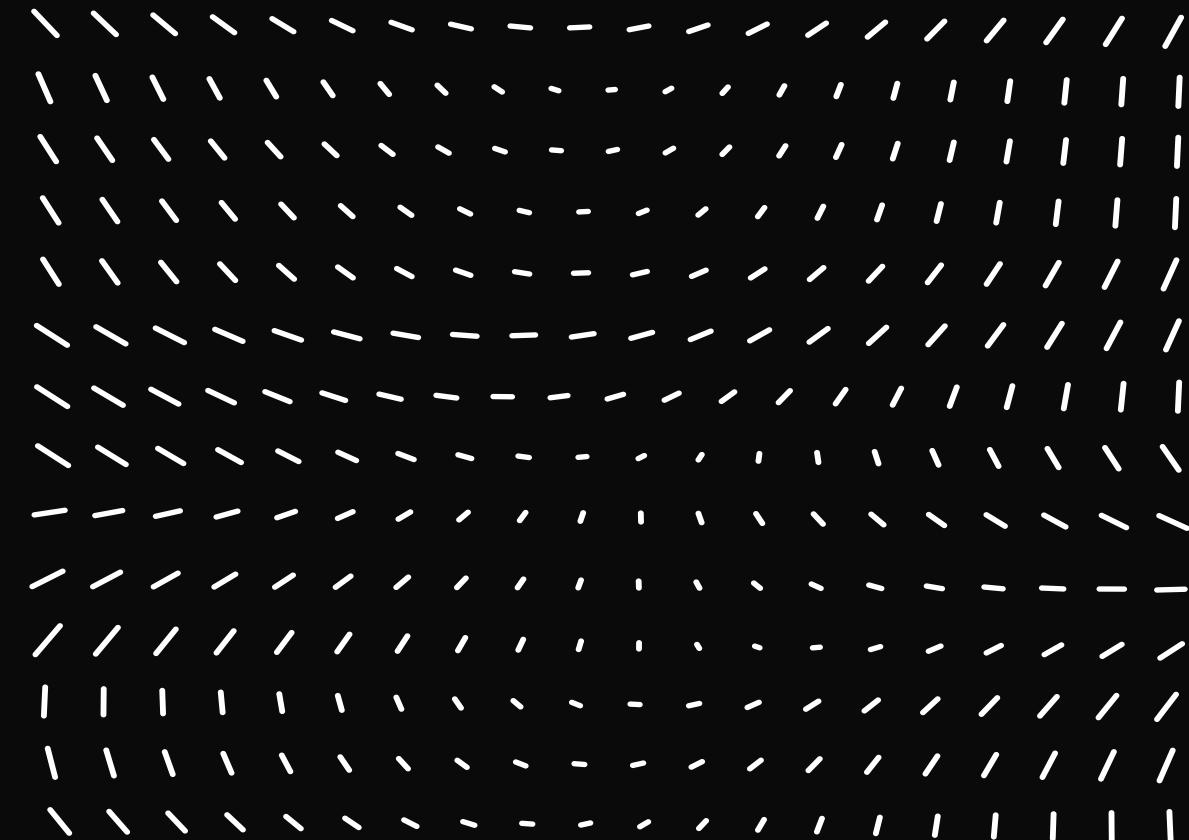


# Geometric Numerical Integration

## An algebraic-geometric introduction



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## Chapter I: The flow of an evolution differential equation

Let  $f \in C^1(\mathbb{R}^d)$  (vector fields on  $\mathbb{R}^d$ ) or  $f \in C^1(M)$  ( $M$  manifold)

Assume  $f$  is Lipschitz (globally) and smooth ( $C^\infty$ ) for simplicity. The ODE  $\begin{cases} \gamma'(t) = f(\gamma(t)) \\ \gamma(0) = \gamma_0 \end{cases}$

is well defined by Cauchy-Lipschitz/Picard/Lindelöf.

We denote  $\varphi_t(\gamma_0) = \gamma(t)$  the exact flow of (c)

Prop: •  $\varphi_0 = \text{id}$   
•  $\varphi_s \circ \varphi_t = \varphi_{s+t}$   
•  $\varphi_{-t} \circ \varphi_t = \text{id}$

$\left( \{\varphi_t, t \in \mathbb{R}\}, \circ \right)$  is a group.

