# Hamiltonian and Metriplectic Descriptions of Plasma and other Matter

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<u>Survey</u> the Hamiltonian and dissipative structure of plasma models. Describe uses: model consistency, stability, and computation. Two methods GEMPIC a Poisson integrator and simulated annealing/metriplectic relaxation for MHD equilibria.

#### Hamiltonian and Metriplectic Descriptions of Plasma and other Matter

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Physical models that describe the dynamics of matter, whether they be discrete, like those for interacting particles or dust, or continuum models, like those for fluids and plasmas, possess structure. The structure may be of *Hamiltonian* type (see [1, 2] for review) and/or posses dissipation and exhibit *metriplectic* structure [3] (see [4] for review). The structure may give rise to conservation laws resulting from Galilean, Poincare, or other invariance, or it may assure the property of entropy production giving relaxation to thermal equilibrium. On a basic level, all structure ultimately arises from an underlying Hamiltonian form that may or may not be maintained in approximations and/or reductions of various kinds.

I will survey the structure and its uses for a variety of models, with an emphasis on general magnetofluid models [5, 6, 7, 8, 9, 10, 11] and Vlasov-Maxwell theory [1, 12]. In particular, I will discuss structure preserving numerical algorithms and how structure can be used to design algorithms for specific purposes [13, 14, 15, 16]. Although symplectic integration has been well studied and widely used for finite-dimensional systems, the preservation of the structure that occurs in continuum models such as extended magnetohydrodynamics with generalized helicities, is considerably more difficult to implement. Progress in developing a discrete version of the Maxwell-Vlasov system that preserves its Hamiltonian structure, and its numerical implementation will be discussed [14].

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A Survey of

- Hamiltonian Structure of Ideal Plasma Dynamics
- Metriplectic Dynamics of Dissipative Plasma Dynamics
- Structure Preserving Computation

For long list of references see abstract.

# Hamilton's Equations

Phase Space with Canonical Coordinates: (q, p)Hamiltonian function:  $H(q, p) \leftarrow$  the energy

Equations of Motion:

$$\dot{p}_i = -\frac{\partial H}{\partial q^i}, \qquad \dot{q}^i = \frac{\partial H}{\partial p_i}, \qquad i = 1, 2, \dots N$$

Phase Space Coordinate Rewrite:  $z = (q, p), \quad \alpha, \beta = 1, 2, ... 2N$ 

$$\dot{z}^{\alpha} = J_{c}^{\alpha\beta} \frac{\partial H}{\partial z^{\beta}} = \{ z^{\alpha}, H \}, \qquad (J_{c}^{\alpha\beta}) = \begin{pmatrix} 0_{N} & I_{N} \\ -I_{N} & 0_{N} \end{pmatrix},$$

 $J_c := \underline{\text{Poisson tensor}}, \text{ Hamiltonian bi-vector, cosymplectic form}$ symplectic 2-form = (cosymplectic form)<sup>-1</sup>:  $\omega_{\alpha\beta}^c J_c^{\beta\gamma} = \delta_{\alpha}^{\gamma},$ 

#### **Noncanonical Hamiltonian Dynamics**

Sophus Lie (1890)

Noncanonical Coordinates:

$$\dot{z}^{\alpha} = J^{\alpha\beta} \frac{\partial H}{\partial z^{\beta}} = \{z^{\alpha}, H\}, \quad \{f, g\} = \frac{\partial f}{\partial z^{\alpha}} J^{\alpha\beta}(z) \frac{\partial g}{\partial z^{\beta}}, \quad \alpha, \beta = 1, 2, \dots M$$
Poisson Bracket Properties:

antisymmetry  $\longrightarrow \{f, g\} = -\{g, f\},\$ 

Jacobi identity  $\longrightarrow \{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$ 

G. Darboux:  $detJ \neq 0 \implies J \rightarrow J_c$  Canonical Coordinates Sophus Lie:  $detJ = 0 \implies$  Canonical Coordinates plus <u>Casimirs</u>

$$J \to J_d = \begin{pmatrix} 0_N & I_N & 0\\ -I_N & 0_N & 0\\ 0 & 0 & 0_{M-2N} \end{pmatrix}$$

