A thermostat model for unresolved dynamics

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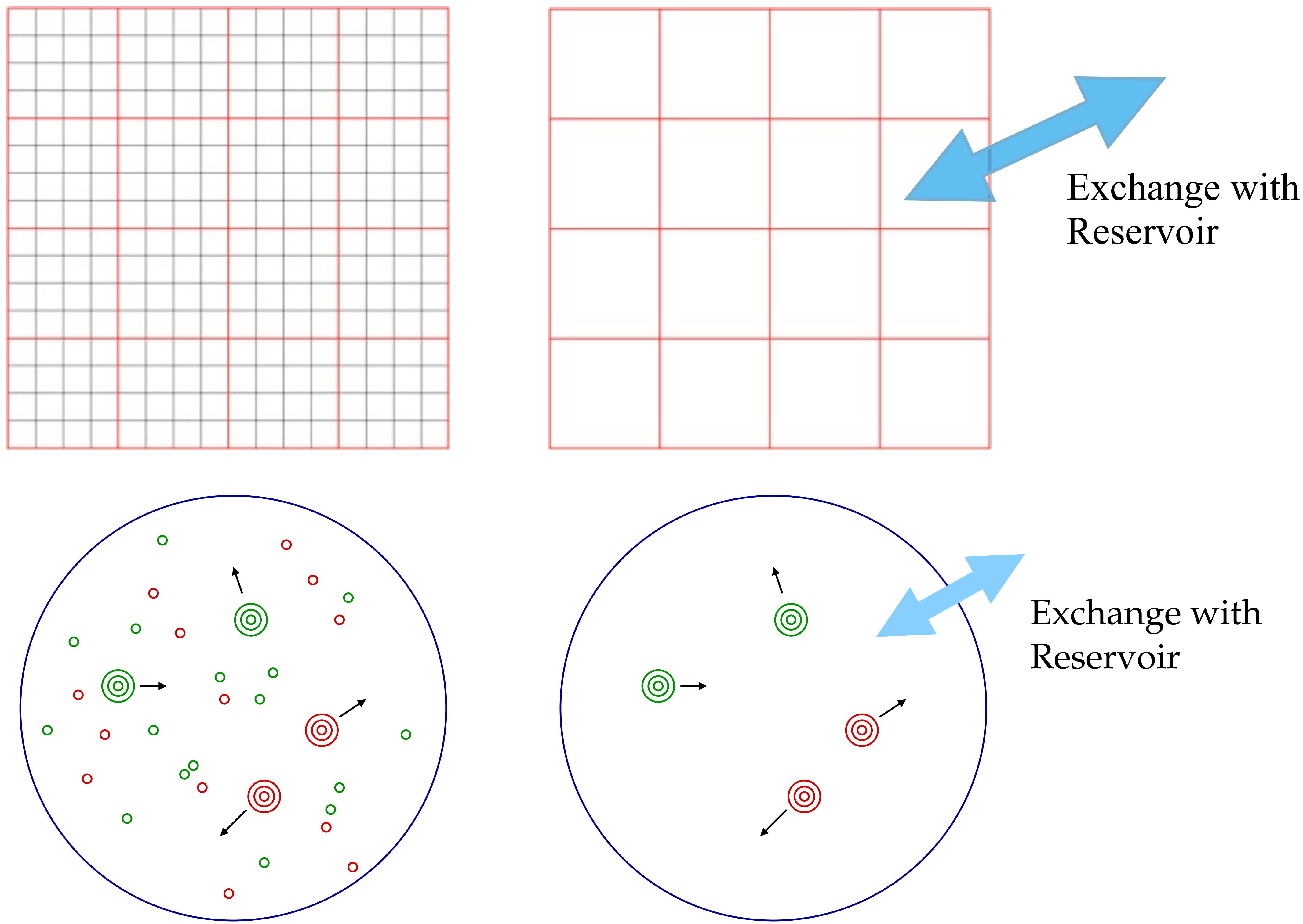
Reservoir of unresolved dynamics

Grid-based model

Particle/point-vortex model



Canonical sampling

Our models are described by Hamiltonian systems

$$\dot{X} = J\nabla H(X)$$

This can be integrated with a symplectic integrator and the energy will be well conserved.

The system samples (≈) 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. Canonical ensemble:

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

Need a mechanism to perturb the dynamics

Interlude:
Mean fields for discretizations

Equilibrium Statistical Mechanics of Discretizations

QG potential vorticity model - incompressible flow over topography

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

Hamiltonian PDE with Poisson structure and energy functional

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

Family of Casimirs

$$\mathcal{C}_f[q] = \int f(q)\, dx \qquad \mathcal{C}_r[q] = \int q^r\, dx \qquad \mathcal{Z} \equiv C_2$$

Area preservation

$$\frac{\partial G}{\partial t} = 0, \qquad G(\sigma, t) = \text{meas}\{x \in \Omega \,|\, q(x,t) \le \sigma\}$$

Equilibrium statistical theories for ideal fluids

A lot* of work has been done on determining the equilibrium distribution for 2D ideal fluids. The various theories differ in their treatment of vorticity conservation laws.

The fine scale vorticity field is modelled by a probability distribution

$$p(x, \sigma) = \text{probability of observing PV value near } \sigma \text{ at } x$$

The coarse-grain, or mean vorticity field is the ensemble average

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

The mean fields are functionally related (steady states)

$$\langle q \rangle = F(\langle \psi \rangle)$$

* 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*

Mean field predictions

Ignoring PV altogether, E conservation leads to a mean field prediction

$$\langle \psi \rangle \equiv 0$$

Energy-enstrophy theory (E-Z) yields a linear mean field relation

$$\langle q \rangle = \mu \langle \psi \rangle$$

Robert/Miller theory enforces conservation of PV level set 'area':

$$\int p(x,\sigma)\, dx = g(\sigma), \quad p(x,\sigma) \propto e^{-\beta\langle\psi\rangle\sigma - \mu(\sigma)}$$

(microcanonical)

Ellis, Haven & Turkington enforce only energy and circulation, but include a prior distribution on fine scale vorticity (canonical)

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

Mean fields for discretizations

- Problem setup of Abramov & Majda (2003)

$$L = 2\pi, \quad M = 22, \quad h(x,y) = 0.2\cos x + 0.4\cos 2x, \quad E_M = 7, \quad Z_M = 20$$

- Instead of ensemble averages, we look at the time average over an interval $[10^3, T]$ for $T = 10^6$

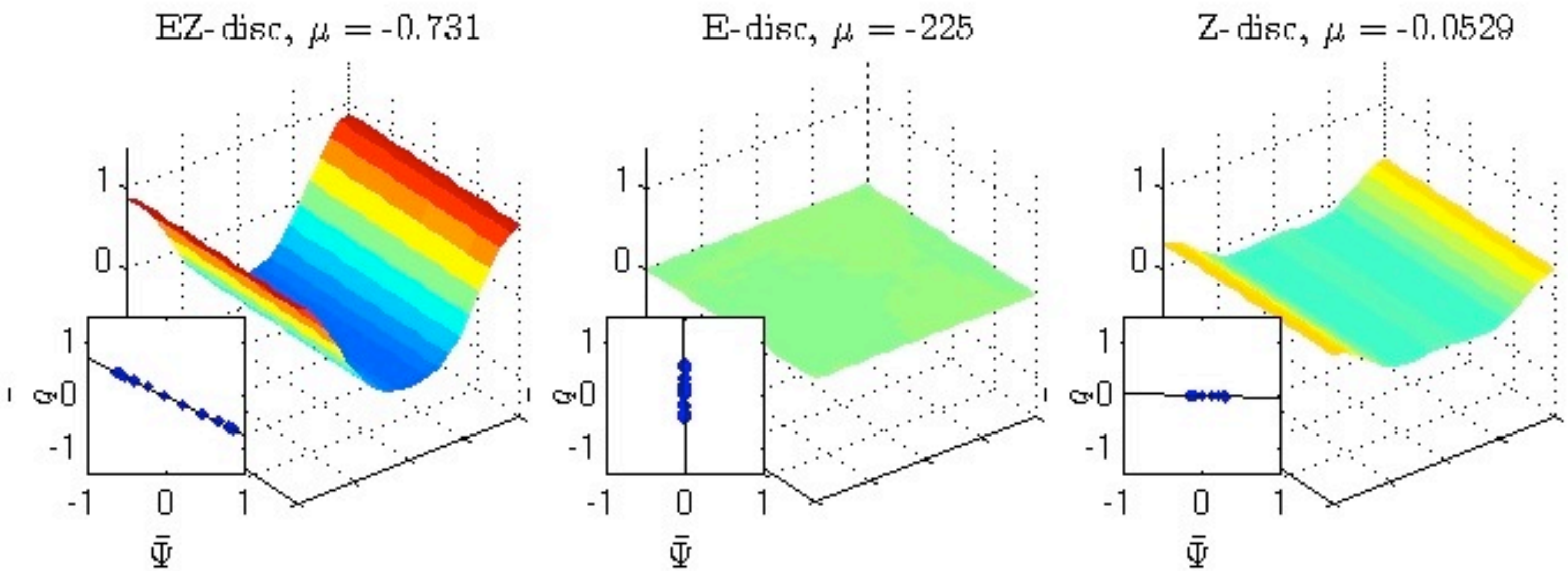
$$\bar{q}_T = \frac{1}{N_T}\sum_n q^n, \quad \bar{\psi}_T = \frac{1}{N_T}\sum_n \psi^n, \quad N_T \Delta t = T - 10^3$$

