Butcher series for Hamiltonian Poisson integrators through symplectic groupoids

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Abstract

We introduce a pre-Lie formalism of Butcher trees for the approximation of Hamilton-Jacobi solutions on any symplectic groupoid $\mathcal{G} \rightrightarrows M$. The impact of this new algebraic approach is twofold. On the geometric side, it yields algebraic operations to approximate Lagrangian bisections of $\mathcal{G}$ using the Butcher-Connes-Kreimer Hopf algebra and, in turn, aims at a better understanding of the group of Poisson diffeomorphisms of M. On the computational side, we define a new class of Poisson integrators for Hamiltonian dynamics on Poisson manifolds.

Keywords: Butcher series, Poisson geometry, mathematical physics, geometric numerical integration, symplectic groupoids, Hamilton-Jacobi equation, pre-Lie algebra, Hopf algebra.

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1 Introduction

1.1 Context

A Poisson bracket on a smooth manifold M equips the space of smooth functions of this manifold $\mathcal{C}^\infty(M)$ with a Lie algebra structure $(\mathcal{C}^\infty(M), \{.,.\})$. Therefore, it is natural to ask about the existence of a Lie group integrating it. In the context of Poisson manifolds, there exists an extremely profitable approach to this question: instead of looking for a infinite-dimensional Lie group, we can try to construct a finite-dimensional Lie groupoid $\mathcal{G}$ over M. This Lie groupoid turns out to have a natural symplectic structure. Therefore, symplectic Lie groupoids are the global counterpart to Poisson structures. They encode in particular three different aspects of Poisson geometry: foliation theory (the partition of any Poisson manifold into leaves), symplectic geometry (the geometry along any leave) and Lie theory. Concerning the question of integrating the Lie algebra of smooth functions, there exists a group object keeping track of this integration inside the symplectic groupoid: the group of Lagrangian bisections. A major interest of symplectic groupoids in mechanics is the deep relation between Lagrangian bisections of the Lie groupoid $\mathcal{G}$ and Hamiltonian dynamics on M.

Another interest of Lagrangian bisections lies in mathematical physics purposes. In [18], a formal correspondence is spelled between symplectic groupoids and C^*-algebra theory, where Lagrangian submanifolds are the elements of the non-commutative algebra. The groupoid inverse

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corresponds to the conjugation and the product law corresponds to the tensor product. There, Lagrangian bisections are unitary elements. This correspondence started a research program on deformation theory and the quantisation of Poisson manifold through symplectic groupoids. This brought in turn a considerable attention on the topic ([43, 10, 33, 30]).

Symplectic groupoids have also been used for computational purposes. Indeed, the relation between Hamiltonian dynamics on M and Lagrangian bisections has been applied to the numerical approximation of Hamiltonian flows on the Poisson manifold M ([15]). The idea appears first in [24], while the case of fiberwise linear Poisson structures has been studied in [22]. More precisely, given any Hamiltonian $H \in \mathcal{C}^\infty(M)$, a Hamilton-Jacobi equation is used to relate its Hamiltonian flow $(\phi_t^H)_t$ to a smooth family of Lagrangian bisections $(L_t)_t$, provided that t is small enough. A truncation at any order of the solution of this Hamilton-Jacobi equation allows to recover the initially considered Hamiltonian dynamics in an approximated way, and this approximation has been proved to be numerically satisfying compared to traditional methods ([17]). The relation with previous paragraphs lies at the comparison between the time-step in numerical purposes and the parameter of deformation in the mathematical physics context. An analogy seems to hold in-between both situations, and we expect tools from one field to become fruitful when applied to the other one.

With that respect, a colossal algebraic formalism has been developed since the sixties in order to deal with the approximation of solutions of ordinary differential equations. Butcher-series were first introduced in [5, 28] (see also [27, 40, 6]) for the study of order conditions for Runge-Kutta methods in numerical analysis. They were later applied successfully to a variety of different fields such as geometric numerical integration [31, 27], quantum field theory [14], rough paths [26, 29], or stochastic numerics [4, 36, 35]. The modern approach to such algebraic formalism relies extensively on Hopf algebras [13, 39, 3, 2] that we shall identify in the context of Hamiltonian systems on Poisson manifolds.

Let us also mention that Hopf algebras have been used already to approximate geometric objects in Poisson geometry. A relation between deformation of symplectic groupoids and high-order Runge-Kutta numerical methods has been explained in [11] and formulated in terms of operads in [12]. Symplectic realizations are constructed using the Butcher group in [9], while [7] gave a detailed construction of local symplectic groupoids using Butcher series of Hamilton-Jacobi generating functions.

It is therefore natural to look for a proper algebraic formalism for the approximation of Hamiltonian dynamics on a Poisson manifold. This article answers this question and explores the algebraic, geometric and computational consequences.

1.2 Content of the paper

In Section 2, we recall how the Hamiltonian dynamics of $H \in \mathcal{C}^\infty(M)$ is recovered by Lagrangian bisections of a symplectic groupoid $\mathcal{G}$ of the Poisson manifold M through a Hamilton-Jacobi equation. Jets are used to introduce the various groups involved and to deduce an approximation of the Hamiltonian dynamics at any arbitrary order. In Section 3, we provide a new pre-Lie combinatorial formalism to compute formal solutions of Hamilton-Jacobi equations. We give two applications of this pre-Lie algebra formalism. First, we use in Section 4 the Butcher-Connes-Kreimer Hopf algebra to provide a new algebraic description of the group of Lagrangian bisections at the identity section, see Theorem 4.2 for a precise statement. In Section 5, we explain how the new algebraic formalism applies to high order approximations of Lagrangian bisections using Runge-Kutta numerical methods. It delivers as a byproduct new Hamiltonian Poisson integrators.

2 Preliminaries

2.1 Reminders on Poisson geometry

In this section, we give a concise summary of various notions of Poisson geometry. We do not intend to give any introduction of the topic. Instead, the reader may consult [38] about Hamiltonian dynamics and symplectic geometry and [19, 20] about Poisson structures and symplectic groupoids.

Let $(M, \{.,.\})$ be a Poisson manifold. In this article, we are interested in Hamiltonian dynamics on M : for any Hamiltonian $H \in \mathcal{C}^\infty(M)$, we study the differential equation on M

$$\dot{x}(t) = X_H\big(x(t)\big) \tag{2.1}$$

where $X_H \colon f \in \mathcal{C}^\infty(M) \mapsto \{H, f\} \in \mathcal{C}^\infty(M)$ is the Hamiltonian vector field[1] of H. Since one main motivation of the present work is the construction of new numerical methods, let us recall the notion of Hamiltonian Poisson integrator.

Definition 2.1 ([17]). *A Hamiltonian Poisson integrator for the Hamiltonian $H \in \mathcal{C}^\infty(M)$ at order $k \in \mathbb{N}$ is a family of map $\varphi_t \colon M \to M$, $t \in I$ a small real parameter, with the following property: there exists a time-dependent Hamiltonian $(\tilde{H}_t)_{t\in I} \in \mathcal{C}^\infty(M \times I)$ such that φ is the time-dependent Hamiltonian flow of $\tilde{H}$. The Hamiltonian Poisson integrator is said to be of order k if for any test function $f \in \mathcal{C}^\infty(M)$,*

$$\forall\ 0 \leqslant i \leqslant k,\ \frac{\partial^i (f \circ \varphi_t)}{\partial t^i}_{|t=0} = \frac{\partial^i (f \circ \phi_t^H)}{\partial t^i}_{|t=0}. \tag{2.2}$$

Symplectic methods are an important particular case of Hamiltonian Poisson integrators and they are a major motivation for this work. An other remark is that h is an approximation of the Hamiltonian H of the same order as the integrator: $\tilde{H}_t = H + o\big(t^k\big)$. As we can see in the equation (2.2), Taylor series with respect to the time t play an important role in our context to count the order of approximation of a dynamics.

We introduce now a geometric space used to construct Hamiltonian Poisson integrators. To any Poisson manifold $(M, \{.,.\})$ is associated a local symplectic groupoid $\mathcal{G} \rightrightarrows M$ over M ([18, 34]). We write $\alpha \colon \mathcal{G} \to M$ and $\beta \colon \mathcal{G} \to M$ for the source and target maps respectively. The tubular neighborhood theorem of [42] provides a local model around the identity section of $\mathcal{G} \rightrightarrows M$ to realize $\mathcal{G}$ as a neighborhood of the zero section inside T^*M. With a slight abuse of notation, we keep the same letters: the tubular neighborhood we call again $\mathcal{G}$ and α and β denote again the resulting maps from $\mathcal{G}$ to M.

