Backward Error Analysis of Isospectral Integrators via Lie–Poisson Reduction of Butcher Series

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Incompressible Inviscid Fluid on a 2-Sphere

Equations for the velocity field $\mathbf{v}(x, t)$ of an incompressible inviscid fluid,[1]

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla_{\mathbf{v}} \mathbf{v} = -\nabla p \,, \quad \mathrm{div}(\mathbf{v}) = 0 \,.$$

Consider the *vorticity* function $\omega := \mathrm{curl}(\mathbf{v})$, then,

$$\dot{\omega} + \{\psi, \omega\} = 0 \,, \quad -\Delta \psi = \omega \,, \tag{1}$$

where ψ is called the *stream function* and $\{\cdot, \cdot\}$ is the Poisson bracket on the sphere,[2]

Equation (1) is a *Lie–Poisson system* with the Hamiltonian given by the kinetic energy of the fluid,

$$H(\omega) = \frac{1}{2} \int_{\mathbb{S}^2} \omega (-\Delta)^{-1} \omega \,.$$

[1] L. Euler. Principes généraux de l'état d'équilibre d'un fluide. Académie Royale des Sciences et des Belles-Lettres de Berlin, Mémoires, 11:217–273, 1757.

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Matrix Hydrodynamics

The PDE for the vorticity ω,

$$\dot{\omega} + \{\psi, \omega\} = 0\,, \quad -\Delta\psi = \omega\,,$$

is discretized in space by the Euler-Zeitlin equation,

$$\dot{W} + \frac{1}{\hbar}[W, P] = 0\,, \quad -\Delta_d P = W\,,$$

where $W \in \mathfrak{u}(d)$.[3]

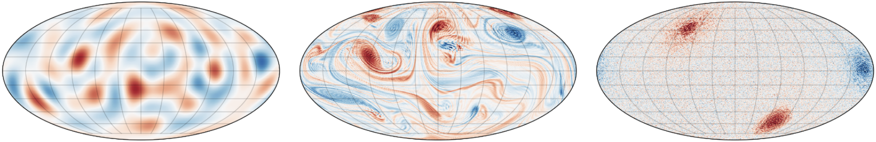
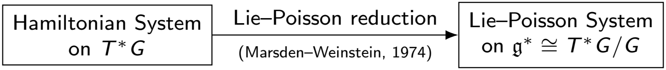


Figure: Vorticity field of a 2D fluid flow on a sphere.[3]

[3] K. Modin and M. Viviani. Two-dimensional fluids via matrix hydrodynamics (arXiv:2405.14282).

Lie–Poisson reduction



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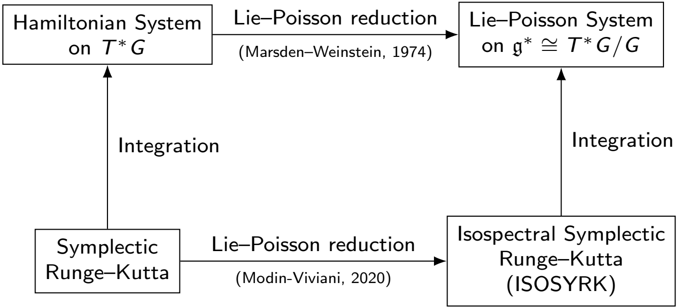