- 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 (Z), or both (EZ). $T = 10^6$



Hamiltonian particle-mesh (HPM) 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]

Poisson integrator with N conserved quantities

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

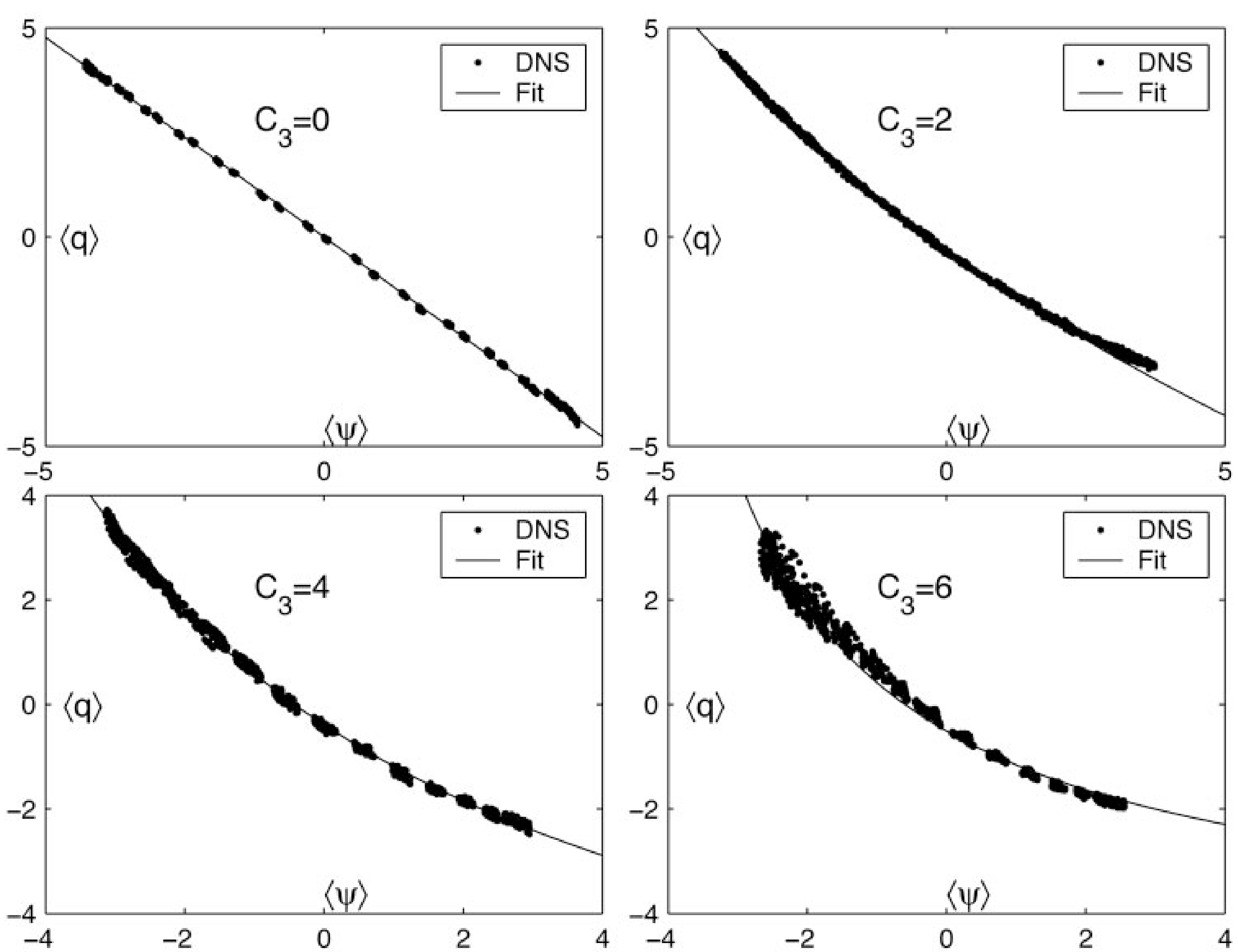


Fig. 3. The scatter plots $\bar{q}$ vs. $\bar{\psi}$ for the 23 × 23 sine-bracket truncation, layered topography, $\hat{C}_3 = 0, 2, 4, 6$.

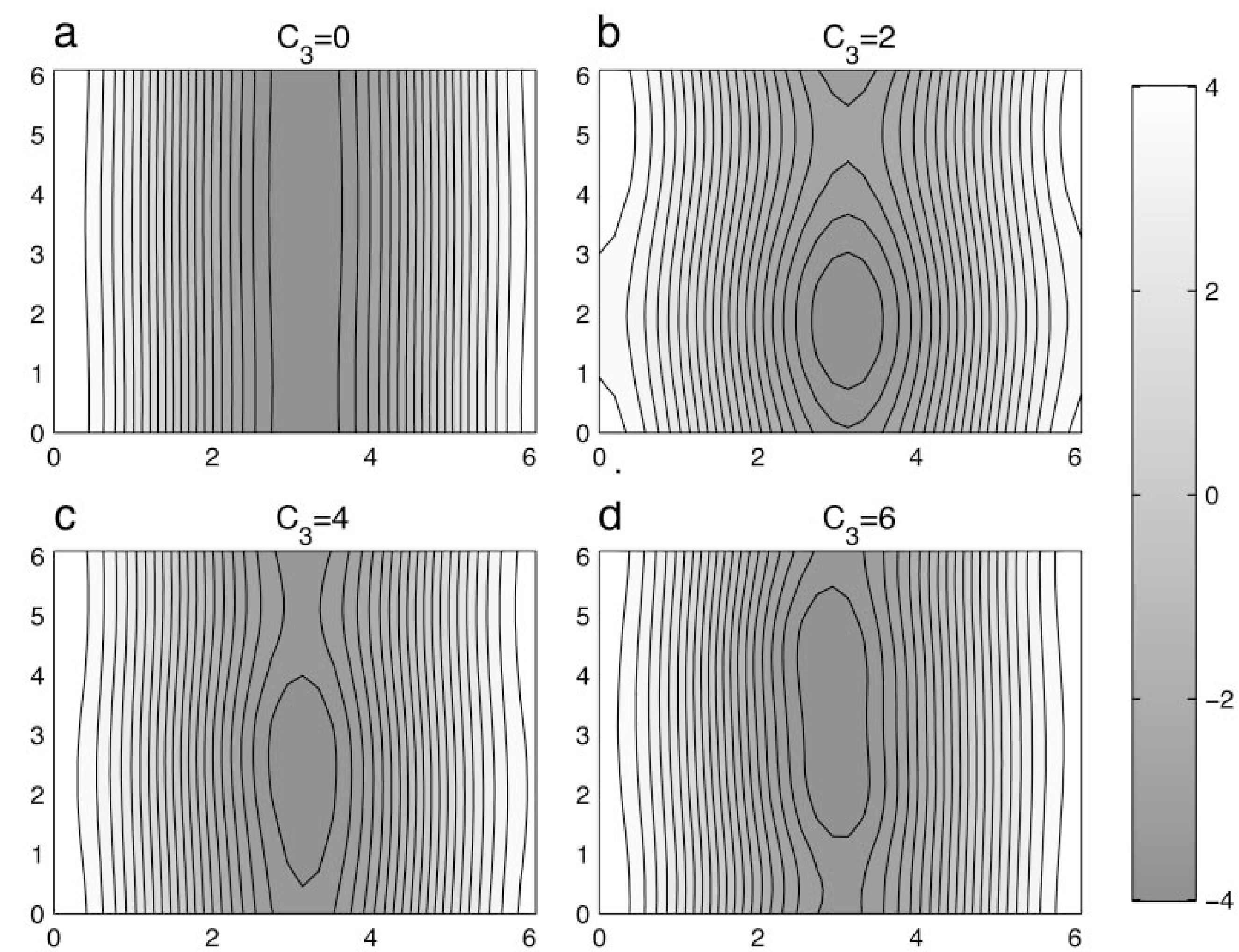


Fig. 4. The contour plots of the mean stream function, 23 × 23 sine-bracket truncation, layered topography, $\hat{C}_3 = 0, 2, 4, 6$.

