Simulated Annealing Using Hamiltonian Structure with Dirac Constraint Theory

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Goals: Describe formal dissipation structures and their use for calculating stationary states using Eulerian Hamiltonian structure (noncanonical Poisson bracket) with Dirac brackets. With Flierl (MIT), Bloch (UM), Ratiu (EPFL).

Overview

(Dissipation, Dirac, Vortices)

1. Dissipative Structures

   (a) Rayleigh, Cahn-Hilliard

   (b) Hamilton Preliminaries

   (c) Hamiltonian Based Dissipative Structures

      i. Double Bracket Dynamics $\longrightarrow$ Computations

      ii. Metriplectic Dynamics $\longrightarrow$ Collision operator

2. Computations

   (a) 2D Euler Vortex States

   (b) Vlasov-Poisson BGK?

Rayleigh Dissipation Function

Introduced for study of vibrations, stable linear oscillations, in 1873 (see e.g. Rayleigh, Theory of Sound, Chap. IV §81)

Linear friction law for n-bodies, $\mathbf{F}_i = -b_i(\mathbf{r}_i)\mathbf{v}_i$, with $\mathbf{r}_i \in \mathbb{R}^3$. Rayleigh was interested in linear vibrations, $\mathcal{F} = \sum_i b_i \, ||\mathbf{v}_i||^2/2$.

Coordinates $\mathbf{r}_i \to q_\nu$ etc. $\Rightarrow$

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_\nu}\right) - \left(\frac{\partial \mathcal{L}}{\partial q_\nu}\right) + \left(\frac{\partial \mathcal{F}}{\partial \dot{q}_\nu}\right) = 0$$

Ad hoc, phenomenological, yet is generalizable, geometrizable (e.g. Bloch et al.,...)

Cahn-Hilliard Equation

Models phase separation, nonlinear diffusive dissipation, in binary fluid with ‘concentrations’ n, $n = 1$ one kind $n = -1$ the other

$$\frac{\partial n}{\partial t} = \nabla^2 \frac{\delta F}{\delta n} = \nabla^2 \left(n^3 - n - \nabla^2 n \right)$$

Lyapunov Functional

$$F[n] = \int d^3x \left[\frac{1}{4} \left(n^2 - 1 \right)^2 + \frac{1}{2} |\nabla n|^2 \right]$$

$$\frac{dF}{dt} = \int d^3x \frac{\delta F}{\delta n} \frac{\partial n}{\partial t} = \int d^3x \frac{\delta F}{\delta n} \nabla^2 \frac{\delta F}{\delta n} = -\int d^3x \left| \nabla \frac{\delta F}{\delta n} \right|^2 \leq 0$$

For example in 1D

$$\lim_{t \to \infty} n(x,t) = \tanh(x/\sqrt{2})$$

Ad hoc, phenomenological, yet generalizable and very important (Otto, Ricci Flows, Poincarè conjecture on S^3, ...)

Hamiltonian Preliminaries

Finite $\longrightarrow$ Infinite degrees of freedom

Canonical Hamiltonian Dynamics

Hamilton's Equations:

$$\dot{p}_i = -\frac{\partial H}{\partial q^i}, \qquad \dot{q}^i = \frac{\partial H}{\partial p_i},$$

Phase Space Coordinates: $z = (q, p)$

$$\dot{z}^i = J_c^{ij} \frac{\partial H}{\partial z^j}, \qquad (J_c^{ij}) = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix},$$

Symplectic Manifold $\mathcal{Z}_s$:

$$\dot{z} = Z_H = [z, H]$$

with Hamiltonian vector field generated by Poisson bracket

$$[f, g] = \frac{\partial f}{\partial z^i} J_c^{ij} \frac{\partial g}{\partial z^j}$$

symplectic 2-form = (cosymplectic form)$^{-1}$: $\omega^c_{ij} J_c^{jk} = \delta_i^k$,

Noncanonical Hamiltonian Dynamics

Noncanonical Coordinates:

$$\dot{z}^i = J^{ij}\frac{\partial H}{\partial z^j} = [z^i, H]\,, \qquad\qquad [A,B] = \frac{\partial A}{\partial z^i} J^{ij}(z) \frac{\partial B}{\partial z^j}$$

Poisson Bracket Properties:

antisymmetry $\longrightarrow$ $[A,B] = -[B,A]\,,$

Jacobi identity $\longrightarrow$ $[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$