Rb: recall that an ODE of the form  $\gamma'(t) = f(t, \gamma(t))$  can be rewritten in the form (c) with  $Y(t) = \begin{pmatrix} \gamma(t) \\ 1 \end{pmatrix}$  and  $F(Y) = \begin{pmatrix} f(t, \gamma) \\ 1 \end{pmatrix}$

# 1) Examples of differential systems

## a) Linear systems

$$\rightarrow f(\gamma) = A\gamma, \quad A \in \mathbb{R}^{d \times d}$$

$$q_t(\gamma) = e^{tA}\gamma, \text{ where } e^{tA} = \sum_{b=0}^{+\infty} \frac{t^b A^b}{b!} \quad \begin{array}{l} (\text{Power series}) \\ R = +\infty \end{array}$$

$$\rightarrow f(t, \gamma) = A(t)\gamma \quad \text{and} \quad [A(t), A(s)] := A(t)A(s) - A(s)A(t) = 0$$

then  $q_t(\gamma) = e^{\int_0^t A(s)ds} \gamma$

$$\rightarrow f(\gamma) = A(\gamma)\gamma$$

↳ see  DM

Rk: if  $f(\gamma) = A(\gamma)\gamma$  and

$$\hookrightarrow A^T(\gamma) = -A(\gamma), \text{ then } q_t \in SO(d)$$

Ex: Rigid body  $f \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{pmatrix} = \begin{pmatrix} 0 & -\gamma_3 & \gamma_2 \\ \gamma_3 & 0 & \gamma_1 \\ -\gamma_2 & \gamma_1 & 0 \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{pmatrix}$

$$\frac{d}{dt} (q_t^\top(\gamma) \quad q_t(\gamma)) = q_t^\top(\gamma) (A^\top(q_t(\gamma)) + A(q_t(\gamma))) q_t(\gamma)$$

$$= 0$$

So that  $|\varphi_t(\gamma)| = |\gamma|$ , that is  $\underline{|\varphi_t(\gamma)| \in |\gamma| \mathbb{S}^{d-1}}$

$\hookrightarrow$  More generally, if  $A(\gamma) \in \mathbb{G}$  and  $\gamma_0 \in G$  where  $G$  a lie group and  $\mathbb{G}$  its lie algebra, then,

$\varphi_t(\gamma_0) \in G, \forall t.$



## (b) Hamiltonian systems

Consider  $q$  the position and  $p$  the momentum (mass  $\times$  speed), a force deriving from a potential  $F(q) = -\nabla V(q)$ ,  $V: \mathbb{R}^d \rightarrow \mathbb{R}$ .

$$\begin{pmatrix} -\frac{\partial V}{\partial q_1}(q) \\ \vdots \\ -\frac{\partial V}{\partial q_d}(q) \end{pmatrix}$$

Then the equations of motion are  $\ddot{q}(t) = -\nabla V(q)$ , or alternatively:

$$\begin{cases} \dot{q}(t) = p(t) \\ \dot{p}(t) = -\nabla V(q(t)) \end{cases} \quad (H)$$

Let the Hamiltonian  $H: \mathbb{R}^{2d} \rightarrow \mathbb{R}$

$$(q, p) \longrightarrow \frac{p^2}{2} + V(q)$$

$(H)$  reduces as

$$\begin{cases} \dot{q}(t) = \nabla_p H(q(t), p(t)) \\ \dot{p}(t) = -\nabla_q H(q(t), p(t)) \end{cases}$$

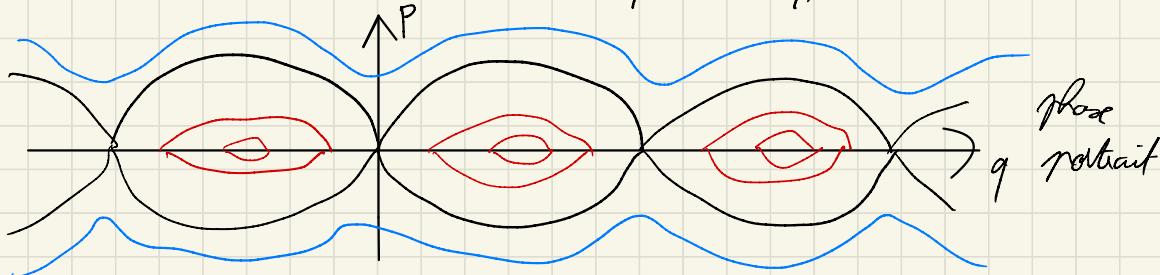
or equivalently  $\gamma'(t) = J \nabla H(\gamma(t))$ ,  $J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}$ .

