them. So the science is just beginning. Beginning, that is, to face up to the challenge of building a climate information system that tracks the current climate and the agents of change, that initializes models and makes predictions, and that provides useful climate information on many time scales regionally and tailored to many sectoral needs…

Of course one can initialize a climate model, but a biased model will immediately drift back to the model climate and the predicted trends will then be wrong. Therefore the problem of overcoming this shortcoming, and facing up to initializing climate models means not only obtaining sufficient reliable observations of all aspects of the climate system, but also overcoming model biases."

- Curse of the Kudzu
- Picture post: 'hottest April ever'
- Costa Rican to become new UN climate chief

RECENT COMMENTS

Out of 1548 total comments, the most recent were:
Vernon on Predictions of climate
Macnerdzcare on Predictions of climate
gary on Predictions of climate

ARCHIVES

- November 2010
- September 2010
- May 2010
- April 2010

However, the science is not done because we do not have reliable or regional predictions of climate. But we need them. Indeed it is an imperative! So the science is just beginning. Beginning, that is, to face up to the challenge of building a climate information system that tracks the current climate and the agents of change, that initializes models and makes predictions, and that provides useful climate information on many time scales regionally and tailored to many sectoral needs.

We will adapt to climate change. The question is whether it will be planned or not? How disruptive and how much loss of life will there be because we did not adequately plan for the climate changes that are already occurring?

Kevin Trenberth
Climate Analysis Section, NCAR

Geometric numerical integration

- Numerical errors not small and random: the discrete flow solves a different problem with its own statistics.
- Geometric integration: exactly preserve symmetries, invariants, group structures. These influence statistics.
- Example: Symplectic methods generate the exact solution of a perturbed Hamiltonian system (phase volume, energy).

Outline

- Part I - Statistical mechanics of geophysical fluids, and numerical methods that sample well.

- Part II - A statistically consistent approach to model reduction.

  - Any truncation is model reduction from infinite to finite d.o.f.
  - Part I - how to truncate such that equilibrium stat. mech. is preserved
  - Part II - accept the truncation, and ask how we can correct statistics

Geophysical fluid dynamics

The atmosphere is well approximated by a fluid that is:

- inviscid ($Re^{-1} = 10^{-6}$ viscosity)
- 2D (10 km vertical vs. 1000-10000 km horizontal scale)
- incompressible (only approximate in 2D)

A particularly simple model is the quasigeostrophic potential vorticity model (QG).

$$\nabla \cdot u(x,t) = 0, \quad u \in R^2, \quad x \in \mathcal{D}$$
$$\frac{dq}{dt} \equiv \frac{\partial q}{dt} + u \cdot \nabla q = 0$$
$$q(x,t) = \nabla \times u(x,t) + h(x)$$

Stream function formulation: $(u = \nabla^{\perp}\psi)$

$$q_t + \nabla^{\perp}\psi \cdot \nabla q = 0, \qquad \Delta\psi = q - h$$

Geophysical fluid dynamics

The QG model is a Hamiltonian PDE with Poisson structure and energy functional

$$\{\mathcal{F}[q], \mathcal{G}[q]\} = \int \frac{\delta \mathcal{F}}{\delta q} \cdot (q_x \partial_y - q_y \partial_x) \frac{\delta \mathcal{G}}{\delta q} \, dx$$

$$\mathcal{H}[q] = -\frac{1}{2} \int \psi(q - h) \, dx$$

The equations of motion are generated by the Hamiltonian in the Poisson bracket

$$q_t = \{q, \mathcal{H}[q]\}$$

Infinite family of Casimir functionals $\{\cdot, \mathcal{C}[q]\} = 0$

i.e. the moments of vorticity:

$$\mathcal{C}(f)[q] = \int f(q) \, dx \qquad\qquad \mathcal{C}_k[q] = \int q^k \, dx$$

Geophysical fluid dynamics

The Casimirs

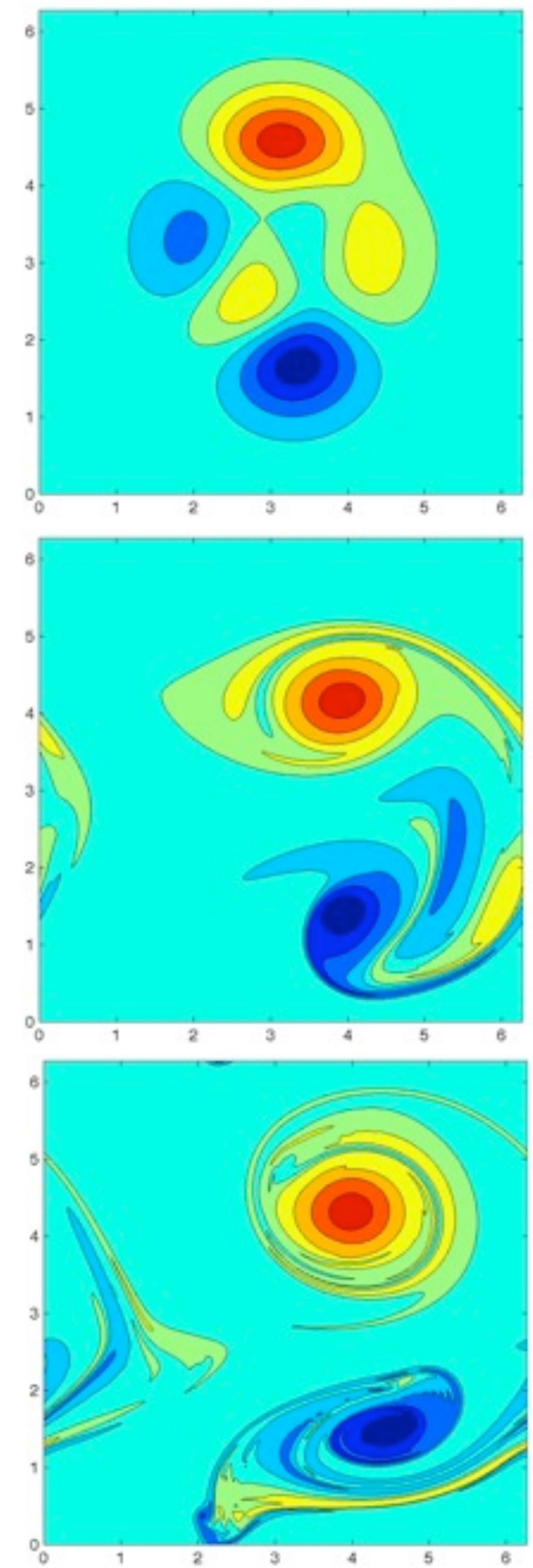
$$\mathcal{C}(f)[q] = \int f(q)\,dx \qquad \mathcal{C}_k[q] = \int q^k\,dx$$

are a consequence of **area preservation:**

$$\frac{\partial \Gamma}{\partial t} = 0, \qquad \Gamma(\sigma, t) = \mathrm{meas}\{x \in \mathcal{D} \,|\, q(x,t) \leq \sigma\}$$

$$\gamma(\sigma) = \frac{1}{|\mathcal{D}|}\frac{d\Gamma}{d\sigma}$$ “area of vortex patch”

Each “patch” of vorticity evolves at constant area under the energy-preserving flow



Equilibrium statistical mechanics of fluids*

Invariant measure: a Young measure on the space of vorticity fields

$$p(x,\sigma) = \mathrm{Prob}\,\{q(x) \in [\sigma, \sigma + d\sigma]\}$$

- $\displaystyle\int p(x,\sigma)\,d\sigma = 1, \quad \forall x$
- $\displaystyle\int p(x,\sigma)\,dx = \gamma(\sigma), \quad \text{area preservation}$

Mean field assumption: distinct points in the domain are coupled only via a *mean field*

$$\langle q\rangle = \int \sigma p(x,\sigma)\,d\sigma, \quad \Delta\langle\psi\rangle = \langle q\rangle - h$$

Miller-Robert-Sommeria measure:

$$p(x,\sigma) \propto e^{-\beta\langle\psi\rangle\sigma - \alpha(\sigma)} \quad \left(= e^{-\beta\langle\psi\rangle\sigma}\Pi(\sigma)\right)$$

Mean field relation:

$$\langle q\rangle = g(\langle\psi\rangle), \quad \forall x$$

* Kraichnan 75, Salmon et al. 76, Carnevale & Frederiksen 87, Miller 91, Miller, Weichman & Cross 92, Robert 91, Robert & Sommeria 91, Ellis, Haven & Turkington 02, *Majda & Wang 2006*

Numerical discretizations

If a numerical method is to have any hope of reproducing even the mean equilibrium statistics it should conserve:

- volume (phase space sense: Liouville)
- energy (quadratic)
- vorticity + moments

- Galerkin methods (FEM and spectral) & Arakawa FD schemes conserve volume, energy and enstrophy (C_2 quadratic moment of q)
- A method of McLachlan ('99) preserves all Casimirs by permuting the discrete vorticity field (but not energy!)
- Sine-bracket truncation (Zeitlin '91) conserves volume, energy, and N Casimirs on an NxN grid
- Hamiltonian Particle-Mesh method

Hamiltonian Particle-Mesh Method*

A set of K discrete particles with lumped vorticity (circulation)

$$\{X_k(t) \in \mathbf{R}^2,\ Q_k(t) = Q_k(0);\ k = 0, \ldots, K\}$$

Coarse-grain vorticity on a uniform grid obtained by summing the overlapping particle distributions

$$q_i = \sum_k Q_k \phi(x_i - X_k(t)), \quad \Delta_{ij}\Psi_j = q_i - h_i$$

Hamiltonian dynamics with $H(X_1, \ldots X_K) = -\frac{1}{2}\sum_i \Psi_i(q_i - h_i)$

$$Q_k \dot{X}_k = J\tfrac{\partial H}{\partial X_k}, \quad J = \left[\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right]$$