G. Darboux: $det J \neq 0 \Longrightarrow J \rightarrow J_c$ Canonical Coordinates

Sophus Lie: $det J = 0 \Longrightarrow$ Canonical Coordinates plus Casimirs

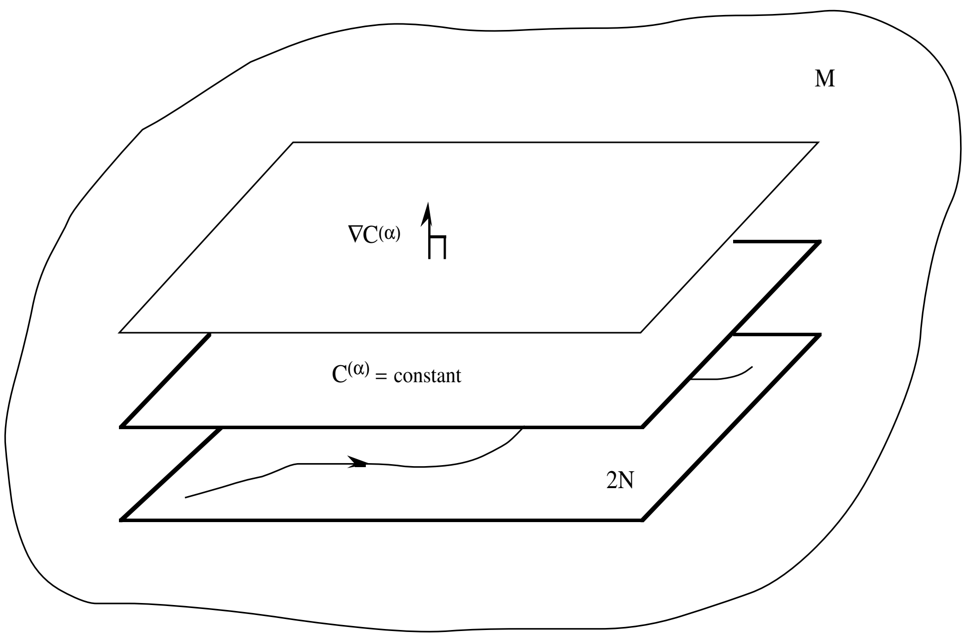
Eulerian Media: $J^{ij} = c_k^{ij} z^k$ $\longleftarrow$ Lie – Poisson Brackets

Poisson Manifold $\mathcal{Z}_p$

Degeneracy $\Rightarrow$ Casimir Invariants:

$$[C, g] = 0 \quad \forall g : \mathcal{Z}_p \rightarrow \mathbb{R}$$

Foliation by Casimir Invariants:



Leaf Hamiltonian vector fields:

$$Z_f^p = [z, f]$$

Example 2D Euler

Noncanonical Poisson Brackets:

$$\{F,G\} = \int dxdy\, \zeta \left[\frac{\delta F}{\delta \zeta}, \frac{\delta G}{\delta \zeta}\right] = -\int dxdy\, \frac{\delta F}{\delta \zeta}\, [\zeta, \cdot]\, \frac{\delta G}{\delta \zeta}$$

$\zeta(x,y,t)$ = vorticity, $\psi = \triangle^{-1}\zeta$ = streamfunction $= -\delta H/\delta\zeta$

$$[f,g] = J(f,g) = f_x g_y - f_y g_x = \frac{\partial(f,g)}{\partial(x,y)}$$

Hamiltonian & Casimirs:

$$H[\zeta] = \int dxdy\, v^2/2 = \int dxdy\, |\nabla\psi|^2/2\,, \qquad C[\zeta] = \int dxdy\, \mathcal{C}(\zeta)$$

Equation of Motion:

$$\zeta_t = \{\zeta, H\}$$

PJM (1981) and P. Olver (1982)

Example Vlasov-Poisson

Noncanonical Poisson Brackets:

$$\{F, G\} = \int dx dv\, f \left[\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f}\right] = -\int dx dv\, \frac{\delta F}{\delta f}\, [f, \cdot]\, \frac{\delta G}{\delta f}$$

$f(x, v, t)$ = distribution fn, $\mathcal{E} = v^2/2 - \phi$ = particle energy $= \delta H/\delta f$

$$[f, g] = f_x g_v - f_v g_x\,, \qquad \phi_{xx} = \int dv\, f - 1$$

Hamiltonian & Casimirs:

$$H[\zeta] = \int dx dv\, f v^2/2 + \int dx\, |\nabla\phi|^2/2\,, \qquad C[f] = \int dx dv\, \mathcal{C}(f)$$

Equation of Motion:

$$f = \{f, H\} = [\mathcal{E}, f]$$

PJM (1980)

Dirac Constrained Hamiltonian Dynamics

Ingredients:

Two functions $D_{1,2} : \mathcal{Z} \to \mathbb{R}$ and good Poisson bracket

Generalized Dirac:

$$[f,g]_D = \frac{1}{[D_1, D_2]}\Big([D_1, D_2][f,g] - [f, D_1][g, D_2] + [g, D_1][f, D_2]\Big)$$

Degeneracy $\Rightarrow$ D's are Casimir Invariants:

$$[D_{1,2}, g]_D = 0 \quad \forall \; g : \mathcal{Z}_p \to \mathbb{R}$$

Foliation again and Dirac Hamiltonian vector fields:

$$Z^d_f = [z, f]_D$$

Hamiltonian Based Dissipation

Double Brackets and Simulated Annealing

Good Idea:

Brockett; Vallis, Carnevale, and Young; Shepherd, (1989)

'Simulated Annealing' Bracket:

$$((f,g)) = [f, z^\ell][z^\ell, g] = \frac{\partial f}{\partial z^i} J^{i\ell} J^{\ell j} \frac{\partial g}{\partial z^j}\,,$$

Use bracket dynamics to do extremization $\Rightarrow$ Relaxing Rearrangement

$$\frac{d\mathcal{F}}{dt} = ((\mathcal{F}, H)) = ((\mathcal{F}, \mathcal{F})) \geq 0$$

Lyapunov function, $\mathcal{F}$, yields asymptotic stability to rearranged equilibrium.

- Maximizing energy at fixed Casimir: Works fine sometimes, but limited to circular vortex states ....