Theorem 2.2. *There exists a tubular neighborhood $\mathcal{G} \subset T^*M$ of the zero section of T^*M and two surjective submersions α and β from $\mathcal{G}$ to M such that*

1. *$\alpha \circ 0 = \beta \circ 0 = Id_M$, where $0 \colon M \to T^*M$ is the zero section of the vector bundle T^*M,*
2. *α is a Poisson morphism and β is an anti-Poisson morphism, where $\mathcal{G}$ is equipped with $\{.,.\}_\omega$ the Poisson bracket of the canonical symplectic form on $\mathcal{G} \subset T^*M$,*
3. *α and β have symplectically orthogonal fibers: $\forall\ f, g \in \mathcal{C}^\infty(M),\ \{\alpha^* f, \beta^* g\}_\omega = 0$.*

[1] We denote derivations of $\mathcal{C}^\infty(M)$ and vector fields the same way.

This realization of the local symplectic groupoid inside T^*M was named *birealization* in [15]. The zero section is the identity for the groupoid product. Following [7], one can show that the inverse is the multiplication by -1 on each cotangent fiber. We emphasize that the symplectic form of $\mathcal{G} \rightrightarrows M$ becomes the canonical symplectic form ω. $\mathcal{G}$ is therefore a Poisson manifold endowed with the Poisson bracket $\{.,.\}_\omega$. We also recall that the cotangent projection $\tau\colon \mathcal{G} \twoheadrightarrow M$ is in general different from the structural maps α and β.

2.2 Hamilton-Jacobi equation for Hamiltonian Poisson integrators

In this section, we recall after [15] how a Hamilton-Jacobi equation allows to lift up Hamiltonian dynamics on M to a birealization $\mathcal{G}$ by describing Hamiltonian flows in terms of generating functions.

First, let us consider a dynamics that is a bit more general than Hamiltonian dynamics. Let θ be a 1-form $\theta \in \Omega^1(M)$. Denoting by $\pi \in \Gamma(\bigwedge^2 TM)$ the bivector field of the Poisson brackets $\{.,.\}$, we write $X_\theta = \pi(\theta,\cdot) \in \mathfrak{X}(M)$ for the vector field generated by θ and ϕ_t^θ the flow of X_θ at time t. In the sequel, we always assume flows to be integrable. The following properties are classical ([38], chapter III).

Proposition 2.3.

1. *For any $x \in M$ and for any time t, $\phi_t^\theta(x)$ belongs to the same symplectic leaf as x.*
2. *Let us assume that θ is closed. Then, ϕ_t^θ is a Poisson automorphism that admits any symplectic leaf as an invariant set and preserves θ. In equation, denoting $\mathcal{F}_x$ the symplectic leaf of $x \in M$,*
$$\forall x \in M, \phi_t^\theta(x) \in \mathcal{F}_x \text{ and } (\phi_t^\theta)_*\pi = \pi \text{ and } (\phi_t^\theta)^*\theta = \theta. \tag{2.3}$$

This classical result justifies the notion of Hamiltonian Poisson integrator. Indeed, following the flow of a time-dependent Hamiltonian guarantees to stay on a symplectic leaf and to preserve the Poisson structure.

Let us leave the case of general 1-forms on M apart and from now on, we assume θ closed. We state now the main result of this reminder section.

Theorem 2.4 (Hamilton-Jacobi equation on a local symplectic groupoid, [15])**.** *Let $\theta \in \Omega_0^1(M)$, I be a small open interval containing 0 and $(\zeta_t)_{t\in I} \in \Omega^1(M)^I$. For any $t \in I$, set*

$$L_t = \mathit{Graph}(\zeta_t) \tag{2.4}$$

and

$$\varphi_t = \beta \circ (\alpha_{|L_t})^{-1}. \tag{2.5}$$

Then, $\forall t \in I$, $\varphi_t = \phi_t^\theta$ if and only if

$$\zeta_0 = 0 \text{ and } \forall t \in I,\ \frac{\partial \zeta_t}{\partial t} = (\zeta_t)^*\alpha^*\theta. \tag{2.6}$$

2.3 Jets of Lagrangian bisections

In this article, we will develop tools to approximate solutions of the Hamilton-Jacobi equation, e.g. (2.6), at high order with respect to the variable t. For this precise reason, we will need an appropriate notion of jets. In this section, we thus explain some geometry of the previous Hamilton-Jacobi equation using jets and Taylor series.

It will be useful in the sequel to keep in mind two properties of the graph L_t of ζ_t for small $t \in I$. First, since L_0 is the zero section, L_t is transverse to the fibers of α and turns the restriction of α to L_t into a diffeomeorphism $\alpha_{|L_t} \colon L_t \to M$. L_t is thus said to be a *bisection*[2]. The set of bisections of a groupoid forms a group ([10], section 15.2). In our local groupoid context, let us introduce the analog objects.

First, in our smooth setting, we need a notion of family of bisections, all being close to the identity section. They can be understood as smooth perturbation of the identity section.

Definition 2.5 (Smooth family of bisections)**.** *We denote by smooth family of bisections of $\mathcal{G}$ the following data:*

- *a real open interval I containing* 0,
- *a family $L = (L_t)_{t\in I}$ of bisections of $\mathcal{G}$, where $L_0 = 0$ is the image of the identity section and the surjective map $\coprod_{t\in I} L_t \twoheadrightarrow I$ is a submersion.*

Example 2.6. *Since the fibers of α are transverse to the zero section, a generic example of smooth family of bisections of $\mathcal{G}$ is provided by any smooth family of 1-forms $(\zeta_t)_{t\in I} \in \Omega^1(M)$ for some small interval I.*

Now, we introduce a notion of ∞-jets for such objects. To achieve this, let $f \in \mathcal{C}^\infty(\mathcal{G})$ be a test function and L a smooth family of bisections. For any $t \in I$, let us set $\Psi_t = \left(\alpha_{|L_t}\right)^{-1} : M \xrightarrow{\sim} L_t$. We consider the Taylor series at $t = 0$ of $f \circ \Psi_t \colon M \to \mathbb{R}$. This provides a map

$$\mathcal{J}^L \colon \begin{array}{ccc} \mathcal{C}^\infty(\mathcal{G}) & \to & \mathcal{C}^\infty(M)\big[[t]\big] \\ f & \mapsto & f \circ \Psi_t \end{array} \tag{2.7}$$

where $f \circ \Psi_t \in \mathcal{C}^\infty(M)\big[[t]\big]$ stands for its Taylor series $\sum_{j=0}^{\infty} \frac{t^j}{j!} \frac{\partial^j f\circ\Psi_t}{\partial t^j}_{|t=0}$ at $t = 0$.

Definition 2.7 (∞-jets of bisections of $\mathcal{G}$)**.** *The map $\mathcal{J}^L \colon \mathcal{C}^\infty(\mathcal{G}) \to \mathcal{C}^\infty(M)\big[[t]\big]$ is said to be the ∞-jet of the smooth family of bisections L. In the sequel, we denote by $\mathbb{B}$ the space of such maps:*

$$\mathbb{B} = \{\mathcal{J}^L \colon \mathcal{C}^\infty(\mathcal{G}) \to \mathcal{C}^\infty(M)\big[[t]\big],\ L \textit{ smooth family of bisections}\}.$$

Example 2.8. *Following Example 2.6, if $L = (Graph(\zeta_t))_{t\in I}$, the data of the ∞-jet of the smooth family of bisections L is equivalent to the one of the Taylor series of $(\zeta_t)_{t\in I}$ with respect to t at $t = 0$. With a slight abuse of terminology, we will then write that the jet of L equals the Taylor series of $(\zeta_t)_{t\in I}$ at $t = 0$.*

$\mathbb{B}$ is a space of equivalence classes of smooth family of Lagrangian bisections. In the following, one defines naturally a product on $\mathbb{B}$. Let $L^1 = (L^1_t)_{t\in I}$ and $L^2 = (L^2_t)_{t\in J}$ two smooth families of Lagrangian bisections. Locally on $\mathcal{G}$, there exists $t_0 > 0$ such that for $|t| < t_0$, the product $L^1_t \cdot L^2_t$ is defined in the local symplectic groupoid $\mathcal{G}$. Then, we set the product to be the pointwise product with respect to the real infinitesimal parameter t :

$$\mathcal{J}^{L^1_t} \cdot \mathcal{J}^{L^2_t} \colon \begin{array}{ccc} \mathcal{C}^\infty(\mathcal{G}) & \to & \mathcal{C}^\infty(M)\big[[t]\big] \\ f & \mapsto & f \circ \left(\alpha_{|L^1_t \cdot L^2_t}\right)^{-1} \end{array}. \tag{2.8}$$

The following property is a straightforward consequence of Definition 2.7 and is left to the reader.