Ex: The simplest example is with  $V(q) = \frac{q^2}{2}$ , the linearized pendulum

$$\begin{cases} \dot{q} = p \\ \dot{p} = -q \end{cases} \rightarrow \gamma'(t) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \gamma(t)$$

$$\varphi_t(\gamma_0) = e^{tJ} \gamma_0 = \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix} \gamma_0$$

The simple pendulum corresponds to  $V(q) = -\cos(q)$ .



Prop: The solution of  $(H)$  satisfies  $H(\gamma(t)) = H(\gamma_0)$ ,  $\forall t$

Proof:  $\frac{d}{dt} (H(\varphi_t(\gamma_0))) = \langle \nabla H(\varphi_t(\gamma_0)), \frac{d}{dt} \varphi_t(\gamma_0) \rangle$

$$= \langle \nabla H(\varphi_t(\gamma_0)), J \nabla H(\varphi_t(\gamma_0)) \rangle \\ = 0 \quad \square$$

Rb: this type of systems appears also in molecular dynamics for instance with the Lennard-Jones potential

$$V(q_i - q_j) = \frac{C_1}{r^{12}} - \frac{C_2}{r^6}$$



In this context, the dimension  $d$  is very high (theoretically,  $d \sim N_{\text{atoms}} \approx 10^{24}$ ).

### © Constrained equations, dynamics on manifolds

Let  $J: \mathbb{R}^d \rightarrow \mathbb{R}^q$ ,  $q < d$ , and define

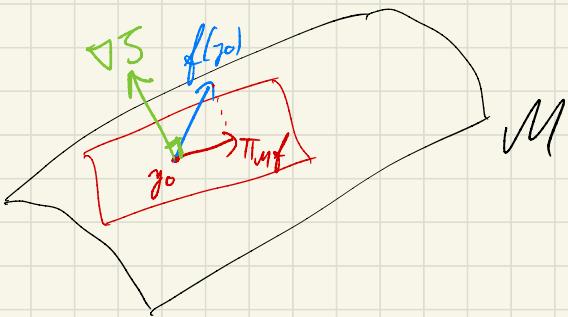
$$M = \{x \in \mathbb{R}^d, J(x) = 0\}$$

and  $\Pi_M(x) = Id - \frac{\nabla J \cdot \nabla J^T}{\nabla J^T \cdot \nabla J}(x)$ , assuming  $|\nabla J(x)| > 0, \forall x$ .

Prop: the solution of

$$\dot{\gamma}'(t) = \Pi_M(\dot{\gamma}(t)) f(\gamma(t)) \text{ satisfies}$$

satisfies  $\varphi_t(\gamma_0) \in M, \forall t$ .



Proof:  $\frac{d}{dt} (\mathcal{J}(\gamma(t))) = \underbrace{(\nabla \mathcal{J}^T \cdot \Pi_M f)}_{=0} (\gamma(t)) .$

□

One could directly define  $f \in \mathcal{X}(M)$  a  $\alpha$  differentiable manifold  $M$ . Then the flow of  $\gamma' = f(\gamma)$  is on  $M$ .  
 $\Rightarrow$  No need for an embedding in a space of higher dimension.

Necessary tools of diff geometry

## 2) Geometric properties of the flow

### @ First integrals

def: a non-constant function  $I(y)$  is called a first integral of  $(C)$  if

$$I'(y) f(y) = 0, \forall y$$

Prop:  $I$  first integral  $\Leftrightarrow \forall t, I(Q_t(y_0)) = I(y_0)$

Ex:  $H$  is a first integral of  $y' = J \nabla H(y)$ .

- rigid body  $y \mapsto |y|^2$  is a first integral.
- $J$  is a first integral of constrained systems.