Generalized Simulated Annealing

'Simulated Annealing' Bracket:

$$((f,g))_D = [f, z^m]_D \, g_{mn} \, [z^n, g]_D = \frac{\partial f}{\partial z^i} J_D^{in} \, g_{mn} \, J_D^{nj} \frac{\partial g}{\partial z^j} \,,$$

Relaxation Property: $\frac{dH}{dt} = ((H,H))_D \geq 0$ at constant Casimirs

<u>General Geometric Construction</u>:

Suppose manifold $\mathcal{Z}$ has both Riemannian and Symplectic structure: Given two vector fields $Z_{1,2}$ the following is defined:

$$\mathbf{g}(Z_1, Z_2)$$

If the two vector fields are Hamiltonian, e.g., Z_f, then we have the bracket

$$((f,g)) = \mathbf{g}(Z_f, Z_g)$$

which produces a 'relaxing' flow. Such flows exist for Kähler manifolds.

Metriplectic Dynamics - Complete

Natural hybrid Hamiltonian and dissipative flow on that embodies the first and second laws of thermodynamics;

$$\dot{z} = (z, S) + [z, H]$$

where Hamiltonian, H, is the energy and entropy, S, is a Casimir.

Degeneracies:

$$(H, g) \equiv 0 \quad \text{and} \quad [S, g] \equiv 0 \quad \forall\ g$$

First and Second Laws:

$$\frac{dH}{dt} = 0 \qquad \text{and} \qquad \frac{dS}{dt} \geq 0$$

Seeks equilibria $\equiv$ extremization of Free Energy $F = H + S$:

$$\delta F = 0$$

2D Euler Calculations

Four Types of Dynamics

$$\begin{aligned}
\text{Hamiltonian}: \frac{\partial F}{\partial t} &= \{F, \mathcal{F}\} && (1)\\
\text{Hamiltonian Dirac}: \frac{\partial F}{\partial t} &= \{F, \mathcal{F}\}_D && (2)\\
\text{Simulated Annealing}: \frac{\partial F}{\partial t} &= \sigma\{F, \mathcal{F}\} + \alpha((F, \mathcal{F})) && (3)\\
\text{Dirac Simulated Annealing}: \frac{\partial F}{\partial t} &= \sigma\{F, \mathcal{F}\}_D + \alpha((F, \mathcal{F}))_D && (4)
\end{aligned}$$

F an arbitrary observable, $\mathcal{F}$ generates time advancement. Equations (1) and (2) are ideal and conserve energy. In (3) and (4) parameters σ and α weight ideal and dissipative dynamics: $\sigma \in \{0, 1\}$ and $\alpha \in \{-1, 1\}$. $\mathcal{F}$, can have form

$$\mathcal{F} = H + \sum_i C_i + \lambda^i P_i \,,$$

Cs Casimirs and Ps dynamical invariants.

DSA is Dressed Advection

$$\frac{\partial \zeta}{\partial t} = -[\Psi, \zeta]\,,$$

$$\Psi = \psi + A^i c_i \quad \text{and} \quad A^i = -\frac{\int d\mathbf{x}\, c_j [\psi, \zeta]}{\int d\mathbf{x}\, \zeta [c_i, c_j]}\,.$$

with constraints

$$C_j = \int d\mathbf{x}\, c_j\, \zeta\,.$$

"Advection" of ζ by Ψ, with A^i just right to force constraints.

Easy to adapt existing vortex dynamics codes!!

DSA is Dressed Advection Numerics

All runs were done at a resolution of 256×256 points with a total domain size of 8 or 16 units with the scale of the initial condition being on the order of one unit. A pseudospectral code was used with integrals evaluated as sums and time advancement accomplished by second order Adams-Bashforth.