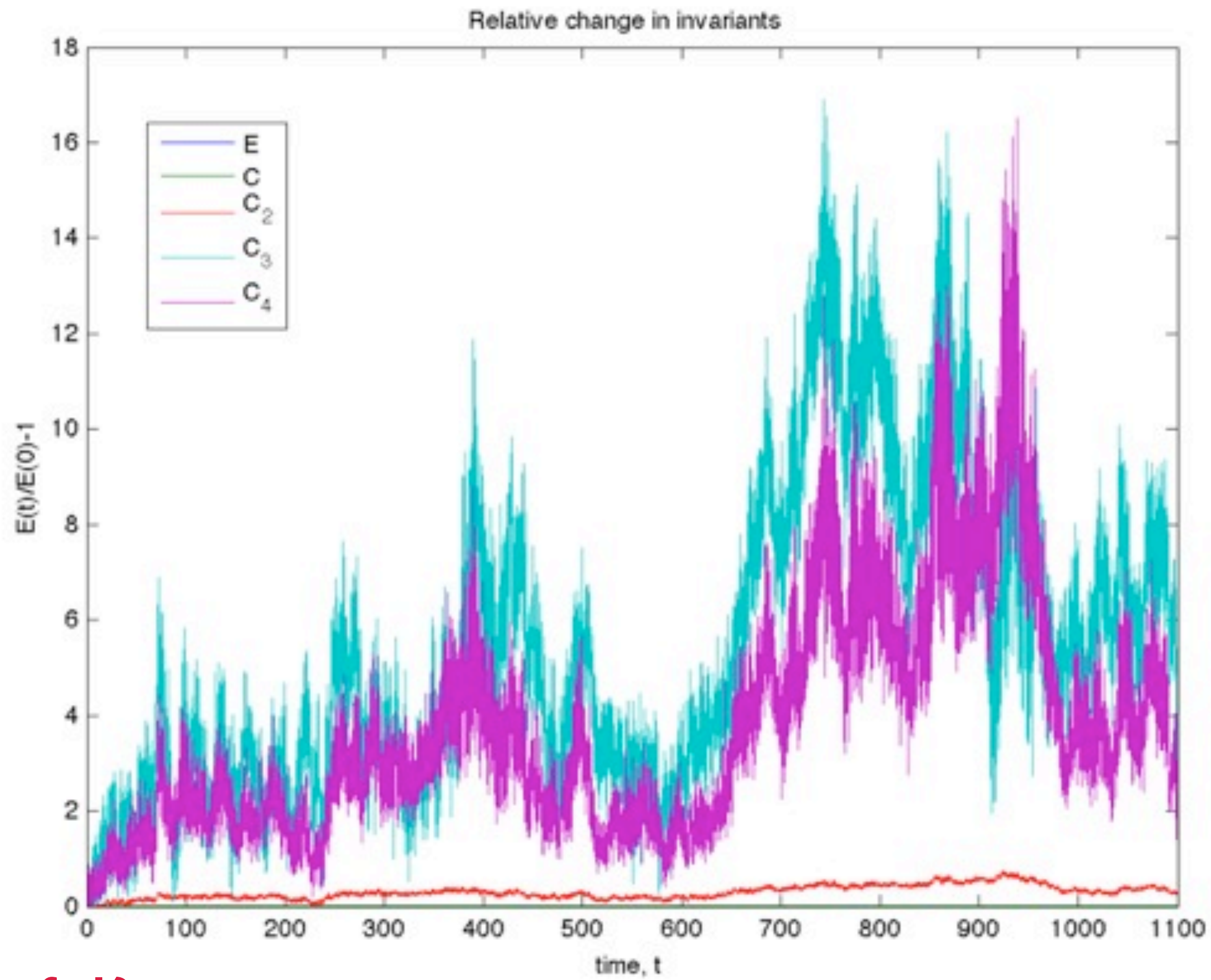
Time integration with a symplectic integrator (implicit midpoint)

* Developed in the context of SWEs: [F., Gottwald & Reich 02, F. & Reich '03, Cotter & Reich 03 04 06, Cotter, F. & Reich 04]

Coarse-grain PV conservation

Potential vorticity trivially conserved on particles, hence all Casimirs.

On the other hand the grid-based vorticity moments typically exhibit significant drift:



The only coarse-grain conserved quantities are the energy

$$H = -\frac{1}{2}\sum_i \Psi_i (q_i - h_i)$$

and circulation

$$C_1 = \sum_i q_i$$

Is the PV/area conservation meaningful?

Numerical results

- Problem setup of Abramov & Majda (2003)

$$h(x,y) = 0.2\cos x + 0.4\cos 2x, \quad E = 7, \quad C_2 = 20$$

- Computer time average over an interval $[10^3, T]$, for $T = 10^6$

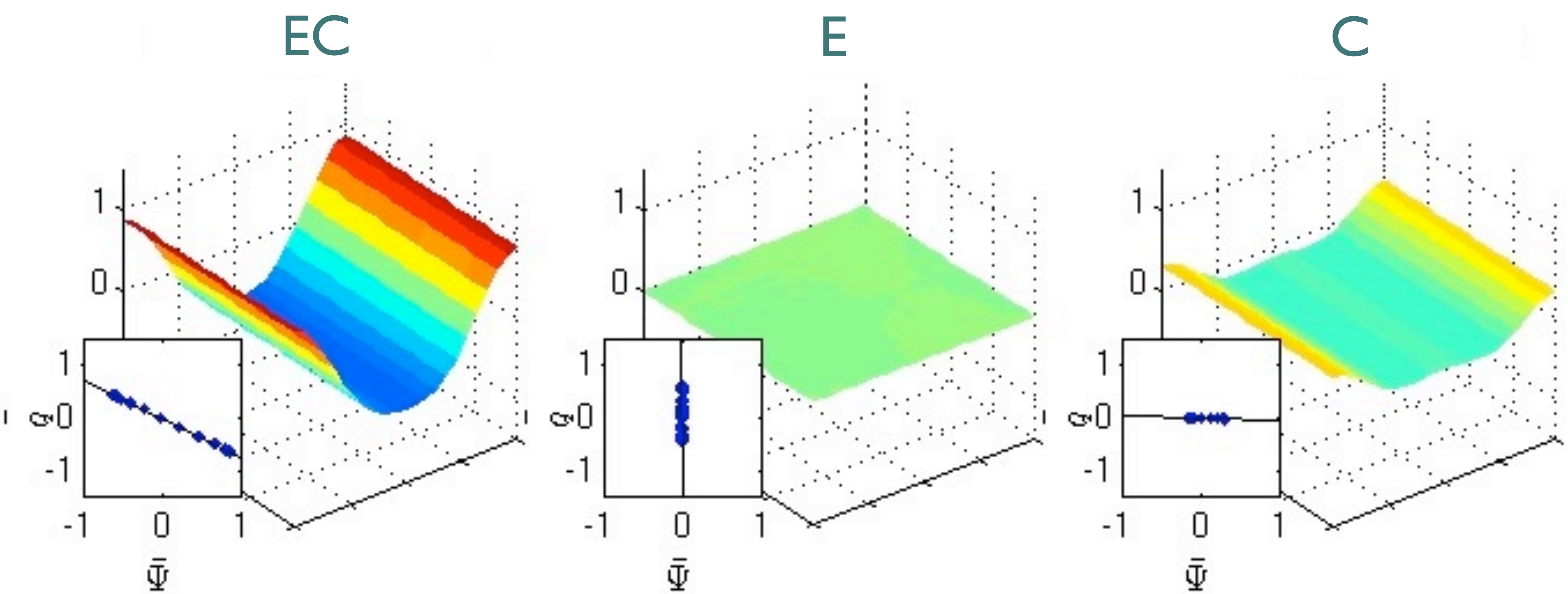
$$\bar{q}_T = \frac{1}{N_T}\sum_n q^n, \quad \bar{\psi}_T = \frac{1}{N_T}\sum_n \psi^n, \quad N_T \Delta t = T - 10^3$$

- Assuming sufficient ergodicity,

$$\lim_{T\to\infty} \bar{q}_T = \langle q \rangle, \quad \lim_{T\to\infty} \bar{\psi}_T = \langle \psi \rangle$$

Mean fields for Arakawa '66 schemes

- Comparison of classical schemes by Arakawa '66 conserving discrete approximations of energy (E), enstrophy (C), or both (EC). $T = 10^6$



- Only quadratic invariants conserved ⇒ Gaussian statistics
- Linear mean-field relations ⇒ 1D flow $\langle q \rangle = g(\langle \psi \rangle), \quad \forall x$
- Very distinct statistics!

