An algebraic approach to conservation of first integrals in numerical integration

Ander Murua

Many results from joint work with P. Chartier and E. Faou

FoCM'05

Santander, July 2005

Overview of the talk

- Integration schemes over the set $\mathcal{R}$ of smooth vector fields.
  - Definitions related to general integration schemed over $\mathcal{R}$
  - Characterization of order conditions
  - Conservation of first integrals, with results for B-series methods.
  - Conjugate methods and modified first integrals
- Extension to integration schemes over a more general reference set $\mathcal{R}$.
  - Definitions and extension of previous results.
  - Characterization of conservation of first integrals
  - Conservation of first integrals and backward error analysis

Integrators

Definition 1 Given an open set $\mathcal{U} \subset \mathbb{R}^d$, an integrator ψ_f on $\mathcal{U}$ is a map

$$\begin{aligned} \psi_f \quad : \quad & \mathcal{V} \subset \mathbb{R}^{d+1} \rightarrow \mathcal{U} \\ & (h, y) \rightarrow \psi_{f,h}(y) \end{aligned}$$

such that $\mathcal{V}$ is an open neighbourhood of $\{0\} \times \mathcal{U}$ and $\psi_{f,0}(y) \equiv y$.

The purpose of such integrators is to compute approximations $y(t_n) = y_n$, $n = 1, 2, \ldots$ of the solution $y(t)$ of initial value problems of the form

$$\dot{y} = f(y), \quad y(t_0) = y_0, \tag{1}$$

by means of $y_n = \psi_{f,h_n}(y_{n-1})$, where $h_n = t_n - t_{n-1}$.

Definition 2 An integration scheme over

$$\mathcal{R} = \bigcup_{d\geq 1} \{f : \mathcal{U}_f \subset \mathbb{R}^d \to \mathbb{R}^d : \ f \text{ smooth}\}$$

is a map ψ that associates a smooth integrator $\psi_f : \mathcal{V}_f \subset \mathbb{R}^{d+1} \to \mathcal{U}_f$ to each $f \in \mathcal{R}$. We write $\psi_f(h, y)$ as $\psi_{f,h}(y)$ for each $(h, y) \in \mathcal{U}_f$.

Example 1 An ERK scheme with parameters $b_i, a_{ij} \in \mathbb{R}$ gives an integrator

$$\begin{aligned} \psi_{f,h}(y) &= y + h\sum_{i=1}^{s} b_i f(Y_i), \\ Y_i &= y + h\sum_{j=1}^{i-1} a_{ij} f(Y_j), \quad j = 1, \ldots, s, \end{aligned}$$

to each $f \in \mathcal{R}$.

Definition 3 The exact integration scheme ϕ over $\mathcal{R}$ is such that $\phi_{f,h}(y(t)) = y(t + h)$ for every solution $y(t)$ of $\dot{y} = f(y)$.

Definition 4 Given two integration schemes ψ and $\widehat{\psi}$ over $\mathcal{R}$, $\psi \overset{(n)}{\equiv} \widehat{\psi}$ if $\psi_{f,h}(y) = \widehat{\psi}_{f,h}(y) + \mathcal{O}(h^{n+1})$ as $h \to 0$ for all $f \in \mathcal{R}$.

The integration scheme ψ is consistent if $\psi \overset{(1)}{\equiv} \phi$, and ψ is of order n if $\psi \overset{(n)}{\equiv} \phi$.

Definition 5 Given a set $\mathcal{G}$ of integration schemes over $\mathcal{R}$, the closure $\overline{\mathcal{G}}$ of $\mathcal{G}$ is the set of integration schemes over $\mathcal{R}$

$$\overline{\mathcal{G}} = \{\overline{\psi} : \ \forall n \geq 1, \ \exists \psi \in \mathcal{G} \text{ such that } \overline{\psi} \overset{(n)}{\equiv} \psi\}.$$

Assumption 1 $\mathcal{G}$ is a set of integration schemes over $\mathcal{R}$ satisfying that

1. $\mathcal{G}$ is closed under composition.
2. If $\psi \in \mathcal{G}$, $\lambda \in \mathbb{R}$, then $\psi^{[\lambda]} \in \mathcal{G}$, where $\psi^{[\lambda]}_{f,h}(y) := \psi_{f,\lambda h}(y)$.
3. For each $\psi \in \mathcal{G}$, $n \geq 1$, there exists $\widehat{\psi} \in \mathcal{G}$ such that $\psi\widehat{\psi} \overset{(n)}{\equiv} \text{id}$ and $\widehat{\psi}\psi \overset{(n)}{\equiv} \text{id}$.