#### Poisson Manifold $\mathcal{M}$ Cartoon

Degeneracy in  $J \Rightarrow$  Casimirs:  $\{f, C\} = 0 \quad \forall f : \mathcal{M} \rightarrow \mathbb{R}$ 

Lie-Darboux Foliation by Casimir (symplectic) leaves:



Leaf vector fields,  $Z_f = \{z, f\} = Jdf$  are tangent to leaves.

#### **Noncanonical Poisson Brackets**

• All nondissipative (correct!) plasma models have them: Ideal fluid flow, two-fluid theory, MHD, shearflow, variety of reduced fluid models, extended MHD, Vlasov-Maxwell, BBGKY, etc.

Yoshida + pjm exotic ones

$$\{f,g\} = \frac{\partial f}{\partial z^{\alpha}} J^{\alpha\beta}(z) \frac{\partial g}{\partial z^{\beta}} \quad \rightarrow$$
$$\{F,G\} = \int d\mu \, \frac{\delta F}{\delta \psi} \, \mathbb{J}(\psi) \, \frac{\delta G}{\delta \psi}$$

with  $\mathbb{J}$  and operator.

For example:  $\psi = (v, B, \rho, p)$  for MHD.

Magnetohydrodynamics (MHD)

# MHD

#### Equations of Motion:

Energy:

$$H = \int_D d^3x \, \left(\frac{1}{2}\rho |v|^2 + \rho U(\rho, s) + \frac{1}{2}|B|^2\right)$$

Thermodynamics:

$$p = \rho^2 \frac{\partial U}{\partial \rho}$$
  $T = \frac{\partial U}{\partial s}$  or  $p = \kappa \rho^{\gamma}$ 

Noncanonical Lie-Poisson Bracket (pjm & Greene 1980):

$$\{F,G\} = -\int_{D} d^{3}x \left[ M_{i} \left( \frac{\delta F}{\delta M_{j}} \frac{\partial}{\partial x^{j}} \frac{\delta G}{\delta M_{i}} - \frac{\delta G}{\delta M_{j}} \frac{\partial}{\partial x^{j}} \frac{\delta F}{\delta M_{i}} \right) \right. \\ + \rho \left( \frac{\delta F}{\delta M} \cdot \nabla \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta M} \cdot \nabla \frac{\delta F}{\delta \rho} \right) + \sigma \left( \frac{\delta F}{\delta M} \cdot \nabla \frac{\delta G}{\delta \sigma} - \frac{\delta G}{\delta M} \cdot \nabla \frac{\delta F}{\delta \sigma} \right) \\ + \left. B \cdot \left[ \frac{\delta F}{\delta M} \cdot \nabla \frac{\delta G}{\delta B} - \frac{\delta G}{\delta M} \cdot \nabla \frac{\delta F}{\delta B} \right] \\ + \left. B \cdot \left[ \nabla \left( \frac{\delta F}{\delta M} \right) \cdot \frac{\delta G}{\delta B} - \nabla \left( \frac{\delta G}{\delta M} \right) \cdot \frac{\delta F}{\delta B} \right] \right],$$

Dynamics:

$$\frac{\partial \rho}{\partial t} = \{\rho, H\}, \quad \frac{\partial s}{\partial t} = \{s, H\}, \quad \frac{\partial v}{\partial t} = \{v, H\}, \text{ and } \frac{\partial B}{\partial t} = \{B, H\}.$$

Densities:

$$M := \rho v \qquad \qquad \sigma := \rho s$$

## **Casimir Invariants**

Helicities are Casimir Invariants:

 $\{F, C\}^{MHD} = 0 \quad \forall \text{ functionals } F.$ 

Casimirs Invariants (helicities):

$$C_B = \int d^3x \, \boldsymbol{B} \cdot \boldsymbol{A}, \qquad C_V = \int d^3x \, \boldsymbol{B} \cdot \boldsymbol{v}$$

Topological content, linking etc.