Skew and Flat distributions - HPM method

Draw the vorticity from

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

with skewness

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

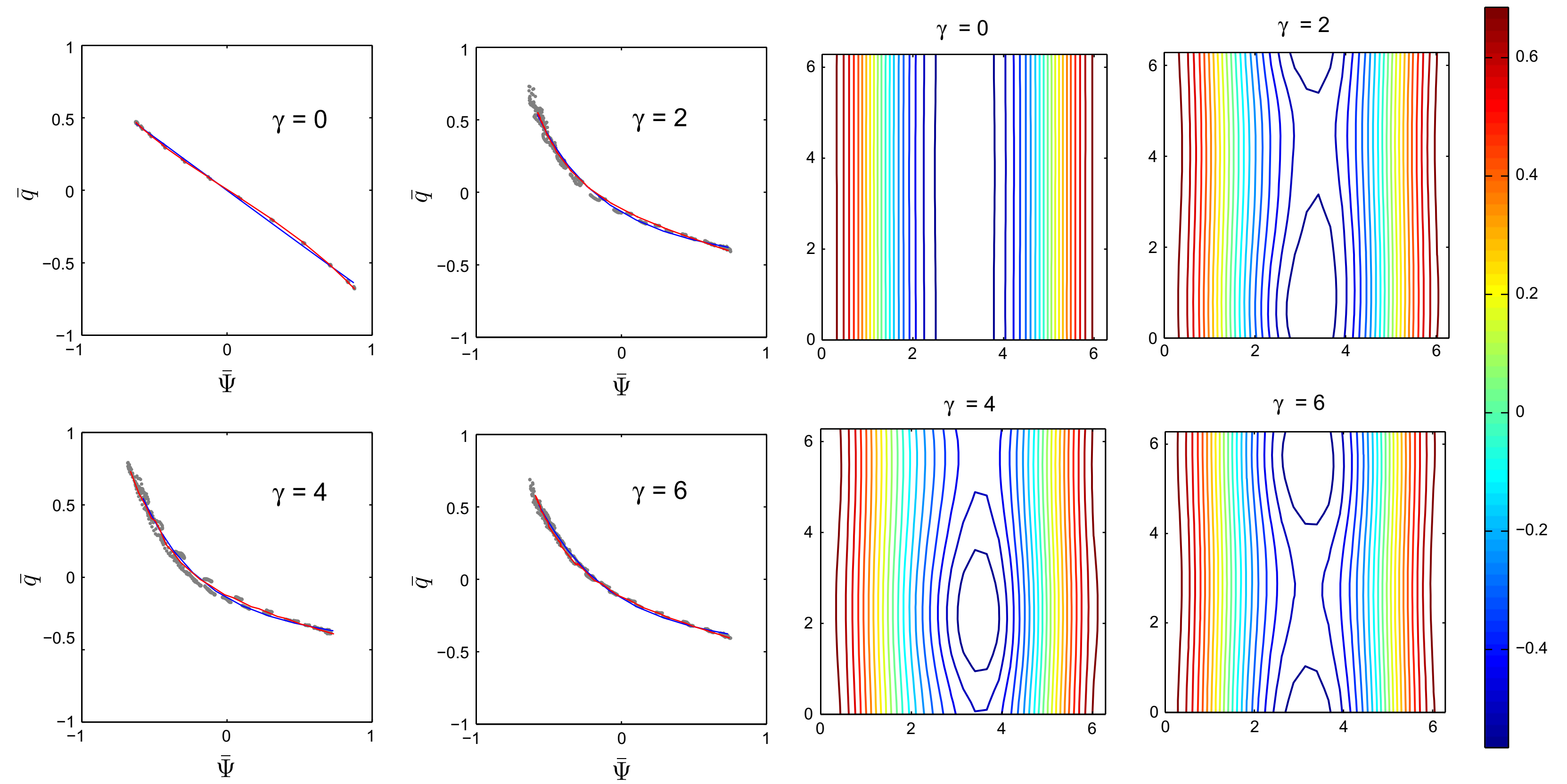
or excess kurtosis (no skew.)

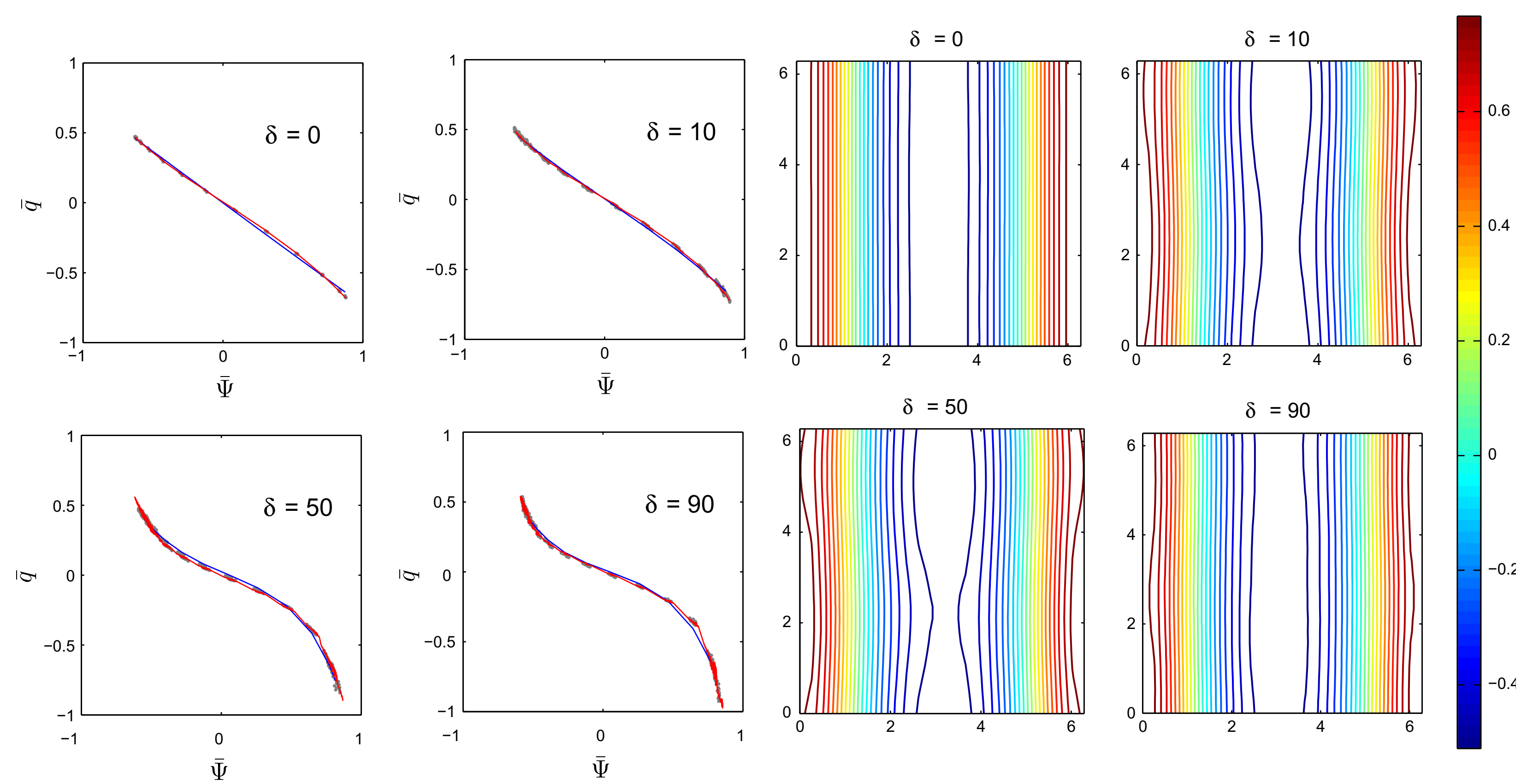
$$\delta = \frac{C_4}{C_2^2} - 3$$

We derived and compare with Lagrangian and Eulerian analytical models.

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

Refutes the conjecture, but only with large δ.