Under such conditions, if there exists $\psi \in \mathcal{G}$ such that $\psi \overset{(1)}{\equiv} \phi$, then $\phi \in \overline{\mathcal{G}}$ (technique of Suzuki, Yoshida).

Theorem 1 Under Assumption 1, there exists a family of disjoint sets $\{\mathcal{T}_n : \ n \geq 1\}$ of functions $u : \overline{\mathcal{G}} \to \mathbb{R}$ satisfying the following:

1. Let $\mathcal{F} = \cup_{n\geq 0}\mathcal{F}_n$ be the set of functions on $\overline{\mathcal{G}}$ defined by
   $\mathcal{F}_n = \{u_1 \cdots u_m : \ m \geq 1, \ u_i \in \mathcal{T}_{n_i}, \ i = 1, \ldots, m, \ n_1 + \cdots + n_m = n - 1\}$,
   For each $f \in \mathcal{R}$, there exists a family of linear operators $\{X_f(u) : \ u \in \mathcal{F}\}$ acting on $C^\infty(\mathcal{U}_f)$ such that, for arbitrary $\psi \in \overline{\mathcal{G}}$,
   $$g(\psi_{f,h}(y)) = g(y) + \sum_{n\geq 1} h^n \sum_{u\in\mathcal{F}_n} u(\psi)\, X_f(u)[g](y), \quad \forall g \in C^\infty(\mathcal{U}_f), \quad \forall y \in \mathcal{U}_f.$$

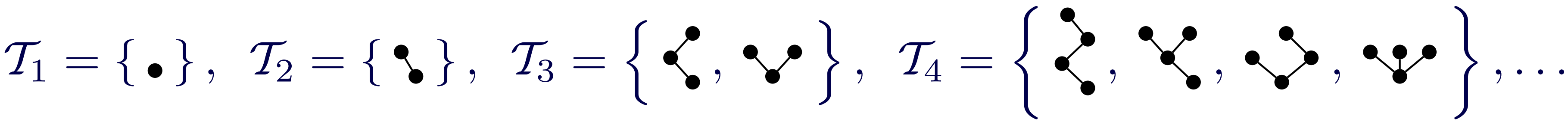
2. For an arbitrary finite subset $\mathcal{T}' \subset \mathcal{T}$ and a map $\alpha : \mathcal{T}' \to \mathbb{R}$, there exists $\psi \in \mathcal{G}$ such that $u(\psi) = \alpha(u)$ for each $u \in \mathcal{T}'$.

First statement implies that, given arbitrary $\psi, \widehat{\psi} \in \overline{\mathcal{G}}$, $n \geq 1$,

$$\psi \overset{(n)}{\equiv} \widehat{\psi} \quad \Longleftrightarrow \quad u(\psi) = u(\widehat{\psi}) \quad \forall u \in \cup_{k=1}^{n}\mathcal{T}_k. \tag{2}$$

Second statement implies that such conditions are independent

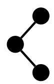
Example: Let $\mathcal{G}$ be the set of ERK schemes over $\mathcal{R}$. Then, its closure $\overline{\mathcal{G}}$ includes: implicit RK, multi-derivative RK, Rossembrock, elementary differential RK, and any ψ that can be expanded as a B-series. Theorem 1 holds with a set $\mathcal{T} = \cup_{n\geq 1}\mathcal{T}_n$ of functions on $\overline{\mathcal{G}}$ identified with the set of rooted trees.

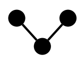


For each $\psi \in \mathcal{G}$,

$$\bullet(\psi) = \sum_{i}^{s} b_i,$$

 $(\psi) = \sum_{i,j} b_i a_{ij},$

 $(\psi) = \sum_{i,j,k} b_i a_{ij} a_{jk},$

 $(\psi) = \sum_{i,j,k} b_i a_{ij} a_{ik},$

For each $\psi \in \mathcal{G}$,

$$\bullet(\psi) = \sum_{i}^{s} b_i, \qquad [\bullet](\psi) = \sum_{i,j} b_i a_{ij},$$

$$[[\bullet]](\psi) = \sum_{i,j,k} b_i a_{ij} a_{jk}, \qquad [\bullet,\bullet](\psi) = \sum_{i,j,k} b_i a_{ij} a_{ik},$$