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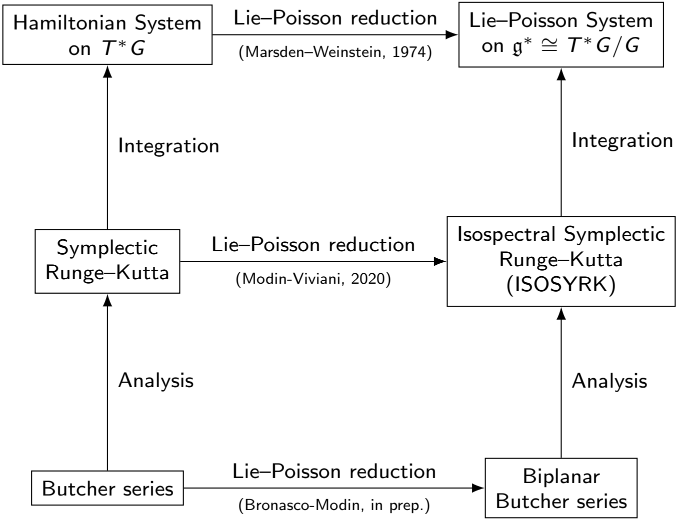

Outline

1. Lie–Poisson reduction and ISOSYRK methods
2. Biplanar Butcher series
   1. Biplanar forests and forest momentum map
   2. Biplanar Butcher series and Lie–Poisson reduction
   3. Composition and substitution laws
   4. Comparison with RKMK methods

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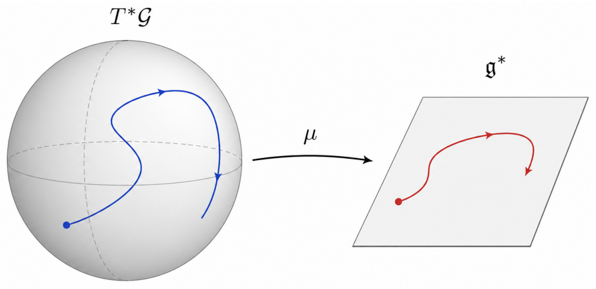
Part 1

Lie–Poisson reduction



Consider the following isospectral equation with linear $f : \mathfrak{u}(d)^* \to \mathfrak{u}(d)^*$,

$$\dot{W} = \mathrm{ad}^*_{f(W)}(W) = [f(W), W] , \quad W(0) = W_0 ,$$

where we assume $f(W) = \nabla H(W)^\dagger$ with the inner product on $\mathfrak{u}(d)$ given by $\langle A, B \rangle = \mathrm{Tr}(A^\dagger B)$ and Hamiltonian $H : \mathfrak{u}(d)^* \to \mathbb{R}$.

The flow of this equation lives on the coadjoint orbit of $U(d)$,

$$\mathcal{O}(W_0) := \{ \mathrm{Ad}^*_Q W_0 \mid Q \in U(d) \} ,$$

where $\mathrm{Ad}^*_Q W = Q W Q^\dagger$ is the coadjoint action of $U(d)$ on $\mathfrak{u}(d)^* \cong \mathfrak{u}(d)$.

Let the *momentum map* $\mu : T^*U(d) \to \mathfrak{u}(d)^*$ be $\mu(Q, P) := Q^\dagger P$,

$$\left.\begin{aligned} \dot{Q} &= Q \nabla H(Q^\dagger P) \\ \dot{P} &= -P \nabla H(Q^\dagger P)^\dagger \end{aligned}\right\} \mu_\sharp f .$$

is a Hamiltonian system on $T^*U(d)$ with the Hamiltonian $H \circ \mu$.

The flow $W(t)$ is given by $W(t) = \mu\big(Q(t), P(t)\big) = Q(t)^\dagger P(t)$.

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Isospectral Symplectic Runge–Kutta methods

Consider a symplectic Runge–Kutta method $(Q_n, P_n) \mapsto (Q_{n+1}, P_{n+1})$, the corresponding ISOSYRK[4] method is obtained by

$$W_{n+1} = Q_{n+1}^{\dagger} P_{n+1}\,, \quad \text{where } (Q_n, P_n) = (I, W_n)\,.$$