[2]In general, the target map β is also required to be invertible on the submanifold $L \subset \mathcal{G}$ for L to be a bisection. Here, since t is assumed sufficiently small, this condition is automatically fulfilled.

Proposition 2.9. $\mathbb{B}$ *is a group, with the neutral element being the jet constantly equal to the identity section:*

$$\mathcal{J}^{Id}\colon \begin{array}{ccc} \mathcal{C}^\infty(\mathcal{G}) & \to & \mathcal{C}^\infty(M)\big[[t]\big] \\ f & \mapsto & f\circ 0 \end{array}. \tag{2.9}$$

Let us now remark a second property of the bisection L_t by adding the symplectic geometry up. Since ζ_t is closed, its graph L_t is Lagrangian in $\mathcal{G}$. This leads us to consider the space of jets of Lagrangian bisections. We denote it by $\overline{\mathbb{L}}$. Again, this set carries a natural structure.

Proposition 2.10. $\overline{\mathbb{L}}$ *is a subgroup of the group* $\mathbb{B}$ *of* ∞*-jets of bisections.*

Now, we recall from [18] that for any two L_1 and L_2 bisections of a groupoid, denoting $L_1\cdot L_2$ the bisection being the product of L_1 and L_2, the induced diffeomorphisms on the base verify

$$\big(\beta\circ(\alpha_{|L_1})^{-1}\big)\circ\big(\beta\circ(\alpha_{|L_2})^{-1}\big)=\beta\circ(\alpha_{|L_1\cdot L_2})^{-1}. \tag{2.10}$$

In our context, the correspondence spelled by the Hamilton-Jacobi equation in Theorem 2.4 interprets as the direct relation inbetween the group $\overline{\mathbb{L}}$ and the dynamics generated by closed 1-forms on the base. Let us be more precise. Since the bisections $(L_t)_t$ are Lagrangian and close to the zero section of T^*M, the induced Poisson diffeomorphisms on the base manifold M $\beta\circ\big(\alpha_{|L_t}\big)^{-1}$ are flows of time-dependent closed forms. It follows from Proposition 2.3 that these Poisson diffeomorphisms stay on a leaf of the symplectic foliation. Furthermore, as explained in the following remark, these closed forms are exact if and only if the Lagrangian bisections are graphs of exact one-forms.

Remark 2.11 (Generating functions)**.** *The closedness of θ is equivalent to the one of ζ_t for all $t\in I$. The same equivalence holds of course about exactedness and leads us to Hamiltonian dynamics. Let us assume θ to be exact and $H\in\mathcal{C}^\infty(M)$ a Hamiltonian being a primitive of θ. As a consequence, there exists $S\in\mathcal{C}^\infty(M\times I)$ such that $dS_t=\zeta_t$. Equation* (2.6) *becomes*

$$\begin{cases} \frac{\partial S_t}{\partial t} = & (dS_t)^*\alpha^* H+\chi(t) \\ dS_0 = & 0 \end{cases} \tag{2.11}$$

where $\chi\in\mathcal{C}^\infty(I)$ is an arbitrary time-dependent constant. In the following, we chose χ to be 0 *and* $S_0=0$*. Using equation* (2.5)*, the graph of dS recovers the Hamiltonian dynamics generated by H. S is thus said to be a generating function for H.*

After a classical terminology for generating functions, let us call these Lagrangian bisections exact. Their jets form a group again.

Proposition 2.12. *We set*

$$\mathbb{L}=\{B^L\colon\mathcal{C}^\infty(G)\to\mathcal{C}^\infty(M)\big[[t]\big], L \textit{ smooth family of exact Lagrangian bisections}\}. \tag{2.12}$$

Then, $\mathbb{L}$ *is a subgroup of* $\overline{\mathbb{L}}$.

Proof. Let $\mathcal{J}^{L^1},\mathcal{J}^{L^2}\colon\mathcal{C}^\infty(\mathcal{G})\to\mathcal{C}^\infty(M)\big[[t]\big]$ two jets of exact Lagrangian bisections. We show that $\mathcal{J}^{L^1\cdot L^2}$ is a jet of exact Lagrangian bisections. Using Remark 2.11 and the Hamilton-Jacobi correspondence of Theorem 2.4, there exists two time-dependent Hamiltonians $\tilde H^1,\tilde H^2\in\mathcal{C}^\infty(M\times I)$ such that for any test function $f\in\mathcal{C}^\infty(\mathcal{G})$, $\mathcal{J}^{L^1}(f)=f\circ\phi_t^{\alpha^*\tilde H^1_t}\circ 0$ and $\mathcal{J}^{L^2}(f)=f\circ\phi_t^{\alpha^*\tilde H^2_t}\circ 0$. Now, the composition of two time-dependent Hamiltonian flows is a Hamiltonian flow.

$$\mathcal{J}^{L^1\cdot L^2}(f)=f\circ\phi_t^{\alpha^*\tilde H^2_t}\circ\phi_t^{\alpha^*\tilde H^1_t}\circ 0 \tag{2.13}$$

$$= f \circ \phi_t^{\alpha^* \tilde{H}_t} \circ 0, \tag{2.14}$$

where $\tilde{H}_t = \tilde{H}_t^2 + \tilde{H}_t^1 \circ \phi_t^{\tilde{H}_t^2}$. The same computation proves the existence of an inverse. Its neutral element is clearly the jet coming from the smooth family being constantly equal to the identity section. □

As already mentioned, the importance of Lagrangian bisections in mechanics is due to their relation with Hamiltonian dynamics. We define the analog in our context of the Hamiltonian group of, e.g., [19, Def. 1.11.], and of the group of diffeomorphisms generated by closed 1-forms.

Definition 2.13 (∞-jets Hamiltonian group)**.** *We call $\mathcal{H}$ the group of ∞-jets of pull-backs of time-dependent Hamiltonian flows:*

$$\mathcal{H} = \left\{ \mathcal{F} \colon \begin{array}{ccc} \mathcal{C}^\infty(M) & \to & \mathcal{C}^\infty(M)\big[[t]\big] \\ f & \mapsto & f \circ \phi_t^{\tilde{H}_t} \end{array}, \tilde{H} \in \mathcal{C}^\infty(M \times I) \right\}. \tag{2.15}$$

and $\overline{\mathcal{H}}$ the group of ∞-jets of pull-backs of flows generated by time-dependent closed 1-forms:

$$\overline{\mathcal{H}} = \left\{ \mathcal{F} \colon \begin{array}{ccc} \mathcal{C}^\infty(M) & \to & \mathcal{C}^\infty(M)\big[[t]\big] \\ f & \mapsto & f \circ \phi_t^{\tilde{\theta}_t} \end{array}, \tilde{\theta} \in \Omega_0^1(M)^I \right\}. \tag{2.16}$$

where, as before, $f \circ \phi_t^{\tilde{H}_t}$ and $f \circ \phi_t^{\tilde{\theta}_t}$ stand for their Taylor series with respect to t.

By adding these definitions to the remark 2.11 on exact Lagrangian bisections, we obtain the following corollary of Theorem 2.4. The proof relies on the same interpolation technique as the one of the proposition 2.12 and is left as an exercise.

Corollary 2.14. *There is a surjective group morphism from the group $\overline{\mathbb{L}}$ of ∞-jets of exact Lagrangian bisections of $\mathcal{G}$ to the group $\overline{\mathcal{H}}$ of ∞-jets of Hamiltonian flows of $(M, \{.,.\})$.*

This morphism restricts to a surjective group morphism from the group $\mathbb{L}$ of ∞-jets of exact Lagrangian bisections of $\mathcal{G}$ to the group $\mathcal{H}$ of ∞-jets of Hamiltonian flows of $(M, \{.,.\})$.

2.4 Approximations in the group of jets of Lagrangian bisections

One other consequence of Theorem 2.4 is the following corollary, yielding the existence of approximations of ϕ_t^θ at arbitrary order that preserve the Poisson geometry in the sense of 2.3.