And for $f \in \mathcal{R}$, $g \in C^\infty(\mathcal{U}_f)$,

$$\begin{aligned} g \circ \psi_{f,h} &= g + \sum_{n\geq 1} h^n \sum_{u \in \mathcal{F}_n} u(\psi)\, X_f(u)[g] \\ &= g + h\{\bullet(\psi)\}\, g' f + h^2 \left(\{[\bullet](\psi)\}\, g' f' f + \{\bullet(\psi)\}^2 \frac{1}{2} g''(f,f) \right) \\ &\quad + h^3 \Big(\{[[\bullet]](\psi)\}\, g' f' f' f + \{[\bullet,\bullet](\psi)\}\, \frac{1}{2} g' f''(f,f) \\ &\quad + \{\bullet(\psi)\}\{[\bullet](\psi)\}\, g''(f, f'f) + \{\bullet(\psi)\}^3 \frac{1}{6} g'''(f,f,f) \Big) + \cdots \end{aligned}$$

For each $\psi \in \mathcal{G}$,

$$\bullet(\psi) \;=\; \sum_{i}^{s} b_i, \qquad [\bullet](\psi) = \sum_{i,j} b_i a_{ij} - \frac{1}{2}\left(\sum_{i}^{s} b_i\right)^2,$$

$$[[\bullet]](\psi) \;=\; \sum_{i,j,k} b_i a_{ij} a_{jk} - \frac{1}{6}\left(\sum_{i}^{s} b_i\right)^3, \qquad [\bullet\bullet](\psi) = \sum_{i,j,k} b_i a_{ij} a_{ik} - \frac{1}{3}\left(\sum_{i}^{s} b_i\right)^3,$$

And for $f \in \mathcal{R}$, $g \in C^\infty(\mathcal{U}_f)$,

$$\begin{aligned}
g \circ \psi_{f,h} &= g + \sum_{n \geq 1} h^n \sum_{u \in \mathcal{F}_n} u(\psi)\, X_f(u)[g] \\
&= g + h\{\bullet(\psi)\}\, L_f[g] + h^2 \left(\{[\bullet](\psi)\}\, g' f' f + \{\bullet(\psi)\}^2 \frac{1}{2} L_f^2[g]\right) \\
&\quad + h^3 \Bigg(\{[[\bullet]](\psi)\}\, g' f' f' f + \{[\bullet\bullet](\psi)\}\, \frac{1}{2} g' f''(f, f) \\
&\quad + \{\bullet(\psi)\}\{[\bullet](\psi)\}\, g''(f, f' f) + \{\bullet(\psi)\}^3 \frac{1}{6} L_f^3[g]\Bigg) + \cdots
\end{aligned}$$

where $L_f[g] := g' f$.

Proposition 1 There exists a unique graded algebra $\mathcal{H} = \bigoplus_{n\geq 0} \mathcal{H}_n$ of functions on $\overline{\mathcal{G}}$ satisfying that, Theorem 1 holds for $\{\mathcal{T}_n : \ n \geq 1\}$ if and only if $\mathcal{T}_n \subset \mathcal{H}_n$ $(n \geq 1)$ and the algebra $\mathcal{H}$ is freely generated by $\mathcal{T} = \cup_{n\geq 1}\mathcal{T}_n$.

Theorem 2 If in addition to Assumption 1, each $\mathcal{H}_n$ is finite dimensional,

1. Given an arbitrary integration scheme ψ over $\mathcal{R}$, if $\exists\alpha : \mathcal{F} \to \mathbb{R}$ such that, for each $f \in \mathcal{R}$, each $g \in C^\infty(\mathcal{U}_f)$, and each $y \in \mathcal{U}_f$,

$$g(\psi_{f,h}(y)) = g(y) + \sum_{h\geq 1} h^n \sum_{u\in\mathcal{F}_n} \alpha(u) X_f(u)[g](y),$$

   then $\psi \in \overline{\mathcal{G}}$.

2. For each $g_1, g_2 \in C^\infty(\mathcal{U}_f)$,

$$X_f(u)[g_1 g_2] = \sum_{vw=u} X_f(v)[g_1] X(w)[g_2]. \qquad (3)$$

according to (3) $X_f(u)$, $u \in \mathcal{T}$, are first order differential operators.