Feature presentation: Thermostats for unresolved dynamics

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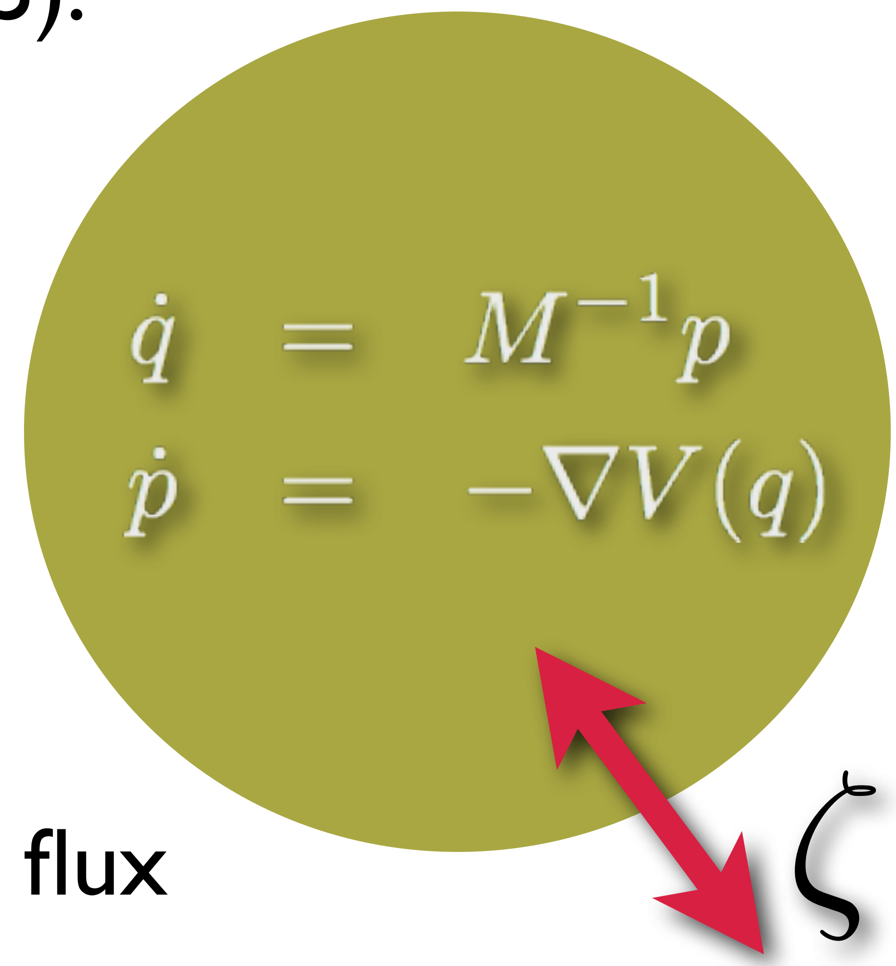
Need a mechanism to perturb the dynamics

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:

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

Sampling of arbitrary distribution F

Extended system:

$$\begin{aligned} \dot{X} &= J\nabla H(X) + g(X,\zeta) \\ \dot{\zeta} &= h(X,\zeta) \end{aligned}$$

Ask that the augmented distribution

$$\tilde{\rho}(X,\zeta) \propto \exp(-\beta F(X) - \alpha G(\zeta))$$

be invariant under the Liouville flow

$$\mathcal{L}\tilde{\rho} := -\nabla_X \cdot \tilde{\rho}(f+g) - \nabla_\zeta \cdot \tilde{\rho} h = 0$$

Simplifying assumptions:

$$G = \frac{\zeta^T \zeta}{2} \quad h = h(X) \quad g(X,\zeta) = s(X)\zeta \quad F(X) = F(H(X))$$

Solve for $h(X) = \frac{1}{\alpha}(\nabla \cdot s(X) - \beta \nabla F \cdot s(X))$

Generalized thermostats

For the canonical distribution:

$$
\begin{aligned}
\dot{X} &= J\nabla H(X) + \zeta s(X) \\
\dot{\zeta} &= \alpha^{-1}\left[\beta \nabla H \cdot s(X) - \nabla \cdot s(X)\right]
\end{aligned}
$$

Mixing can be ‘encouraged’ by adding Langevin noise & diss.

$$
\begin{aligned}
\dot{X} &= J\nabla H(X) + \zeta s(X) \\
\dot{\zeta} &= \alpha^{-1}\left[\beta \nabla H \cdot s(X) - \nabla \cdot s(X)\right] - \frac{\alpha\sigma^2}{2}\zeta + \sigma \dot{w}
\end{aligned}
$$

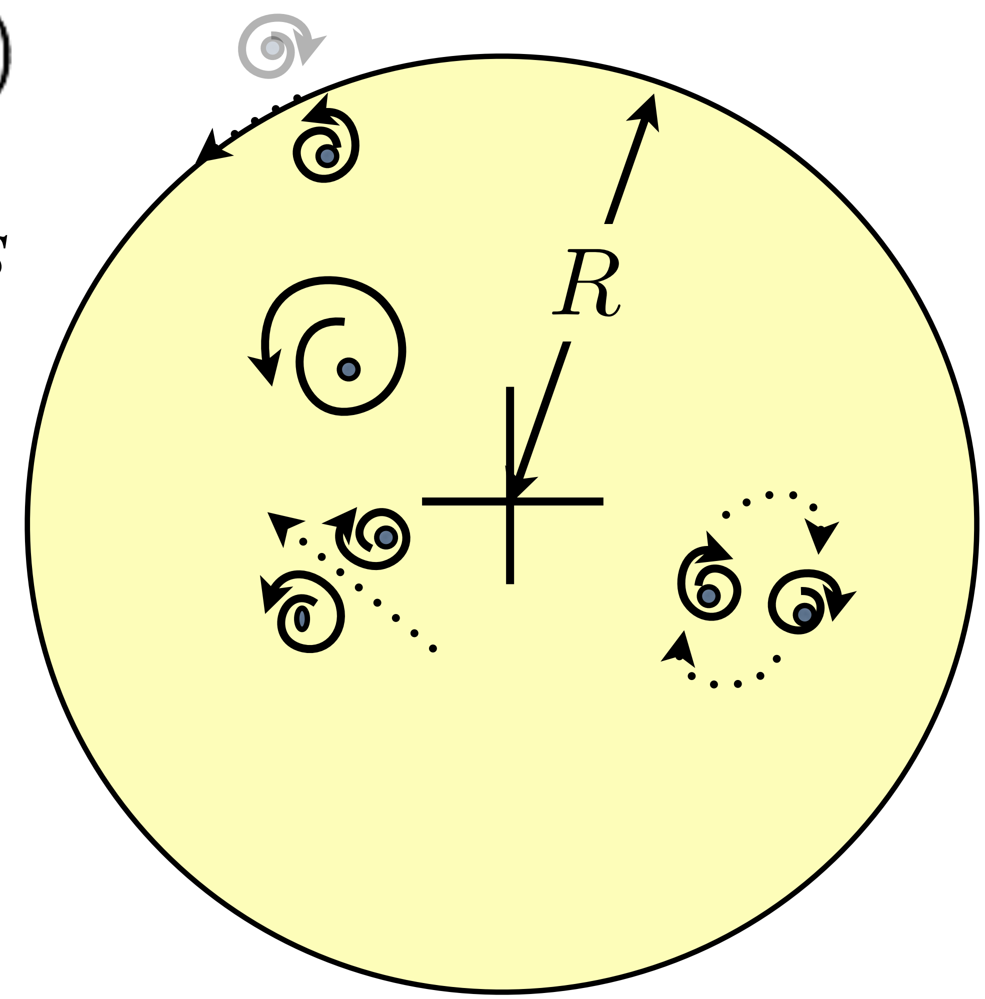
$$
\nabla \cdot s(X) = 0 \quad \Rightarrow \quad \text{Langevin (degenerate)}
$$