$\longrightarrow$ Possibilities? DG for VP

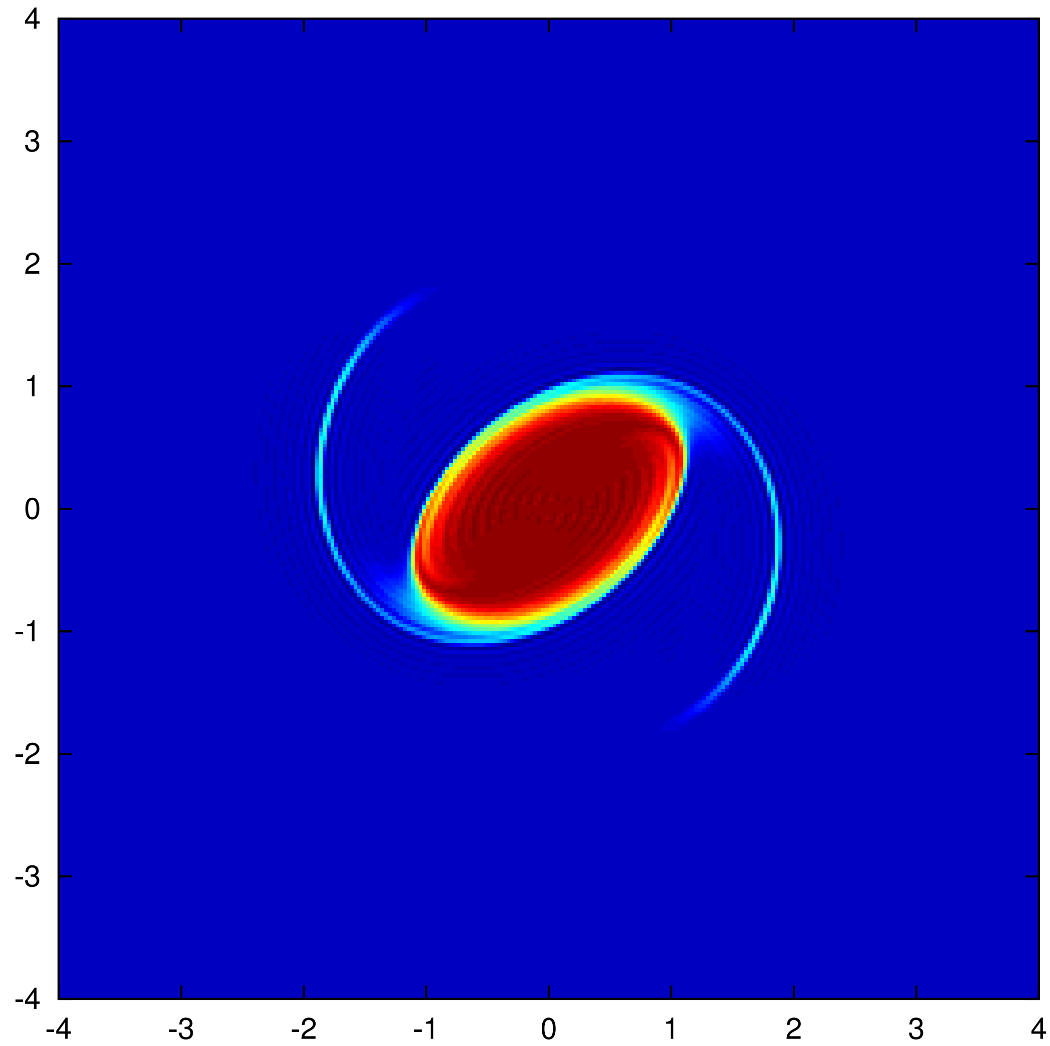
2D Euler Clip, 2-fold Symmetry – H

Initial Condition:

$$q = e^{-(r/r_0)^{10}}\,, \qquad r_0 = 1 + \epsilon \cos(2\theta)\,, \qquad \epsilon = 0.4$$

{(fig3)els-1-m0}

Filamentation leading to 'relaxed state'. How much? Which state?



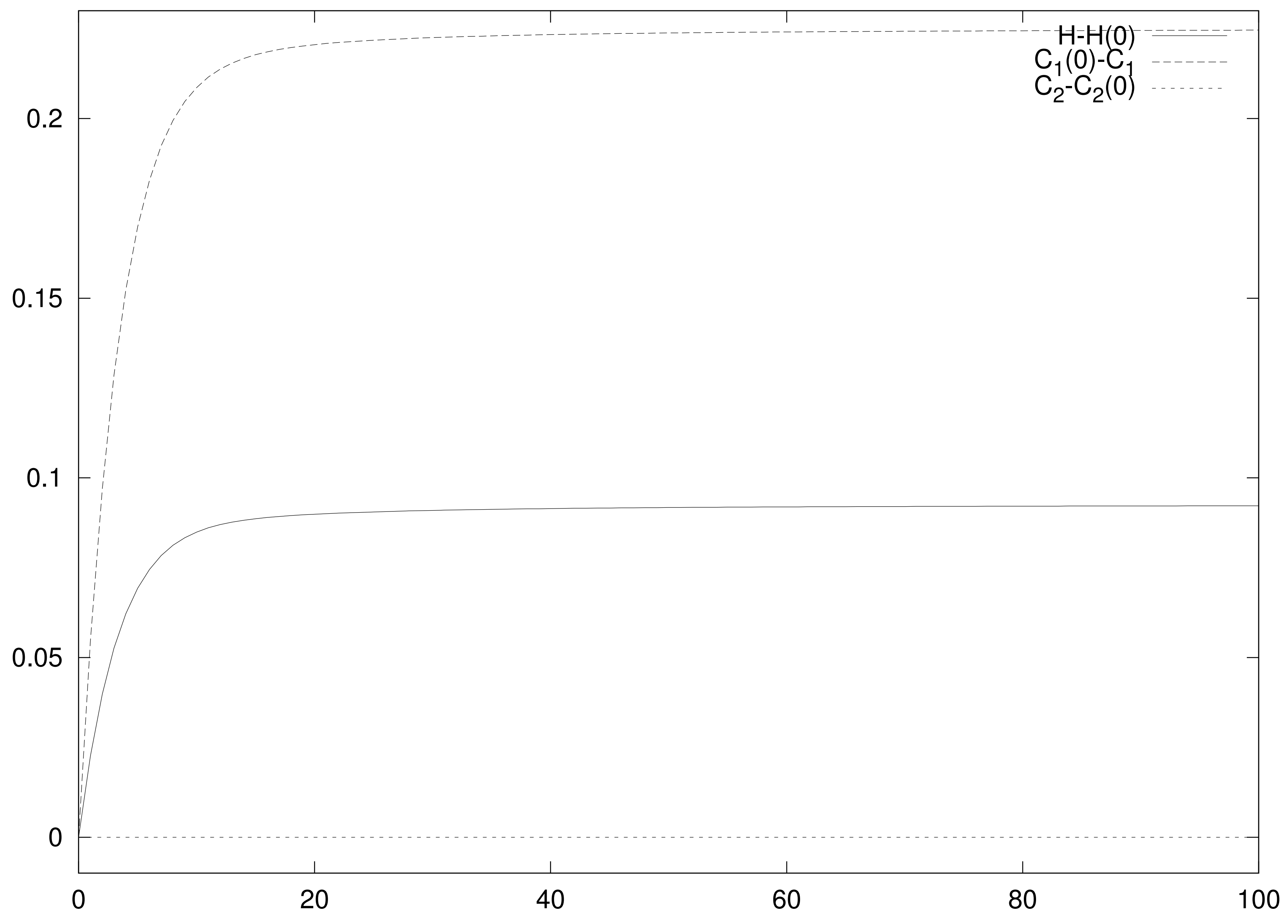
2D Euler Clip, 2-fold Symmetry – SA$_{\sigma=0}$