Corollary 2.15. *Let $k \in \mathbb{N}$ and $(\zeta_t^k)_{t\in I} \in \Omega^1(M)^I$. Set $(L_t^k)_{t\in I} = \big(Graph(\zeta_t^k)\big)_{t\in I}$ and*

$$\varphi_t^k = \beta \circ (\alpha_{|L_t^k})^{-1}, \; t \in I. \tag{2.17}$$

If for all $t \in I$,

$$\left\{ \begin{array}{rcl} \frac{\partial \zeta_t^k}{\partial t} = & (\zeta_t^k)^* \alpha^* \theta + o(k) \\ \zeta_0 = & 0 \end{array} \right. , \tag{2.18}$$

then $(\varphi_t^k)_{t\in I}$ is the flow of a time-dependent closed 1-form $(\theta_t^k)_{t\in I} \in \Omega_0^1(M)$ such that $\theta_t^k = \theta + o(k)$. In particular, $(\varphi_t^k)_{t\in I}$ is an approximation of $(\phi_t^\theta)_{t\in I}$ at order at least k such that

- *for any $x \in M, \varphi_t^k(x)$ and x belong to the same symplectic leaf of $(M, \{.,.\})$,*
- *φ_t^k is a Poisson diffeomorphism for all $t \in I$.*

The family of Lagrangian bisections $L^k = (L^k_t)_{t\in I}$ is an approximation at order k of the family of Lagrangian bisections $L = (L_t)_{t\in I}$ given by the equation (2.4). The jet formalism of Section 2.3 provides a rigorous framework.

Proposition 2.16. *With the notations of Corollary 2.15, we have:*

$$\forall f \in \mathcal{C}^\infty(\mathcal{G}),\ \mathcal{J}^L(f) = \mathcal{J}^{L^k}(f) + o\left(t^k\right). \tag{2.19}$$

Using Corollary 2.15, this Hamilton-Jacobi equation has been applied to computational mechanics in [17]: the purpose was there to truncate solutions of this equation to approximate Hamiltonian dynamics on the base. Indeed, if S^k_t is a solution of equation (2.11) at order k, then the map

$$\phi^k_{\Delta t} = \beta \circ \left(\alpha_{|\mathrm{Graph}(\mathrm{d}S^k_{\Delta t})}\right)^{-1} \tag{2.20}$$

is a Hamiltonian Poisson integrator for H at order k and time-step Δt. This article is devoted to explain an algebraic formalism for the construction of high order Hamiltonian dynamics approximations. We also hope this to be of interest for a better understanding of the group of Lagrangian bisections of a symplectic groupoid and, in turn, a better understanding of the group of Poisson diffeomorphisms of a Poisson manifold. For that reason, let us consider an equation being a bit more general that (2.6). Namely, we consider the same one with a generic initial condition $\zeta_0 \in \Omega^1_0(M)$ such that its graph belongs to $\mathcal{G}$:

$$\begin{cases} \frac{\partial \zeta_t}{\partial t} = & (\zeta_t)^*\alpha^*\theta \\ \zeta_0 \in & \Omega^1_0(M) \end{cases} \tag{2.21}$$

Regarding equation (2.10), equation (2.21) is of interest while one looks at composition of Hamiltonian flows on M. We will come back to that in Section 4.

Since we aim at understanding high order approximations of Hamiltonian dynamics on M, let us study truncated solutions of (2.21). For this, we introduce the Lie-algebroid bracket $[.,.]$ on $\Omega^1(T^*M)$ defined by

$$[\zeta_1, \zeta_2] = \mathcal{L}_{X_{\zeta_1}}\zeta_2 - \mathcal{L}_{X_{\zeta_2}}\zeta_1 - d\omega(X_{\zeta_1}, X_{\zeta_2}) \tag{2.22}$$

where X_{ζ_i}, $i = 1, 2$, are the vector fields on T^*M generated by the canonical symplectic form out of the 1-forms ζ_i. Out of the following lemma, this Lie bracket allows us to compute approximations at arbitrary order of Hamilton-Jacobi equation.

Lemma 2.17. *Let $(\zeta_t)_{t\in I}$ and $(\theta_t)_{t\in I} \in \Omega^1(M)^I$ such that the graph of ζ_t is in $\mathcal{G}$ for all $t \in I$. Then,*

$$\frac{\partial}{\partial t}\left((\zeta_t)^*\alpha^*\theta_t\right) = (\zeta_t)^*\left([\alpha^*\theta_t, \tau^*\frac{\partial \zeta_t}{\partial t}] + \alpha^*\frac{\partial \theta_t}{\partial t}\right). \tag{2.23}$$

Similarly, for any $(S_t)_{t\in I} \in \mathcal{C}^\infty(M \times I)$ and any $(f_t)_{t\in I} \in \mathcal{C}^\infty(T^*M)$,

$$\frac{\partial}{\partial t}\left((dS_t)^* f_t\right) = (dS_t)^*\left(\{f_t, \tau^*\frac{\partial S_t}{\partial t}\}_\omega + \frac{\partial f_t}{\partial t}\right). \tag{2.24}$$

Proof. We start by proving equation (2.24). Let $x \in M$. It follows from classical symplectic geometry of the cotangent bundle that the curve $\gamma\colon t \in I \mapsto d_xS_t \in T^*M$ is the flow of the time-dependent Hamiltonian vector field of $\tau^* \frac{\partial S_t}{\partial t}$ starting at $d_x S_0$. Equation (2.24) is then a plain consequence of the chain rule. Since

$$\forall f, g \in \mathcal{C}^\infty(T^*M),\ d\{f,g\}_\omega = [df, dg], \tag{2.25}$$

equation (2.23) is obtained by usual extension from smooth functions to exact 1-forms, and then from closed forms to generic 1-forms using the Leibniz rule. $\square$

Let us illustrate Lemma 2.17. The algebroid bracket $[.,.]$ allows us to obtain iterated derivations of the Hamilton-Jacobi equation (2.21). We spell out the order 2 :

$$\frac{\partial^2 \zeta_t}{\partial t^2} = (\zeta_t)^*[\alpha^*\theta, \tau^*\zeta_t\alpha^*\theta], \tag{2.26}$$

After applying Lemma 2.17 a second time, we obtain an order 3 derivation:

$$\frac{\partial^3 \zeta_t}{\partial t^3} = (\zeta_t)^* \left([\alpha^*\theta, \tau^*(\zeta_t)^*[\alpha^*\theta, \tau^*(\zeta_t)^*\alpha^*\theta]] + [[\alpha^*\theta, \tau^*(\zeta_t)^*\alpha^*\theta], \tau^*(\zeta_t)^*\alpha^*\theta] \right). \tag{2.27}$$

3 A Pre-Lie approach to Hamiltonian Poisson integrators

Since $\mathcal{G} \subset T^*M$, the Lagrangian bisections of $\mathcal{G}$ that are close to the identity section are described by graphs of time-dependent closed 1-forms. We can approximate them by using the notion of jets we developed in the previous section. In order to approximate a given Lagrangian bisection by 1-forms, we now introduce an appropriate space J_ξ^∞ and a pre-Lie algebra structure on it. We then explain how this pre-Lie algebra encodes expansions of solutions of the Hamilton-Jacobi equation (2.21) through the introduction of Butcher series. In Section 3.3, we exhibit some algebraic simplifications arising in this expansion if the initial condition is chosen to be zero.

3.1 Pre-Lie formalism for Hamilton-Jacobi flows

In full generality, for $\xi \in \Omega^1(\mathcal{G})$, we are interested in the expansion of the general Hamilton-Jacobi flow

$$\frac{\partial \zeta}{\partial t} = \zeta_t^*\xi, \quad \zeta_0 \in \Omega_0^1(M). \tag{3.1}$$

We consider the infinite dimensional real vector subspace $J_\xi^\infty \subset \Omega^1(\mathcal{G})$ spanned by ξ and stable w.r.t. the following maps: for any $f, g \in J_\xi^\infty$,

$$\eta(f,g) \colon \begin{array}{ccc} \Omega_0^1(M) & \to & \Omega_0^1(M) \\ \zeta & \mapsto & \zeta^*[f, \tau^*\zeta^*g] \end{array}. \tag{3.2}$$

The space J_ξ^∞ is naturally equipped with the product $\rhd$

$$h \rhd \xi(\zeta) = \zeta^*[\xi, \tau^*\zeta^*g], \quad h \rhd \eta(f,g) = \eta(h \rhd f, g) + \eta(f, h \rhd g). \tag{3.3}$$

This yields a non-associative non-commutative magmatic structure on $(J_\xi^\infty, \rhd)$. Note that $(J_\xi^\infty, \rhd)$ is not a Lie algebra as $\rhd$ is not antisymmetric.

