The Inclusive Metriplectic Form of Nonequilibirum Thermodynamics

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WORKING ACROSS SCALES IN COMPLEX SYSTEMS

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Overview: Theory of theories/models.

Dynamics – Theories – Models

Goal:

Predict the future or explain the past $\Rightarrow$

$$\dot{z} = V(z)\,, \qquad z \in \mathcal{Z}\,, \ \text{Phase Space}$$

A dynamical system. ODEs, PDEs, etc.

Whence V?

• Fundamental parent theory (microscopic, N interacting gravitating or charged particles, BBGKY hierarchy, Vlasov-Maxwell system, ...). Identify small parameters, rigorous asymptotics $\rightarrow$ Reduced Computable Model V.

• Phenomena based modeling using known properties, constraints, etc. used to intuit $\rightarrow$
Reduced Computable Model V.

Types of Vector Fields, V

Natural Split:

$$V(z) = V_H + V_D$$

- Hamiltonian vector fields, V_H: conservative, properties, etc.
- Dissipative vector fields, V_D: not conservative, relaxation, etc.

General Forms:

$$V_H = J \cdot \nabla H \qquad \text{and} \qquad V_D = G \cdot \nabla F \,,$$

where $J(z)$ is Poisson tensor/operator, H Hamiltonian, $G(z)$ metric tensor/operator, F 'free energy' generator/Lyapunov function. Hamiltonian flows + gradient flows.

Noncanonical Hamiltonian Vector Fields V_H - Poisson Bracket Dynamics

Sophus Lie (1890) $\longrightarrow$ pjm (1980) $\longrightarrow$ Poisson Manifolds etc.

Noncanonical Coordinates:

$$\dot{z}^a = \{z^a, H\} = J^{ab}(z)\frac{\partial H}{\partial z^b}\,, \qquad a, b = 1, 2, \ldots M$$

Noncanonical Poisson Bracket:

$$\{A, B\} = \frac{\partial A}{\partial z^a} J^{ab}(z) \frac{\partial B}{\partial z^b}\,, \qquad \{\,,\}: C^\infty(\mathcal{Z}) \times C^\infty(\mathcal{Z}) \to C^\infty(\mathcal{Z})$$

Poisson Bracket Properties:

antisymmetry $\longrightarrow$ $\{A, B\} = -\{B, A\}$

Jacobi identity $\longrightarrow$ $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$

Leibniz $\longrightarrow$ $\{AC, B\} = A\{C, B\} + \{C, B\}A$

G. Darboux: $det J \neq 0 \Longrightarrow J \to J_c$ Canonical Coords $z = (q, p)$

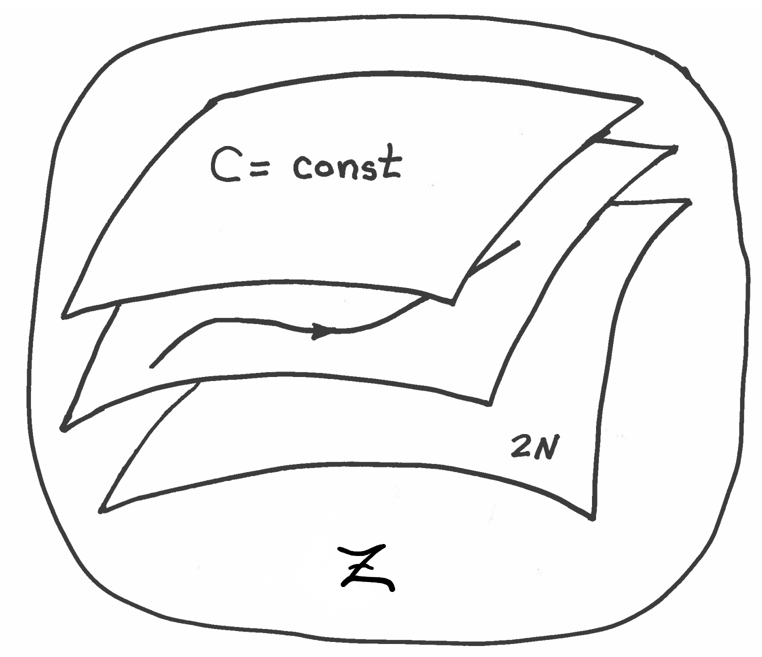
Sophus Lie: $det J = 0 \Longrightarrow$ Canonical Coordinates plus Casimirs
(Lie's distinguished functions!)