### (b) Volume preservation

def: the flow of an ODE  $y' = f(y)$  preserves volume if for all measurable set  $\Omega \subset \mathbb{R}^d$ , for all  $t \geq 0$ , we have  $\text{Vol}(Q_t(\Omega)) = \text{Vol}(\Omega)$ , that is,

$$\int_{\varphi_t(\Omega)} dy = \int_{\Omega} dy.$$

Thm (Liouville): The flow of  $\gamma' = f(\gamma)$  is VP iff  $\operatorname{div}(f) = 0$ .

Proof:  $\int_{\varphi_t(\Omega)} dy = \int_{\Omega} |\det\left(\frac{\partial \varphi_t}{\partial \gamma}\right)| dy$  ← Jacobian

As this is valid for any  $\Omega$ , we have:

$$VP \Leftrightarrow \left| \det\left(\frac{\partial \varphi_t}{\partial \gamma}\right) \right| = 1, \forall t, \gamma$$

$$\Leftrightarrow \det\left(\frac{\partial \varphi_t}{\partial \gamma}\right) = 1, \forall t, \gamma \quad (\text{exp value at } t=0)$$

$$\Leftrightarrow \frac{d}{dt} \left( \det\left(\frac{\partial \varphi_t}{\partial \gamma}\right) \right) = 0$$

We find  $\frac{d}{dt} (\varphi_t(\gamma)) = f(\varphi_t(\gamma))$ ,

so that by differentiating in  $\gamma$ :

$$\frac{\partial}{\partial \gamma} \left( \frac{d}{dt} \varphi_t(\gamma) \right) = f'(\varphi_t(\gamma)) \frac{\partial \varphi_t}{\partial \gamma}$$

By Schowy, we find the Variational equation

$$\boxed{\frac{d}{dt} \left( \frac{\partial \varphi_t}{\partial \gamma} \right) = f'(\varphi_t(\gamma)) \frac{\partial \varphi_t}{\partial \gamma}}$$

Puis la différentielle du déterminant pour une matrice inversible

$$\text{est : } \det'(A)(H) = T_A \left( \text{Cor}(A)^T H \right) \\ = T_A (A^{-1} H) \det(A)$$

$$\text{donc } \frac{d}{dt} \left( \det \left( \frac{\partial \varphi_t}{\partial \gamma} \right) \right) = \det' \left( \frac{\partial \varphi_t}{\partial \gamma} \right) \left( \frac{d}{dt} \frac{\partial \varphi_t}{\partial \gamma} \right) \\ = T_{\varphi_t} \left( \left( \frac{\partial \varphi_t}{\partial \gamma} \right)^T f'(\varphi_t(\gamma)) \frac{\partial \varphi_t}{\partial \gamma} \right) \det \left( \frac{\partial \varphi_t}{\partial \gamma} \right) \\ = \text{div}(f)(\varphi_t(\gamma)) \cdot \det \left( \frac{\partial \varphi_t}{\partial \gamma} \right)$$

Soit,  $\frac{d}{dt} \left( \det \left( \frac{\partial \varphi_t}{\partial \gamma} \right) \right) = 0 \iff \boxed{\text{div}(f) = 0}$

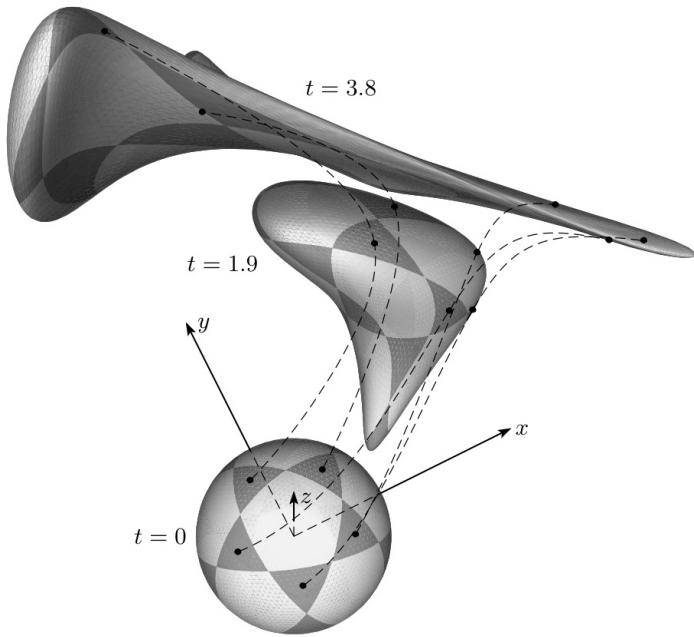
□

Ex: (ABC plane)  $x = A \sin(\gamma) + C \cos(\gamma)$   
 $y = B \sin(x) + A \cos(x)$   
 $z = C \sin(y) + B \cos(y)$