Characterization of conservation of first integrals up to order n

Given $\mathcal{S} \subset \{(f, I) : \; f \in \mathcal{R}, \; I \in C^{\infty}(\mathcal{U}_f), \; I'(y)f(y) \equiv 0\}$, there exists a unique graded ideal $\mathcal{I} = \bigoplus_{n \geq 1} \mathcal{I}_n$ of $\mathcal{H}$ such that, given $\psi \in \overline{\mathcal{G}}$,

$$I(\psi_{f,h}(y)) = I(y) + \mathcal{O}(h^{n+1}) \quad \text{as} \quad h \to 0 \tag{4}$$

for all $(f, I) \in \mathcal{S}$ if and only if, $u(\psi) = 0$ for all $u \in \bigoplus_{k=1}^{n} \mathcal{I}_k$.

Let $\widehat{\mathcal{G}} = \{\psi \in \overline{\mathcal{G}} : \; u(\psi) = 0 \; \forall u \in \mathcal{I}\}$, then $\widehat{\mathcal{G}}$ satisfies Assumption 1, $\overline{\widehat{\mathcal{G}}} = \widehat{\mathcal{G}}$ and $\widehat{\mathcal{H}} \simeq \mathcal{H}/\mathcal{I}$ for the algebra $\widehat{\mathcal{H}}$ given by Proposition 1 for $\widehat{\mathcal{G}}$ (thus, $\mathcal{H} \simeq \widehat{\mathcal{H}} \oplus \mathcal{I}$).

Example: Let $\mathcal{S} = \{(f, I) : \; f \in \mathcal{R}, \; I'(y)f(y) \equiv 0, \; I(y) \text{ quadratic}\}$, and $\mathcal{G}$ the set of ERK schemes over $\mathcal{R}$. then, $\mathcal{I}$ is the ideal of $\mathcal{H}$ generated by the set of functions $\{u_1 \circ u_2 + u_2 \circ u_1 - u_1 u_2 : \quad u_1, u_2 \in \mathcal{T}\}$. Here, $\widehat{\mathcal{G}}$ is the set of symplectic B-series integration schemes. If $\widehat{\mathcal{T}} = \cup_{n \geq 1} \widehat{\mathcal{T}}_n$ freely generates $\widehat{\mathcal{H}}$, then $\#\widehat{\mathcal{T}}_n =$ number of free trees with n vertices.

Some results on conservation of first integrals of B-series methods

Consider the set $\mathcal{G}$ of ERK schemes ($\overline{\mathcal{G}}$ are thus B-series integration schemes).

$$
\begin{aligned}
\mathcal{S}^Q &= \{(f, I):\ f \in \mathcal{R},\ I'(y)f(y) \equiv 0,\ I(y) \text{ quadratic}\} &\longrightarrow\ \mathcal{I}^Q,\\
\mathcal{S}^C &= \{(f, I):\ f \in \mathcal{R},\ I'(y)f(y) \equiv 0,\ I(y) \text{ cubic}\} &\longrightarrow\ \mathcal{I}^C,\\
\mathcal{S}^A &= \{(f, I):\ f \in \mathcal{R},\ I'(y)f(y) \equiv 0,\ I(y) \text{ arbitrary}\} &\longrightarrow\ \mathcal{I}^A,\\
\mathcal{S}^H &= \{(f, H):\ f \in \mathcal{R},\ \text{Hamiltonian } f(y) = J^{-1}\nabla H(y)\} &\longrightarrow\ \mathcal{I}^H.
\end{aligned}
$$

Then it holds the following. Let $\mathcal{H}^\bullet$ be the subalgebra of $\mathcal{H}$ generated by the consistency function $\bullet \in \mathcal{T}_1$.

- [Chartier, Faou, M. 2005]: $\mathcal{I}^Q \oplus \mathcal{I}^H \oplus \mathcal{H}^\bullet = \mathcal{H}$. Thus, consistent $\psi \in \overline{\mathcal{G}}$ that preserve quadratic invariants and Hamiltonian functions up to order n, are methods of order n.

- [Ch., F., M. 2005]+[M. 2003]: $\mathcal{I}^C = \mathcal{I}^A$, and $\mathcal{I}^A \oplus \mathcal{H}^\bullet = \mathcal{H}$. Consistency and preservation of cubic invariants up to order n imply that $\psi \overset{(n)}{\equiv} \phi$.