Poisson (phase space) Manifold $\mathcal{Z}$ Cartoon

Degeneracy in J $\Rightarrow$ Casimirs:

$$\{A, C\} = 0 \quad \forall\ A\colon \mathcal{Z} \to \mathbb{R}$$

Lie-Darboux Foliation by Casimir (symplectic) leaves:



Examples of Dissipative Vector Fields V_D - Symmetric Bracket Dynamics

Two Types:

- Gradient flows of metriplectic dynamics (pjm 1984, ...).
  Builds in basic thermodynamics and computational tool.

- Double bracket dynamics Vallis et al. 1989.
  Computational tool.

Mixed Flows:

$$\dot{z} = V_H + V_D = J \cdot \nabla H + G \cdot \nabla F = \{z, H\} + (z, F)$$

where $(A, B) = (B, A)$ is a symmetric bracket on functions.

Metriplectic Dynamics – Entropy, Degeneracies, and 1st and 2nd Laws

- Casimirs of noncanonical PB $\{\, ,\, \}$ are 'candidate' entropies. Election of particular $S \in \{\text{Casimirs}\} \Rightarrow$ thermal equilibrium (relaxed) state.

- Generator: $F = H + S$

- 1st Law: identify energy with Hamiltonian, H, then

$$\dot{H} = \{H, F\} + (H, F) = 0 + (H, H) + (H, S) = 0$$

Foliate $\mathcal{Z}$ by level sets of H, with $(H, A) = 0 \ \forall \ A \in C^{\infty}(\mathcal{Z})$.

- 2nd Law: entropy production

$$\dot{S} = \{S, F\} + (S, F) = (S, S) \geq 0$$

Lyapunov relaxation to the equilibrium state. Dynamics solves the equilibrium variational principle: $\delta F = \delta(H + S) = 0$.

Double Bracket Dynamics

Square of Poisson tensor is positive definite:

$$\dot{z} = V_D = JGJ \cdot \nabla H = (z, H)_{DB}$$

Dissipates H but conserves all Casimirs because

$$(C, A)_{DB} = 0 \quad \forall A\,.$$

Examples

Vlasov-Landau Kinetic Theory

System:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f + \frac{e}{m}\boldsymbol{E} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = C_{Landau}[f]\,, \qquad \nabla \cdot \boldsymbol{E} = 4\pi e \int d^3v f\,,$$

$f(\boldsymbol{x}, \boldsymbol{v}, t)$ phase space density, $\boldsymbol{E}$ electric field, $C_{Landau}(f)$ is a complicated nonlinear Fokker-Planck operator.

Hamiltonian:

$$H[f] = \frac{1}{2}\int d^3x d^3v\, mv^2 f + \frac{1}{4\pi}\int d^3x\, |\boldsymbol{E}|^2$$

Dynamics (pjm 1980,1984):

$$\frac{\partial f}{\partial t} = \{f, F\} + (f, F) = \mathcal{J}\frac{\delta H}{\delta f} + \mathcal{G}\frac{\delta S}{\delta f}$$

Casimir:

$$S[f] = c\int d^3x d^3v\, f \ln f$$

Thermodynamic Equilibrium:

$$\dot{S} \geq 0 \Rightarrow \delta F = \delta H + \delta S = 0 \quad \Rightarrow \quad \text{Maxwellian Distribution}$$

Lotka-Volterra – Preditor-Prey

Lotka-Volterra system:

$$\frac{dx}{dt} = \mu x(1-y) \quad \text{and} \quad \frac{dy}{dt} = y(1-x)\,,$$

$x = \#$ prey (rabbits) and $y = \#$ number of predators (foxes).

Noncanonical PB: (Nutku 1990, Shadwick et al. 1999)

$$\{A, B\} = xy\left(\frac{\partial A}{\partial x}\frac{\partial B}{\partial y} - \frac{\partial B}{\partial x}\frac{\partial A}{\partial y}\right)$$