$$\text{div}(f) = 0$$

Ex:  $\dot{\gamma} = A(t) \gamma$

$$VP \iff T_A(A(t)) = 0, \forall t$$



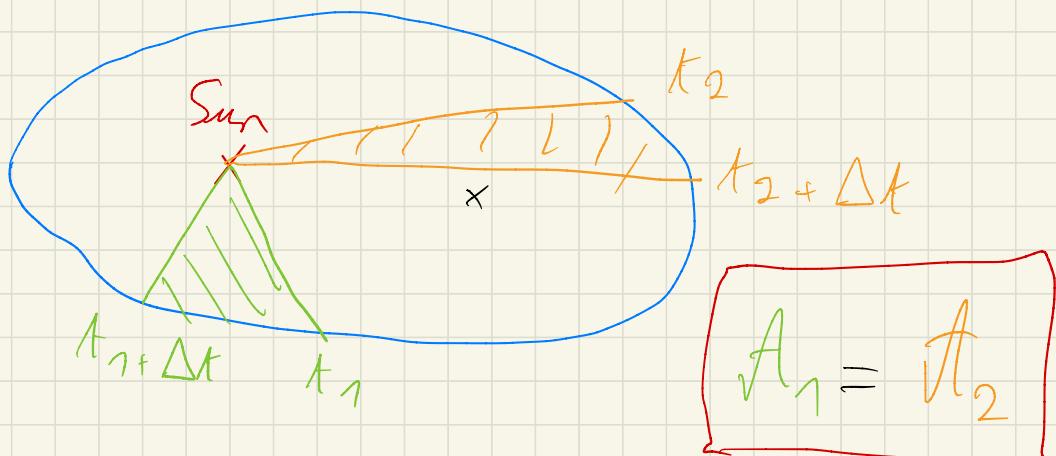
**Fig. 9.1.** Volume preserving deformation of the ball of radius 1, centred at the origin, by the ABC flow;  $A = 1/2$ ,  $B = C = 1$

## ⑥ Symplecticity

Idea: Motion of the earth around the sun  
given by a Hamiltonian system.

Kepler second law says:

"A line segment joining a planet and the sun  
sweeps out equal areas during equal intervals  
of time."



def: let the 2-form  $w$  be given by

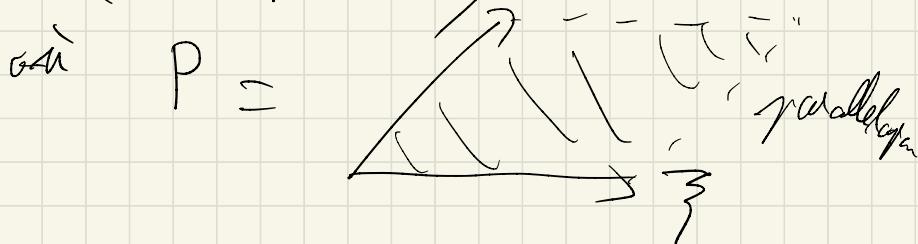
$$w: \mathbb{R}^{2d} \times \mathbb{R}^{2d} \longrightarrow \mathbb{R}$$

$$w: (\xi, \eta) \longrightarrow \sum_{i=1}^d \det \begin{pmatrix} \xi^1 & \eta^1 \\ \xi^P & \eta^P \end{pmatrix}$$

$$\begin{pmatrix} \xi^1 \\ \vdots \\ \xi^P \end{pmatrix} \quad \begin{pmatrix} \eta^1 \\ \vdots \\ \eta^P \end{pmatrix}$$

↳ Matrix form  $w(\xi, \eta) = \xi^T J \eta$ ,  $J = \begin{pmatrix} 0 & \mathbb{I}_d \\ -\mathbb{I}_d & 0 \end{pmatrix}$