Conjugate schemes and modified first integrals

Assume that $\psi, \widehat{\psi}, \chi \in \overline{\mathcal{G}}$ are such that $\psi \circ \chi = \chi \circ \widehat{\psi}$ (ψ and $\widehat{\psi}$ are conjugate). If for a $f \in \mathcal{R}$, and $I \in C^{\infty}(\mathcal{U}_f)$, $I(\widehat{\psi}_{f,h}(y)) \equiv I(y) + \mathcal{O}(h^{n+1})$, then,

$$\tilde{I}_h(\psi_{f,h}(y)) \equiv \tilde{I}_h(y) + \mathcal{O}(h^{n+1}),$$

where

$$\tilde{I}_h(y) := I(\chi_{f,h}(y)) = \sum_{u \in \mathcal{F}} h^{|u|} u(\chi)\, X_f(u)[I](y).$$

More generally: Given $\psi \in \overline{\mathcal{G}}$, $\exists \tilde{I}_h(y)$ of the form

$$\tilde{I}_h(y) := \sum_{u \in \mathcal{F}} h^{|u|} \alpha(u)\, X_f(u)[I](y)$$

such that $\tilde{I}_h(\psi_{f,h}(y)) \equiv \tilde{I}_h(y) + \mathcal{O}(h^{n+1})$? If ψ is conjugate to a scheme $\widehat{\psi} \in \overline{\mathcal{G}}$ such that $I(\widehat{\psi}_{f,h}(y)) \equiv I(y) + \mathcal{O}(h^{n+1})$, yes. And otherwise? We have answered that for some particular cases of interest.

Let $\mathcal{R} = \{f: \ f: \mathcal{U}_f \subset \mathbb{R}^d \to \mathbb{R}^d \text{ smooth }, \ d \geq 1\}$, and let $\mathcal{G}$ be the set of ERK schemes.

Theorem 3 [Faou, Chartier, M. 2005] Given $\psi \in \overline{\mathcal{G}}$, $f \in \mathcal{R}$, $I(y)$ quadratic such that $I'(y)f(y) \equiv 0$. Assume that $\exists \tilde{I}_h(y)$ of the form

$$\tilde{I}_h(y) := \sum_{u \in \mathcal{F}} h^{|u|} \alpha(u) \, X_f(u)[I](y)$$

such that $\tilde{I}_h(\psi_{f,h}(y)) \equiv \tilde{I}_h(y) + \mathcal{O}(h^{n+1})$. Then ψ is conjugate to a scheme $\widehat{\psi} \in \overline{\mathcal{G}}$ such that $I(\widehat{\psi}_{f,h}(y)) \equiv I(y) + \mathcal{O}(h^{n+1})$.

Theorem 4 [Faou, Chartier, M. 2005] Given $\psi \in \overline{\mathcal{G}}$, $f \in \mathcal{R}$, $f = J^{-1} \nabla H$ Hamiltonian. Assume that $\exists \tilde{H}_h(y)$ of the form

$$\tilde{H}_h(y) := \sum_{u \in \mathcal{F}} h^{|u|} \alpha(u) \, X_f(u)[H](y)$$

such that $\tilde{H}_h(\psi_{f,h}(y)) \equiv \tilde{H}_h(y) + \mathcal{O}(h^{n+1})$. Then ψ is conjugate to a scheme $\widehat{\psi} \in \overline{\mathcal{G}}$ such that $H(\widehat{\psi}_{f,h}(y)) \equiv H(y) + \mathcal{O}(h^{n+1})$.

Both are true also when $\mathcal{G}$ is the set of partitioned RK methods ($\overline{\mathcal{G}}$ =P-series).

A more general setting

Assume that we want to integrate numerically

$$\dot{y} = f_1(y) + f_2(y), \quad y(t_0) = y_0, \tag{5}$$

with smooth maps $f^{[i]} : \mathcal{U} \subset \mathbb{R}^d \to \mathbb{R}^d$ $(i = 1, 2)$. It then seems reasonable to modify Definition 2 by considering the reference set $\mathcal{R}$ as a subset

$$\mathcal{R} \ \subset \ \{f = (f_1, f_2) : \ f_i : \mathcal{U}_f \subset \mathbb{R}^d \to \mathbb{R}^d \text{ smooth } \ (i = 1, 2), \ d \geq 1\}.$$

Definition 6 An integration scheme over $\mathcal{R}$ is a map ψ that associates a smooth integrator $\psi_f : \mathcal{V}_f \subset \mathbb{R}^{d+1} \to \mathcal{U}_f$ to each $f \in \mathcal{R}$.