(Dubinkina & Frank 2007)

Sine-bracket Poisson integrator

- Abramov & Majda (2003) used Zeitlin's (1991) Poisson truncation of the ideal fluid, which preserves N+1 integrals on an NxN grid, to study the statistical relevance of the higher moments of vorticity
- A nonzero third moment C_3 is "statistically relevant"
- Experimental setup suggests that higher moments could be irrelevant

$$\langle q \rangle = g(\langle \psi \rangle), \quad \forall x$$

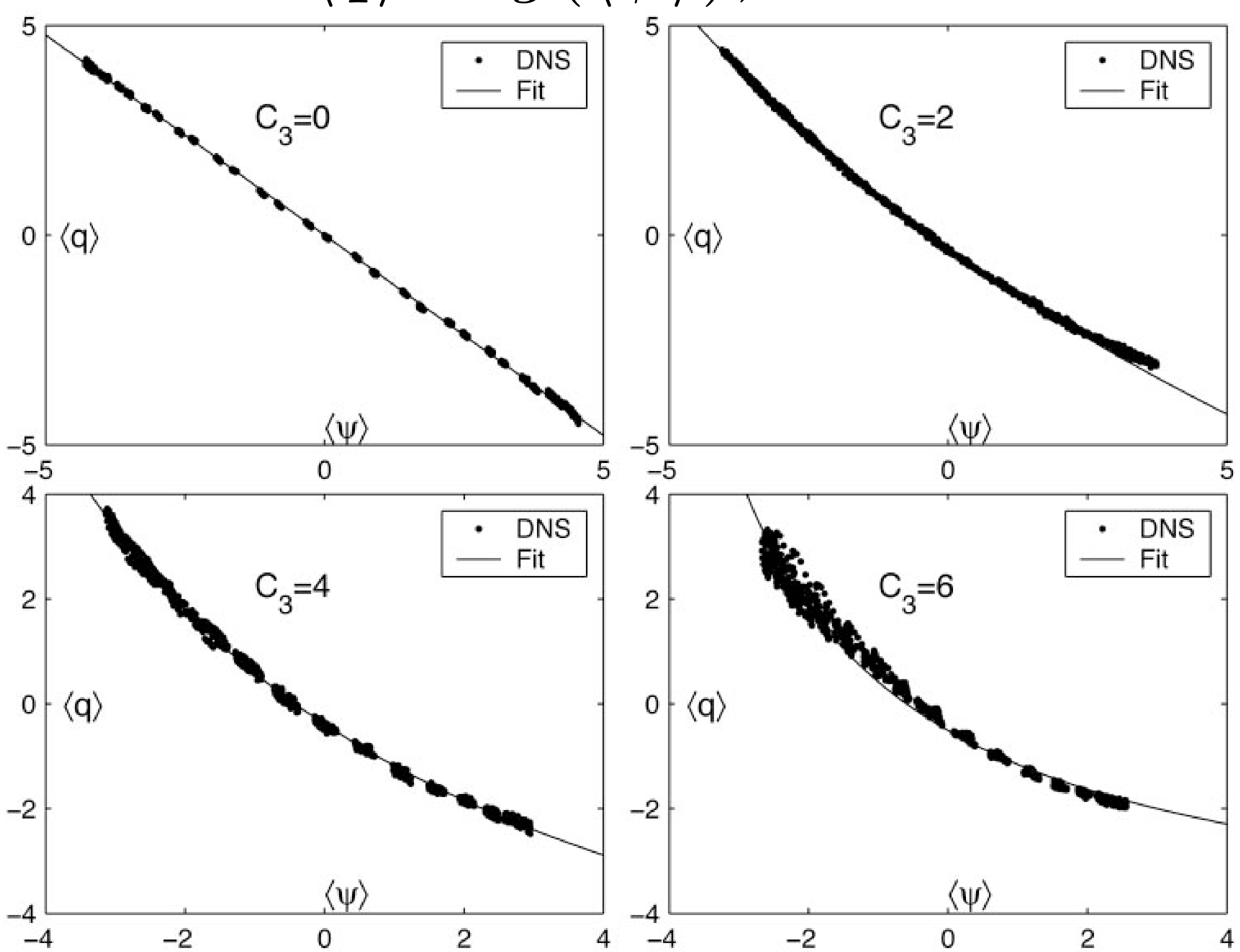


Fig. 3. The scatter plots $\bar{q}$ vs. $\bar{\psi}$ for the 23 × 23 sine-bracket truncation, layered topography, $\hat{C}_3 = 0, 2, 4, 6$.

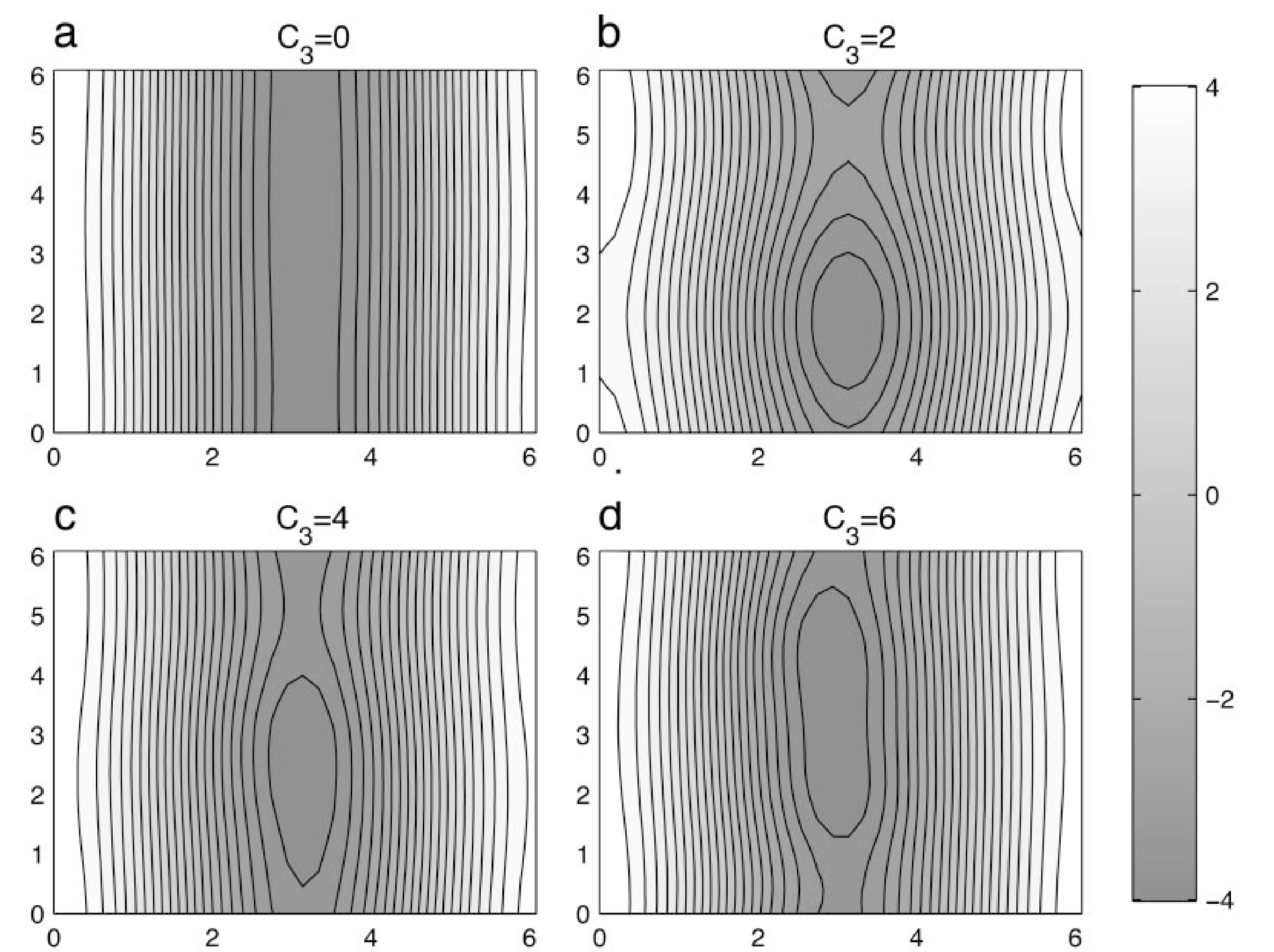


Fig. 4. The contour plots of the mean stream function, 23 × 23 sine-bracket truncation, layered topography, $\hat{C}_3 = 0, 2, 4, 6$.

Skew and Flat distributions - HPM

$$\langle q \rangle = g(\langle \psi \rangle), \quad \forall x$$

Draw the vorticity from

$$Q_k \sim \Pi(\sigma)$$

with skewness

$$\gamma = \frac{C_3}{C_2^{3/2}}$$

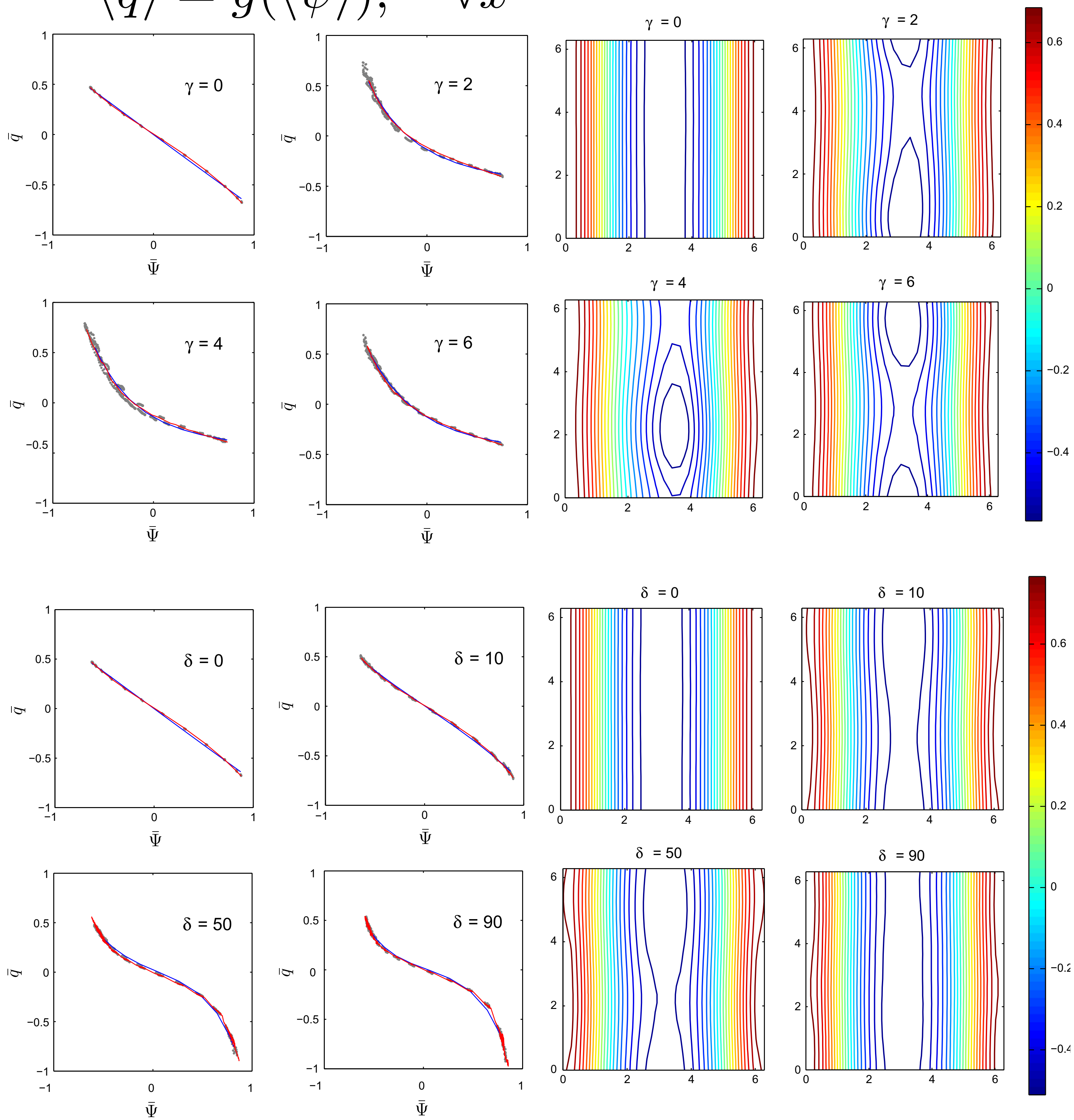
or excess kurtosis (no skew.)

$$\delta = \frac{C_4}{C_2^2} - 3$$

We derived and compare with Lagrangian and Eulerian analytical models.