Extended MHD (XMHD)

#### **XMHD** Scaled

Ohm's Law:

$$egin{aligned} m{E} + m{V} imes m{B} &= rac{d_e^2}{
ho} \left( rac{\partial m{J}}{\partial t} + 
abla \cdot ig( m{V} m{J} + m{J} m{V} - rac{d_i}{
ho} m{J} m{J} ig) 
ight) \ &+ rac{d_i}{
ho} ig( m{J} imes m{B} - 
abla p_e ig). \end{aligned}$$

Momentum:

$$\rho\left(\frac{\partial V}{\partial t} + (V \cdot \nabla)V\right) = -\nabla p + J \times B$$
$$-d_e^2 J \cdot \nabla\left(\frac{J}{\rho}\right)$$

Two parameters,  $d_e = \frac{c}{\omega_{p_e}L}$  measures electron inertia and  $d_i = \frac{c}{\omega_{p_i}L}$  accounts for current carried by electrons mostly ... .

#### **Energy Conservation**

Candidate Hamiltonian:

$$H = \int d^3x \left[ \rho \frac{|V|^2}{2} + \rho U(\rho) + \frac{|B|^2}{2} + d_e^2 \frac{|J|^2}{2\rho} \right]$$

Kimura and pjm 2014 on energy conservation

*H* is conserved. Pressure,  $p = \rho^2 \partial U / \partial \rho$ .

What is the Poisson bracket? Casimirs? Helicities?

# **XMHD** Hamiltonian Structure

Yoshida, Abdelhamid, Kawazura, pjm, Lingam, Miloshevich, D'Avignon

Poisson Bracket:

$$\{F,G\}^{XMHD} = \{F,G\}^{MHD} + d_e^2 \int_D d^3x \left[ \frac{\nabla \times \mathbf{V}}{\rho} \cdot \left( \left( \nabla \times F_{\mathbf{B}^\star} \right) \times \left( \nabla \times G_{\mathbf{B}^\star} \right) \right) \right] + d_i \int_D d^3x \frac{\mathbf{B}^\star}{\rho} \cdot \left[ \left( \nabla \times F_{\mathbf{B}}^\star \right) \times \left( \nabla \times G_{\mathbf{B}}^\star \right) \right]$$

where we introduce the 'inertial' magnetic field

$$\mathbf{B}^{\star} = \mathbf{B} + d_e^2 \, \nabla \times \left( \frac{\nabla \times \mathbf{B}}{\rho} \right) \,,$$

Hamiltonian:

$$H = \int_D d^3x \left[ \frac{\rho |\mathbf{V}|^2}{2} + \rho U(\rho) + \frac{\mathbf{B} \cdot \mathbf{B}^*}{2} \right] \,.$$

# **XMHD** Hamiltonian Structure (cont)

Casimirs;

$$C_{XMHD}^{\pm} = \int_D d^3x \, \left( \mathbf{V} + \lambda_{\pm} \mathbf{A}^* \right) \cdot \left( \nabla \times \mathbf{V} + \lambda_{\pm} \mathbf{B}^* \right) \,,$$

where

$$\lambda_{\pm} = \frac{-d_i \pm \sqrt{d_i^2 + 4d_e^2}}{2d_e^2}.$$

Jacobi Identity:

Directly Abdelhamid et al.; remarkable transformations Lingam et al. which lead to **normal fields.** 

### **Normal Fields**

Normal Fields:

$$\boldsymbol{\mathcal{B}}_{\pm} := \mathbf{B} + d_e^2 \, \nabla \times \left[ \frac{\nabla \times \mathbf{B}}{\rho} \right] + \lambda_{\pm} \nabla \times \mathbf{V}$$

XMHD remarkably yields:

 $\frac{\partial \mathcal{B}_{\pm}}{\partial t} + \pounds_{V_{\pm}} \mathcal{B}_{\pm} = 0 \quad \leftarrow \quad \text{Lie dragging} \Rightarrow 2 \text{ frozen fluxes!}$ Hamiltonian Reconnection  $\rightarrow \text{Kawazura}$ 

Dragging velocities:

$$\mathbf{V}_{\pm} = \mathbf{V} - \lambda_{\mp} \nabla \times \mathbf{B} / \rho$$

Helicities:

$$K_{\pm} = \int \mathsf{A}_{\pm} \wedge d\mathsf{A}_{\pm}, \qquad \mathcal{B}_{\pm} = \nabla \times \mathbf{A}_{\pm} \sim d\mathsf{A}_{\pm}$$

Maxwell-Vlasov

#### **Maxwell Part**



#### **Coupling to Vlasov**

$$\frac{\partial f_s}{\partial t} = -\boldsymbol{v} \cdot \nabla f_s - \frac{e_s}{m_s} \left( \mathbf{E} + \frac{\boldsymbol{v}}{c} \times \mathbf{B} \right) \cdot \frac{\partial f_s}{\partial \boldsymbol{v}}$$

$$\rho_e(\boldsymbol{x},t) = \sum_s e_s \int f_s(\boldsymbol{x},\boldsymbol{v},t) \, d^3 v \,, \quad \boldsymbol{J}_e(\boldsymbol{x},t) = \sum_s e_s \int \boldsymbol{v} \, f_s(\boldsymbol{x},\boldsymbol{v},t) \, d^3 v$$

 $f_s(x, v, t)$  is a phase space density for particles of species s with charge and mass,  $e_s, m_s$ .

$$\psi = \left( \mathbf{E}(\boldsymbol{x},t), \, \mathbf{B}(\boldsymbol{x},t), \, f_s(\boldsymbol{x},\boldsymbol{v},t) \right)$$

#### Maxwell-Vlasov Hamiltonian Structure

Hamiltonian:

$$H = \sum_{s} \frac{m_s}{2} \int |v|^2 f_s \, d^3 x \, d^3 v + \frac{1}{8\pi} \int (|\mathbf{E}|^2 + |\mathbf{B}|^2) \, d^3 x \, ,$$

Bracket:

$$\{F, G\} = \sum_{s} \int \left( \frac{1}{m_{s}} f_{s} \left( \nabla F_{f_{s}} \cdot \partial_{v} G_{f_{s}} - \nabla G_{f_{s}} \cdot \partial_{v} F_{f_{s}} \right) \right. \\ \left. + \frac{e_{s}}{m_{s}^{2}c} f_{s} \mathbf{B} \cdot \left( \partial_{v} F_{f_{s}} \times \partial_{v} G_{f_{s}} \right) \right. \\ \left. + \frac{4\pi e_{s}}{m_{s}} f_{s} \left( G_{\mathbf{E}} \cdot \partial_{v} F_{f_{s}} - F_{\mathbf{E}} \cdot \partial_{v} G_{f_{s}} \right) \right) d^{3}x d^{3}v \\ \left. + 4\pi c \int \left( F_{\mathbf{E}} \cdot \nabla \times G_{\mathbf{B}} - G_{\mathbf{E}} \cdot \nabla \times F_{\mathbf{B}} \right) d^{3}x ,$$

where  $\partial_v := \partial/\partial v$ ,  $F_{f_s}$  means functional derivative of F with respect to  $f_s$  etc.

pjm 1980,1982; Marsden and Weinstein 1982

# Maxwell-Vlasov Structure (cont)

Equations of Motion:

$$\frac{\partial f_s}{\partial t} = \{f_s, H\}, \quad \frac{\partial \mathbf{E}}{\partial t} = \{\mathbf{E}, H\}, \quad \frac{\partial \mathbf{B}}{\partial t} = \{\mathbf{B}, H\}.$$