↳ In dim 2,  $\det \begin{pmatrix} \xi^1 & \eta^1 \\ \xi^P & \eta^P \end{pmatrix} = \text{Area}(P)$  (oriented)



def: a smooth map  $g: \mathcal{U} \subset \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$

is symplectic iff

$$g'(\gamma)^T J g'(\gamma) = J, \forall \gamma$$

that is,  $w(g'(g_P)\xi, g'(g_P)\eta) = w(\xi, \eta), \forall g_P \in \mathcal{U}$

E.g.: for  $g(\gamma) = A\gamma$ ,  $g$  is symplectic

$$\Leftrightarrow \omega(A\beta, A\gamma) = \omega(\beta, \gamma)$$

$$\Leftrightarrow A^T J A = J$$

That is,  $A$  preserves the areas  
(rotation for instance)

Thm (Poincaré): let  $H: \mathbb{R}^{2d} \rightarrow \mathbb{R}$  be  $C^2$ ,  
then the flow of  $\gamma' = J \nabla H(\gamma)$  is symplectic.

Proof: variational equation for  $\psi_t = \frac{\partial \Psi_t}{\partial \gamma}$

$$\frac{d}{dt} \psi_t(\gamma) = J \nabla^2 H(\varphi_t(\gamma)) \cdot \psi_t(\gamma)$$

$$\begin{aligned} \text{Then } \frac{d}{dt} (\psi_t^T J \psi_t) &= \left( \frac{d}{dt} \psi_t \right)^T J \psi_t + \psi_t^T J \left( \frac{d}{dt} \psi_t \right) \\ &= \psi_t^T \left[ \underbrace{(\nabla^2 H)^T}_{=\nabla^2 H} \underbrace{J^T J}_{=J_{2d}} + \underbrace{J J^T}_{=-J_{2d}} \nabla^2 H \right] \psi_t \\ &\quad \text{Schwarz} \\ &= 0 \end{aligned}$$

□ /

$$\text{Let } J: \mathbb{R}^{d \times d} \times \mathbb{R}^{d \times d} \rightarrow \mathbb{R}^{d \times d} \text{, then}$$

$$(q, \psi) \rightarrow \psi^T J \psi$$

!

$J$  is a quadratic first integral of the augmented ODE:

$$\begin{cases} \frac{d}{dt} q_t(\gamma) = f(q_t(\gamma)) \\ \frac{d}{dt} \psi_t(\gamma) = f'(q_t(\gamma)) \cdot \psi_t(\gamma) \end{cases}$$

Thm: let  $f: U \subset \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$

the flow of  $\dot{\gamma} = f(\gamma)$  is symplectic for  $t$  small iff it is locally Hamiltonian, that is,

$\forall \gamma_0 \in U, \exists V(\gamma_0), \exists H: V(\gamma_0) \rightarrow \mathbb{R}$  st  $f = J \nabla H$   
in  $V(\gamma_0)$

Proof:  $\Leftarrow$ : OK

$\Rightarrow$ : for  $t$  small enough, we have

$$\frac{d}{dt} (\Psi_t^\top J \Psi_t) = 0$$

that is  $\Psi_t^\top [(\mathbf{f}'(\varphi_t))^\top J + J \mathbf{f}'(\varphi_t)] \Psi_t = 0$

$t=0$  gives  $\mathbf{f}'(\gamma)^\top J + J \mathbf{f}'(\gamma) = 0, \forall \gamma \in U$

that is  $J \mathbf{f}'(\gamma)$  is symmetric  
 $(J \mathbf{f}' \text{ as well})$

Define  $g = J^{-1} \mathbf{f}$  and assume  $\gamma_0 = 0$  for simplicity.

let  $H(\gamma) = \int_0^1 \gamma^\top g(t\gamma) dt$  for  $\gamma \in B(\gamma_0, \varepsilon) \cap U$

$$\begin{aligned} \text{then } \nabla H(\gamma) &= \int_0^1 \left( g(t\gamma) + t (\gamma^\top g'(t\gamma))^\top \right) dt \\ &= \int_0^1 (g(t\gamma) + t g'(t\gamma)^\top \gamma) dt \\ &= \int_0^1 \frac{d}{dt} (t g(t\gamma)) dt \\ &= g(\gamma) \end{aligned}$$

That is  $f(\gamma) = \int \nabla H(\gamma), \forall \gamma \in B(\gamma_0, \varepsilon)$  □