Comparison with time averaged loci. T = 10^4.

Fourth moment C_4 is statistically relevant, for large δ.



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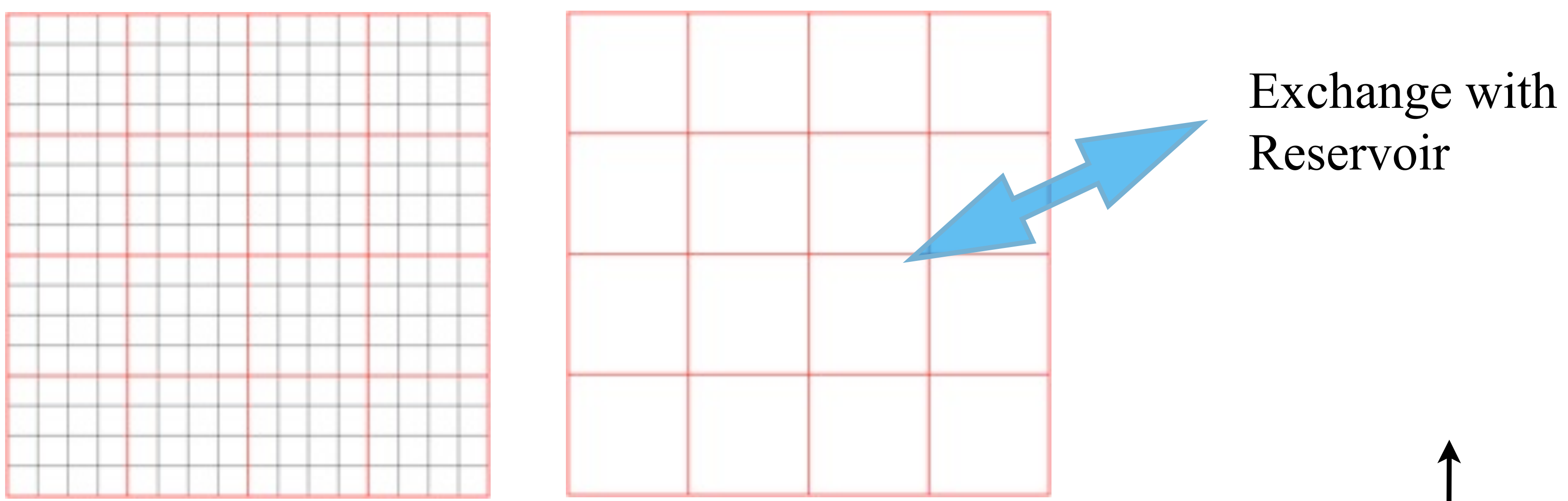
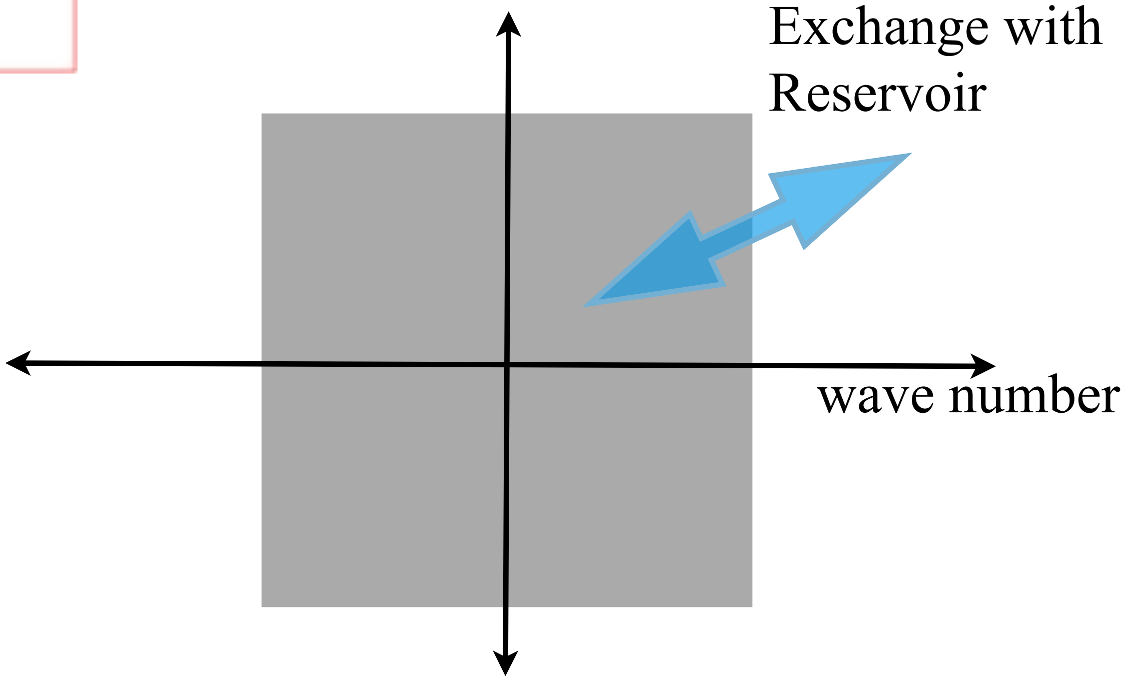
Reservoir of unresolved dynamics

