On the Hamiltonian Structure of the Low Rank Method for Vlasov-Poisson

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Plasma Models with Common Noncanonical (Lie-Poisson) Hamiltonian Structure

- Particles in Given Fields (α-particles)
- Fluid Models (MHD, XMHD, 2-fluid, gyrofluid ...)
- Kinetic Theories
  - Maxwell-Vlasov
  - Gyrokinetics
  - Drift Kinetic
  - **Vlasov-Poisson** $\leftarrow$ **can do** $\Rightarrow$ **can do all!**
- Wigner-Weyl Quantum Mechanics (also Wigner-Poisson)

Structure Preserving Numerics

Process for Initial Value Problem Numerics: **PDE** $\rightarrow$ **ODE** $\rightarrow$ **time stepping**

- Hamiltonian
  - Conservative integrators (energy, other invariants)
  - Symplectic integrators (measure, Poincaré invariants, ...)
  - Poisson integrators (Symplectic plus leaf preservation, e.g., GEMPIC)
- Dissipative
  - Metriplectic integrator (thermodynamic consistency, $\dot{H} = 0, \dot{S} \geq 0$)

Hamilton's Canonical Equations

Phase Space with Canonical Coordinates: (q, p)

Hamiltonian function: $H(q, p)$ $\leftarrow$ the energy

Equations of Motion:

$$\boxed{\dot{p}_i = -\frac{\partial H}{\partial q^i} \quad \text{and} \quad \dot{q}^i = \frac{\partial H}{\partial p_i}} \qquad i = 1, 2, \ldots N$$

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

$$\dot{z}^\alpha = J_c^{\alpha\beta} \frac{\partial H}{\partial z^\beta} = \{z^\alpha, H\}_c \quad \text{where} \quad (J_c^{\alpha\beta}) = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix}$$

$J_c :=$ Poisson tensor, Hamiltonian bi-vector, cosymplectic form

Noncanonical Hamiltonian Structure

Sophus Lie (1890) $\longrightarrow$ PJM (noncanonical 1980) $\longrightarrow$ Weinstein (1982) Poisson Manifolds

Noncanonical Coordinates:

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

Noncanonical Poisson Bracket:

$$\{f, g\} = \frac{\partial f}{\partial z^\alpha} J^{\alpha\beta}(z) \frac{\partial g}{\partial z^\beta}$$

Bilinear Poisson Bracket Properties:

antisymmetry $\rightarrow$ $\{f, g\} = -\{g, f\}$ $\rightarrow$ $J^{\alpha\beta} = -J^{\beta\alpha}$

Jacobi identity $\rightarrow \{f, \{g, h\}\} + \{b, \{h, f\}\} + \{h, \{f, g\}\} = 0 \rightarrow$ Jacobiator $S^{\alpha\beta\gamma} = J^{\alpha\ell}\partial_\ell J^{\beta\gamma} + cyc \equiv 0$

Leibniz $\rightarrow$ $\{fh, g\} = f\{h, g\} + \{h, g\}f\,, \qquad fg$ pointwise

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

Sophus Lie: $detJ = 0 \Longrightarrow$ Canonical Coordinates plus Casimirs $\leftarrow$ G. Sudarshan
(Lie's distinguished functions!)

Noncanonical Poisson Brackets – Flows on Poisson Manifolds

Definition. A Poisson manifold $\mathcal{Z}$ has bracket

$$\{\,,\}\colon C^\infty(\mathcal{Z})\times C^\infty(\mathcal{Z})\to C^\infty(\mathcal{Z})$$

st $C^\infty(\mathcal{Z})$ with $\{\,,\}$ is a Lie algebra realization, i.e., is

- $\mathbb{R}$-bilinear,
- antisymmetric,
- Jacobi identity
- Leibniz, i.e., acts as a derivation $\Rightarrow$ vector field.