Previous definitions make sense in this more general setting: Exact integration scheme ϕ (giving exact solution of (5)), $\psi \overset{(n)}{\equiv} \widehat{\psi}$, closure $\overline{\mathcal{G}}$ of a set $\mathcal{G}$ of integration schemes over $\mathcal{R}$, and under Assumption 1, the graded algebra $\mathcal{H} = \bigoplus_{n\geq 0} \mathcal{H}_n$. Theorems 1 and 2 and Proposition 1 still hold. Actually, they also hold for an arbitrary reference set $\mathcal{R}$ of objects such that, each $f \in \mathcal{R}$ has assigned an open set $\mathcal{U}_f \subset \mathbb{R}^d$.

Definition 7 Given $\alpha \in \mathcal{H}^*$ (i.e. a linear form $\alpha : \mathcal{H} \to \mathbb{R}$, determined by the values $\alpha(u)$ for $u \in \mathcal{F}$, where $\mathcal{F}$ is a basis of $\mathcal{H}$), we consider for each $f \in \mathcal{R}$

$$S_f(\alpha) = \sum_{u \in \mathcal{F}} h^{|u|} \alpha(u) X_f(u).$$

where, given $u \in \mathcal{H}$, we denote $|u| = n$ if $u \in \mathcal{H}_n$.

For each $\psi \in \overline{\mathcal{G}}$, consider $\Psi \in \mathcal{H}^*$ given by $\Psi(u) := u(\psi)$. Then, the composition $g \circ \psi_{f,h}$ can be expanded as $S_f(\Psi)[g]$.

Theorem 5 For each $u \in \mathcal{H}$, there exist $v_1, \ldots, v_k, w_1, \ldots, w_k \in \mathcal{H}$ such that $|v_i| + |w_i| = |u|$ for all i, and

$$u(\psi \circ \widehat{\psi}) = \sum_{i=1}^{k} v_i(\widehat{\psi}) w_i(\psi), \quad \forall \psi, \widehat{\psi} \in \overline{\mathcal{G}}.$$

Furthermore, given $\alpha, \beta \in \mathcal{H}^*$, for each $f \in \mathcal{R}$

$$S_f(\alpha) S_f(\beta) = S_f(\alpha\beta), \quad \text{where} \quad \alpha\beta(u) = \sum_{i=1}^{k} \alpha(v_i)\beta(w_i).$$

This gives an algebra structure to $\mathcal{H}^*$

Characterization of conservation of first integrals up to order n

Theorem 6 Let $\mathcal{G}$ be a set of integration schemes over an arbitrary reference set $\mathcal{R}$, which satisfies the assumptions of Theorem 2. Given

$$\mathcal{S} \subset \{(f, I): \ f \in \mathcal{R}, \ I \in C^{\infty}(\mathcal{U}_f), \ I(\psi_{f,h}(y)) \equiv I(y) + \mathcal{O}(h^2) \ \forall \psi \in \mathcal{G}\},$$

there exists a unique graded ideal $\mathcal{I} = \bigoplus_{n \geq 1} \mathcal{I}_n$ of $\mathcal{H}$ such that, given $\psi \in \overline{\mathcal{G}}$,

$$I(\psi_{f,h}(y)) = I(y) + \mathcal{O}(h^{n+1}) \quad \text{as} \quad h \to 0 \tag{6}$$

for all $(f, I) \in \mathcal{S}$ if and only if, $u(\psi) = 0$ for all $u \in \bigoplus_{k=1}^{n} \mathcal{I}_k$.

How to construct $\mathcal{I}$? Consider

$$\mathcal{J} = \{\alpha \in \bigoplus_{n \geq 0} \mathcal{H}_n^* : \ S_f(\alpha)[I] = 0 \ \forall (f, I) \in \mathcal{S}\}$$

($\mathcal{J}$ is a left-sided ideal of the algebra $\mathcal{H}^*$), and

$$\mathcal{J}^{\perp} = \{u \in \mathcal{H} : \ \alpha(u) = 0 \ \forall \alpha \in \mathcal{J}\},$$

then $\mathcal{I}$ is the ideal generated by $\mathcal{J}^{\perp}$.