Hamiltonian:

$$H = x - \ln x + \mu y - \mu \ln y$$

Canonization:

$$q = \ln x \quad \text{and} \quad p = \ln y$$

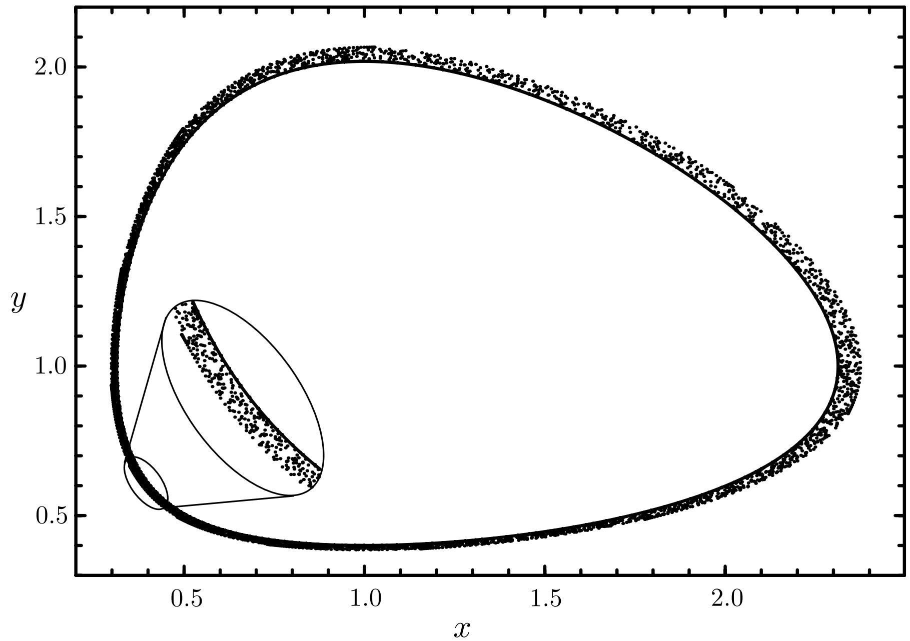


FIG. 8. *Integration of the Lotka–Volterra problem using a standard second-order PC method and a C-PC algorithm, each with* 8×10^5 *time steps of size* 0.02. *A point is plotted every* 200 *time steps. The solid line represents the energy surface containing the initial condition. The points obtained from C-PC all lie on this curve. The dramatic effect of the* 1.2% *energy gain by the standard algorithm is clearly visible.*

Consequence:
Any area in (q, p) space is conserved. Liouville theorem is needed for statistical mechanics.

Metriplectic:
Add entropy degree of freedom to create relaxation to extinction of rabbits, while conserving H

SIR Model of Epidemiology

Reduced SIR model:

$$\dot{S} = -\beta I S\,, \quad \dot{I} = \beta I S - \gamma I\,, \quad \dot{R} = \gamma I\,.$$

Three populations: S for the number of susceptible, I for the number of infected, and R for the number recovered (immune) individuals. $R_0 = \beta/\gamma$ is *reproduction rate*, the expected number of new infections from a single infection for susceptible subjects.

Hamiltonian system?

Total number of people:

$$H = I + S + R \qquad \to \qquad \dot{H} = 0$$

SIR is Hamiltonian

Hamiltonian $\dot{z} = J \cdot \nabla H$:

$$\begin{bmatrix} \dot{S} \\ \dot{I} \\ \dot{R} \end{bmatrix} = \begin{bmatrix} 0 & V_3 & -V_2 \\ -V_3 & 0 & V_1 \\ V_2 & -V_1 & 0 \end{bmatrix} \begin{bmatrix} \partial H/\partial S \\ \partial H/\partial I \\ \partial H/\partial R \end{bmatrix}$$

Jacobi:

$$\boldsymbol{V} \cdot \nabla \times \boldsymbol{V} = 0\,.$$

Poisson Tensor:

$$J = \begin{bmatrix} 0 & -\beta I S & 0 \\ \beta I S & 0 & -\gamma I \\ 0 & \gamma I & 0 \end{bmatrix}$$

Casimir $\{A, C\} = 0\ \forall A$:

$$C = \gamma \ln(S) + \beta R$$

Metriplectic SIR for Optimal Outcome

Find symmetric bracket st

$$\dot{H} = 0 \quad \text{and} \quad \lim_{t \to \infty} I = 0$$

What is G?

$$G = c\Big(\nabla H \otimes \nabla H - |\nabla H|^2 I\Big) = c \begin{bmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{bmatrix}$$

Design dissipation to decrease infection at fixed populationn!

Conclusion

- Structure is important, i.e., the split: $V = V_H + V_D$.

- There exist generalizations, e.g., driven/control extensions.