Geometrically $C^\infty(\mathcal{Z})\equiv\Lambda^0(\mathcal{Z})$ and $\boldsymbol{d}$ exterior derivative.

$$\{f,g\}=\langle \boldsymbol{d}f, J\boldsymbol{d}g\rangle = J(\boldsymbol{d}f,\boldsymbol{d}g)=\frac{\partial f}{\partial z^\alpha}J^{\alpha\beta}\frac{\partial g}{\partial z^\beta}\,.$$

J the Poisson tensor/operator. Flows are integral curves of noncanonical Hamiltonian vector fields, $J\boldsymbol{d}H$, i.e.,

$$\dot z^\alpha = J^{\alpha\beta}(z)\frac{\partial H(z)}{\partial z^\beta}\,,\qquad \mathcal{Z}'s \text{ coordinate patch } z=(z^1,\dots,z^N)$$

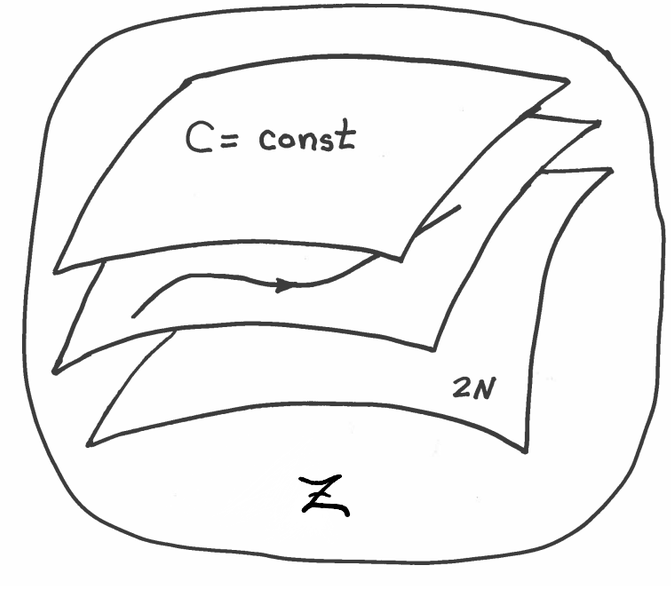
Because of degeneracy, $\exists$ functions C st $\{f,C\}=0$ for all $f\in C^\infty(\mathcal{Z})$, called Casimir invariants.

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

Degeneracy in $J \Rightarrow$ Casimirs:

$$\{f, C\} = 0 \quad \forall\ f : \mathcal{Z} \to \mathbb{R}$$

Lie-Darboux Foliation by Casimir (symplectic) leaves:



Whence Noncanonical? Reduction.

Free Rigid Body Example

Euler angles and conjugate momenta to angular velocities:

$$z = (\chi_1, \chi_2, \chi_3, p_1, p_2, p_3) \to (\omega_1, \omega_2, \omega_3)$$

Bracket Reduction:

$$\left\{\omega_i(\chi_1, \chi_2, \chi_3, p_1, p_2, p_3), \omega_j(\chi_1, \chi_2, \chi_3, p_1, p_2, p_3)\right\}_c = \frac{\partial \omega_i}{\partial z^\alpha} J_c^{\alpha\beta} \frac{\partial \omega_i}{\partial z^\alpha} = \epsilon_{ijk}\omega_k \frac{\partial f}{\partial \omega_i}\frac{\partial j}{\partial \omega_g}$$

Hamiltonian Reduction:

$$H(\alpha, \beta, \gamma, p_\alpha, p_\beta, p_\gamma) = \frac{1}{2} I_1 \omega_1^2 + \frac{1}{2} I_2 \omega_2^2 + \frac{1}{2} I_3 \omega_3^2$$

Equation of Motion: $\dot{\omega}_i = \{\omega_i, H\}, i = 1, 2, 3 \Rightarrow$

$$\begin{aligned} I_1 \dot{\omega}_1 &= (I_2 - I_3)\, \omega_2\, \omega_3 \\ I_2 \dot{\omega}_2 &= (I_3 - I_1)\, \omega_3\, \omega_1 \\ I_3 \dot{\omega}_3 &= (I_1 - I_2)\, \omega_1\, \omega_2 \end{aligned}$$

