Towards symplectic Lie-group integrators!

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Lie group integrators

(Cambridge-Trondheim-Bergen 1995 -> ...)

LGI generalizes classical integrators, based on the commutative action of translations on $\mathbb{R}^n$

$$y_{n+1} = y_n + \Phi(h, F, y_n, \ldots),$$

to methods based on Lie group actions on a manifold $\mathcal{M}$

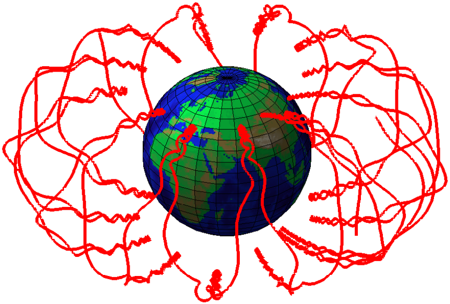
$$y_{n+1} = g(h, f, y_n, \ldots)\cdot y_n, \quad g \in G, y \in \mathcal{M}.$$

Common families of methods:

- Methods based on commutators.
- Commutator-free methods.
- Magnus series methods.

Example: An oscillatory problem

Carl Størmer explains Aurorae (1907).



Størmer developed an excellent symplectic integrator.
He 'ran' his scheme on human compuers (students),
4500 CPU hours! Three steps per hour ...

Aurora example (cont.)

Equation of motion:

$$\begin{pmatrix} y(t) \\ v(t) \end{pmatrix}' = \begin{pmatrix} v(t) \\ v(t) \times B(y) \end{pmatrix}, \quad B(y): \text{ magnetic field}$$

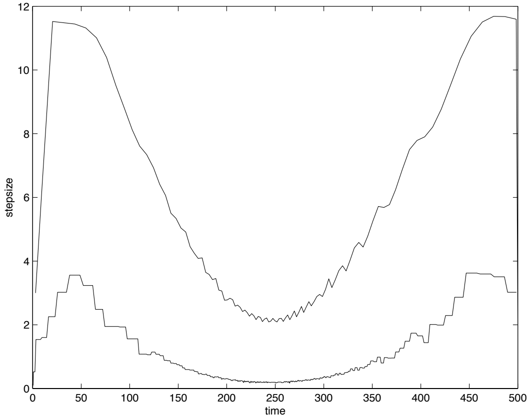
Lie group action by freezing magnetic field (⇒ helical motion):

$$\begin{pmatrix} y(t) \\ v(t) \end{pmatrix}' = \begin{pmatrix} v(t) \\ v(t) \times B(y_0) \end{pmatrix}.$$

Equations rewritten by action of GL(6) on $\mathbb{R}^6$. $f\colon \mathcal{M} \to \mathfrak{gl}(6)$

$$\begin{pmatrix} y \\ v \end{pmatrix}' = \begin{pmatrix} v \\ v \times B(y) \end{pmatrix} = \begin{pmatrix} 0 & I \\ 0 & -\widehat{B(y)} \end{pmatrix} \cdot \begin{pmatrix} y \\ v \end{pmatrix} = f(y) \cdot \begin{pmatrix} y \\ v \end{pmatrix}.$$

Størmers problem integrated with an LGI



Stepsize in LGI and RK-45.

LGI is more efficient, since it can take 8-10 times longer steps with same accuracy.

Analysis of time integration methods

Questions:

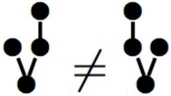
- Order theory. Taylor expansion of numerical solution and analytical solution, $\Rightarrow$ algebraic conditions on coefficients of method by matching as many terms as possible.
- Backward error analysis. What differential equation does the numerical solution solve?
- Geometric properties of the numerical integrator. Preservation of first integrals? Preservation of symplecticity?

Tools for classical integrators: B-series, S-series
(J. Butcher, Hairer, Wanner, Murua, ++).

Tools for LGI: Generalization of B-series to non-commutative actions:
Lie-Butcher theory, LS-series
(MK, Owren-Marthinsen, Owren-Berland, MK-Krogstad, MK-Wright).

Tree-Expansions, brief history:

- *Trees, B-series*: Cayley 1857, Merson 1957, Butcher 1963-1972, Hairer-Wanner 1974.
- *Connections to Hopf*: A. Dür 1986, Connes, Moscovici, Kreimer 1998, Brouder 2000, Murua 1999.
- *B-series and symplecticity*: Sanz-Serna Abia (91), Hairer (93), Calvo Sanz-Serna (94),..., Murua, Chartier Hairer Vilmart (05).
- *Lie-Butcher theory* (1995-present): Extension of B-theory to general non-commutative group actions on manifolds.
  MK (95,98), Owren-Marthinsen (99), MK-Krogstad (03), Owren-Berland (03), Owren (06), MK-Wright (07).