Casimirs invariants:

$$\begin{aligned} \mathcal{C}_{s}^{f}[f_{s}] &= \int \mathcal{C}_{s}(f_{s}) d^{3}x d^{3}v \\ \mathcal{C}^{E}[\mathbf{E}, f_{s}] &= \int h^{\mathbf{E}}(x) \left( \nabla \cdot \mathbf{E} - 4\pi \sum_{s} e_{s} \int f_{s} d^{3}v \right) d^{3}x \,, \\ \mathcal{C}^{B}[\mathbf{B}] &= \int h^{\mathbf{B}}(x) \, \nabla \cdot \mathbf{B} \, d^{3}x \,, \end{aligned}$$

where  $C_s$ ,  $h^E$  and  $h^B$  are arbitrary functions of their arguments. These satisfy the degeneracy conditions

$$\{F,C\} = 0 \quad \forall F.$$

# **Summary**

Poisson brackets defined by  $\mathbb{J}$ , dynamics  $\partial \psi / \partial t = \{\psi, H\}$ :

$\mathbb{J}_{MHD}$	$\rightarrow$	Casimirs
$\mathbb{J}_{XMHD}$	$\rightarrow$	Casimirs
$\mathbb{J}_{V-M}$	$\rightarrow$	Casimirs

**Good theories** in their ideal limit  $(\nu, \eta, \dots \rightarrow 0)$  conserve energies, *H*, and have **Poisson brackets**. Bad theories do bad things: unaccounted energy, unphysical instabilities, etc.

# **Other Models**

• **Reduced Fluid Models**: aspect ratio expansion, 4-field model, fluid models with gyroviscosity, Hall physics, etc.

Hazeltine et al., Waelbroeck, Tassi, Grasso, Pegoraro et al., ...

• Hybrid Models: hot particle species, kinetic MHD, gyro-fluid models , etc.

Tronci, Tassi, et al., Burby et al., etc. ...

**The good theories** in their ideal limit  $(\nu, \eta, \dots \rightarrow 0)$  conserve energies, *H*, and have **Poisson brackets**. Bad theories do bad things: unaccounted energy, unphysical instabilities, etc. **Bonus**: Casimir invariants emerge.

# **Energy Principles**

All good theories have energy principles, akin to  $\delta W$  of MHD.

$$\frac{\partial \psi}{\partial t} = \{\psi, H\} = \{\psi, H + C\} = 0 \quad \rightarrow$$

- Variational principle for equilibrium,  $\delta F = \delta(H + C) = 0$
- Dirichlet energy theorem:  $\delta^2 F$  definite  $\Rightarrow$  stability
- Lagrange iff energy theorem:  $\delta^2 F = \text{Kinetic} + \text{Potential}$

MHD: e.g. Andreussi, et al. 2010 – 2019 XMHD: e.g. Kaltsas et al. 2019

Explains "mysterious" ad hoc discoveries over the years and leads to new results.

# **Dissipation and Metriplectic Dynamics**

# **Metriplectic Dynamics**

General dynamical framework making thermodynamics dynamical.

Captures:

- First Law: conservation of energy
- Second Law: entropy production

pjm, ... 1982,1984. ... Generic 1998

## **Prototypes and Examples**

- Finite-dimensional systems: rigid body ,,, Materassi, Tassi, ...
- Kinetic theories: Vlasov Fokker-Planck equation, Lenard-Balescu equation, etc.
- Fluid flows: various nonideal fluids, Navier-Stokes, MHD, XMHD, etc.
- Many more ...

# Entropy, Degeneracies, and 1st and 2nd Laws

- Casimirs of  $\{,\}$  are 'candidate' entropies. Election of particular  $S \in \{\text{Casimirs}\} \Rightarrow \text{thermal equilibrium (relaxed) state.}$
- Generator (free energy):  $\mathcal{F} = H + S$
- <u>1st Law</u>: identify energy with Hamiltonian, H, then  $\dot{H} = \{H, \mathcal{F}\} + (H, \mathcal{F}) = 0 + (H, H) + (H, S) = 0$ Degeneracy such that  $(H, f) = 0 \forall f$
- <u>2nd Law</u>: entropy production

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

Lyapunov relaxation to the equilibrium state:  $\delta \mathcal{F} = 0$ .

