On Geometric PIC-like Discretizations of Lie-Poisson Brackets

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Methodology:

PIC algorithms for a general class of **Lie-Poisson** Hamiltonian systems following the **GEMPIC** technology (Poisson integrator) for the Maxwell-Vlasov system. Explain **Dual PIC** for 2D Euler vorticity fluid dynamics.

*with William Barham (Oden Institute) and E. Sonnendruecker (Max Planck NMPP)

Overview

- What is **Lie-Poisson** Hamiltonian Structure?

- What are **PIC** & Vlasov **GEMPIC**?

- What is basic idea of **Dual PIC**?

Noncanonical Hamiltonian Systems – Flows on Poisson Manifolds Generated by Poisson Brackets

A phase space $\mathcal{M}$ diff. manifold with binary bracket operation on $C^\infty(\mathcal{P})$ functions $f, g \colon \mathcal{P} \to \mathbb{R}$, s.t. $\{\cdot\,,\cdot\} \colon C^\infty(\mathcal{P}) \times C^\infty(\mathcal{P}) \to C^\infty(\mathcal{P})$ satisfies

- Bilinear: $\{f + \lambda g, h\} = \{f, h\} + \lambda\{g, h\}\,, \quad \forall f, g, h$ and $\lambda \in \mathbb{R}$
- Antisymmetric: $\{f, g\} = -\{g, f\}\,, \qquad \forall f, g$
- Jacobi: $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} \equiv 0\,, \qquad \forall f, g, h$
- Leibniz: $\{fg, h\} = f\{g, h\} + \{f, h\}g\,, \qquad \forall f, g, h$.

Above is a Lie algebra realization on functions. Take fg to be pointwise multiplication.

Eqs. Motion: $\frac{\partial O}{\partial t} = \{O, H\}$, O an observable & H a Hamiltonian.

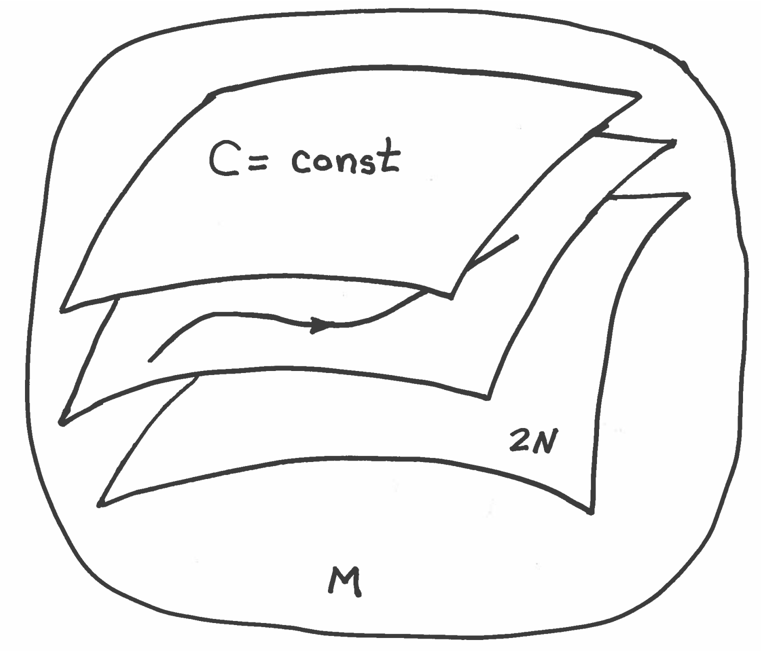
Example: flows on Poisson manifolds, e.g. Weinstein 1983 ....

Poisson Manifold $\mathcal{M}$ Cartoon

Degeneracy in J $\Rightarrow$ Casimirs:

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

Lie-Darboux Foliation by Casimir (symplectic) leaves:



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

Lie-Poisson Brackets

Coordinates:

$$\{f,g\} = \frac{\partial f}{\partial z^\alpha} J^{\alpha\beta} \frac{\partial g}{\partial z^\beta} \qquad \text{where} \qquad J^{\alpha\beta} = c_\gamma^{\alpha\beta} z^\gamma$$

where $c_\gamma^{\alpha\beta}$ are the structure constants for some Lie algebra.