B-series and symplecticity, backward error style:

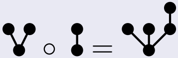
Consider $\mathbb{R}^{2n}$ with standard symplectic structure $\Omega = \sum_{i=1}^{n} dp_i \wedge dq_i$ and let f be a symplectic vectorfield.

Theorem (CHV05)

An autonomous vectorfield $g(y)$, defined by B-series

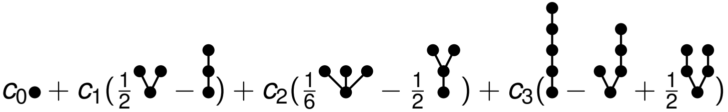
$$g(y) = B_f(b, y) = \sum_{\tau \in T} \frac{b(\tau)}{\sigma(\tau)} \mathcal{F}_f(\tau)(y)$$

is symplectic iff $b(\tau_1 \circ \tau_2) + b(\tau_2 \circ \tau_1) = 0$ for all $\tau_1, \tau_2 \in T$, where



(Butcher product)

Example:



Goals in development of symplectic LGIs:

Let (P, Ω) be a general Poisson manifold.
Let a Hamiltonian group action

$$\cdot : G \times P \to P$$

define Lie–Butcher LS-series on P.

Main Goals:

1. Characterize all LS-series representing (autonomous) symplectic vectorfields on P.
2. Characterize all *elementary Hamiltonian vectorfields*.
3. Construct symplectic Lie group integrators.

Today: (1) and (2), a'la Chartier Hairer Vilmart (05) (backward error).

Motivating examples

1. Classical case: $P = \mathbb{R}^{2n}$, $\Omega = \sum dp_i \wedge dq_i$, $G = R^{2n}$ acting by translation. (G is action of all linear Hamiltonians).
2. Quadratic hamiltonian action: $P = \mathbb{R}^{2n}$, $\Omega = \sum dp_i \wedge dq_i$, $G = \mathrm{SP}(2n) \rtimes \mathbb{R}^{2n}$ the action induced by all linear and quadratic Hamiltonians.
3. Lie-Poisson systems: G any Lie group with Lie algebra $\mathfrak{g}$, $P = \mathfrak{g}^*$, G acts by coadjoint action on P. Symplectic form: $\Omega(f,g)(y) = y([f(y), g(y)])$ for vectorfields $f, g \colon P \to \mathfrak{g}$ and $y \in P = \mathfrak{g}^*$.
   (Poisson bracket Ω is linear in y).

Basic operations in Lie–Butcher theory [MK-Wright 07]

Given vectorfields $f, g\colon P \to \mathfrak{g}$, written in terms of a rigid frame as

$$f(y) = \sum_i f_i(y)E_i, \quad g(y) = \sum_j g_j(y)E_j, \text{where } \{E_i\}_i \text{ is a basis for } \mathfrak{g}.$$

Basic operations:

- Frozen concatenation, *fg* defined as:

$$(fg)(y) = f(y)g(y) = \sum_{ij} f_i(y)g_j(y)E_iE_j \in U(\mathfrak{g}).$$

- Covariant derivation wrt. flat connection (absolute parallelism), $f[g]$ defined as

$$f[g](y) = \sum_{ij} f_i(y)E_i[g_j]E_j.$$

... basic operations

- Torsion bracket, $[f, g]$ defined as:

$$[f, g](y) = [f(y), g(y)] = (fg - gf)(y).$$

- Operator composition, $f \circ g$ defined as:

$$f \circ g = fg + f[g].$$

- Jacobi bracket $[f, g]_J$, defined as

$$[f, g]_J = f \circ g - g \circ f = [f, g] + f[g] - g[f].$$

Note:

$$\begin{aligned} (f \circ g)[h] &= f[g[h]] \quad \text{for any } h\colon P \to U(\mathfrak{g}). \\ [f, g] &= [f, g]_J - f[g] + g[f], \end{aligned}$$

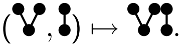
thus $[f, g]$ is the torsion of the (flat) absolute-parallelism-connection.

Basic operations on trees

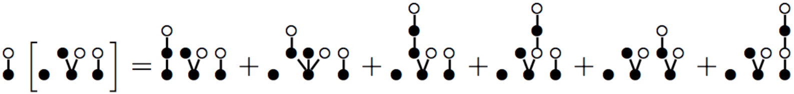
Note:

All basic operations have nice geometric interpretations, and all of these can be lifted to the algebra of LS series over trees and forests. (Universal property of LS series).