Remark 3.1 (J_ξ^∞ and jet spaces)**.** *The space J_ξ^∞ is analogous to the infinite jet space [1, 41, 37] on $\mathfrak{X}(M)$ used for the analysis of Runge-Kutta and Lie-group methods. In [31, 27], the accuracy of numerical integrators is studied via the use of Taylor expansions of ODE flows. Given a vector* *field $f \in \mathfrak{X}(M)$, the associated flow is expanded in terms of the partial derivatives of f at all order. The jet space over f is the vector space spanned by f, f', f'', ... We follow here a similar approach by fixing a one form $\xi \in \Omega^1(\mathcal{G})$ and considering the iterated derivatives appearing in the expansion of the flow. As a result, we shall use flows whose Taylor expansion is written with repeated compositions of the operator $\rhd$ on the space J^∞_ξ. For $\xi = \alpha^*\theta$, $\theta \in \Omega^1(M)$,these flows define a subspace of the jet of bisections.*

Lemma 2.17 provides an interpretation of the product $\rhd$ as a variational derivation in the sense of [41]. In that framework, considering jet spaces to iterate derivatives is therefore a natural idea. Let us notice that it is in general delicate to extend the product $\rhd$ on the whole $\Omega^1(\mathcal{G})$, as the definition of $\rhd$ is tied to the choice of the form $\xi \in \Omega^1(\mathcal{G})$. For instance, we raise the following remark.

Remark 3.2. *Given two spaces $(J^\infty_{\xi_1}, \rhd_1)$ and $(J^\infty_{\xi_2}, \rhd_2)$ and a map $\varphi\colon J^\infty_{\xi_1} \to J^\infty_{\xi_2}$ satisfying*

$$\varphi\Big(\eta(f,g)\Big) = \eta\Big(\varphi(f), \varphi(g)\Big), \quad f, g \in J^\infty_{\xi_1},$$

One can show that φ is a morphism, that is $\varphi(f \rhd_1 g) = \varphi(f) \rhd_2 \varphi(g)$ if and only if $\varphi(\xi_1) = \xi_2$.

We then obtain the following algebraic structure on J^∞_ξ.

Proposition 3.3. *The space $(J^\infty_\xi, \rhd)$ is a pre-Lie algebra, that is, for all $f, g, h \in J^\infty_\xi$,*

$$(f \rhd g) \rhd h - f \rhd (g \rhd h) = (g \rhd f) \rhd h - g \rhd (f \rhd h). \tag{3.4}$$

Proof. In the case $h = \xi$, equation (3.4) is a consequence of the Jacobi identity and that $\{\tau^*\zeta^* f, \tau^*\zeta^* g\}_\pi = 0$ for all f, $g \in \mathcal{C}(\mathcal{G})$. By induction, assume that the identity (3.4) holds for f, g, h_1 and f, g, h_2. Let $h = \eta(h_1, h_2)$, then

$$\begin{aligned}(f \rhd g) \rhd h - f \rhd (g \rhd h) &= \eta((f \rhd g) \rhd h_1 - f \rhd (g \rhd h_1), h_2) - \eta(f \rhd h_1, g \rhd h_2) \\ &\quad + \eta(h_1, (f \rhd g) \rhd h_2 - f \rhd (g \rhd h_2)) - \eta(g \rhd h_1, f \rhd h_2) \\ &= (g \rhd f) \rhd h - g \rhd (f \rhd h).\end{aligned}$$

Hence the result. □

Remark 3.4. *Following [21, 25], the product $\rhd$ can be seen as a flat connection on J^∞_ξ (see also the previous remark 3.1). A relation is expected in between the geometric interpretation of $\rhd$ and our use of a Weinstein tubular neighborhood. Indeed, the very existence of $\rhd$ is a consequence of the embedding of the local symplectic groupoid consisting in a neighborhood of the identity section of $\mathcal{G}$ inside T^*M.*

As stated in Theorem 2.4, the Lagrangian bisections are represented by the solution of Hamilton-Jacobi equations of the general form provided by equation (2.21) and Hamiltonian Poisson integrators rely on efficient discretizations of the exact Hamilton-Jacobi equation (2.11). The present pre-Lie formalism allows to conveniently give an explicit expression of the Taylor expansion of the solution of equation (2.21).

Proposition 3.5. *For $\xi \in \Omega^1(\mathcal{G})$, the solution of the Hamilton-Jacobi equation* (3.1) *satisfies*

$$\begin{aligned}\zeta_t &= (\zeta_0)^* \exp^{\rhd}(t\xi) = (\zeta_0)^* \sum_{n=0}^{\infty} \frac{t^n}{n!} \xi^{\rhd n} \qquad (3.5)\\ &= (\zeta_0)^* \Big(\operatorname{id} + t\xi + \frac{t^2}{2} \xi \rhd \xi + \frac{t^3}{3!} \xi \rhd (\xi \rhd \xi) + \frac{t^4}{4!} \xi \rhd (\xi \rhd (\xi \rhd \xi)) + \dots\Big).\end{aligned}$$

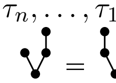
Proof. The result is proven by induction, in the spirit of [39]. □

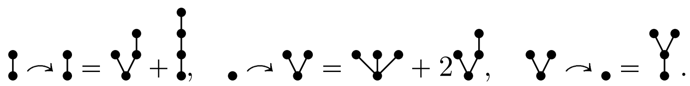
3.2 Butcher series expansion of a solution of Hamilton-Jacobi equation

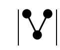
The expansion (3.5) is concise and simple as each order has only one Taylor term. However, the expansion of the iterations of $\rhd$ is not trivially represented. In this section, we further expand the Taylor expansion of (3.1), relying on a pre-Lie formalism of Butcher trees.

A non-planar Butcher tree in T is an oriented graph defined recursively by

$$\bullet \in T, \quad (\tau_n, \dots, \tau_1)_\bullet \in T, \quad \tau_1, \dots, \tau_n \in T,$$

where the root is graphically represented at the bottom. $(\tau_n, \dots, \tau_1)_\bullet$ denotes the tree with the root $\bullet$ and the n trees $\tau_n, \dots, \tau_1$ plugged to the root, $\mathcal{T} = \mathrm{Span}_{\mathbb{R}}(T)$, and the order of the branches does not matter: . The grafting of trees $\curvearrowright$ is defined as a product on $\mathcal{T}$ returning the sum of all possibilities (counted with multiplicity) of grafting the root of one tree on the nodes of another tree. For instance:



This defines the pre-Lie algebra $(\mathcal{T}, \curvearrowright)$ of Butcher trees. A natural grading on $\mathcal{T}$ is given by the number of nodes:  $= 3$.

The translation between the geometric structure $(J_\xi^\infty, \rhd)$ and the algebraic structure $(\mathcal{T}, \curvearrowright)$ is obtained through the elementary differential map. Given $\xi \in \Omega^1(\mathcal{G})$, define

$$\mathbb{F}^\xi(\bullet) = \xi \text{ and for } \zeta \in \Omega^1(M),\ \zeta^*\mathbb{F}^\xi((\tau_n, \dots, \tau_1)_\bullet) = \zeta^*[[\dots[\xi, \zeta^*\mathbb{F}^\xi(\tau_1)], \dots], \zeta^*\mathbb{F}^\xi(\tau_n)].$$

The following result is a straightforward consequence of the definition of the product $\rhd$.

Proposition 3.6. *The elementary differential* $\mathbb{F}^\xi \colon J_\xi^\infty \to \mathcal{T}$ *is a pre-Lie algebra morphism:*

$$\mathbb{F}^\xi(\tau_2 \curvearrowright \tau_1) = \mathbb{F}^\xi(\tau_2) \rhd \mathbb{F}^\xi(\tau_1). \tag{3.6}$$

This morphism allows to transport Proposition 3.5 and to rewrite it naturally in terms of trees. Let ζ_t be the solution of the Hamilton-Jacobi equation (3.1). Then, its expansion satisfies

$$\begin{aligned}\zeta_t &= (\zeta_0)^*\mathbb{F}^\xi(\exp^{\curvearrowright}(t\bullet)) = (\zeta_0)^* \sum_{n=0}^{\infty} \frac{t^n}{n!}\mathbb{F}^\xi(\bullet^{\curvearrowright n}) \\ &= (\zeta_0)^*\mathbb{F}^\xi\Big(\mathrm{id} + t\bullet + \frac{t^2}{2}\bullet \curvearrowright \bullet + \frac{t^3}{3!}\bullet \curvearrowright (\bullet \curvearrowright \bullet) + \frac{t^4}{4!}\bullet \curvearrowright (\bullet \curvearrowright (\bullet \curvearrowright \bullet)) + \dots\Big).\end{aligned} \tag{3.7}$$

Now, we use trees to encode explicitly the expansion $\exp^{\curvearrowright}$. The appropriate concept for such formal expansions is the one of Butcher series, often called B-series.