Examples:

• 3-dimensional Bianchi algebras for free rigid body, Kida vortex, & rattleback toy. See Jayawarda, pjm, Ohsawa, arXiv:2106.12552v1 to appear in J. Geom. Mech. for general **Lie-Poisson integrator**.

• Infinite-dimensional theories - matter models: Ideal fluid flow, MHD, shearflow, extended MHD, Vlasov-Maxwell, BBGKY, etc.

Lie-Poisson Geometry

Lie Algebra: $\mathfrak{g}$, a vector space with

$$[\ ,\ ] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}\,,$$

antisymmetric, bilinear, satisfies Jacobi identity

Pairing:

$$\langle\ \ ,\ \rangle : \mathfrak{g}^* \times \mathfrak{g} \to \mathbb{R}$$

with $\mathfrak{g}^*$ vector space dual to $\mathfrak{g}$

Lie-Poisson Bracket:

$$\{f, g\} = \left\langle z, \left[\frac{\partial f}{\partial z}, \frac{\partial g}{\partial z}\right]\right\rangle\,, \qquad z \in \mathfrak{g}^*,\ \frac{\partial f}{\partial z} \in \mathfrak{g}$$

Vlasov-Maxwell System

Maxwell:

$$\frac{\partial \mathbf{B}(\boldsymbol{x},t)}{\partial t} = -c\,\nabla \times \mathbf{E}\,, \qquad \frac{\partial \mathbf{E}(\boldsymbol{x},t)}{\partial t} = c\,\nabla \times \mathbf{B} - 4\pi \boldsymbol{J}_e(\boldsymbol{x},t)$$

$$\nabla \cdot \mathbf{B} = 0\,, \qquad \nabla \cdot \mathbf{E} = 4\pi\rho_e(\boldsymbol{x},t)$$

Vlasov:

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

Coupling:

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

$\mathbf{E}$ & $\mathbf{B}$ electric & magnetic fields, $f_s(\boldsymbol{x},\boldsymbol{v},t)$ is a phase space density for particles of species s with charge and mass, e_s, m_s.

Maxwell-Vlasov Structure

Hamiltonian:

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

Bracket:

$$\begin{aligned}\{F,G\} \;=\; & \sum_s \int \Bigg(\frac{1}{m_s} f_s \left(\nabla F_{f_s}\cdot\partial_{\boldsymbol{v}} G_{f_s} - \nabla G_{f_s}\cdot\partial_{\boldsymbol{v}} F_{f_s}\right) \\ & + \frac{e_s}{m_s^2 c} f_s\, \mathbf{B}\cdot\left(\partial_{\boldsymbol{v}} F_{f_s}\times\partial_{\boldsymbol{v}} G_{f_s}\right) \\ + \; & \frac{4\pi e_s}{m_s} f_s \left(G_{\mathbf{E}}\cdot\partial_{\boldsymbol{v}} F_{f_s} - F_{\mathbf{E}}\cdot\partial_{\boldsymbol{v}} G_{f_s}\right)\Bigg) d^3x\, d^3v \\ + \; & 4\pi c\int (F_{\mathbf{E}}\cdot\nabla\times G_{\mathbf{B}} - G_{\mathbf{E}}\cdot\nabla\times F_{\mathbf{B}})\, d^3x\,,\end{aligned}$$

where $\partial_{\boldsymbol{v}} := \partial/\partial\boldsymbol{v}$, 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:

$$\begin{aligned}
\mathcal{C}_s^f[f_s] &= \int \mathcal{C}_s(f_s)\, d^3x d^3v \\
\mathcal{C}^E[\mathbf{E}, f_s] &= \int h^{\mathbf{E}}(x) \left(\nabla \cdot \mathbf{E} - 4\pi \sum_s e_s \int f_s\, d^3v \right) d^3x\,, \\
\mathcal{C}^B[\mathbf{B}] &= \int h^{\mathbf{B}}(x)\, \nabla \cdot \mathbf{B}\, d^3x\,,
\end{aligned}$$

where $\mathcal{C}_s$, $h^{\mathbf{E}}$ and $h^{\mathbf{B}}$ are arbitrary functions of their arguments. These satisfy the degeneracy conditions

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

PIC (particle in cell)

overcoming the curse of dimensions
Plasma Physics Technique

(Buneman, Dawson, Hockney, Birdsall, ...)