- Frozen concatenation $\leftrightarrow$ word concatenation:



- Covariant derivation $\leftrightarrow$ Left grafting:



- Operator composition $\leftrightarrow$ Grossman-Larson product $\tau_1 \circ \tau_2 = \tau_1 \tau_2 + \tau_1[\tau_2]$.

Main result

Result

Under the *Symplectic Torsion Assumption*, we can achieve our goals (1) and (2), i.e. characterizing symplectic LS series and elementary Hamiltonian vectorfields.

Symplectic Torsion Assumption (STA)

A hamiltonian vectorfield f satisfies STA if for all frozen vectorfields U we have that also the torsion $[U, f] = Uf - fU$ is symplectic.

Note: $[U, f]_J = [U, f] + U[f]$, thus STA implies $U[f]$ symplectic.

Basic techniques for proving symplecticity

Definition

A vectorfield f is symplectic if $d(\imath_f \Omega) = 0$, where d is exterior derivation and i inner product.

Lemma

Suppose that G acts transitively on the symplectic leaves of P. Then a vectorfield f is symplectic iff

$$\Omega(U[f], V) = -\Omega(U, V[f]) \quad \textit{for all frozen } U, V.$$

Proof

is based on Cartan Magic Formula $\imath_V \mathrm{d}\alpha = \mathcal{L}_V \alpha - \mathrm{d}\imath_V \alpha$, and the Jacobi rule for symplectic vectorfields g, h, k:

$$\Omega([g,h]_J, k) + \Omega([h,k]_J, g) + \Omega([k,g]_J, h) = 0. \tag{1}$$

... proving symplecticity

Example

Show that the LS series $h = 2\begin{smallmatrix}\bullet\\|\\\bullet\\|\\\bullet\end{smallmatrix} - \begin{smallmatrix}\bullet\ \ \bullet\\\vee\\\bullet\end{smallmatrix} - [\bullet, \begin{smallmatrix}\bullet\\|\\\bullet\end{smallmatrix}]$ is symplectic.

Evaluate $\Omega(U[h], V)$ at $y \in \mathcal{P}$. Open nodes denote freezing at y.

$$
\begin{aligned}
U[2\begin{smallmatrix}\bullet\\|\\\bullet\\|\\\bullet\end{smallmatrix}] &= 2U[\begin{smallmatrix}\circ\\|\\\circ\\|\\\bullet\end{smallmatrix}] + 2U[\begin{smallmatrix}\circ\\|\\\bullet\end{smallmatrix}][\bullet] + 2U[\bullet][\bullet][\bullet]\\
U[-\begin{smallmatrix}\bullet\ \ \bullet\\\vee\\\bullet\end{smallmatrix}] &= -U[\begin{smallmatrix}\circ\ \ \circ\\\vee\\\bullet\end{smallmatrix}] - 2U[\bullet][\begin{smallmatrix}\circ\\|\\\bullet\end{smallmatrix}] - U[[\circ,\bullet]][\bullet]\\
U[-[\bullet,\begin{smallmatrix}\bullet\\|\\\bullet\end{smallmatrix}]] &= U[[\begin{smallmatrix}\circ\\|\\\bullet\end{smallmatrix},\circ]] - U[\bullet][[\circ,\bullet]] + U[[\begin{smallmatrix}\circ\\|\\\circ\end{smallmatrix},\bullet]]\\
0 &= \Omega(U[\begin{smallmatrix}\circ\ \ \circ\\\vee\\\bullet\end{smallmatrix}] + U[[\circ,\bullet]][\bullet] + U[\bullet][[\circ,\bullet]], V) \quad \text{(Jacobi++)}.
\end{aligned}
$$

$$
\begin{aligned}
\Omega(U[h], V) &= \Omega(U, -2V[\begin{smallmatrix}\circ\\|\\\circ\\|\\\bullet\end{smallmatrix}] + 2V[\bullet][\begin{smallmatrix}\circ\\|\\\bullet\end{smallmatrix}] - 2V[\bullet][\bullet][\bullet] - 2V[\begin{smallmatrix}\circ\\|\\\bullet\end{smallmatrix}][\bullet]) +\\
&\quad \Omega(U, V[[\begin{smallmatrix}\circ\\|\\\bullet\end{smallmatrix},\circ]] + V[[\begin{smallmatrix}\circ\\|\\\circ\end{smallmatrix},\bullet]]) = \Omega(U, -V[h]).
\end{aligned}
$$