Point Vortex Model

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

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

$$+\ \textit{boundary terms}$$

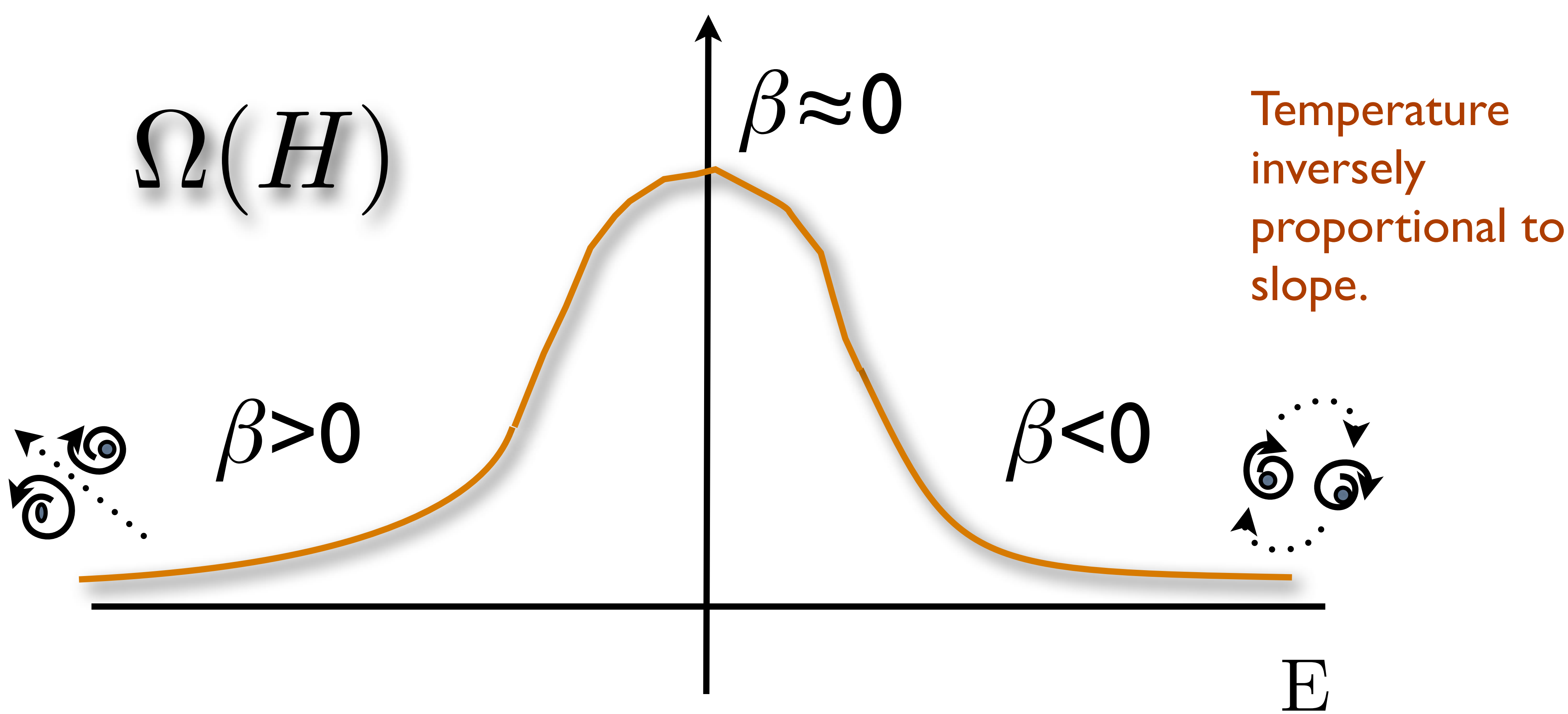


$$\longrightarrow \quad \Gamma_i \dot{x}_i = J\nabla_{x_i} H$$

Onsager, 1949 "Statistical Hydrodynamics"
Oliver Bühler, 2002: a numerical study

Statistical Mechanics

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



Onsager's Predictions

"... vortices of the same sign will tend to cluster---preferably the strongest ones---so as to use up excess energy at the least possible cost in terms of degrees of freedom ... the weaker vortices, free to roam practically at random will yield rather erratic and disorganized contributions to the flow."

Positive temperatures:

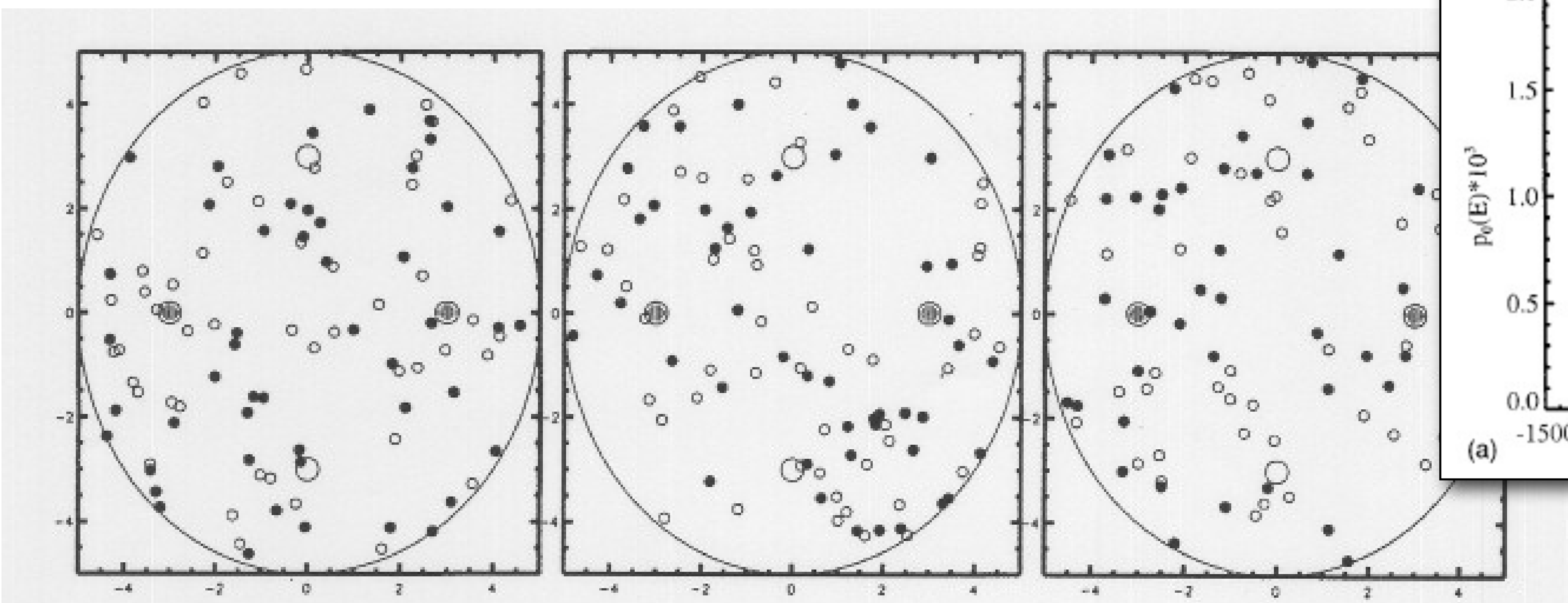
Strong vortices of opposite sign tend to approach each other

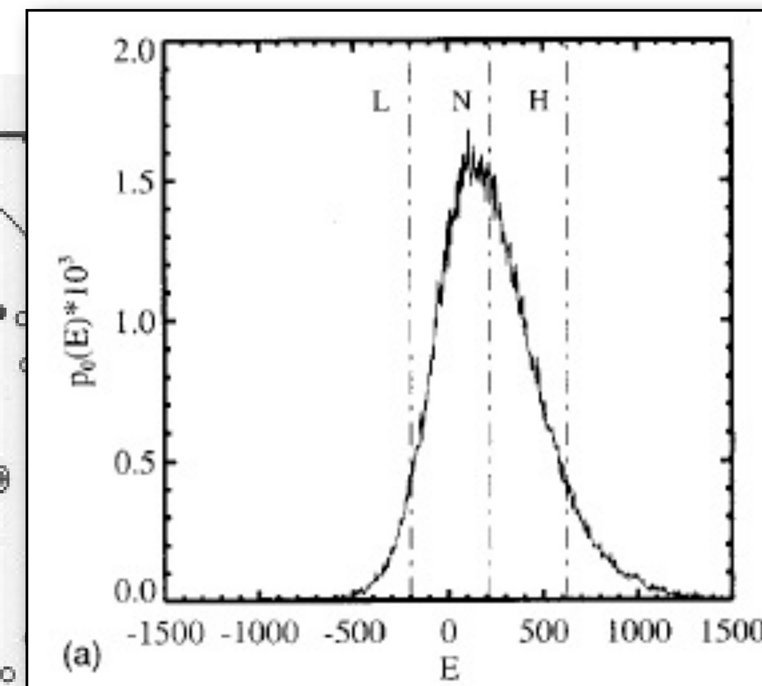
Negative temperatures:

Strong vortices of the same sign will cluster

Oliver Bühler's (2002) simulation

4 strong, 96 weak vortices, sign indefinite,
0 net circulation in each group, fixed ang. mom.





β>0 $\beta\approx$0 β<0

Simulation results support Onsager's predictions

Canonical Statistical Mechanics

Bühler discusses his simulations in terms of canonical statistical mechanics, i.e. *the system of strong vortices in contact with a reservoir of weak ones.*

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

We replaced the 96 small vortices by the stochastic-dynamic thermostat, achieving very similar phenomenologies for the large vortices.

Infinite reservoir allows arbitrarily close approaches of same sign vortex pairs, not observed in Bühler's simulations. β is restricted to a finite interval.

Derivation of canonical ensemble

Assume the subsystem and reservoir variables decoupled in the Hamiltonian

$$H(X_A, X_B) = H_A(X_A) + H_B(X_B)$$

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

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

Then:
$$\begin{aligned}\mathrm{Prob}\{X_A | H = E\} &\propto \Omega_B(E - H_A(X_A)) \\ &= \exp(S_B(E - H_A)) \\ &= \exp(S_B(E) - S_B'(E)H_A + S_B''(E)H_A^2 + \cdots) \\ &\propto \exp(-\beta H_A + \gamma H_A^2 + \cdots)\end{aligned}$$

To apply the Taylor expansion, we need the reservoir entropy to be slowly varying over the energy range of the resolved dynamics.

Finite reservoir effects

Assume the subsystem and reservoir variables decoupled in the Hamiltonian

$$E = E_A + E_B$$

Central limit Thm: $$p_0(E_B) = \frac{1}{\sigma_B\sqrt{2\pi}} \exp\left(\frac{-E_B^2}{2\sigma_B^2}\right)$$

Then:
$$\begin{aligned}
\mathrm{Prob}\{X_A|H=E\} &\propto p_0(E_B = E - E_A) \\
&\propto \exp\left(\frac{-(E-E_A)^2}{2\sigma_B^2}\right) \\
&\propto \exp\left(\frac{EE_A}{\sigma_B^2} - \frac{E_A^2}{2\sigma_B^2}\right) = \exp(-\beta E_A - \gamma E_A^2)
\end{aligned}$$

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

Finite reservoir model

$$\rho_{\text{finite}} \propto e^{-\beta H - \gamma H^2} \qquad F = H + \frac{\gamma}{\beta} H^2$$

Modified control law:

$$\begin{aligned} \dot{X} &= J\nabla H(X) + \zeta s(X) \\ \dot{\zeta} &= \alpha^{-1}\left[\beta \nabla H \cdot s(X) - \nabla \cdot s(X)\right] \end{aligned}$$

+ noise + diss.