Lie-Poisson Brackets

$\mathfrak{g}$ a dim-n Lie algebra with basis $\{e_i\}_{i=1}^n$ and structure constants $\{c_{ij}^k\}$, i.e., $[e_i, e_j] = c_{ij}^k e_k$

$\mathfrak{g}^*$ dual algebra with pairing $\langle \cdot, \cdot \rangle \colon \mathfrak{g}^* \times \mathfrak{g} \to \mathbb{R}$ and basis $\{e_*^i\}_{i=1}^n$ st $\langle e_*^i, e_j \rangle = \delta_j^i$

For smooth $f \colon \mathfrak{g}^* \to \mathbb{R}$, $\boldsymbol{d}f(\mu) \in \mathfrak{g}$ evaluated at $\mu \in \mathfrak{g}^*$ for any $\delta\mu \in \mathfrak{g}^*$,

$$\frac{d}{d\epsilon} f(\mu + \epsilon\delta\mu)\Big|_{\epsilon=0} \langle \delta\mu, \boldsymbol{d}f(\mu) \rangle \qquad \to \qquad \boldsymbol{d}f(\mu) = \frac{\partial f}{\partial \mu_i}(\mu)\, e_i.$$

Lie–Poisson bracket for any $f, g \colon \mathfrak{g}^* \to \mathbb{R}$ is

$$\boxed{\{f, g\}_{\mathfrak{g}}(\mu) := \langle \mu, [\boldsymbol{d}f(\mu), \boldsymbol{d}g(\mu)] \rangle = \mu_k c_{ij}^k \frac{\partial f}{\partial \mu_i} \frac{\partial g}{\partial \mu_j} = J_{ij} \frac{\partial f}{\partial \mu_i} \frac{\partial g}{\partial \mu_j}}$$

Lie–Poisson dynamics for a Hamiltonian $H \colon \mathfrak{g}^* \to \mathbb{R}$ is given by

$$\dot{\mu}_i = \{\mu_i, H\}_{\mathfrak{g}} = \mu_k c_{ij}^k \frac{\partial H}{\partial \mu_j}, \qquad \Leftrightarrow \qquad \dot{\mu} = -\operatorname{ad}^*_{\boldsymbol{d}h(\mu)} \mu.$$

Clebsch Canonization (pjm 1980, Jayawardana et al. 2022)

Associated with Lie–Poisson bracket $\exists$ special canonical system for $\bar{f}, \bar{g} \colon T^*\mathbb{R}^n \to \mathbb{R}$:

$$\left\{\bar{f}, \bar{g}\right\} = \frac{\partial \bar{f}}{\partial q^i}\frac{\partial \bar{g}}{\partial p_i} - \frac{\partial \bar{g}}{\partial q^i}\frac{\partial \bar{f}}{\partial p_i},$$

where $\mu = \mu_i e^i_* \in \mathfrak{g}^*$ and $(q, p) \in T^*\mathbb{R}^n$ are related as follows:

$$\mu_i = c^k_{ij} q^j p_k \,.$$

$f, g \colon \mathfrak{g}^* \to \mathbb{R}$, we define $\bar{f}, \bar{g} \colon T^*\mathbb{R}^n \to \mathbb{R}$ by $\bar{f}(q, p) := f(\mu)$. Then the chain rule $\Rightarrow$

$$\frac{\partial \bar{f}}{\partial q^i} = \frac{\partial f}{\partial \mu_j}\frac{\partial \mu_j}{\partial q^i} = \frac{\partial f}{\partial \mu_j} c^k_{ji} p_k, \qquad \frac{\partial \bar{f}}{\partial p_i} = \frac{\partial f}{\partial \mu_j}\frac{\partial \mu_j}{\partial p_i} = \frac{\partial f}{\partial \mu_j} c^i_{jk} q^k$$

using the Jacobi identity $\Rightarrow$

$$\left\{\bar{f}, \bar{g}\right\}(q, p) = \frac{\partial \bar{f}}{\partial q^i}\frac{\partial \bar{g}}{\partial p_i} - \frac{\partial \bar{g}}{\partial q^i}\frac{\partial \bar{f}}{\partial p_i} = \mu_i c^i_{jk}\frac{\partial f}{\partial \mu_j}\frac{\partial g}{\partial \mu_k} = \{f, g\}_{\mathfrak{g}}(\mu),$$

If the canonical system is solved with Hamiltonian $\bar{H}(q, p) = H(\mu)$ for $(q(t), p(t))$, then $\mu(t)$ solves the Lie–Poisson system!