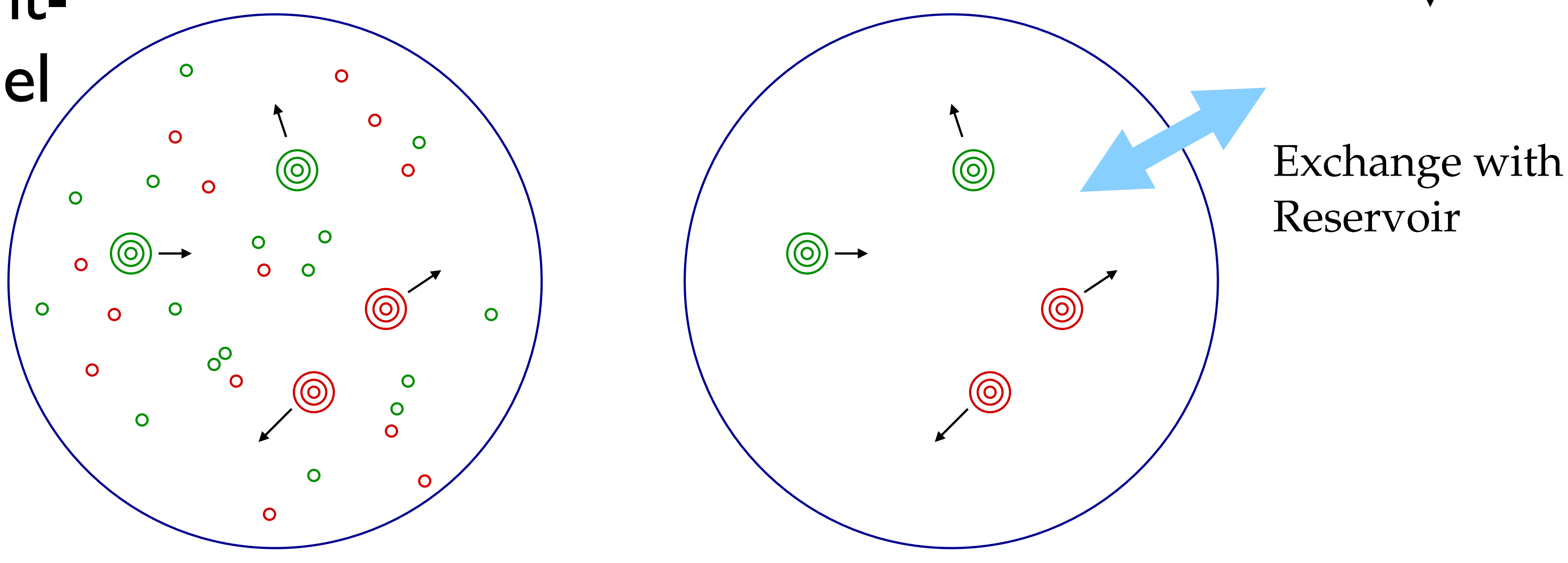
Grid-based model



Truncated spectral model

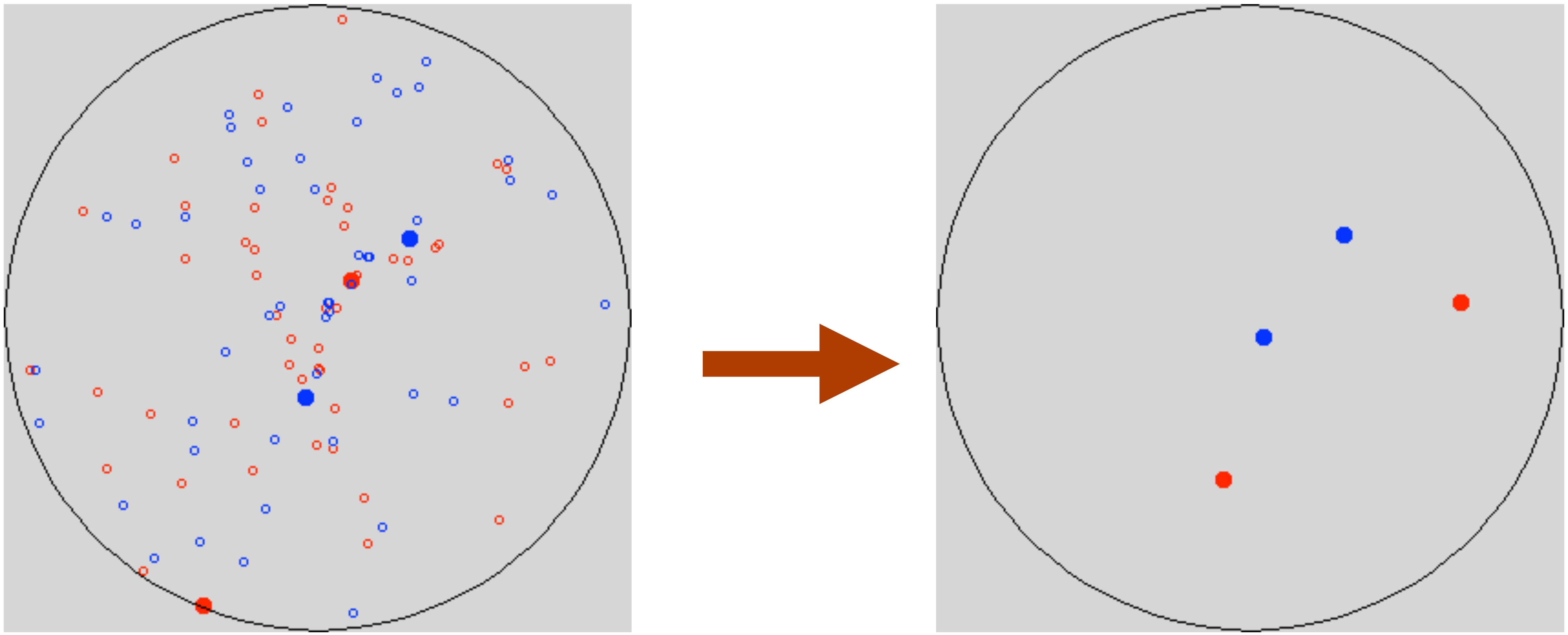


Particle/point-vortex model



Model reduction with thermostats

specific model: point vortex system



- Singular point vorticity field
- Heterogeneous: +/- orientation, strong/weak
- Reduce to only strong vortices, preserve their statistics
- Weak vortices → reservoir (canonical ensemble)

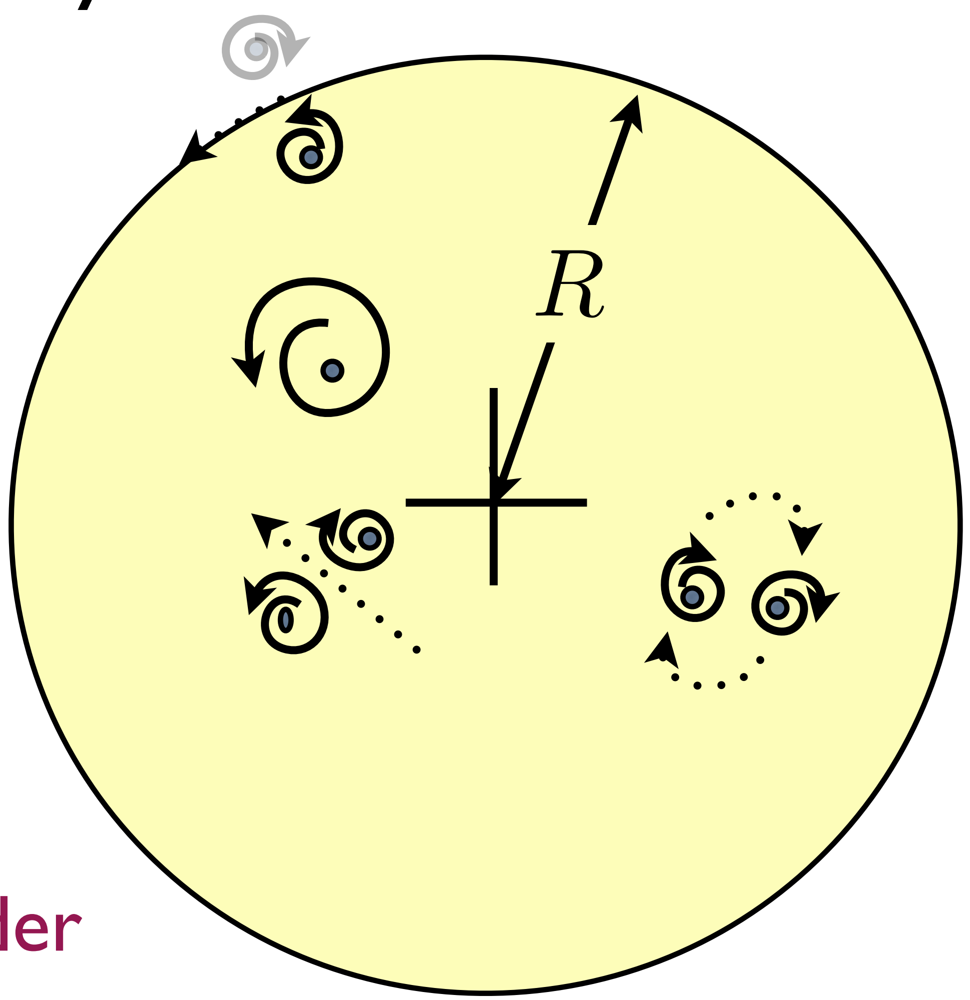
(Dubinkina, Frank & Leimkuhler 2010)

Point Vortex Model

A point vortex model for *N* vortices in a cylinder

$$H = -\frac{1}{4\pi}\sum_{i<j}\Gamma_i\Gamma_j \ln(|r_i - r_j|^2)$$
$$+ \; boundary\ terms$$

$$\Gamma_i \dot{r}_i = J\nabla_{r_i} H$$



$$q(x,t) = \sum_i \Gamma_i \delta(x - r_i(t))$$
$$\Delta\psi(x,t) = q(x,t)$$
$$u(x,t) = \nabla^{\perp}\psi(x,t)$$

H unbounded under collisions

Onsager, 1949 "Statistical Hydrodynamics"

Oliver Bühler, 2002 canonical theory & numerics

Statistical Mechanics

Onsager, 1949 "Statistical Hydrodynamics"

Unbounded energy range, bounded phase space gives rise to positive and negative temperature states.

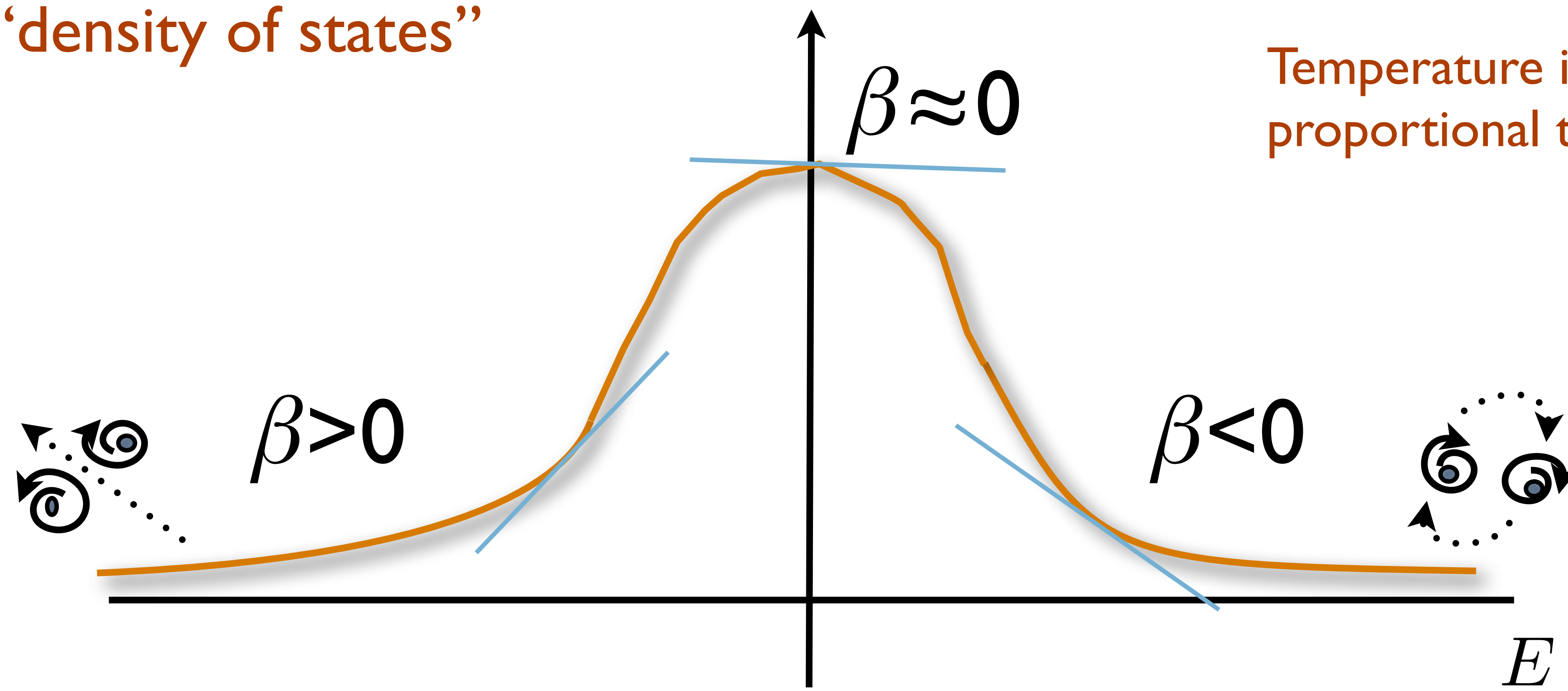
$$H = -\frac{1}{4\pi}\sum_{i<j}\Gamma_i\Gamma_j\ln(|r_i - r_j|^2)$$

Entropy $\quad S(E) = \ln\Omega$

Inverse Stat. Temp. $\quad \beta = S'(E)$

$$\Omega(E) = \mathrm{vol}\{X \mid H(X) \in [E, E+dE)\}$$

"density of states"



Temperature inversely proportional to slope.