Distribution function f as particles

$$f(\boldsymbol{x},\boldsymbol{v},t) = \sum_{a=1}^{N} w_a\,\delta(\boldsymbol{x}-\boldsymbol{x}_a(t)\,\delta(\boldsymbol{v}-\boldsymbol{v}_a(t))$$

also with shape functions

- Time step particle equations of motion (e.g. Boris)

Maxwell Fields $\boldsymbol{E},\boldsymbol{B}$ on mesh

- Interpolated sources $\rho,\boldsymbol{J}$ on field mesh and compute $\boldsymbol{E},\boldsymbol{B}$

- Obtain $\boldsymbol{E},\boldsymbol{B}$ on particle locations

GEMPIC

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

A Poisson integrator: preserves Casimir leaves exactly; symplectic on a leaf.

Michael Kraus, Katharina Kormann, pjm, and Eric Sonnendrücker, Journal of Plasma Physics **83**, 905830401 (2017).

See William Barham, June 7, MS145 Buskerud (1F).

Discretizing the Noncanonical Maxwell-Vlasov Hamiltonian Structure

- Discretize fields: f (particles), $\boldsymbol{E}$, $\boldsymbol{B}$ (FEEC, Arnold et al.)

- Discretize Vlasov-Maxwell noncanonical Poisson bracket

- Discretize Hamiltonian $\widehat{\mathcal{H}}$

- Obtain finite-dimensional noncanonical Hamiltonian system for

$$z = (z^1, z^2, \ldots, z^N) = (\boldsymbol{Z}, \boldsymbol{V}, \mathbf{E}, \mathbf{B})$$

$$\dot{z}^i = \{z^i, \widehat{\mathcal{H}}\}$$

with N very large. Solve e.g. by Lie-Trotter splitting.
A structure preserving discretization, a flow on Poisson manifold.

de Rham complex

- Spaces of electromagnetics form a de Rham complex

$$H^1(\Omega) \xrightarrow{\text{grad}} H(\text{curl}, \Omega) \xrightarrow{\text{curl}} H(\text{div}, \Omega) \xrightarrow{\text{div}} L^2(\Omega)$$

with $\phi \in H^1(\Omega)$, $\mathbf{E}, \mathbf{A} \in H(\text{curl}, \Omega)$, $\mathbf{B}, \mathbf{J} \in H(\text{div}, \Omega)$, $\rho \in L_2(\Omega)$.

- Equivalent formulation of de Rham complex with differential forms

$$H\Lambda^0(\Omega) \xrightarrow{\text{d}} H\Lambda^1(\Omega) \xrightarrow{\text{d}} H\Lambda^2(\Omega) \xrightarrow{\text{d}} H\Lambda^3(\Omega)$$

Form	integrands	quantity	unit
0-form	point evaluation	ϕ	V
1-form	line integral	$\mathbf{E}$	V/m
2-form	surface integral	$\mathbf{B}$	$(\text{Vs})/\text{m}^2$
3-form	volume integral	ρ	C/m^3

- Exactness: Im(grad) $=$ Ker(curl), Im(curl) $=$ Ker(div).