Poisson Integrator

Def. A Poisson integrator exactly preserves symplectic leaves and is symplectic on leaf.

Thm. *For a class of Lie algebras, a symplectic integrator on* $T^*\mathbb{R}^n$ is Poisson on $\mathfrak{g}^*$.

Comment. Although the dimension is doubled, $\exists$ invariants on $T^*\mathbb{R}^n$ that make it efficient. (dual moment maps)

The Kida Vortex

The Kida vortex is an elliptical patch of constant vorticity in a two-dimensional Euler fluid flow. Dynamical variables are the semi axes a, b and the angle ϕ of orientation:

$$\dot{a} = \frac{\epsilon}{2} a \sin(2\phi), \qquad \dot{b} = -\frac{\epsilon}{2} b \sin(2\phi), \qquad \dot{\phi} = \frac{ab}{(a+b)^2} + \frac{\omega}{2} + \frac{\epsilon}{2} \frac{a^2+b^2}{a^2-b^2} \cos(2\phi),$$

where $\epsilon > 0$ is strain of the background shear flow.

Kida is Lie-Poisson for $\mathfrak{so}(2,1)$ with basis

$$e_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \qquad e_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \qquad e_3 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

structure constants satisfy, for any $\mu \in \mathfrak{so}(2,1)^* \cong \mathbb{R}^3$,

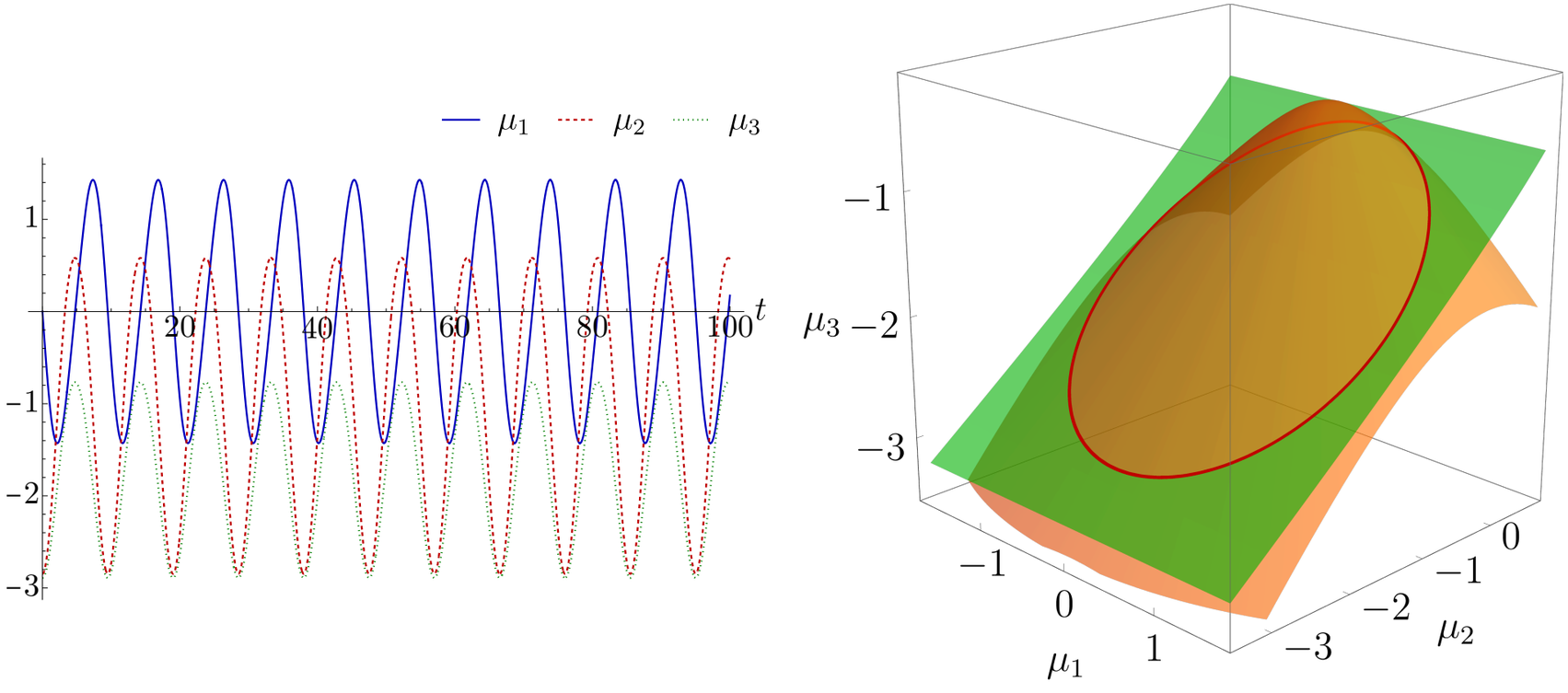
$$\mu_k c_{ij}^k = \begin{bmatrix} 0 & \mu_3 & \mu_2 \\ -\mu_3 & 0 & -\mu_1 \\ -\mu_2 & \mu_1 & 0 \end{bmatrix}.$$