β	E	Coll.
$\beta > 0$	E<0	+/-
$\beta < 0$	E>0	++ - -

Onsager (1949) proposed for a heterogeneous point vortex flow: strong vortices cluster:

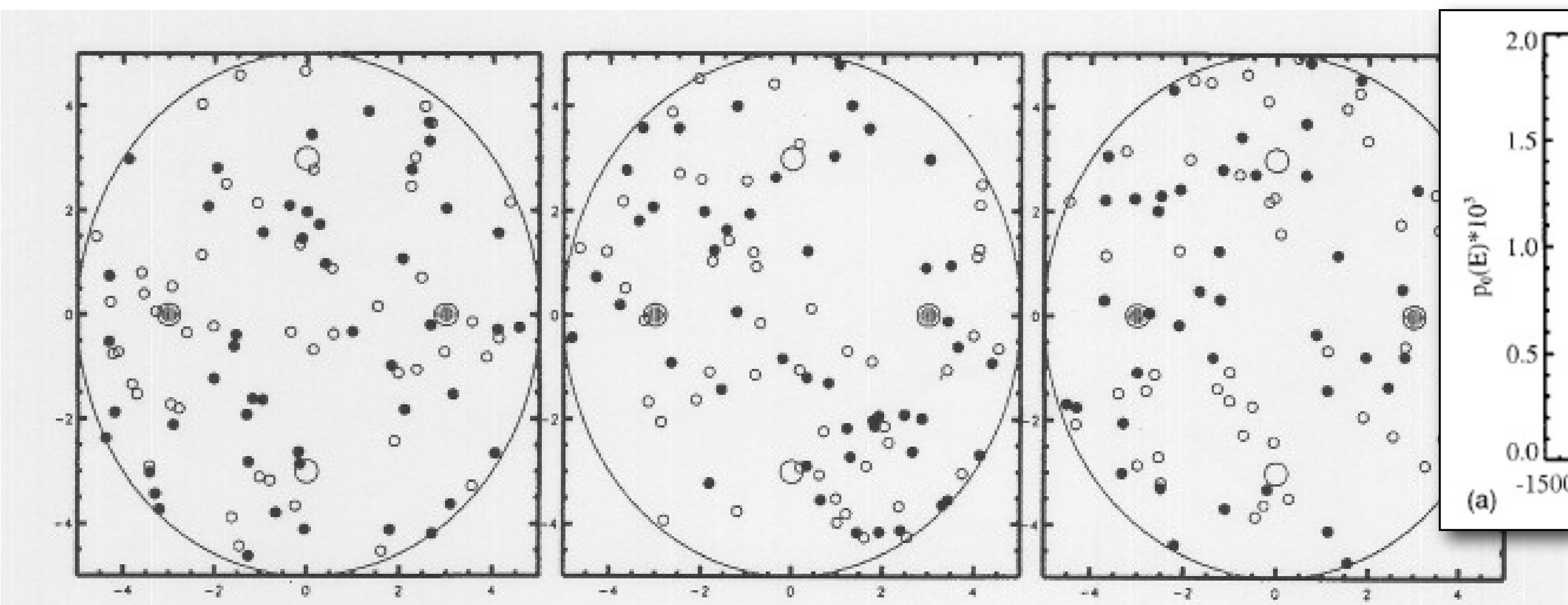
Positive temperature: opposite signed,

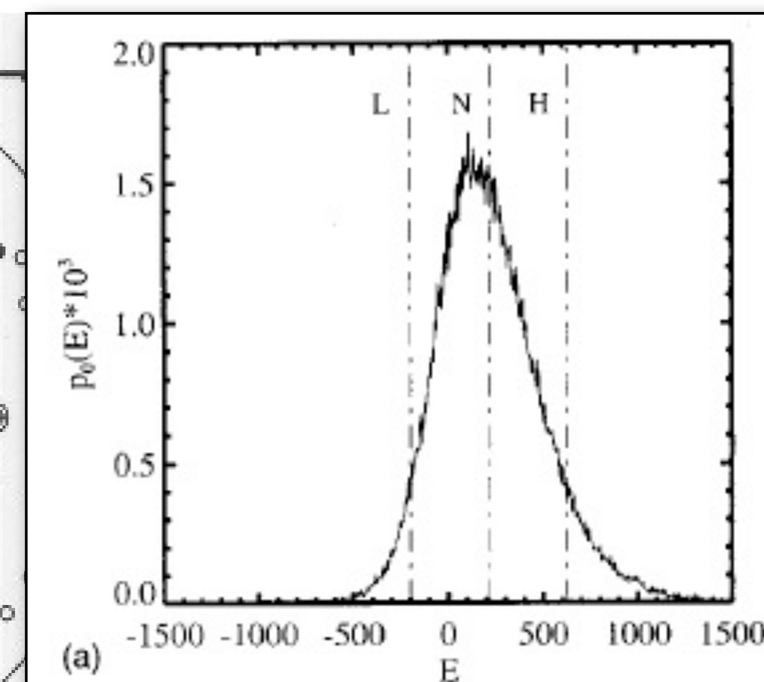
Negative temperature: like-signed,

weak ones behave randomly

Simulations by Oliver Bühler (2002)

4 strong, 96 weak vortices, sign indefinite, 0 ang. mom.





$\beta>0$ $\beta\approx0$ $\beta<0$

Canonical ensemble

The canonical ensemble is the invariant (Gibbs) measure describing a system in thermal equilibrium with an infinite reservoir (heat bath):

$$\rho(X) \propto \exp(-\beta H(X))$$

To compare with Bühler's simulations which were done with a modest number (96) of weak vortices, we must include an additional term in the measure:

$$\rho(X) \propto \exp(-\beta H(X) - \gamma H(X)^2)$$

Parameters depend on the full model:

$$\beta = -\frac{E}{\sigma_B^2} \qquad \gamma = \frac{1}{2\sigma_B^2} = -\frac{\beta}{2E}$$

Canonical sampling

Volume and energy preserving model

$$\dot{X} = f(X), \qquad \nabla \cdot f = 0, \qquad f \cdot \nabla H = 0$$

samples (if ergodic) the microcanonical ensemble:

$$\rho(X) \propto \delta(H(X) - H_0)$$

For a system in thermal equilibrium with a reservoir at temperature β^{-1}, energy is exchanged. Finite reservoir ensemble:

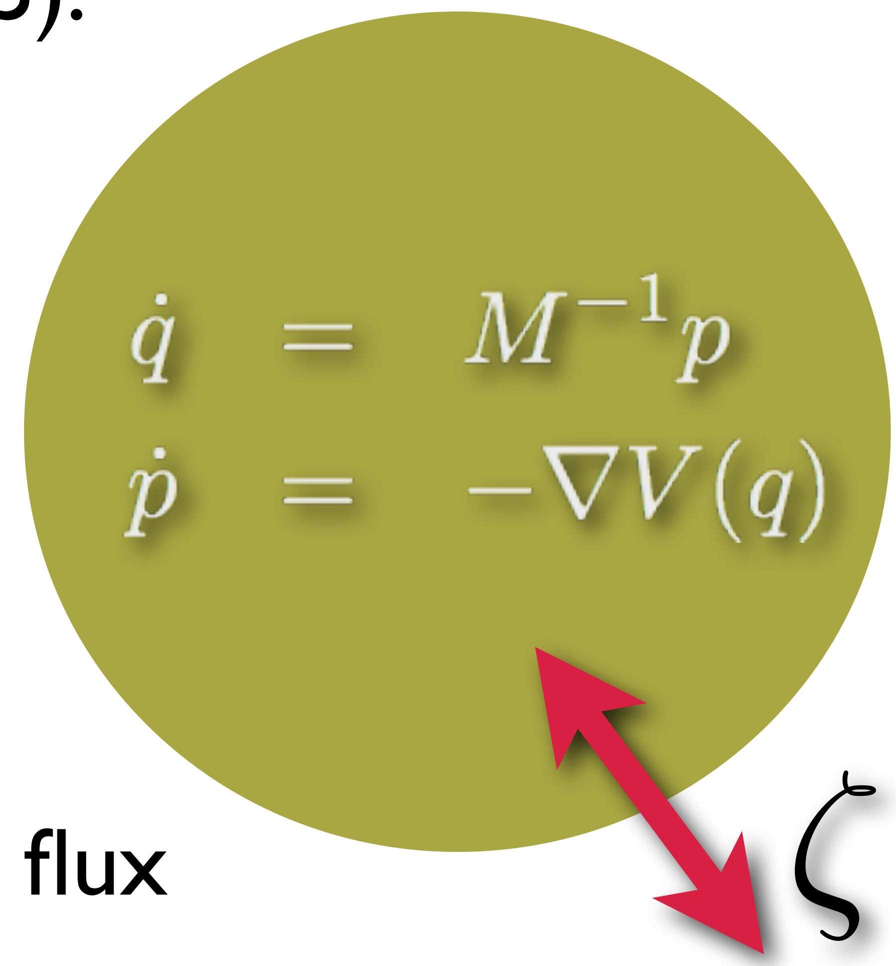
$$\rho(X) \propto \exp(-\beta H(X) - \gamma H(X)^2)$$

Need a mechanism to perturb the dynamics.