Let $\mathcal{R} = \{f = (f_1, f_2): \ f_i : \mathcal{U}_f \subset \mathbb{R}^d \to \mathbb{R}^d \text{ smooth } \ (i = 1,2), \ d \geq 1\}$, and $\mathcal{G}$ the set of additive RK schemes (essentially PRK), so that $\mathcal{T}$ can be identified with the set of rooted trees with vertices in two colours.

$$\begin{array}{rcll} \mathcal{S}^C & = & \{(f, I): \ I'(y)f_i(y) \equiv 0, \ i = 1,2, \ I(y) \text{ cubic}\} & \longrightarrow \ \mathcal{I}^C, \\ \mathcal{S}^A & = & \{(f, I): \ I'(y)f_i(y) \equiv 0, \ i = 1,2, \ I(y) \text{ arbitrary}\} & \longrightarrow \ \mathcal{I}^A, \end{array}$$

In [Chartier, M. 2005, in preparation], we identify the graded ideals $\mathcal{I}^C$ and $\mathcal{I}^A$. Such ideals already appear in the results in [M. 2003] which imply that $I^C = I^A$ and

Theorem 7 [Chartier, M. 2005] Given $\psi \in \overline{\mathcal{G}}$, if for all $(f, I) \in \mathcal{S}^C$ we have that $I(\psi_{f,h}(y)) = I(y) + \mathcal{O}(h^{n+1})$, then, there exists $a_1, \ldots, a_m, b_1, \ldots, b_m \in \mathbb{R}$ such that

$$\psi_{f,h} = \phi_{f_2, b_m h} \circ \phi_{f_1, a_m h} \circ \cdots \circ \phi_{f_2, b_1 h} \circ \phi_{f_1, a_1 h} + \mathcal{O}(h^{n+1}).$$

Characterization of conservation of first integrals and BEA

Proposition 2 Let $\mathcal{G}$ be a set of integration schemes over an arbitrary reference set $\mathcal{R}$, which satisfies the assumptions of Theorem 2, and let

$$\mathcal{S} \subset \{(f, I) : \ f \in \mathcal{R},\ I \in C^\infty(\mathcal{U}_f),\ I(\psi_{f,h}(y)) \equiv I(y) + \mathcal{O}(h^2)\ \forall \psi \in \mathcal{G}\}.$$

Given $\psi \in \overline{\mathcal{G}}$, $f \in \mathcal{R}$, $\psi_{f,h}$ is formally the h-flow of the modified ODE

$$\dot{y} = \sum_{u \in \mathcal{T}} h^{|u|-1} \beta(u)\, F_f(u)(y), \tag{7}$$

where $F_f(u) = X_f(u)[\mathrm{id}_{\mathcal{U}_f}]$ for all $u \in \mathcal{T}$, and $\beta(u) = \log \Psi(u)$ $(\Psi(u) = u(\psi))$, for all $u \in \mathcal{H}$, and it holds that $\beta(u) = 0 \quad \forall u \in \mathcal{F} \backslash \mathcal{T}$.

Furthermore, let $\mathcal{I} = \bigoplus_{n \geq 0} \mathcal{I}_n$ be given by Theorem 6,

$$u(\psi) = 0 \quad \forall u \in \bigoplus_{k=1}^{n} \mathcal{I}_k \quad \Longleftrightarrow \quad \beta(u) = 0 \quad \forall u \in \bigoplus_{k=1}^{n} \mathcal{I}_k. \tag{8}$$

Some results on conservation of first integrals of B-series methods

Consider the set $\mathcal{G}$ of ERK schemes ($\overline{\mathcal{G}}$ are thus B-series integration schemes).

$$
\begin{aligned}
\mathcal{S}^Q &= \{(f,I):\ f\in\mathcal{R},\ I'(y)f(y)\equiv 0,\ I(y) \text{ quadratic}\} &\longrightarrow&\quad \mathcal{I}^Q,\\
\mathcal{S}^C &= \{(f,I):\ f\in\mathcal{R},\ I'(y)f(y)\equiv 0,\ I(y) \text{ cubic}\} &\longrightarrow&\quad \mathcal{I}^C,\\
\mathcal{S}^A &= \{(f,I):\ f\in\mathcal{R},\ I'(y)f(y)\equiv 0,\ I(y) \text{ arbitrary}\} &\longrightarrow&\quad \mathcal{I}^A,\\
\mathcal{S}^H &= \{(f,H):\ f\in\mathcal{R},\ \text{Hamiltonian } f(y)=J^{-1}\nabla H(y)\} &\longrightarrow&\quad \mathcal{I}^H.
\end{aligned}
$$

Then it holds the following. Let $H^\bullet$ be the subalgebra of $\mathcal{H}$ generated by the consistency function $\bullet \in \mathcal{T}_1$.