Dual PIC – Via 2D Euler

Equation of Motion:

$$\frac{\partial \omega}{\partial t} = -\boldsymbol{v} \cdot \nabla \omega = -[\phi, \omega]\,, \qquad \Delta \phi = \omega\,, \quad [\phi, \omega] = \partial_x \phi \partial_y \omega - \partial_y \phi \partial_x \omega$$

vorticity $\omega(x, y, t)$, streamfunction $\phi(x, y, t)$

Lie-Poisson Bracket:

$$\{F, G\} = \int d^2x\ \omega \left[\frac{\delta F}{\delta \omega}, \frac{\delta G}{\delta \omega}\right]$$

Hamiltonian:

$$H[\omega] = -\frac{1}{2} \int d^2x\, \omega \phi$$

Dual PIC Lift

Two copies, dual to each other:

$$\omega \to \omega_1, \omega_2$$

Lifted Poisson Bracket:

$$\{F, G\} = \int d^2x\, \omega_1 \Big([F_1, G_1] + [F_1, G_2] + [F_2, G_1] + [F_2, G_2] \Big)$$

where $F_1 = \delta F / \delta \omega_1$ etc.

Lifted Hamiltonian:

$$H = \int d^2x\, \omega_1 \frac{\delta K}{\delta \omega_2} = -\int d^2x\, \omega_1 \phi_2$$

Casimirs:

$$C_1 = \int d^2x\, \mathcal{C}_1(\omega_1)\,, \qquad C_2 = \int d^2x\, \mathcal{C}_2(\omega_1 - \omega_2)$$

where $\mathcal{C}_{1,2}$ arbitrary. Casimir functions: C_1 weight conservation and C_2 natural interpolator.

Dual PIC Discretization

Dual Discretization:

$$\omega_1 = \sum_{a=1}^{N_p} w_a \delta(\boldsymbol{z}_a - \boldsymbol{z}) \in H^{-1}(\Omega) \quad \text{and} \quad \omega_2 = \sum_{i=1}^{N} \omega_i \psi^i(\boldsymbol{z}) \in H^1(\Omega)$$

$\{\psi_i\}_{i=1}^N$ Galerkin basis, $\boldsymbol{\omega} = \{\omega_i\}_{i=1}^N$, $\boldsymbol{Z} = \{\boldsymbol{z}_a\}_{a=1}^{N_p}$, $\boldsymbol{w} = \{w_a\}_{a=1}^{N_p}$

Discretized Poisson:

$$\{F, G\} = DG(\boldsymbol{Z}, \boldsymbol{\omega})^T \mathbb{J}(\boldsymbol{Z}) DF(\boldsymbol{Z}, \boldsymbol{\omega}).$$

Discretized Hamiltonian:

$$H(\boldsymbol{Z}, \boldsymbol{\omega}) = \frac{1}{2} \mathbf{w}^T \Psi(\boldsymbol{Z}) \frac{\partial K}{\partial \boldsymbol{\omega}}, \quad \text{where } \Psi(\boldsymbol{Z}) = \{\psi_i(z_a)\}_{i,a=1}^{N,N_p}$$

Discretized Dynamics:

$$\dot{O} = \{O, H\}$$

Dual PIC Discretized Casimir

Discretized Casimirs:

$$\mathrm{C}(\boldsymbol{Z}, \boldsymbol{\omega}) = \Psi(\boldsymbol{Z})^T \mathbf{w} - \boldsymbol{\omega}\,, \qquad \text{e.g. choose } \boldsymbol{\omega} = \Psi(\boldsymbol{Z})^T \mathbf{w}$$

Slaved Dynamics:

At any point in the simulation, we may reconstruct the coefficients in the Galerkin basis via $\boldsymbol{\omega} = \Psi(\boldsymbol{Z})^T \mathbf{w}$. Given initial data of vorticity, $\mathring{\omega}(\boldsymbol{z})$, if one draws $\boldsymbol{Z}|_{t=0}$ randomly and uniformly from Ω, and computes $\omega_i|_{t=0} = (\psi_i, \mathring{\omega})$ for $i = 1, \ldots, N$, then one may select the initial weights by finding the least squares solution of $\boldsymbol{\omega} = \Psi(\boldsymbol{Z})^T \mathbf{w}$.

Result is a **Poisson Integrator**.

Dual PIC Generality

- Lie-Poisson systems are ubiquitous in mechanics, fluid mechanics, kinetic theory, plasma physics, ...

- **If** Dual PIC works, it will work for large class of systems!

- To be continued.