↓

$$\dot{\zeta} = \alpha^{-1}\left[\beta(1 + \frac{\gamma}{\beta} H)\nabla H \cdot s(X) - \nabla \cdot s(X)\right]$$

+ noise + diss.

Allows direct comparison with Bühler's results

Angular momentum

$$\begin{aligned} \dot{X} &= J\nabla H(X) + \zeta s(X) \\ \dot{\zeta} &= \alpha^{-1}\left[\beta\nabla H \cdot s(X) - \nabla \cdot s(X)\right] \end{aligned}$$

For point vortices we take:

$$s(X) = \left(\frac{x_1^{\perp}}{|x_1|}, \ldots, \frac{x_N^{\perp}}{|x_N|}\right)$$

- This choice preserves the angular momentum

$$M = \sum_i \Gamma_i |x_i|^2$$

- It yields generalized Langevin dynamics

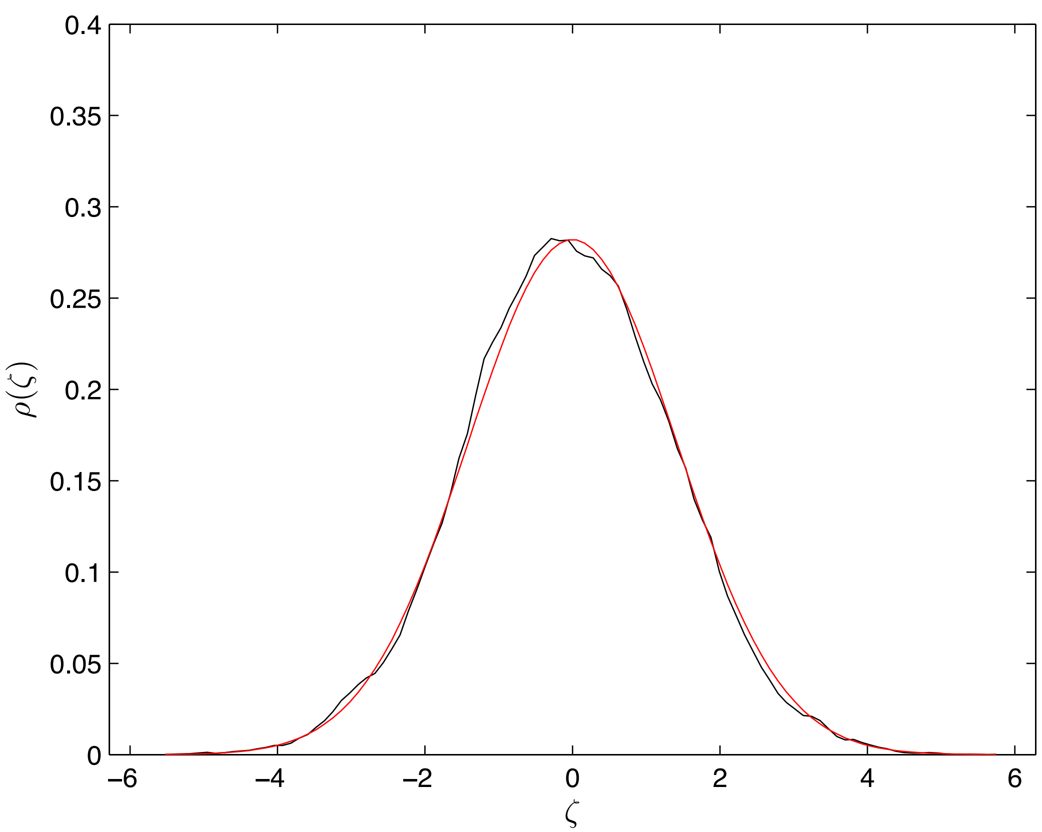
Experimental parameters

$\beta \in \{-0.006, -0.00055, 0.01\}$

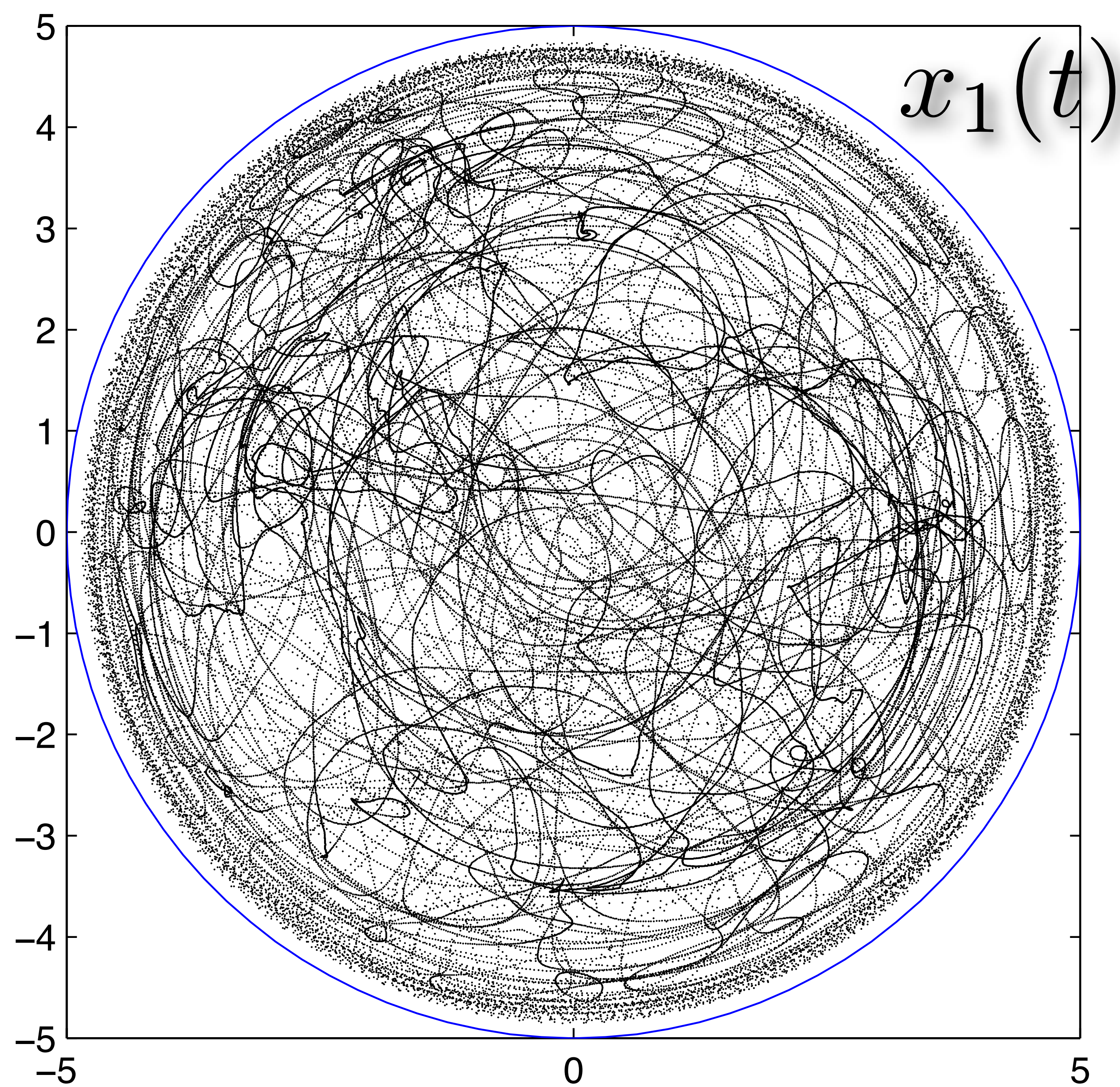
$\gamma = -\frac{\beta}{2E_0}, \quad E_0 \in \{628, 221, -197\}$