Let $A = (a_{ij})_{i,j=1}^{s}$ and $b = (b_i)_{i=1}^{s}$ of a symplectic Runge–Kutta method,

$$\begin{aligned} W_{n+1} &= W_n + h\sum_{i=1}^{s} b_i[f(\tilde{W}_i), \tilde{W}_i]\,, \qquad \tilde{W}_i = W_n + h\sum_{j=1}^{s} a_{ij}(X_j + Y_j + K_{ij})\,, \\ X_i &= -(W_n + h\sum_{j=1}^{s} a_{ij}X_j) f(\tilde{W}_i)\,, \qquad Y_i = f(\tilde{W}_i)(W_n + h\sum_{j=1}^{s} a_{ij}Y_j)\,, \\ K_{ij} &= h\sum_{k=1}^{s} f(\tilde{W}_i)(a_{ik}X_k + a_{jk}K_{ik})\,, \end{aligned} \tag{2}$$

[4] K. Modin and M. Viviani, Lie–Poisson Methods for Isospectral Flows, Foundations of Computational Mathematics, 20 (2020)

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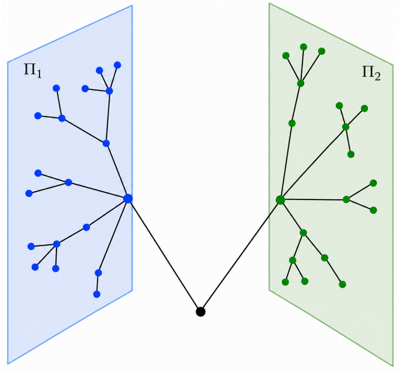
Part 2

Biplanar Butcher series



Runge–Kutta methods

Consider the following ODE where $f : \mathbb{R}^d \to \mathbb{R}^d$ is a smooth vector field:

$$\dot{y}(t) = f(y(t)), \quad y(0) = y_0 \in \mathbb{R}^d.$$

A widely used class of integrators is the Runge–Kutta family

$$\begin{aligned} Y_i &= y_0 + h\sum_{j=1}^{s} a_{ij} f(Y_j), \\ y_1 &= y_0 + h\sum_{i=1}^{s} b_i f(Y_i), \end{aligned} \qquad \text{with} \qquad \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}.$$

We can Taylor expand y_1 around y_0 to obtain

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i \cdot f(y_0) + h^2 \sum_{i=1}^{s} b_i c_i \cdot f'(y_0) f(y_0) + \cdots.$$

Runge–Kutta method is *symplectic* if

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, \quad \text{for } i, j = 1, \ldots, s.$$

Butcher series[5,6]

Consider rooted non-planar trees $T := \{\bullet,\ [\bullet],\ [\bullet,\bullet],\ [[\bullet]],\ \dots\}$.

$$a_{RK}(\bullet) = \sum b_i\,, \qquad a_{RK}([[\bullet]]) = \sum b_i a_{ij} c_j\,,$$

$$a_{RK}([\bullet]) = \sum b_i c_i\,, \qquad a_{RK}([\bullet,\bullet]) = \sum b_i c_i^2\,.$$

Let $a : T \to \mathbb{R}$, then a Butcher series is a formal sum $B(a) : \mathbb{R}^d \to \mathbb{R}^d$:

$$B_f(a)(y_0) := y_0 + h a(\bullet) f(y_0) + h^2 a([\bullet]) f' f(y_0) + h^3 \frac{a([\bullet,\bullet])}{2} f''(f,f)(y_0) + h^3 a([[\bullet]]) f' f' f(y_0) + \cdots\,.$$

RK methods: $y_1 = B_f(a_{RK})(y_0)\,,$ Order conditions:

Exact solution: $y(h) = B_f(e)(y_0)\,,$ $a_{RK}(\tau) = e(\tau)\,.$

[5] J. C. Butcher. Coefficients for the study of Runge-Kutta integration processes. J. Austral. Math. Soc., 3:185–201, 1963.