Rk: if  $V$  is star shaped,  $H$  is globally defined. (for instance)

Reformulation in geometry:

$$\Omega^0 \xrightarrow{\text{"J}\nabla\text{"}} \Omega^1 \xrightarrow{\text{"w"\}} \Omega^2$$

1 forms                                    2 forms

$$H \longmapsto JdH \longmapsto \sum f_i dy_1 \wedge \dots \wedge f_idy_n$$

*Mh*

$\uparrow$

$f_1 dy_1 + \dots + f_n dy_n$

*A collige!*

Then  $f dy \in \text{Ker}(w) \Leftrightarrow f \in \text{Im}(\text{J}\nabla)$

We just showed that a cycle is exact!

The homotopy operator is

$$\Omega^0 \xrightarrow{d} \Omega^1$$

$$h: f \mapsto \int_0^1 \gamma^t f(t\gamma) dt$$

(and  $\gamma^0 = 0$ )

Prop: 1) If  $g$  sym., then  $g$  preserves volume

2) If  $g_1, g_2$  sym., then  $g_2 \circ g_1$  sym.

Proof: 1)  $(g')^T J g' = J$  2) exercise

$$\Rightarrow \det(g')^2 = 1$$

$$\Rightarrow |\det(g')| = 1$$

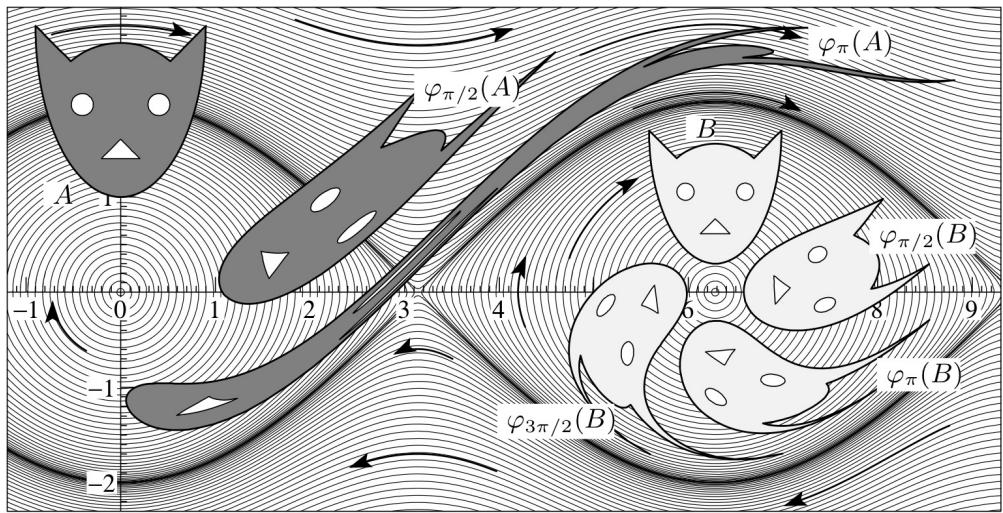
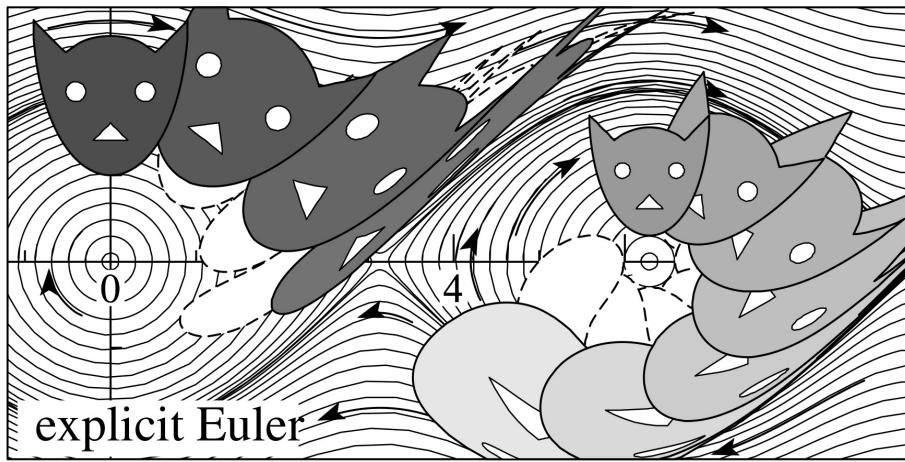
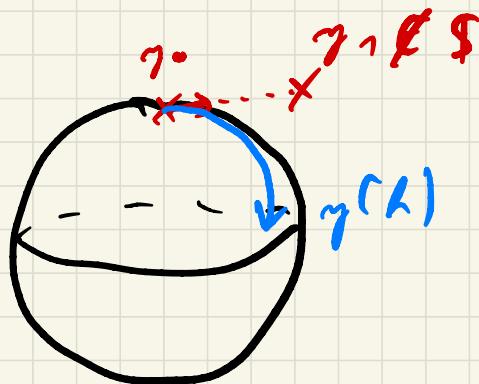