This algebra has the Casimir

$$C(\mu) := \mu_1^2 + \mu_2^2 - \mu_3^2,$$

which is essentially the area of the ellipse.

Poisson Integration for Kida



(Left) Time evolution of μ using the canonized system for $0 \leq t \leq 100$ with time step $\Delta t = 0.1$. (right) Red curve is the Lie–Poisson dynamics in $\mathfrak{g}^* = \mathfrak{so}(2,1)^* \cong \mathbb{R}^3$ computed using the canonized system and momentum mapped by $\mu_i = c_{ij}^k q^j p_k$. Green and orange surfaces are the level sets of the Hamiltonian H and the Casimir C.

Why Poisson Integrator?

Most important plasma basic equations have noncanonical Poisson brackets.

Magnetohydrodynamics pjm & Greene (1980),

Maxwell – Vlasov system (1980, 1982), Marsden & Weinsten (1982)

BBGKY heirarchy: Marsden, pjm, &Weinsetin (1984)

...

GEMPIC, a particle-in-cell (PIC) code Kraus et. al (2017). FEEC builds De Rham cohomology into numerics for Maxwell's equations etc.

Infinite-Dimensional Hamiltonian Systems

Functionals $F\colon \mathcal{B} \to \mathbb{R}$, $\mathcal{B}$ function space, **Functional derivative**: $\partial/\partial z^\alpha \to \delta/\delta\psi$

$$\frac{d}{d\epsilon} F[\psi + \epsilon\delta\psi]\Big|_{\epsilon=0} = \left\langle \frac{\delta F}{\delta \psi}, \delta\psi \right\rangle$$

Wave equation as **canonical** Hamiltonian system:

$$\{F,G\} = \int dx \left(\frac{\delta F}{\delta\psi}\frac{\delta G}{\delta\pi} - \frac{\delta G}{\delta\psi}\frac{\delta F}{\delta\pi} \right), \quad H = \int dx \left(\pi^2 + \psi_x^2\right)/2\,, \quad \text{No Casimirs}$$

$$\partial_t \pi = \{\pi, H\} = \psi_{xx} \quad \text{and} \quad \partial_t \psi = \{\psi, H\} = \pi$$

Vlasov-Poisson as **noncanonical** Hamiltonian system:

$$\{F,G\} = \int dxdv\, f \left[\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right], \quad H = \int dxdv \left(f v^2 + E^2 \right)/2\,, \quad C = \int dxdv\, \mathcal{C}(f)$$

$$[f,g] = \partial_x f \cdot \partial_v g - \partial_x g \cdot \partial_v f$$

$$\partial_t f = \{f, H\} = [\delta H/\delta f, f] = -v \cdot \partial_x f - E \cdot \partial_v f$$