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

$t \in [1500, 12000]$



ζ is Gaussian



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

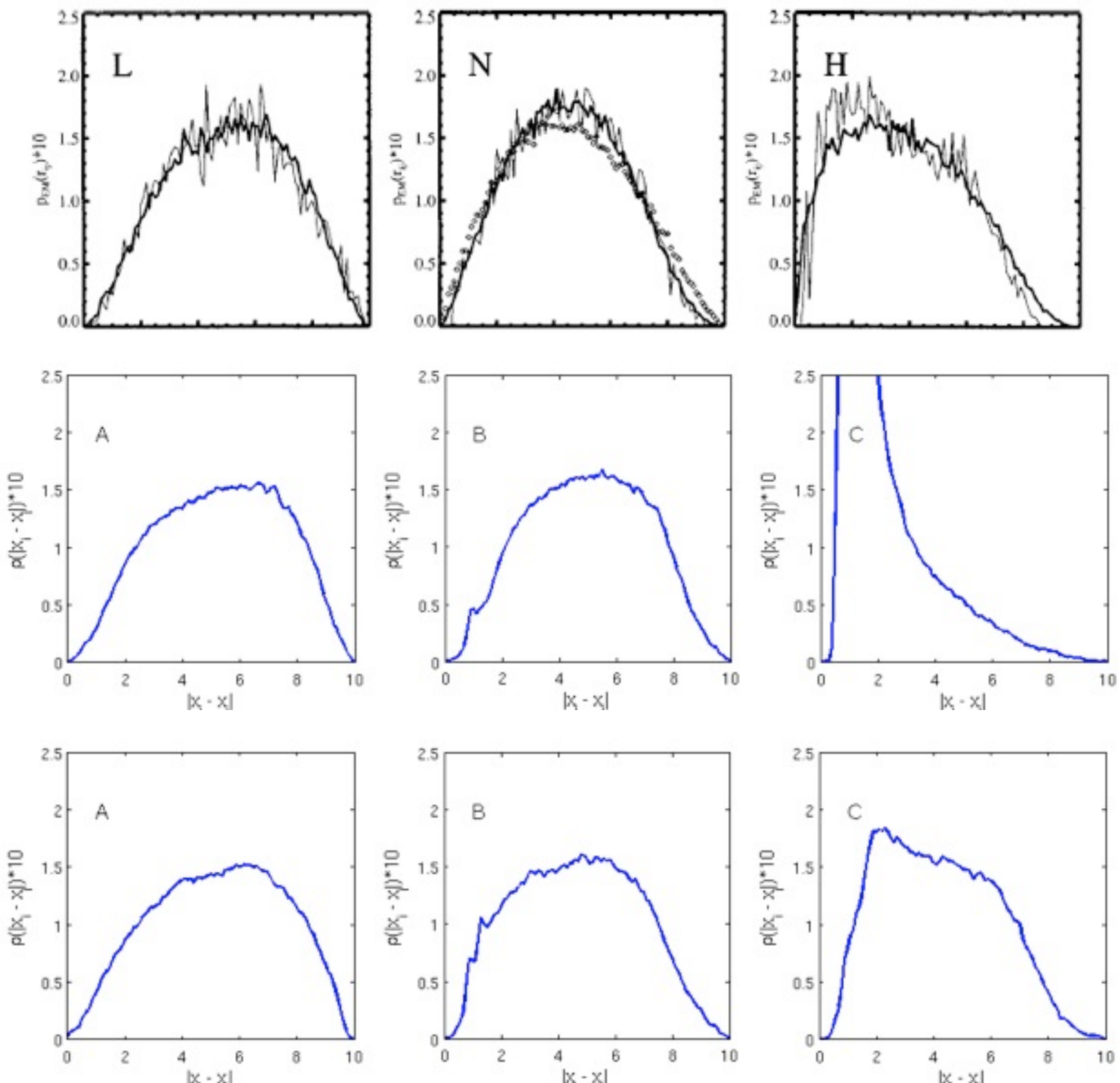
Distance between like signed vortices $|x_i - x_j|_{++}$

β>0 β≈0 β<0

Buhler '02

∞

<∞



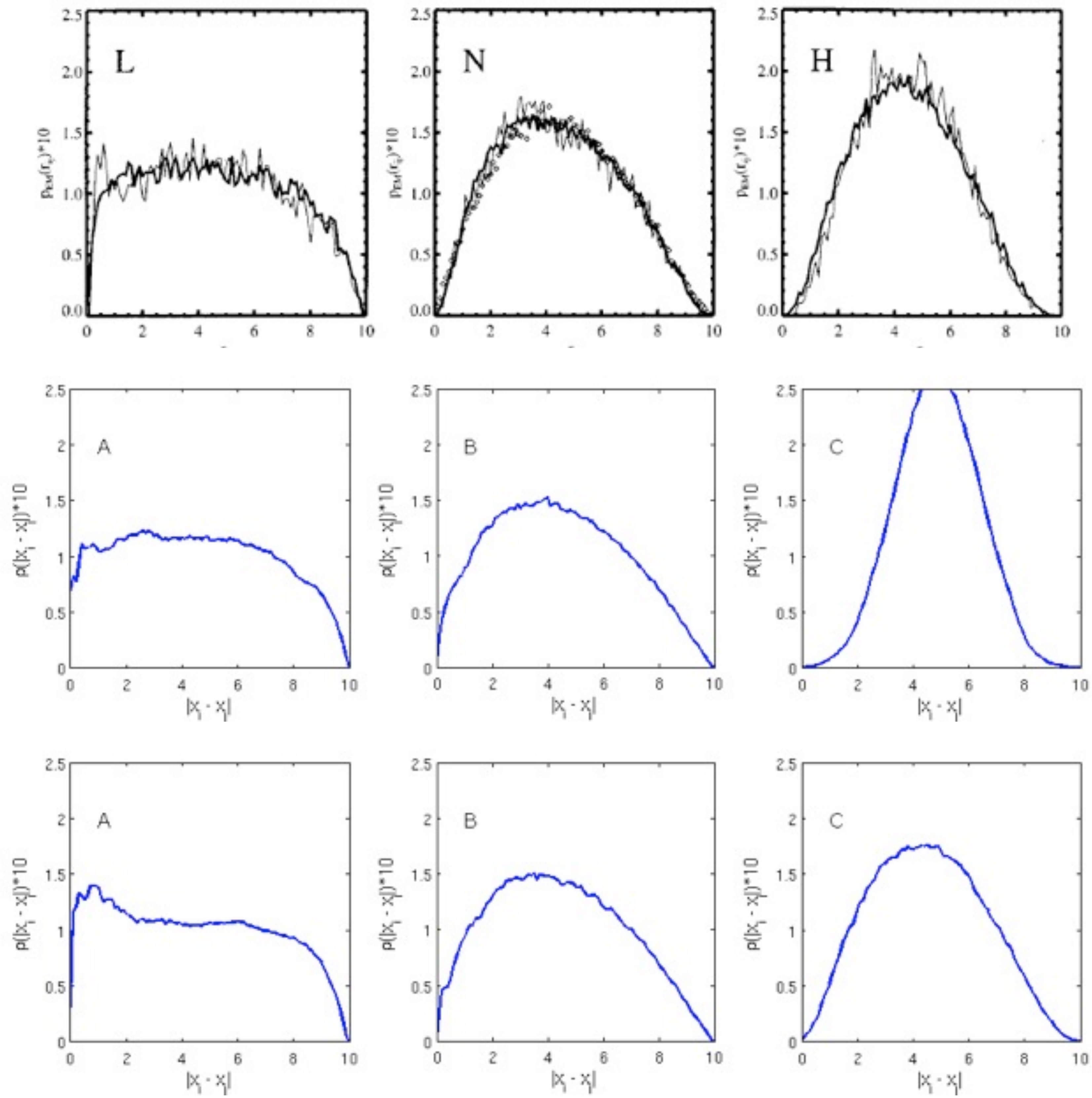
Distance between opposite signed vortices $|x_i - x_j|_{+-}$