#### **Preliminaries**

Entropy/volume:  $\sigma(x,t)$ 

Density of Extensive variable:  $\zeta_a(x,t)$  a = 1, 2, ...

$$d\sigma = \sum_{a} \frac{\partial \sigma}{\partial \zeta_a d\zeta_a} =: \sum_{a} X^a d\zeta_a$$

$$\frac{\partial \zeta_a}{\partial t} + \nabla \cdot \boldsymbol{J}_T = \sum_a \boldsymbol{J}_a \cdot \nabla X^a \,,$$

$$J_T = \sum_a X^a J_a$$
,  $J_a = unknown flux?$ 

Near Equilibrium Assumption:

$$J_a = \sum_b L_{ab} \nabla X^b$$

Onsager for Afifnity  $\nabla X^a$ :

$$L_{ab} = L_{ba} \qquad \Rightarrow \qquad \text{Second Law}$$

# Whence (F, G)?

The Dissipative Bracket:

$$(F,G) = \frac{1}{\mathcal{T}} \int d^3x \, \nabla \frac{\delta F}{\delta \zeta_a} \cdot L_{ab}[\zeta] \cdot \nabla \frac{\delta G}{\delta \zeta_b}$$

Natural Variable  $\mathcal{E}$ :

$$H = \int d^3 x \, \mathcal{E} \qquad \Rightarrow \quad (F, H) = 0 \quad \forall F$$

Hamiltonian  $(M, B^*, \rho, \sigma)$  vs. Metriplectic  $(M, B^*, \rho, \mathcal{E})$ 

**Onsager Pairs** (Force/Flux):

- Current ↔ Temp, etc., in particular
- Viscosity  $\leftrightarrow$  Current

XMHD, Coquinot & pjm 2019

# **Structure and Computation**

- Poisson Integrator
- Simulated Annealing

# **Poisson Integrator**

**Symplectic Integrator:**  $z(t) \rightarrow z(t + \delta t)$  via a canonical transformation  $\Rightarrow$  volume preservation, all Poincare invariants, symplectic invariants. Energy is shadowed.

Noncanonical phase space (Poisson manifold):



#### **Poisson Integrator**:

- Exactly preserves Casimir leaf (constraint surface)
- Symplectic on each leaf.

# GEMPIC

A Maxwell-Vlasov structure preserving particle-in-cell algorithm.

**A** Poisson integrators:

Kraus, et al. 2017.

Other structure preserving: Qin + , Xiao Zhou, ... Shadwick +, etc.

Review: pjm 2017

# Discretizing the Noncanonical Maxwell-Vlasov Hamiltonian Structure

- Discretize fields f (particles), E, B (finite element exterior calculus)
- Discretize Vlasov-Maxwell noncanonical Poisson bracket
- $\bullet$  Discretize Hamiltonian  $\widehat{\mathcal{H}}$
- Obtain finite-dimensional noncanonical Hamiltonian system for

$$z = (z^1, z^2, \dots, z^N) = (X, V, E, B)$$
  
 $\dot{z}^i = \{z^i, \hat{\mathcal{H}}\}_d$ 

with N very large. Splitting method.

# **Simulated Annealing**

Metriplectic integrators: For accurate collision operators, that relax to thermal equilibrium while preserving energy etc. Hirvijoki, Kraus, Burby, ...

Relaxation by False Dynamics: Construct system, metriplectic or other that relaxes to desired equilbrium while conserving desired quantities. MHD equilibria: <u>Furukawa</u>, Bressen, Maj, ... Geophysical Fluid Dynamics: Flierl + pjm

# **Underview**

A Survey of

- Hamiltonian Structure of Ideal Plasma Dynamics
- Metriplectic Dynamics of Dissipative Plasma Dynamics
- Structure Preserving Computation

For long list of references see abstract.