Nosé thermostat (molecular dynamics)

Idea of Nosé (1984), Hoover(1985):

$$\begin{aligned} \dot{q} &= M^{-1}p \\ \dot{p} &= -\nabla V(q) - \zeta\, p \\ \dot{\zeta} &= \beta\, p \cdot M^{-1}p - K \end{aligned}$$



Total energy of subsystem

$$H = \tfrac{1}{2}p \cdot M^{-1}p + V(q)$$

New variable controls the energy flux

$$\frac{dH}{dt} = -\zeta p \cdot M^{-1}p$$

Alternative to Langevin dynamics:

$$\dot{X} = J\nabla H(X) - \frac{\beta}{2}\Sigma\Sigma^T\nabla H + \Sigma\dot{W}$$

Generalized thermostats

Augmented system:

$$\begin{aligned}\dot{X} &= f(X) + \zeta g(X) \\ \dot{\zeta} &= h(X)\end{aligned}$$

Desired distribution:

$$\rho(X) \propto e^{F(H(X))}$$

Require the product distribution

$$\tilde{\rho}(X,\zeta) \propto e^{F(H(X))} e^{-\frac{\alpha}{2}\zeta^2}$$

to be stationary under the Liouville flow

$$\begin{aligned}\mathcal{L}^*\tilde{\rho} = 0 &= \nabla_X \cdot \tilde{\rho}(f + \zeta g) + \partial_\zeta \tilde{\rho} h \\ &= \zeta \nabla_X \cdot \tilde{\rho} g + h \partial_\zeta \tilde{\rho} \\ &= \tilde{\rho}\left[\zeta \nabla_X \cdot g + \zeta F'(H) g \cdot \nabla_X H - \alpha \zeta h\right] \\ h(X) &= \alpha^{-1}\left[\nabla_X \cdot g + F'(H) g \cdot \nabla_X H\right]\end{aligned}$$

Ergodicity

We add noise and dissipation to the thermostat variable only

$$\begin{aligned}\dot{X} &= f(X) + \zeta g(X) \\ \dot{\zeta} &= h(X) - \zeta + \sqrt{2/\alpha}\,\dot{w}\end{aligned}$$

For ergodicity we also need (Hörmander condition)

$$\mathbb{R}^d \subset \mathrm{span}\{f, g, [f,g], [f,[f,g]], [g,[f,g]], \ldots\}$$

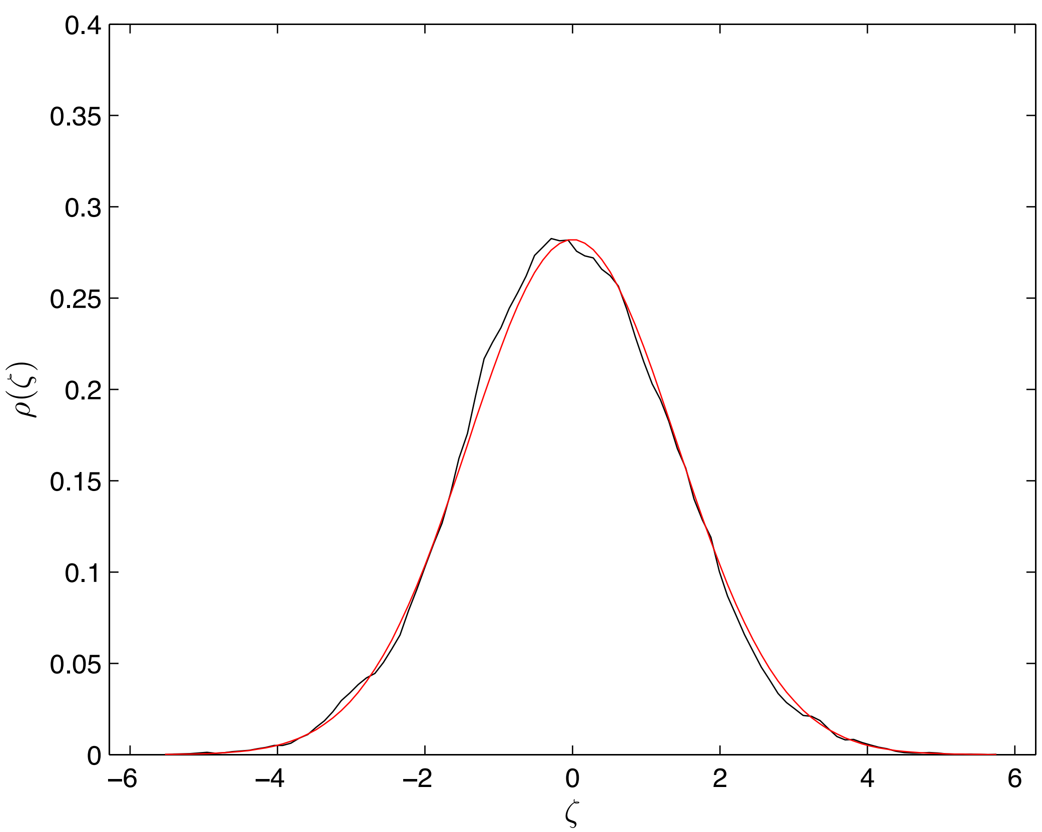
Experimental parameters

$\beta \in \{-0.006, -0.00055, 0.01\}$ $\quad\quad \gamma = -\frac{\beta}{2E_0}, \quad E_0 \in \{628, 221, -197\}$

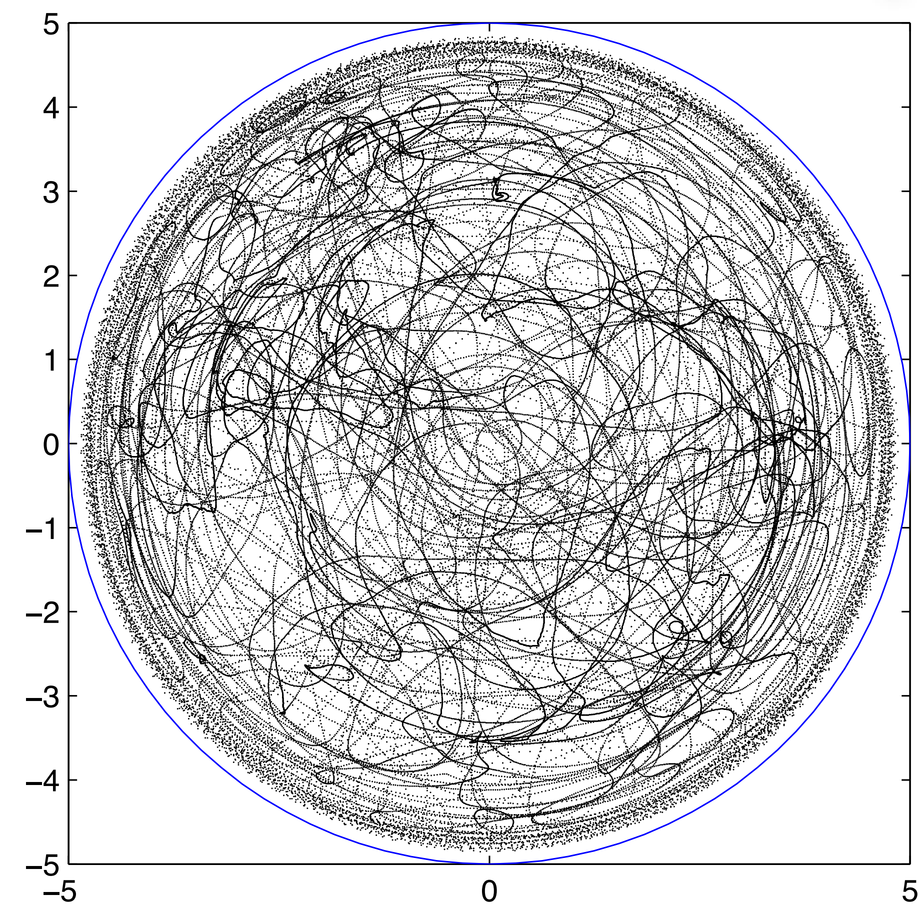
$\alpha = 0.5, \quad \sigma = \sqrt{0.4}$