Basic techniques for finding elementary Hamiltoinans

Definition

A vectorfield X_H is Hamiltonian if there exists a Hamiltonian function H such that

$$\imath_{X_H}\Omega = \mathrm{d}H.$$

Lemma

The Hamiltonian vectorfield X_H satisfies:

$$U[H] = \Omega(X_H, U) \quad \textit{for all frozen } U.$$

Definition

Given a Hamiltonian H and a tree $\tau = B^+(\tau_1 \ldots \tau_k)$ there exists an elementary Hamiltonian vectorfield $X_{\tilde{H}} = \Phi_H(\tau)$ with the Hamiltonian

$$\tilde{H} = (\tau_1 \ldots \tau_k)[H].$$

Computing $\Phi_H(\tau)$

We seek a vectorfield $\Phi_H(\tau)$ satisfying

$$U[(\tau_1 \dots \tau_k)[H]] = \Omega(\Phi_H(\tau), U) \quad \text{for all frozen } U.$$

This is done by computing at an arbitrary point $y \in P$, splitting in frozen vectorfields and using the formula

$$f[\Omega(g, h)] = \Omega([h, g]_J, f)$$

valid for any f and symplectic g, h.

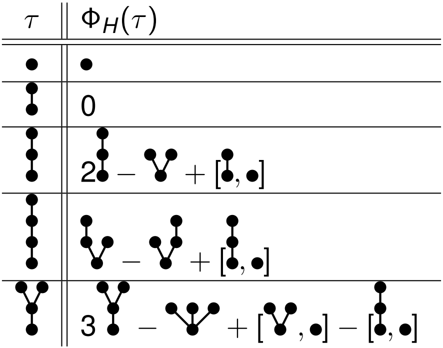
Example:

Find $\Phi_H(\substack{\bullet\,\bullet\\ \bullet})$.

$$
\begin{aligned}
U[(\bullet\bullet)[H]] &= U[\circ[\circ[H]]] + 2U[\bullet][\circ[H]] + U[[\circ,\bullet]][H] \\
&= U[\circ[\Omega(\bullet,\circ)]] + 2U[\bullet][\Omega(\bullet,\circ)] + \Omega(\bullet, U[[\circ,\bullet]]) \\
&= U[\Omega([\circ,\bullet] + \substack{\circ\\ \bullet}, \circ] + 2\Omega([\circ,\bullet] + \substack{\circ\\ \bullet}, U[\bullet]) - \Omega(\bullet[[\circ,\bullet]], U) \\
&= \Omega(2[\circ, \substack{\circ\\ \bullet}] + \substack{\circ\,\circ\\ \bullet}, U) - 2\Omega(\substack{\circ\\ \bullet\\ \bullet}, U) - \Omega([\circ, \substack{\bullet\\ \bullet}], U) \\
&= \Omega([\bullet, \substack{\bullet\\ \bullet}] + \substack{\bullet\,\bullet\\ \bullet} - 2\substack{\bullet\\ \bullet\\ \bullet}, U).
\end{aligned}
$$

Thus $\Phi_H(\substack{\bullet\,\bullet\\ \bullet}) = [\bullet, \substack{\bullet\\ \bullet}] + \substack{\bullet\,\bullet\\ \bullet} - 2\substack{\bullet\\ \bullet\\ \bullet}$.

Some elementary Hamiltonian vectorfields



We recover the classical ones for the commutative case. Note that LS-series are normalized without the tree symmetry $1/\sigma(\tau)$. Note that  yields 0 classically and is non-zero in the general case.

On the Symplectic Torsion Assumption

- The STA condition is *not* true in general. It is related to *choice of isotropy*, in the representation of a vectorfield f as a function $f\colon P \to \mathfrak{g}$.
- In the case of the quadratic Hamiltonian action on $\mathbb{R}^{2n}$, STP is true when
$$f(y) = (F_M(y), f_v(y)) \in \mathfrak{sp}(2n) \rtimes \mathbb{R}^{2n},$$
where the matrix part $F_M(y)$ is the Jacobian of f at y. Such vectorfields can be understood as being horizontal on the principal fiber bundle $SP(2n) \rtimes \mathbb{R}^{2n}$ (with fibre $SP(2n)$).
- In the case of Lie Poisson systems, the torsion $[f, g]$ is vertical (and thus symplectic) if f and g are horizontal (with respect to the Levi–Civita connection $\nabla_f(g) = f[g] + \frac{1}{2}[f, g]$). This is the natural choice of isotropy for f. However, the frozen vectorfields U are *not* horizontal, so STA does not hold for $[U, f]$.

Concluding remarks

- We are seeing the contours of a theory of symplectic Lie group methods.
- The theory seems to work for constant Ω and careful choice of isotropy.
- There are still problems for non-constant Ω (e.g. Lie Poisson). Possible solutions seem to be related to differential geometry (curvature and torsion).
- The algebraic side of Lie Butcher theory has been understood much more in the recent years, and is connecting both to classical Butcher theory and to the free associative algebra.
- Lie Butcher theory is now being tied closer also to mainstream differential geometry.