$\beta>0$ | $\beta\approx 0$ | $\beta<0$

Buhler '02

∞

$<\infty$



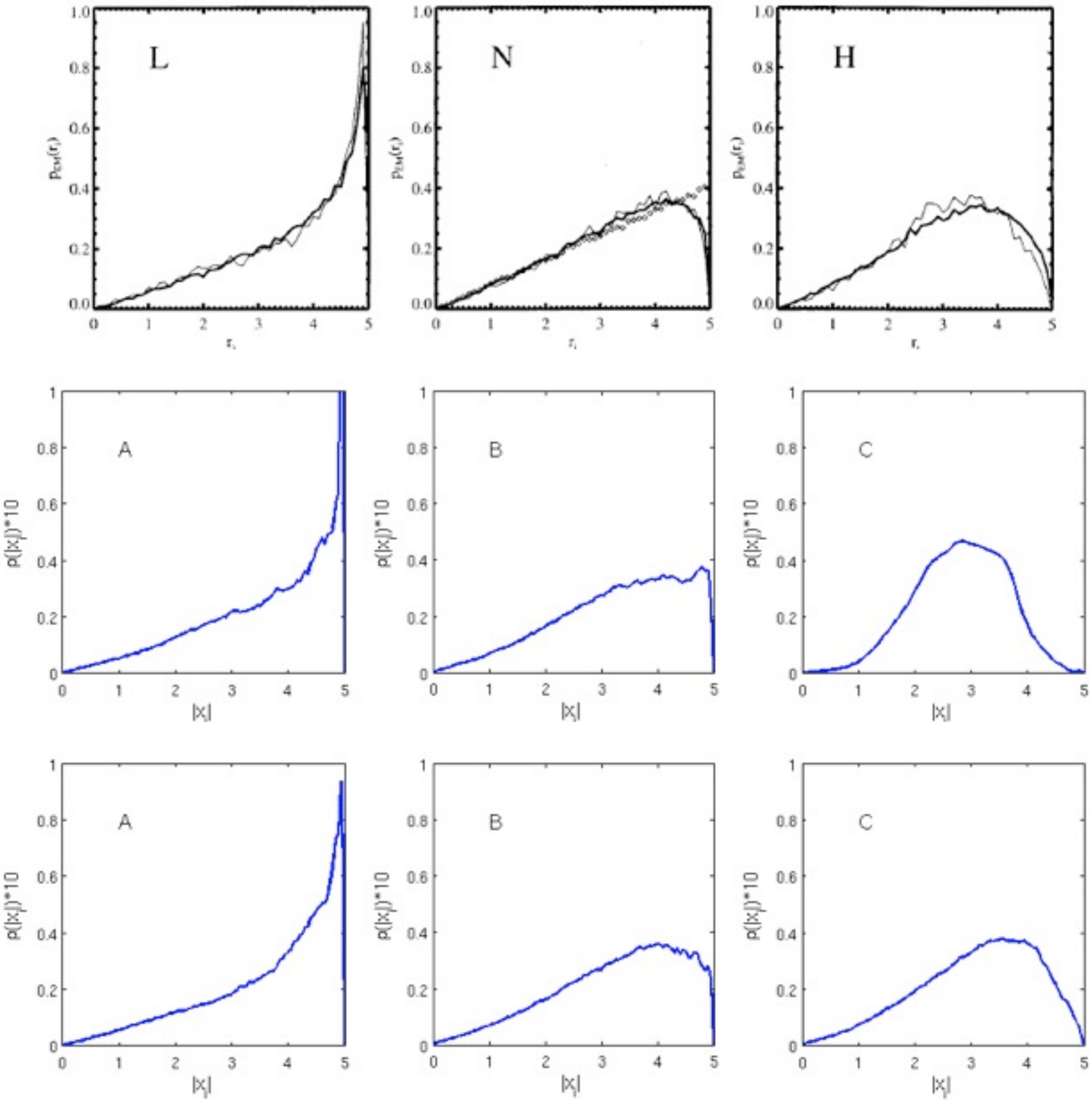
Radial position of vortices $|x_i|$

$\beta > 0$ | $\beta \approx 0$ | $\beta < 0$

Buhler '02

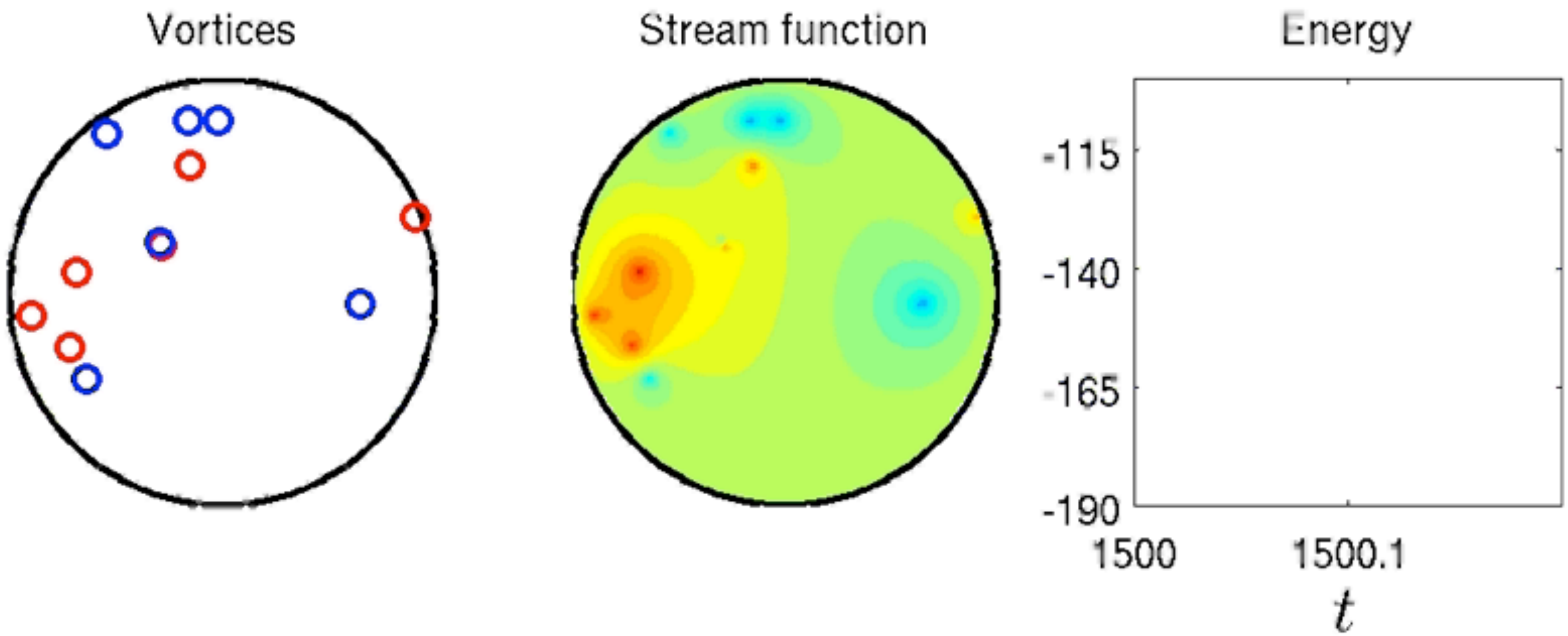
∞

$< \infty$

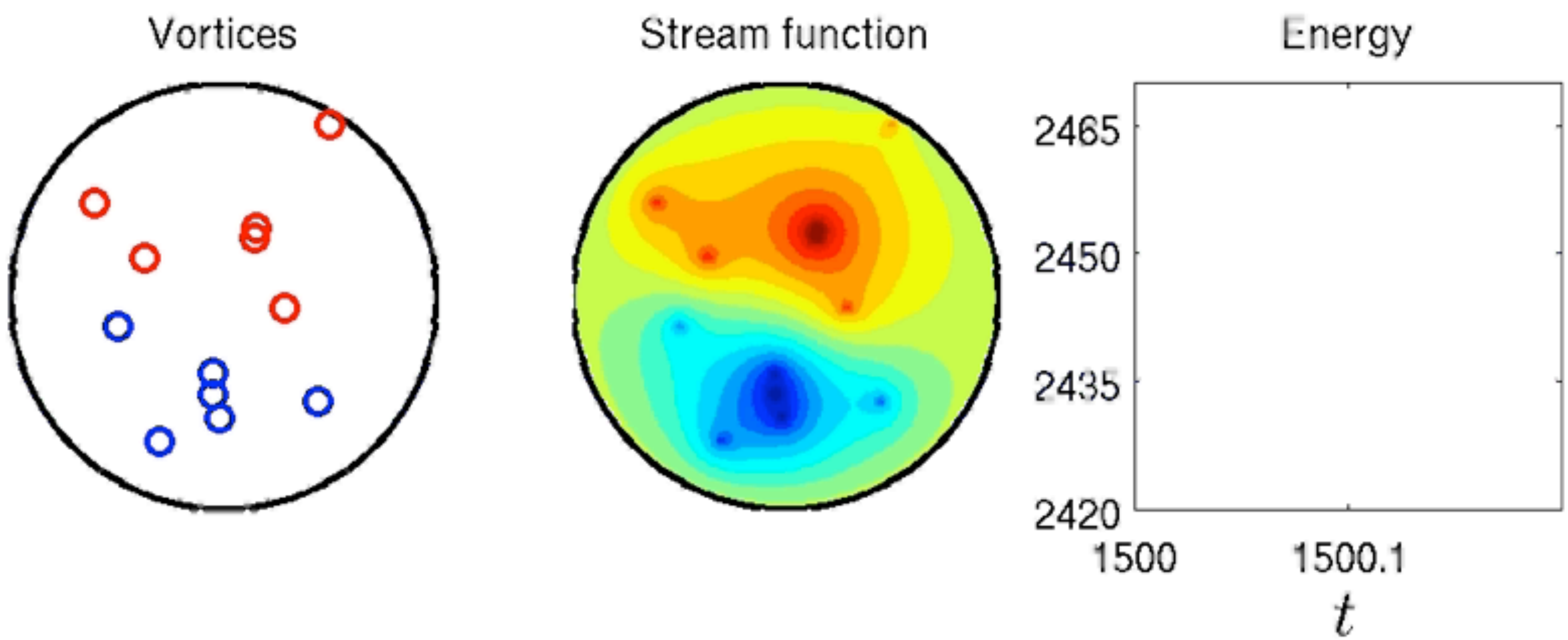


Vortex clustering, N=12

$\beta = 0.01$



$\beta = -0.006$



Summary

- General thermostat for preserving a desired distribution.
- Flexibility of the scheme allows to model either infinite or finite reservoirs.
- Using a simple scalar thermostat, we are able to reproduce the statistical behavior of a set of vortices in ‘thermal’ contact with a reservoir.
- Future work: how this approach can be extended to PDE/grid-point models.

the End