[6] E. Hairer and G. Wanner. On the Butcher group and general multi-value methods. Computing (Arch. Elektron. Rechnen), 13 (1):1–15, 1974

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Biplanar forests

Start with the following recursive definition:

1. a *biplanar tree* is denoted by $B^+(\pi, \eta)$ where (π, η) is a biplanar forest,
2. a *biplanar forest* (π, η) is a pair of ordered monomials π and η of biplanar trees.

The set of trees is denoted by BT, ordered monomials of trees by $T(BT)$ and the set of forests by BF. Note that $(\pi, \eta) = (\eta, \pi)$.

Let the *Butcher product* for $\tau \in T$ and $\pi \in F$ be defined as

$$\tau \triangleright B^+(\pi) = B^+(\tau\pi)\,.$$

The *forest momentum map* $\psi : BF \to T^2$ is given by

$$\psi(\pi, \eta) = \psi(\pi)\psi(\eta)\,, \quad \psi(\pi \cdot \tau) = \psi(\pi) \triangleright \psi(\tau)\,,$$

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Biplanar action

Let $\mathcal{U}^2$ be the commutative product of the universal enveloping algebra of $\mathfrak{u}(d)$, that is, $\mathcal{U}^2 := \mathcal{U} \cdot \mathcal{U}$ with $(A, B) = (B, A)$ where $A, B \in \mathcal{U}$.

Consider the action $\odot : \mathcal{U}^2 \otimes \mathfrak{u}(d) \to \mathfrak{u}(d)$,

$$(A, B) \odot W = AWB^\dagger + BWA^\dagger \,,$$

which generalizes the well-known actions,

$$\mathrm{Ad}^*_Q W = \frac{1}{2}(Q, Q) \odot W \,, \quad \mathrm{ad}^*_{\tilde{W}} W = (\tilde{W}, I) \odot W \,.$$

Elementary differential $\mathbb{F}_f(\pi, \eta)$ is defined as,

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Biplanar Butcher series

Biplanar Butcher series are defined for $\alpha : BF \to \mathbb{R}$ as

$$B_f(\alpha) = \sum_{(\pi,\eta)\in BF} \frac{\alpha(\pi,\eta)}{\sigma(\pi,\eta)} \mathbb{F}_f(\pi,\eta)\,.$$

Theorem (Lie–Poisson reduction of biplanar Butcher series)

Let $a, b : F \to \mathbb{R}$ be such that $a(\mathbf{1}) = 1, a(\pi \cdot \eta) = a(\pi)a(\eta)$ and $b(\mathbf{1}) = 0, b(\pi \cdot \eta) = 0$. Then,

$$\mu \circ B_{\mu_\sharp f}(a) = B_f(a \circ \psi) \circ \mu\,, \quad B_{\mu_\sharp f}(b) = \mu_\sharp B_f(b \circ \psi)\,,$$

The composition and substitution laws follow,

$$B_f(a_1 \circ \psi) \circ B_f(a_2 \circ \psi) = B_f\big((a_2 * a_1) \circ \psi\big)\,,$$
$$B_{\frac{1}{h} B_f(b\circ\psi)}(a \circ \psi) = B_f\big((b \star a) \circ \psi\big)\,.$$

Biplanar Butcher series

Biplanar Butcher series are defined for $\alpha : BF \to \mathbb{R}$ as

$$B_f(\alpha) = \sum_{(\pi,\eta)\in BF} \frac{\alpha(\pi,\eta)}{\sigma(\pi,\eta)} \mathbb{F}_f(\pi,\eta) .$$

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Let $\alpha : BF \to \mathbb{R}$ be a coefficient map and let $\alpha_T := \alpha|_{T(BT)}$.

Corollary (Butcher series of ISOSYRK methods)

Let Φ_h be a symplectic Runge–Kutta method which can be expanded as $B_{\mu_\sharp f}(a)$ and let Ψ_h be the corresponding ISOSYRK method, then,

$$\Psi_h(W_0) = B_f(\alpha) \odot W_0 = Ad^*_{B_f(\alpha_T)(W_0)} W_0\,,$$

where $\alpha = a \circ \psi$ and $B_f(\alpha_T)(W_0) \in U(d)$.