Initial Condition:

$$q = e^{-(r/r_0)^{10}}, \qquad r_0 = 1 + \epsilon \cos(2\theta), \qquad \epsilon = 0.4$$

{(fig6)els-2-m0}

Constants vs. t; Kelvin's H-Maximization



2-fold Symmetry – HD vs. DSA$_{0,1}$

Initial Condition:

$$q = e^{-(r/r_0)^{10}}, \qquad r_0 = 1 + \epsilon \cos(2\theta), \qquad \epsilon = 0.4$$

- Angular momentum:

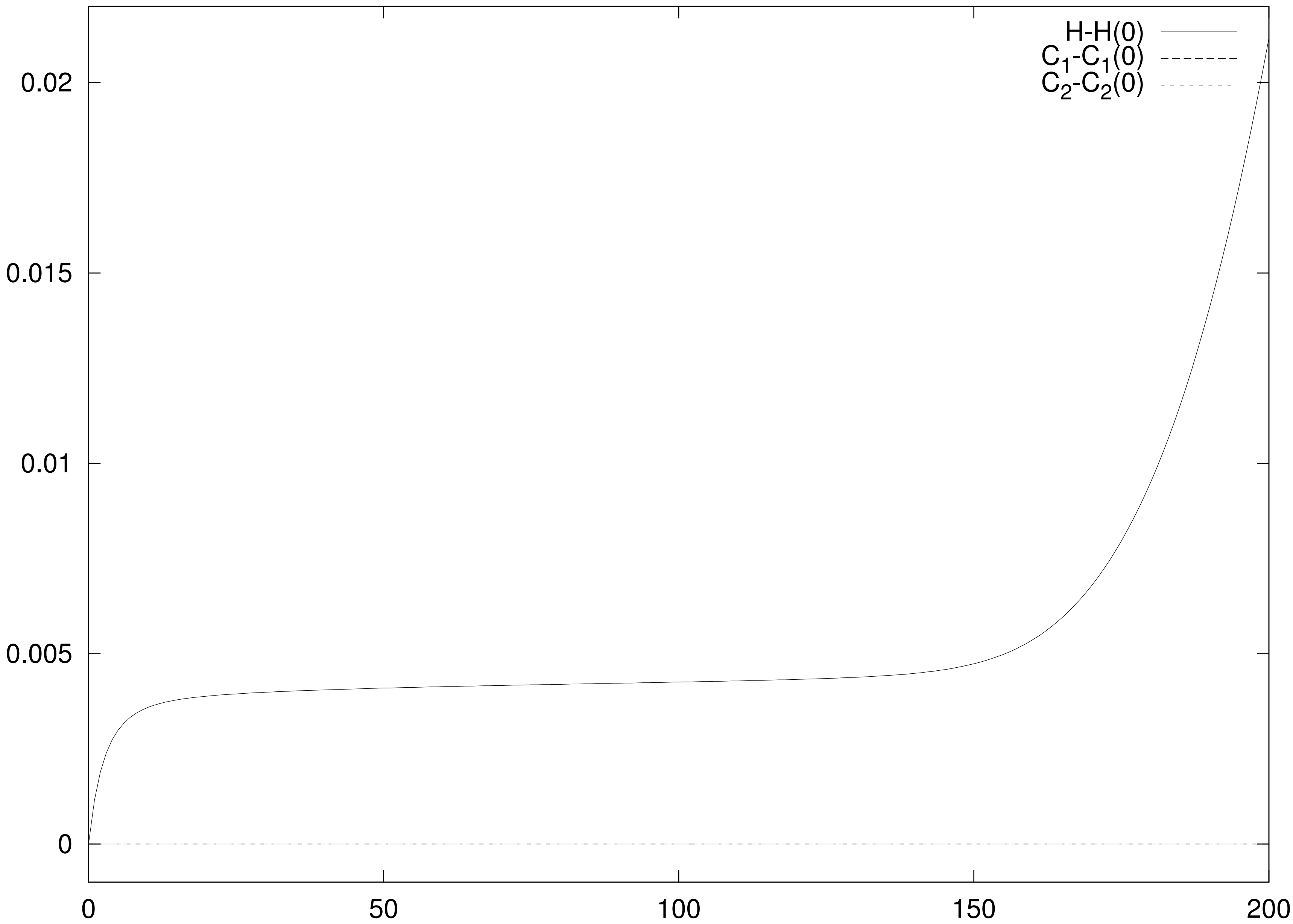
$$L = \int_D (x^2 + y^2)\, d^2x$$

- Strain moment (2-fold symmetry):