Definition 3.7 ([6])**.** *A B-series is a formal power series indexed by a coefficient map* $a \in \mathcal{T}^*$*:*

$$B^\xi(a) = \sum_{\tau \in \mathcal{T}} \frac{a(\tau)}{\sigma(\tau)}\mathbb{F}^\xi(\tau),$$

where $\sigma(\tau)$ *is the number of graph automorphisms of* τ*, also called the symmetry coefficient.*

We refer to [27, Sec. III] for an explicit formula of the symmetry coefficient. Then, the Butcher series of the solution of an Hamilton-Jacobi equation is the following.

Proposition 3.8. *Let $(\zeta_t)_t \in (\Omega^1(M))^I$ be the solution of the Hamilton-Jacobi equation* (3.1). *Then its Taylor expansion is given by the B-series*

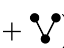
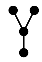
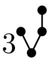
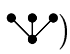
$$(\zeta_0)^* B^{t\xi}(e), \quad e(\tau) = \gamma^{-1}(\tau),$$

where γ is given by

$$\gamma(\bullet) = 1, \quad \gamma(\tau) = |\tau|\,\gamma(\tau_1)\ldots\gamma(\tau_n), \quad \tau = (\tau_n, \ldots, \tau_1)_\bullet.$$

Using Section 2.3, this proposition rephrases in terms of jets: the jet of the smooth family of Lagrangian bisections $(\mathrm{Graph}(\zeta_t)_{t\in I})$ is given by the Taylor series $(\zeta_0)^* B^{t\xi}(e)$ in $\overline{\mathbb{L}}$.

The representation of the Hamilton-Jacobi flow with trees allows us to conveniently provide an explicit expansion of ζ_t at any order. These calculations are called Farmer series in [16], where Hamiltonian Poisson integrators were implemented. Our algebraic formalism simplifies greatly the tedious calculations in [16] and allows to identify the degeneracies for specific choice of forms ξ (see Section 3.3). Using our construction of the appropriate Butcher series provided by Proposition 3.8, we find directly

$\zeta_t = \zeta_0^* \mathbb{F}^\xi \Big(\mathrm{id} + t\bullet + \frac{t^2}{2}$  $+ \frac{t^3}{3!}\big($  $+$  $\big) + \frac{t^4}{4!}\big($  $+$  $+ 3$  $+$  $\big) + \ldots \Big)$

$$\begin{aligned}
&= \zeta_0^* \Big(\mathrm{id} + t\xi + \frac{t^2}{2}[\xi, \tau^*\zeta_0^*\xi] + \frac{t^3}{3!}\big([\xi, \tau^*\zeta_0^*[\xi, \tau^*\zeta_0^*\xi]] + [[\xi, \tau^*\zeta_0^*\xi], \tau^*\zeta_0^*\xi]\big) \\
&+ \frac{t^4}{4!}\big([\xi, \tau^*\zeta_0^*[\xi, \tau^*\zeta_0^*[\xi, \tau^*\zeta_0^*\xi]]] + [\xi, \tau^*\zeta_0^*[[\xi, \tau^*\zeta_0^*\xi], \tau^*\zeta_0^*\xi]] \\
&+ 3[[\xi, \tau^*\zeta_0^*[\xi, \tau^*\zeta_0^*\xi]], \tau^*\zeta_0^*\xi] + [[[\xi, \tau^*\zeta_0^*\xi], \tau^*\zeta_0^*\xi], \tau^*\zeta_0^*\xi]\big) + \ldots \Big).
\end{aligned}$$

Note that in particular, we recover the equations (2.26) and (2.27) straightforwardly.

3.3 Degeneracies and explicit description of Hamilton-Jacobi flows

For the Farmer series in [16], one is interested in the specific case where $\xi = d\alpha^* H$ and $\zeta_0 = 0$. We use the previously introduced formalism of trees to identify vanishing terms and degeneracies corresponding to this particular case. First, let us collect useful observations in the following lemma.

Lemma 3.9. *Let $f \in \mathcal{C}^\infty(M)$. The following degeneracies hold:*

$$0^*\alpha^* f = f, \tag{3.8}$$

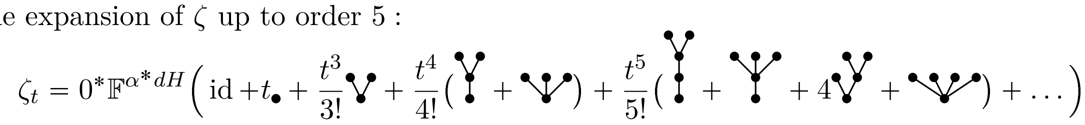
$$0^*\{\alpha^* f, \tau^* f\}_\omega = 0. \tag{3.9}$$

Proof. The first item is trivial. Let us prove the second one. Let $g \in \mathcal{C}^\infty(M)$. Since α is a Poisson morphism, it follows from equation (3.6) of [9] and the first item of the present proposition, that $0^*\{\alpha^* f, \tau^* f\}_\omega$ is colinear to $\{f, g\}$ in $\mathcal{C}^\infty(M)$. Equation (3.9) is deduced from anti-symmetry of $\{-,-\}$. ☐

As (3.9) implies $0^*\{\alpha^* H, \tau^* H\}_\omega = 0$, the differential associated to some specific trees vanishes, in the spirit of superconvergence (see, e.g., [32]).

Lemma 3.10. *Let $\tau \in \mathcal{T}$. If τ contains a descendant of the form* *, then $0^*\mathbb{F}^{\alpha^* dH}(\tau) = 0$.*

With the formalism of Butcher series, we are now able to compute straightforwardly the Farmer series of [16] at high order. Let $(S_t)_t \in \mathcal{C}^\infty(M \times I)$ be a generating function of a Hamiltonian $H \in \mathcal{C}^\infty(M)$ provided by equation (2.11). Let us set $\zeta_t = \mathrm{d}S_t$ for $t \in I$. We write the expansion of ζ up to order 5 :



$$
\begin{aligned}
&= t\mathrm{d}H + \frac{t^3}{3!}0^*[[\alpha^*\mathrm{d}H, \tau^*\mathrm{d}H], \tau^*\mathrm{d}H] \\
&+ \frac{t^4}{4!}\big(0^*[\alpha^*\mathrm{d}H, \tau^*0^*[[\alpha^*\mathrm{d}H, \tau^*\mathrm{d}H], \tau^*\mathrm{d}H]] + 0^*[[[\alpha^*\mathrm{d}H, \tau^*\mathrm{d}H], \tau^*\mathrm{d}H], \tau^*\mathrm{d}H]\big) \\
&+ \frac{t^5}{5!}\big(0^*[\alpha^*\mathrm{d}H, \tau^*0^*[\alpha^*\mathrm{d}H, \tau^*0^*[[\alpha^*\mathrm{d}H, \tau^*\mathrm{d}H], \tau^*\mathrm{d}H]]] \\
&+ 0^*[\alpha^*\mathrm{d}H, \tau^*0^*[[[\alpha^*\mathrm{d}H, \tau^*\mathrm{d}H], \tau^*\mathrm{d}H], \tau^*\mathrm{d}H]] \\
&+ 4 \cdot 0^*[[\alpha^*\mathrm{d}H, \tau^*0^*[[\alpha^*\mathrm{d}H, \tau^*\mathrm{d}H], \tau^*\mathrm{d}H]], \tau^*\mathrm{d}H] \\
&+ 0^*[[[[\alpha^*\mathrm{d}H, \tau^*\mathrm{d}H], \tau^*\mathrm{d}H], \tau^*\mathrm{d}H], \tau^*\mathrm{d}H]\big) + \dots
\end{aligned}
\tag{3.10}
$$

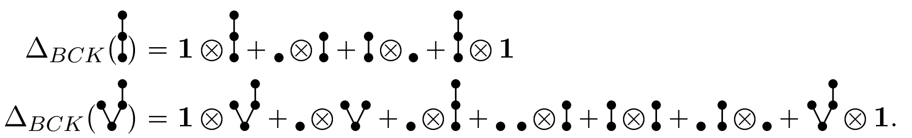
4 Composition of Lagrangian bisections and B-series

In this section, we use Butcher series theory to describe algebraically the group law of Lagrangian bisections. More precisely, we prove that the product of Lagrangian bisections is encoded by the composition of B-series and the Butcher-Connes-Kreimer Hopf algebra. The analysis relies heavily on the notion of jets constructed in Section 2.3. The main result of this section is Theorem 4.2.