$t \in [1500, 12000]$

$x_1(t)$



ζ is Gaussian



$t \in [0, 1000] \quad\quad \beta = -0.00055$

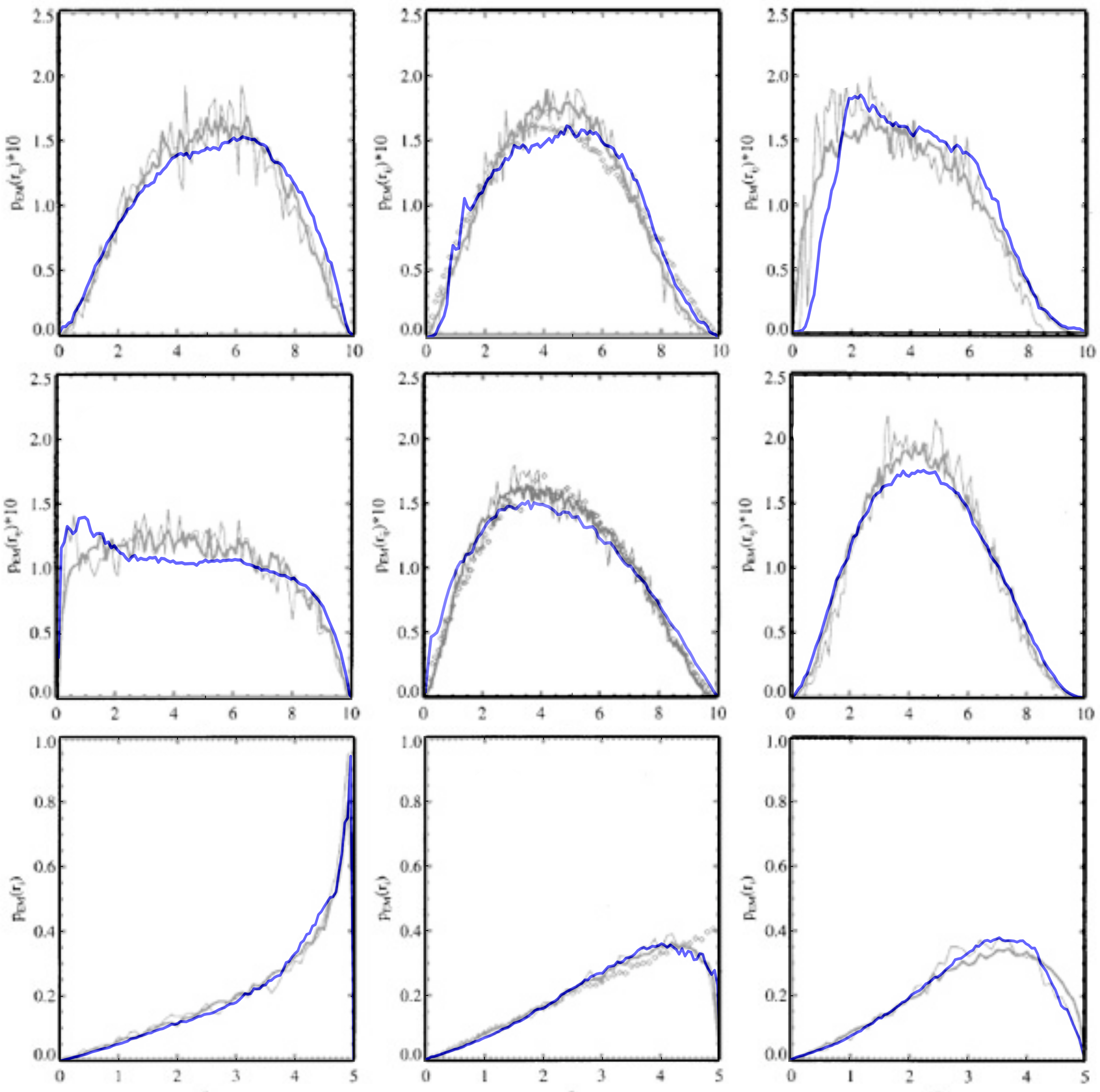
Statistics of strong vortices

β>0 β≈0 β<0

$|x_i - x_j|_{\pm\pm}$

$|x_i - x_j|_{\pm\mp}$

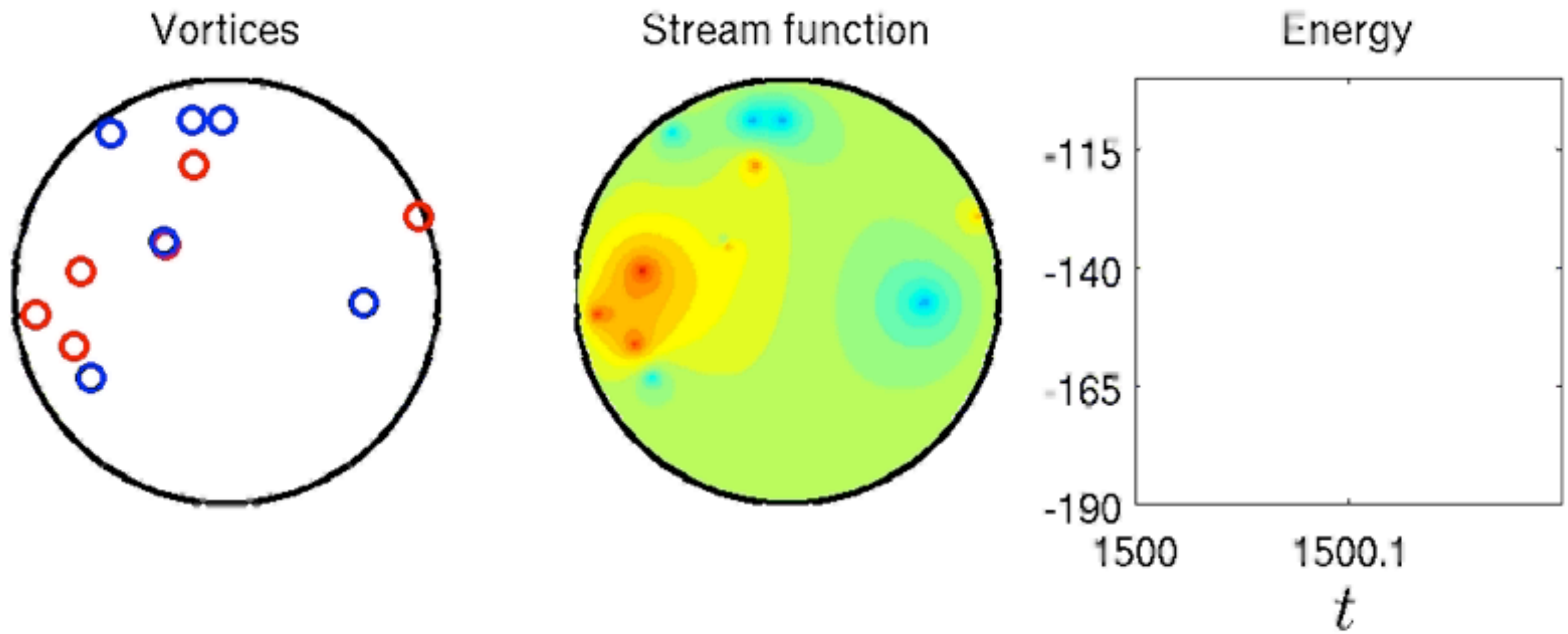
$|x_i|$



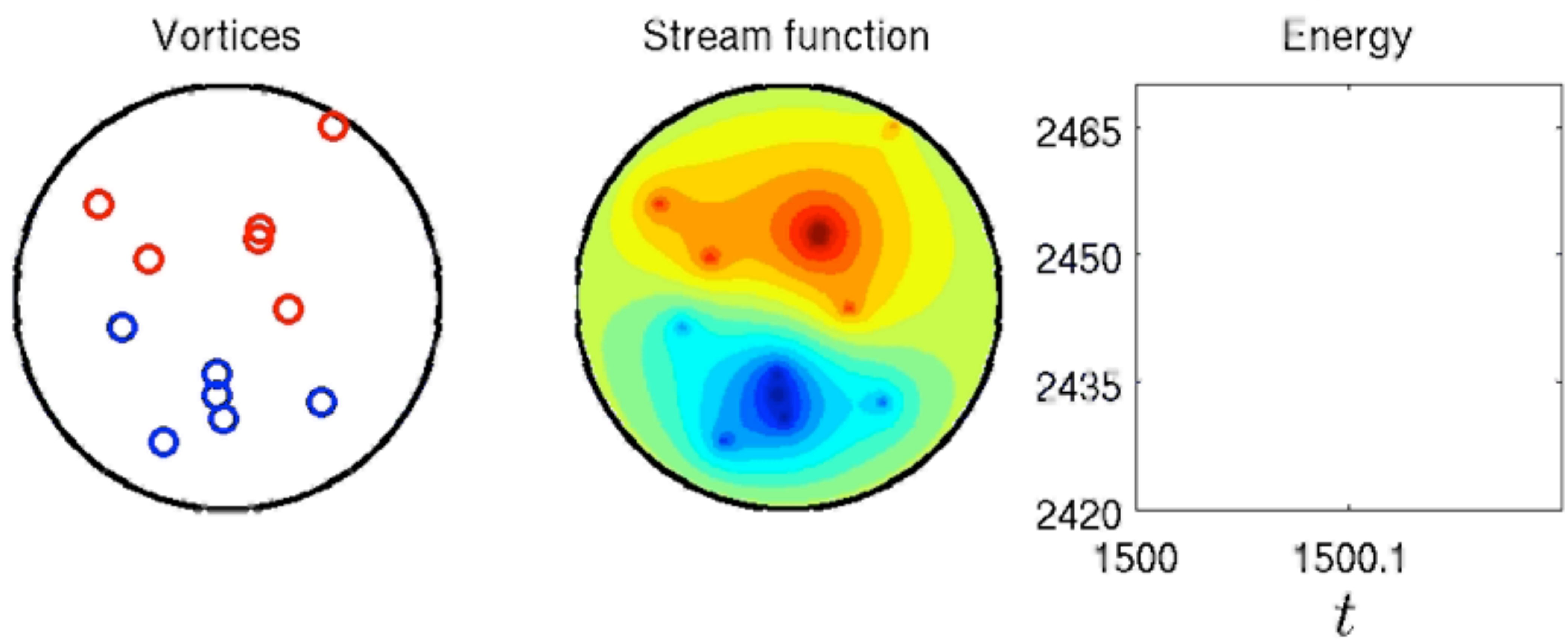
β	E	Coll.
β >0	E<0	+/-
β <0	E>0	++ - -

Vortex clustering, N=12

$\beta = 0.01$



$\beta = -0.006$



Summary

- Numerical bias is an obstacle to accurate statistical prediction of the first and second kinds.
- Numerical schemes should *minimally* conserve phase-space volume and energy.
- For ideal fluids, vorticity conservation is significant. Standard methods limited to Gaussian statistics. Lagrangian methods offer most flexibility here.
- Approach to model reduction:
  - *Start with a high resolution discretization*
  - *Partition into resolved dynamics + 'reservoir'*
  - *Derive canonical ensemble for the resolved variables*
  - *Apply thermostat to model energy exchange with reservoir*

Thank you for your attention.

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