Infinite-Dimensional Clebsch for Vlasov-Poisson

'Potential' Representation:

$$f(x,v,t) = [\chi,\psi] = \partial_x\chi\cdot\partial_v\psi - \partial_x\psi\cdot\partial_v\chi$$

Reduction:

$$\partial_t\chi = \frac{\delta H}{\delta\psi} \qquad \text{and} \qquad \partial_t\psi = -\frac{\delta H}{\delta\chi}$$

Variational principle (integrator), ... Finite elements 1981. Very stiff.

Product structure similar to low rank, but different.

Low Rank for 1D Vlasov-Poisson

Vlasov–Poisson:

$$\partial_t f + v\partial_x f - E\partial_v f = 0$$

Representation:

$$f(t,x,v) = \sum_{i=1}^{r}\sum_{j=1}^{r} X_i(t,x)S_{ij}(t)V_j(t,v)$$

Projections:

$$\langle X_i, X_j\rangle_x = \int dx\, X_i X_j = \delta_{ij}\,, \quad \langle V_i, V_j\rangle = \int dv\, V_i V_j = \delta_{ij} \quad \text{and} \quad \langle f, g\rangle_{xv} = \int dxdv\, fg$$

Alternate Variables:

$$K_j = \sum_i X_i S_{ij}, \qquad L_i = \sum_j S_{ij} V_j \qquad \text{assume } S^{-1} \text{ exists}$$

Low Rank for 1D Vlasov-Poisson (cont)

Equations of Motion:

$$\dot{S}_{ij} = -\sum_{kl}(\langle X_i, \partial_x X_k\rangle_x \langle vV_j, V_l\rangle_v + \langle X_i, EX_k\rangle_x \langle V_j, \partial_v V_l\rangle_v) S_{kl}$$

$$\partial_t K_j = -\sum_{l}\langle vV_j, V_l\rangle_v \partial_x K_l + \sum_{l}\langle V_j, \partial_v V_l\rangle_v E K_l$$

$$\partial_t L_i = -\sum_{k}\langle X_i, \partial_x X_k\rangle_x v L_k + \sum_{k}\langle X_i, EX_k\rangle_x \partial_v L_k$$

or

$$\partial_t S_{ij} = -\sum_{kl}(\langle X_i \partial_x X_k\rangle_x \langle vV_j V_l\rangle_v + \langle X_i EX_k\rangle_x \langle V_j \partial_v V_l\rangle_v) S_{kl}$$

$$\sum_i (\partial_t X_i) S_{ij} = -\sum_{kl}\langle vV_j, V_l\rangle_v S_{kl} \partial_x X_k + \sum_{kl}\langle V_j, \partial_v V_l\rangle_v E S_{kl} X_k - \sum_i X_i (\partial_t S_{ij})$$

$$\sum_j S_{ij} (\partial_t V_j) = -\sum_{kl}\langle X_i, \partial_x X_k\rangle_x v S_{kl} V_l + \sum_{kl}\langle X_i, EX_k\rangle_x S_{kl} \partial_v V_l - \sum_j (\partial_t S_{ij}) V_j$$

Charge density:

$$\rho = 1 - \sum_{ij} X_i S_{ij} \int V_j \, dv = 1 - \sum_{ij} X_i S_{ij} \langle V_j\rangle_v \quad \Rightarrow \; E$$

Problems

Not Hamiltonian!

Does not conserve energy!

Can Fix Via Reduction?