Corollary (Backward error analysis of ISOSYRK methods)

Let Φ_h be a symplectic Runge–Kutta method with the modified equation given by $B_{\mu_\sharp f}(b)$, then, $B_f(\beta)$ is the modified vector field of the corresponding ISOSYRK method Ψ_h with $\beta = b \circ \psi$. Moreover,

$$B_f(\beta) \odot W_0 = ad^*_{B_f(\beta_T)(W_0)} W_0\,,$$

where $B_f(\beta_T)(W_0) \in \mathfrak{u}(d)$.

Moreover, the modified Hamiltonians are related by $\tilde{H} = \tilde{\mathcal{H}} \circ \mu$.

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Let us use the following notation,

$$\epsilon = \frac{h}{\hbar}\,, \quad \delta = f(W)\,, \quad \gamma = \delta^2 + f\big([\delta, W]\big)\,.$$

Modified Hamiltonian of the midpoint ISOSYRK method is given by

$$\begin{aligned}\tilde{H}_h(W) = H(W) &- \frac{1}{12}\epsilon^2\langle \delta W \delta^\dagger, \delta\rangle_d - \frac{1}{24}\epsilon^2\langle [\delta, W], f\big([\delta, W]\big)\rangle_d \\ &+ \frac{1}{80}\epsilon^4\langle \gamma W \gamma^\dagger, \delta\rangle_d \\ &+ \frac{1}{160}\epsilon^4\langle \gamma W + W\gamma^\dagger, f\big(\gamma W + W\gamma^\dagger\big)\rangle_d \\ &+ \frac{1}{240}\epsilon^4\langle \gamma W \delta^\dagger + \delta W \gamma^\dagger, f\big([\delta, W]\big)\rangle_d \\ &+ \frac{1}{240}\epsilon^4\langle \gamma W + W\gamma^\dagger, f(\delta W \delta^\dagger)\rangle_d \\ &+ \frac{7}{480}\epsilon^4\langle \delta W \delta^\dagger, f(\delta W \delta^\dagger)\rangle_d + \mathcal{O}(\epsilon^6)\,.\end{aligned}$$

Engø-Faltinsen[7] introduce Runge–Kutta–Munthe-Kaas methods for Lie–Poisson systems. A Lie–Poisson system can be written as,

$$W(t) = \mathrm{Ad}^*_{\exp(\omega(t))} W_0 \,, \quad \text{where } \dot{\omega} = \mathrm{dexp}_{\omega}^{-1} f\big(W(t)\big) \,.$$

Therefore, given any Runge–Kutta method Φ_h, it can be integrated as

$$W_1 = \mathrm{Ad}^*_{\exp(\Phi_h(\omega_0))} W_0 \,, \quad \text{where } \omega_0 = 0 \,.$$

Proposition

RKMK methods are expanded as biplanar Butcher series with coefficient maps $\alpha : BF \to \mathbb{R}$ satisfying $\alpha_T(\pi \sqcup \eta) = \alpha_T(\pi)\alpha_T(\eta)$.

Corollary

ISOSYRK methods are not RKMK methods.

[7] K. Engø and S. Faltinsen, Numerical Integration of Lie–Poisson Systems While Preserving Coadjoint Orbits and Energy, SIAM Journal on Numerical Analysis, 39 (2001)

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Conclusion

In this talk, we have,

1. introduced biplanar forest and Butcher series,
2. introduced forest momentum map and performed Lie–Poisson reduction of Butcher series,
3. obtained composition and substitution laws for biplanar Butcher series,
4. analysed geometric properties of ISOSYRK methods,
5. compared ISOSYRK methods with RKMK methods for Lie–Poisson systems.

Thank you for your attention!

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Thank you for your attention!