- [Chartier, Faou, M. 2005]: $\mathcal{I}^Q \oplus \mathcal{I}^H \oplus \mathcal{H}^\bullet = \mathcal{H}$. Thus, consistent $\psi \in \overline{\mathcal{G}}$ that preserve quadratic invariants and Hamiltonian functions up to order n, are methods of order n.

- [Ch., F., M. 2005]+[M. 2003]: $\mathcal{I}^C = \mathcal{I}^A$, and $\mathcal{I}^A \oplus \mathcal{H}^\bullet = \mathcal{H}$. Consistency and preservation of cubic invariants up to order n imply that $\psi \overset{(n)}{\equiv} \phi$.

Related result:

Theorem 8 [Iserles,Quispel,Tse (2005)] Given a consistent $\psi \in \overline{\mathcal{G}}$,

$$\det\left(\frac{\partial}{\partial y}\psi_{f,h}(y)\right) \equiv 1 + \mathcal{O}(h^{n+1}) \quad \text{as} \quad h \to 0 \tag{9}$$

for arbitrary divergence free $f \in \mathcal{R}$, if and only if $\psi \overset{(n)}{\equiv} \phi$.

Alternative proof [Chartier & M. 2005]: We show that (9) implies that

$$u(\psi) = 0 \quad \forall u \in \bigoplus_{k=1}^{n} \mathcal{I}_k^C .$$

Let $\mathcal{R} = \{f = (f_1, f_2) : \; f_i : \mathcal{U}_f \subset \mathbb{R}^d \to \mathbb{R}^d \text{ smooth } \; (i = 1, 2), \; d \geq 1\}$, and $\mathcal{G}$ the set of additive RK schemes (essentially PRK), so that $\mathcal{T}$ can be identified with the set of rooted trees with vertices in two colours.

$$\begin{aligned} \mathcal{S}^C &= \{(f, I) : \; I'(y) f_i(y) \equiv 0, \; i = 1, 2, \; I(y) \text{ cubic}\} & \longrightarrow \quad \mathcal{I}^C, \\ \mathcal{S}^A &= \{(f, I) : \; I'(y) f_i(y) \equiv 0, \; i = 1, 2, \; I(y) \text{ arbitrary}\} & \longrightarrow \quad \mathcal{I}^A, \end{aligned}$$

In [Chartier, M. 2005, in preparation], we identify the graded ideals $\mathcal{I}^C$ and $\mathcal{I}^A$. Such ideals already appear in the results in [M. 2003] which imply that $I^C = I^A$ and

Theorem 9 [Chartier, M. 2005] Given $\psi \in \overline{\mathcal{G}}$, if for all $(f, I) \in \mathcal{S}^C$ we have that $I(\psi_{f,h}(y)) = I(y) + \mathcal{O}(h^{n+1})$, then, there exists $a_1, \ldots, a_m, b_1, \ldots, b_m \in \mathbb{R}$ such that

$$\psi_{f,h} = \phi_{f_2, b_m h} \circ \phi_{f_1, a_m h} \circ \cdots \circ \phi_{f_2, b_1 h} \circ \phi_{f_1, a_1 h} + \mathcal{O}(h^{n+1}).$$

Related result:

Theorem 10 [Chartier, M. 2005] Given $\psi \in \overline{\mathcal{G}}$, if for all $f = (f_1, f_2)$ such that f_1 and f_2 are divergence-free, we have that

$$\det\left(\frac{\partial}{\partial y}\psi_{f,h}(y)\right) = 1 + \mathcal{O}(h^{n+1}),$$

then, there exists $a_1, \ldots, a_m, b_1, \ldots, b_m \in \mathbb{R}$ such that

$$\psi_{f,h} = \phi_{f_2, b_m h} \circ \phi_{f_1, a_m h} \circ \cdots \circ \phi_{f_2, b_1 h} \circ \phi_{f_1, a_1 h} + \mathcal{O}(h^{n+1}).$$