Representation:

$$f(t,x,v) = \sum_{i=1}^{r}\sum_{j=1}^{r} X_i(t,x)S_{ij}(t)V_j(t,v) = XSV$$

Variation:

$$\delta f = X\delta SV + \delta XSV + XS\delta V$$

Constraints:

$$\langle \delta X_i, X_j\rangle_x = 0 \quad \text{and} \quad \langle \delta V_i, V_j\rangle_v = 0$$

Variations:

$$\begin{aligned}
\delta S &= \langle X\otimes V, \delta f\rangle_{xv}\\
\delta V &= -S^{-1}\delta SV + S^{-1}\langle X, \delta f\rangle_x = -S^{-1}\langle X\otimes V, \delta f\rangle_{xv}V + S^{-1}\langle X, \delta f\rangle_x\\
\delta X &= -X\delta SS^{-1} + \langle V, \delta f\rangle_v S^{-1} = -X\langle X\otimes V, \delta f\rangle_{xv}S^{-1} + \langle V, \delta f\rangle_v S^{-1}
\end{aligned}$$

Reduction (cont)

Usual Low Rank:

$$\partial_t f = \mathcal{R}(f) = -vX'SV - EXSV'$$

EoMs:

$$\begin{aligned}
\dot{S} &= \langle X \otimes V, \mathcal{R}(XSV)\rangle_{xv} \\
\partial_t V &= -S^{-1}\langle X \otimes V, \mathcal{R}(XSV)\rangle_{xv} V + S^{-1}\langle X, \mathcal{R}(XSV)\rangle_x \\
\partial_t X &= -X\langle X \otimes V, \mathcal{R}(XSV)\rangle_{xv} S^{-1} + \langle V, \mathcal{R}(XSV)\rangle_v S^{-1}\,.
\end{aligned}$$

Chain Rule $F[f] = \hat{F}[X, S, V]$:

$$\begin{aligned}
\delta F[f; \delta f] &= \langle F_f, X\delta SV + \delta XSV + XS\delta V\rangle_{xv} = \delta\hat{F}[X, S, V; \delta X, \delta S, \delta V] \\
&= \hat{F}_S : \delta S + \langle \hat{F}_X, \delta X\rangle_x + \langle \hat{F}_V, \delta V\rangle_v
\end{aligned}$$

Functional Derivative Projections:

$$\begin{aligned}
F_f = \hat{F}_S : (X \otimes V) + \hat{F}_X V : S^{-1} - \left\langle \hat{F}_{X(x')}, X(x')\right\rangle_{x'} X \otimes VS^{-1} \\
+ \hat{F}_V S^{-1} X - \left\langle \hat{F}_{V(v')}, S^{-1}X \otimes VV(v')\right\rangle_{v'}
\end{aligned}$$

Reduction

$$\{F, G\} = \langle f, [F_f, G_f]\rangle_{xv}$$

Poisson Bracket?

Reduced PB:

$$\{\hat{F},\hat{G}\} = \int dxdv\, XSV \Bigg[\Big(\hat{F}_S : (X' \otimes V) + \hat{F}'_X V : S^{-1} - \left\langle \hat{F}_{X(x')}, X(x') \right\rangle_{x'} X' \otimes V S^{-1} + \hat{F}_V S^{-1} X' - \left\langle \hat{F}_{V(v')}, S^{-1} X' \otimes V V(v') \right\rangle_{v'} \Big) \times \Big(\hat{G}_S : (X \otimes V') + \hat{G}_X V' : S^{-1} - \left\langle \hat{G}_{X(x')}, X(x') \right\rangle_{x'} X \otimes V' S^{-1} + \hat{G}'_V S^{-1} X - \left\langle \hat{G}_{V(v')}, S^{-1} X \otimes V' V(v') \right\rangle_{v'} \Big) \Bigg] \quad - \quad \hat{F} \leftrightarrow \hat{G}$$

Above has 50 terms!

Equations of Motion:

$$\dot{S} = \{S, \hat{H}\}, \quad \partial_t X = \{X, \hat{H}\}, \quad \text{and} \quad \partial_t V = \{V, \hat{H}\}$$

Must conserve energy!

Final comments

- Basic plasma systems have noncanonical Hamiltonian form
- Noncanonical form can be maintained for numerics
- What about ML?

$\rightarrow$ Learn vector fields. Learn noncanonical Hamiltonian structure. Learn Casimirs