Let us consider the symmetric tensor algebra $(S(\mathcal{T}), \cdot)$ over trees, that is the vector space spanned by forests, with its unit being the empty forest $\mathbf{1}$. Let the Butcher-Connes-Kreimer coproduct $\Delta_{BCK} \colon \mathcal{T} \to \mathcal{T} \otimes \mathcal{T}$ be given by

$$
\Delta_{BCK}(\tau) = \sum_{s \subset \tau} (\tau \backslash s) \otimes s,
$$

where the sum is indexed on all the subtrees of τ that contain the root (including the empty tree). One finds for instance



(4.1)

The coproduct is extended on $S(\mathcal{T})$ by $\Delta_{BCK}(\pi_1 \cdot \pi_2) = \Delta_{BCK}(\pi_1) \cdot \Delta_{BCK}(\pi_2)$. Then, it is well-known that $(S(\mathcal{T}), \mathbf{1}, \cdot, \mathbf{1}^*, \Delta_{BCK})$ yields the BCK Hopf algebra [14, 23], used in particular to represent differential operators.

We call character a form $a \in S(\mathcal{T})^*$ that satisfies $a(\pi_1 \cdot \pi_2) = a(\pi_1)a(\pi_2)$ and we denote the product $\mu \colon \mathcal{T} \otimes \mathcal{T} \to \mathcal{T}$. Note that given $a \in \mathcal{T}^*$, there is a unique way to extend a as a character on $S(\mathcal{T})$.

The composition of two B-series is detailed by the BCK Hopf algebra [13]. Note that it applies for any Taylor expansion over J^∞_ξ, not just for the exact Hamilton-Jacobi flow.

Proposition 4.1. *Let $B^\xi(a^1)$ and $B^\xi(a^2)$ be two B-series. Their composition is the B-series*

$$(B^\xi(a^1))^* B^\xi(a^2) = B^\xi(a^1 * a^2), \quad a^1 * a^2 = \mu \circ (a^1 \otimes a^2) \circ \Delta_{BCK},$$

where a_1 is extended as a character over $S(\mathcal{T})$ and $*$ is called the composition law. In addition, the set $G_B = \{a \in \mathcal{T}^*, a(\bullet) = 1\}$, equipped with $*$ forms a group, called the Butcher group, with unit $\delta_\bullet$.

From the example (4.1), we find, for instance,

$$a^1 * a^2(\;) = a_2(\;) + a_1(\bullet)a_2(\;) + a_1(\bullet)a_2(\;) + a_1(\bullet)^2 a_2(\;)$$
$$+ a_1(\;)a_2(\;) + a_1(\bullet)a_1(\;)a_2(\bullet) + a_1(\;)$$

Comparing Proposition 4.1 with equation (2.10), we observe that the Butcher group encodes the product of Lagrangian bisections in a local symplectic groupoid, as stated in the following theorem.We use the terminology introduced in the example 2.8, meaning that if $(\mathrm{Graph}(\zeta_t)_{t\in I}$ is a smooth family of bisections, we identify its jet with the Taylor series of $(\zeta_t)_t$ with respect to t.

Theorem 4.2. *Let $\xi \in \Omega^1(\mathcal{G})$ and the map $\Psi^\xi \colon G_B \to \Omega^1(M)[[t]]$ be given by*

$$\Psi^\xi(a) = 0^* B^{t\xi}(a).$$

Then:

- *For any $\theta \in \Omega^1(M)$, $\Psi^{\alpha^*\theta} \colon (G_B, *) \hookrightarrow (\mathbb{B}, \cdot)$ is an injective group morphism.*
- *For any $\theta \in \Omega^1_0(M)$, $\Psi^{\alpha^*\theta} \colon (G_B, *) \hookrightarrow (\bar{\mathbb{L}}, \cdot)$ is an injective group morphism.*
- *For any $H \in \mathcal{C}^\infty(M)$, $\Psi^{\alpha^* dH} \colon (G_B, *) \hookrightarrow (\mathbb{L}, \cdot)$ is an injective group morphism.*

Proof. The fact that these maps are well defined is a consequence of the section 2. Their injectivity follows from the definition of a Butcher series, and the group morphism property is provided by the proposition 4.1. $\square$

We considered for simplicity jet spaces generated by one form ξ, and it is worth mentioning that one could straightforwardly extend the previous formalism for flows driven by several forms $\xi_1, \dots, \xi_n$ by using decorated nodes. The jet space of the section 3 becomes $J^\infty_{\xi_1,\dots,\xi_n}$ and is represented by the algebra of decorated trees spanned by $\bullet_1, \dots, \bullet_n$. The previously described algebra adapts straightforwardly in this setting, in the spirit of P-series for partitioned problems [27].

For instance, let us consider $J^\infty_{\xi_1,\xi_2}$ and bi-coloured trees where $\bullet$ stands for ξ_1 and $\circ$ stands for ξ_2. Let us compose the B-series $B^{t\xi_1}(\delta_\bullet)$ and $B^{t\xi_2}(\delta_\circ)$. The composition is computed with the BCK Hopf algebra as in Proposition 4.1 and we find

$$\begin{aligned}
\zeta_0^*(B^{t\xi_2}(\delta_\circ))^* B^{t\xi_1}(\delta_\bullet) &= \zeta_0^* B^{t\xi_1,t\xi_2}(\delta_\circ * \delta_\bullet) \\
&= \zeta_0^* \mathbb{F}^{t\xi_1,t\xi_2}\Big(\circ + \bullet + \; + \frac{1}{2!}\; + \frac{1}{3!}\; + \frac{1}{4!}\; + \dots\Big) \\
&= \zeta_0^*\Big(t(\xi_1 + \xi_2) + t^2[\xi_1, \tau^*\zeta_0^*\xi_2] + \frac{t^3}{2!}[[\xi_1, \tau^*\zeta_0^*\xi_2], \tau^*\zeta_0^*\xi_2] + \dots\Big).
\end{aligned}$$

5 Numerical methods for Hamiltonian systems on Poisson manifolds

Using the pre-Lie structure of Butcher trees, we present a new class of Hamiltonian Poisson methods based on Taylor and Runge-Kutta discretisations. We emphasize that the framework of pre-Lie algebras and Butcher series is a central tool for the numerical integration of ODEs in $\mathbb{R}^d$. The surprising effect of the birealisations is that they translate a Poisson geometry into a simpler geometry on $\Omega^1_0(M)$, where one can apply Euclidean numerical tools.

Denote $\mathcal{T}_0$ the vector space spanned by trees that do not have a descendant of the form and $\mathcal{T}_0^N$ the subspace containing trees of order at most N. Let $e_0^N(\tau) = \gamma^{-1}(\tau)\mathbb{1}_{\tau\in\mathcal{T}_0^N}$ the restriction of the coefficient map of Proposition 3.8. Following Lemma 3.10, we obtain new Hamiltonian Poisson integrators of arbitrary order N. They are based on truncations of the expansion (3.10) of the Hamilton-Jacobi flow (3.1).

Theorem 5.1. *The following Taylor-Hamiltonian-Poisson integrator is of order N for solving equation* (2.1)*:*

$$y_n = \alpha(0^* B_{x_n}^{\Delta t\alpha^* dH}(e_0^N)), \tag{5.1}$$

$$y_{n+1} = \beta(0^* B_{x_n}^{\Delta t\alpha^* dH}(e_0^N)), \tag{5.2}$$

where $x_n \in M$ denotes an intermediary point implicitly defined by equation (5.1) *and Δt is the timestep of the method.*

By their very constructions, these methods are Hamiltonian Poisson integrators. Therefore, they follow the flow of some time-dependent Hamiltonian and stay on a symplectic leaf (or preserve any Casimir) all along a trajectory. The following method has been benchmarked in [17, Sec. 5.2.] on a Lotka-Volterra system in a neighborhood of a singularity.