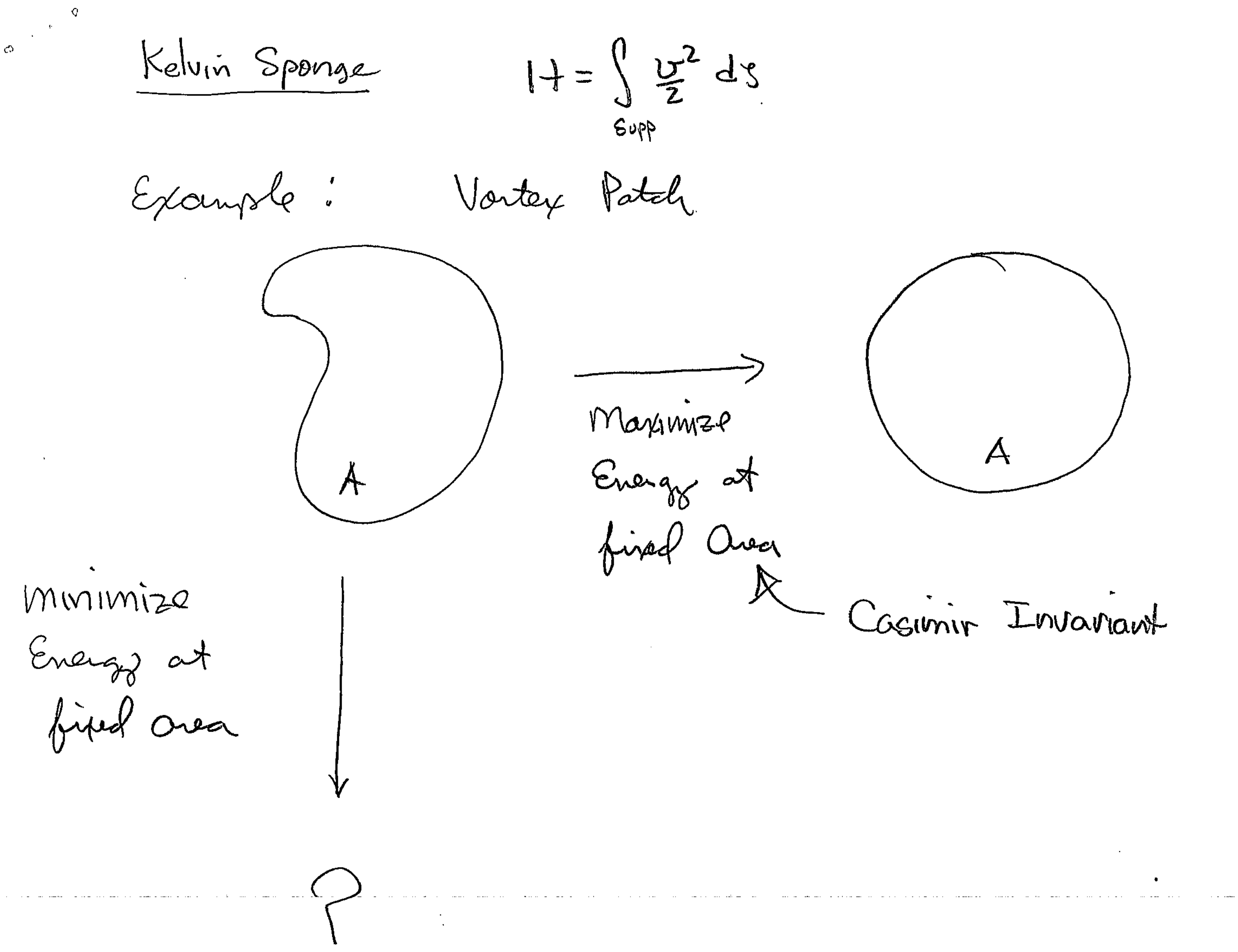
$$K = \int_D xy\, d^2x$$

{(fig8)els-3-m0, (fig10)els-4-m0,(fig12)els-4-m1}

Constants vs. t for DSA_0



Kelvin's Sponge



Uniform positive vorticity inside circle. Net vorticity maintained. But, angular momentum not conserved? With Dirac, angular momentum conserved. Then what?

2-fold Symmetry – Minimizing SA vs. DSA$_0$

Initial Condition:

$$q = e^{-(r/r_0)^{10}}, \qquad r_0 = 1 + \epsilon \cos(2\theta), \qquad \epsilon = 0.4$$

- Angular momentum:

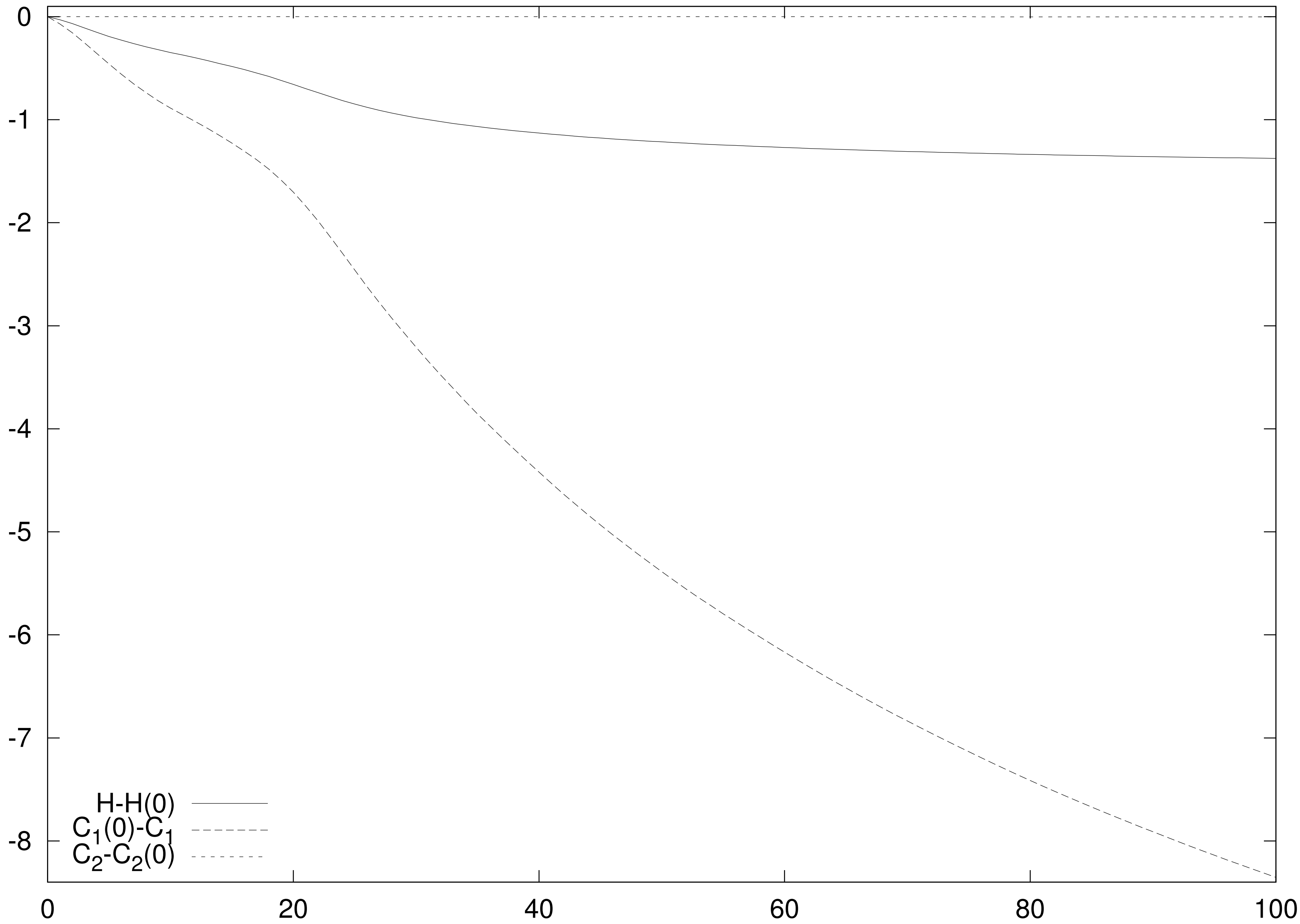
$$L = \int_D (x^2 + y^2)\, d^2x$$

- Strain moment (2-fold symmetry):

$$K = \int_D xy\, d^2x$$

{(fig14)els-2-p0,(fig16)els-4-p0}

Constants vs. t for SA_0



3-fold Symmetry and Dipole DSA

skipping details

{(fig21)tri-db2, (fig27)dip-4-m0}

Underview

1. Dissipative Structures
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   (b) Hamilton Preliminaries
   (c) Hamiltonian Based Dissipative Structures
      i. Double Bracket Dynamics
      ii. Metriplectic Dynamics
2. Computations
   (a) 2D Euler Vortex States
   (b) Vlasov-Poisson BGK?

DG for Vlasov Works

DG for Vlasov

- R. E. Heath, Ph.D. Thesis "Analysis of the Discontinuous Galerkin Method Applied to Collisionless Plasma Physics." (2007)

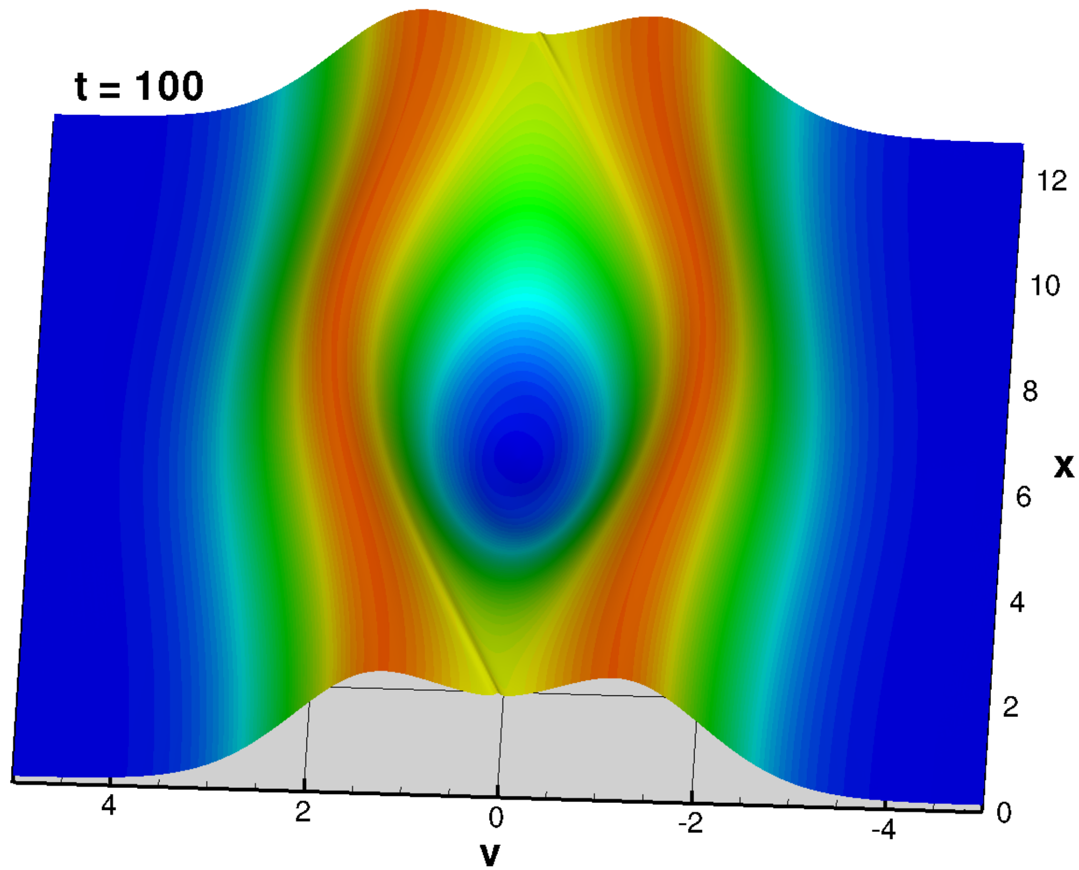
- R. E. Heath, I. M. Gamba, P. J. Morrison, and C. Michler, "A Discontinuous Galerkin Method for the Vlasov-Poisson System, Journal of Computational Physics **231**, 1140–1174 (2012).

- Y. Cheng, I. M. Gamba, and P. J. Morrison, "Study of Conservation and Recurrence of Runge-Kutta Discontinuous Galerkin Schemes for Vlasov-Poisson Systems," Journal of Scientific Computing **56**, 319–349 (2013).

- Y. Cheng, I. M. Gamba, F. Li, and P. J. Morrison, "Discontinuous Galerkin Methods for the Vlasov-Maxwell Equations," submitted (2013).

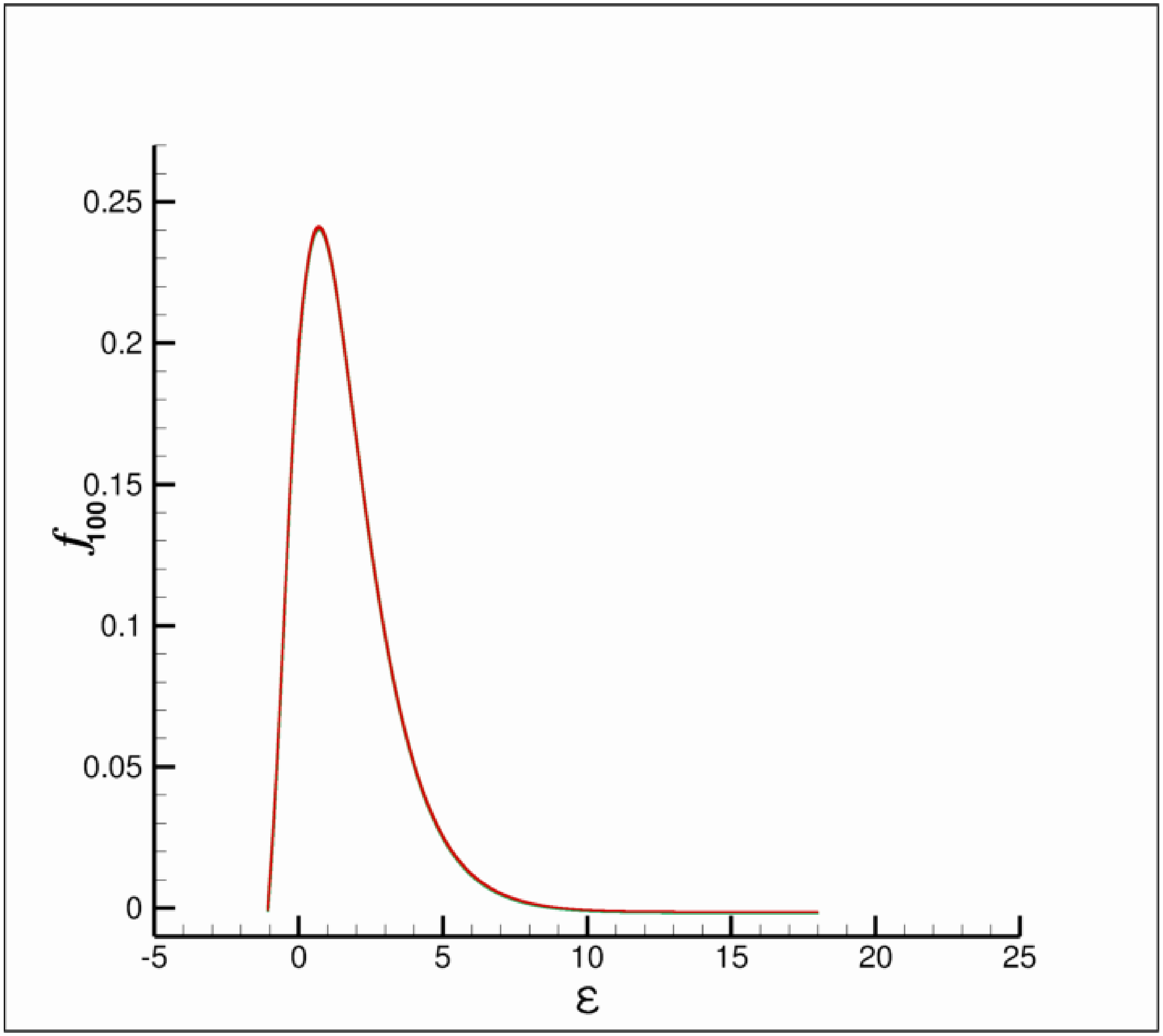
BGK Application?

Symmetric Two-Stream $f \sim v^2 e^{-v^2}$



BGK Application?

Symmetric Two-Stream $f \sim v^2 e^{-v^2}$



$$\mathcal{E} = v^2/2 - \phi$$