Example 5.2 (Euler method)**.** *The simplest method is the Euler method, given by Theorem 5.1 for $N = 1$ or $N = 2$. It is of second order and the associated iteration is*

$$y_n = \alpha(\Delta t d_{x_n} H), \quad y_{n+1} = \beta(\Delta t d_{x_n} H). \tag{5.3}$$

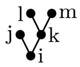
The number of terms in $\mathcal{T}_0^N$ blows up quickly as the order N gets larger, which makes the Taylor approach computationally expensive and often unstable. As a solution, we propose the following class of Runge-Kutta-Hamiltonian-Poisson (RKHP) approximations for the high-order approximation of equation (2.1):

$$\begin{aligned} Z_i &= \zeta_0 + t\sum_{j=1}^s a_{ij}(Z_j)^*\xi, \\ \psi^{t\xi}(\zeta_0) &= \zeta_0 + t\sum_{i=1}^s b_i(Z_i)^*\xi, \\ y_n &= \alpha(0^*\psi_{x_n}^{\Delta t d\alpha^* H}) \\ y_{n+1} &= \beta(0^*\psi_{x_n}^{\Delta t d\alpha^* H}). \end{aligned} \tag{5.4}$$

The a_{ij} and b_i are the coefficients of the method and shall be chosen in order to reach high order of accuracy with a small number of intermediate stages s. We use the notation $c_i = \sum_{j=1}^s a_{ij}$. For t small enough, note that this definition gives a local diffeomorphism $\psi^{t\xi}$ on the space of closed 1-forms $\Omega^1_0(M)$. Similarly to the order theory of Runge-Kutta methods for ODEs, the Taylor expansion of methods of $\psi^{t\xi}(\zeta_0)$ in (5.4) writes as a Butcher series

$$\psi^{t\xi}(\zeta_0) = \zeta_0 + \zeta_0^* B^{t\xi}(a),$$

with the same coefficient map a as for standard Runge-Kutta methods [27, Chap. III]:

$a($ 

$) = \sum_{i,j,k,l,m=1}^{s} b_i a_{ij} a_{ik} a_{kl} a_{km} = \sum_{i,k=1}^{s} b_i c_i a_{ik} c_k^2.$

The algebraic reformulation of Section 3 allows us to take over the classical order theory of Runge-Kutta methods for ODEs [27] and to adapt it in the context of Hamilton-Jacobi approximations.

Theorem 5.3. *Let a RKHP method* (5.4)*, with coefficient map a. Then, if $a(\tau) = e(\tau)$ for all $\tau \in \mathcal{T}_0^N$, the method has order N for solving* (2.1)*. In particular, the order conditions for the first orders are in Table 1.*

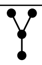
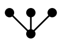
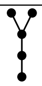
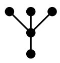
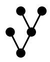
Order	Butcher tree τ	Order condition $a(\tau) = e(\tau)$
1		$\sum_{i=1}^s b_i = 1$
3		$\sum_{i=1}^s b_i c_i^2 = \frac{1}{3}$
4		$\sum_{i,j=1}^s b_i a_{ij} c_j^2 = \frac{1}{12}$
		$\sum_{i=1}^s b_i c_i^3 = \frac{1}{4}$
5		$\sum_{i,j,k=1}^s b_i a_{ij} a_{jk} c_k^2 = \frac{1}{60}$
		$\sum_{i,j=1}^s b_i a_{ij} c_j^3 = \frac{1}{20}$
		$\sum_{i,j=1}^s b_i c_i a_{ij} c_j^2 = \frac{1}{15}$
		$\sum_{i=1}^s b_i c_i^4 = \frac{1}{5}$

Table 1: Order conditions of RKHP integrators.

Remark 5.4. *The idea of approximating birealizations at high order has been explored by [8], where a procedure to asymptotically compute the map $\alpha\colon \mathcal{G} \to M$ is investigated. This relies on a long history research of deformation theory in order to construct the local symplectic groupoid of any Poisson manifold ([11, 7]). We expect an accurate relation inbetween the order of the approximation of the birealization and the one of the dynamics to provide robust numerical methods.*

A collection of explicit RKHP integrators with minimal number of stages for fixed order is the following. The superconvergence property of Lemma 3.10 allows us to reach high order p with less than p evaluations. Note in particular that there is no need to consider discretisations associated to symplectic methods (like the midpoint method) as the geometry has been taken care of by the birealisations. Let us also recall that for any $\theta \in \mathcal{G}$, $\beta(\theta) = \alpha(-\theta)$, where the sign comes from the vector bundle T^*M.

Euler method: The Euler method given by (5.1)-(5.2) is associated to the following Runge-Kutta discretisation.

$$\begin{aligned} y_n &= \alpha(\Delta t d_{x_n} H) \\ y_{n+1} &= \beta(\Delta t d_{x_n} H) \end{aligned} \qquad \begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

Third order method:

$$\begin{aligned} Z &= \tfrac{1}{\sqrt{3}}\Delta t d_{x_n} H \\ y_n &= \alpha(\Delta t d_{x_n} Z^* \alpha^* H) \\ y_{n+1} &= \beta(\Delta t d_{x_n} Z^* \alpha^* H) \end{aligned} \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ \hline & 0 & 1 \end{array}$$

Fourth order method:

$$\begin{aligned} Z_1 &= -\tfrac{\sqrt{3}}{4}\Delta t d_{x_n} H \\ Z_2 &= \tfrac{3}{4}\Delta t d_{x_n} Z_1^* \alpha^* H \\ y_n &= \alpha\left(\Delta t(\tfrac{11}{27} d_{x_n} H + \tfrac{16}{27} d_{x_n} Z_2^* \alpha^* H)\right) \\ y_{n+1} &= \beta\left(\Delta t(\tfrac{11}{27} d_{x_n} H + \tfrac{16}{27} d_{x_n} Z_2^* \alpha^* H)\right) \end{aligned} \qquad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} & 0 & 0 \\ \frac{3}{4} & 0 & \frac{3}{4} & 0 \\ \hline & \frac{11}{27} & 0 & \frac{16}{27} \end{array}$$

Remark 5.5. *If implicit implementations are computationally feasible, a one-stage third order implicit method is*

$$\begin{aligned} Z &= \tfrac{1}{\sqrt{3}}\Delta t d_{x_n} Z^* \alpha^* H \\ y_n &= \alpha(\Delta t d_{x_n} Z^* \alpha^* H) \\ y_{n+1} &= \beta(\Delta t d_{x_n} Z^* \alpha^* H) \end{aligned} \qquad \begin{array}{c|c} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \hline & 1 \end{array}$$

Remark 5.6. *The Butcher-Connes-Kreimer Hopf algebra seen in Section 4 is also relevant to approximations of Lagrangian bisections. As a computational consequence, it allows for the study of composition methods. For instance, let the first order approximation of the Farmer series, analogous to the Euler method, be given by*

$$\psi^{t\xi}(\zeta_0) = \zeta_0 + t\zeta_0^*\xi = \zeta_0^*(\mathrm{id} + B^{t\xi}(\delta_\bullet)).$$

Then the explicit midpoint method is the composition

$$\begin{aligned} \hat{\psi}^{t\xi}(\zeta_0) &= \zeta_0^*(d\psi^{t\xi/2})^*\psi^{t\xi} = \zeta_0 + t\xi(\zeta_0 + \frac{t}{2}d\xi(\zeta_0) = \zeta_0^*(\mathrm{id} + B^{t\xi}(\delta_\bullet \circ (\delta_\bullet/2))) \\ &= t\zeta_0^*\xi + \frac{t^2}{2}\zeta_0^*[\xi, \tau^*\zeta_0^*\xi] + \frac{t^3}{8}\zeta_0^*[[\xi, \tau^*\zeta_0^*\xi], \tau^*\zeta_0^*\xi] + \frac{t^4}{48}\zeta_0^*[[[\xi, \tau^*\zeta_0^*\xi], \tau^*\zeta_0^*\xi], \tau^*\zeta_0^*\xi] + \dots \end{aligned}$$

We observe in particular that $\hat{\psi}$ provides a second order approximation for a general ξ, similarly to the context of ODEs.

6 Conclusion

The algebraic tools of geometric integration extend for the study of Poisson geometry and bring new insights, from both geometric and computational viewpoints. Some possible extensions of the present work could include the creation of a stability analysis in the context of Hamiltonian Poisson integrators. For instance, steep dynamical systems of conservative mechanics may benefit from the formalism we introduced. We also plan to implement implicit methods and benchmark their orders in order to provide numerical illustrations of our algebraic results. This will deserve a more mechanics oriented article. On the algebraic side, a natural extension could adapt the Hopf algebra of substitution for the backward error analysis in this context, and a more general geometric context could yield post-Lie algebras. This is matter for future work.

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