Fig. 2.2. Area preservation of the flow of Hamiltonian systems

The question: the flow satisfies  
a handful of geometric properties. How  
do we create numerical integrals that  
preserve these properties as well?

Example: Euler method



## Chapter II: Splitting and composition methods

### 1) Definition and example

$$\text{ODE } \begin{cases} y' = f(y) \\ y(0) = y_0 \end{cases} \quad \text{flow } y(t) = \varphi_t(y_0)$$

integrate  $y_{n+1} = \psi_L(y_n)$ ,  $t_n = n\Delta$ ,  $RN = T$

If  $f = f^1 + f^2 + \dots + f^P$  and we know the exact flows  $\varphi_t^p$ ,  $1 \leq p \leq P$  (a sufficiently good approximation), then a splitting method is a composition of these flows.

For simplicity, we consider  $f = f^A + f^B$ .

def: A splitting method is given for constants  $a_1, \dots, a_s$  by  $b_1, \dots, b_s$

$$\psi_L = \varphi_{b_s \Delta}^B \circ \varphi_{a_s \Delta}^A \circ \dots \circ \varphi_{b_1 \Delta}^B \circ \varphi_{a_1 \Delta}^A$$

Ex:  $y' = J \nabla H(y)$ ,  $H(q, p) = T(p) + V(q)$   
 $\hookrightarrow$  separable Hamiltonian

Pb A

$$\begin{cases} q' = \nabla T(p) \\ p' = 0 \end{cases} \Rightarrow \varphi_t^A\left(\begin{pmatrix} q_0 \\ p_0 \end{pmatrix}\right) = \begin{pmatrix} q_0 + t \nabla T(p_0) \\ p_0 \end{pmatrix}$$

Pb B

$$\begin{cases} q' = 0 \\ p' = -\nabla V(q) \end{cases} \Rightarrow \varphi_t^B\left(\begin{pmatrix} q_0 \\ p_0 \end{pmatrix}\right) = \begin{pmatrix} q_0 \\ p_0 - t \nabla V(q_0) \end{pmatrix}$$

Idea: we split the pb into multiple single pb.

def: given an integrator  $\mathcal{X}_L(\gamma_0)$ , a composition method is

$$\Psi_L = \mathcal{X}_{\gamma_{0,2}} \circ \dots \circ \mathcal{X}_{\gamma_{1,L}}$$

We obtain methods given by composition of exact/numerical flows.

$\Rightarrow$  If a geometric property is satisfied by

$\gamma' = f(\gamma)$ , if this spt is satisfied by the flows used in the method  $(x_k, \varphi_k^A, \varphi_k^B)$ , then the splitting/cayana method preserves the geometric properties.

$$\text{Ex: } f^A(\gamma) = A\gamma, \quad A^T = -A$$

$$f^B(\gamma) = B\gamma, \quad B^T = -B$$

the  $\varphi_A^A = e^{tA} \gamma \in \mathbb{S}^d$        $\varphi_B^B = e^{tB} \gamma \in \mathbb{S}^d$       for  $\gamma \in \mathbb{S}^d$

Ex: Schrödinger equation

$$\partial_t u = i \Delta u + F(u), \quad F(u) = i P(\mu) u$$

$\mu: \mathbb{R} \rightarrow \mathbb{R}$

discretisation  $\gamma' = A\gamma + g(|\gamma|)\tilde{\gamma}, \quad A^T = -A$

$$\partial_t |\gamma|^2 = 2 \langle \gamma, A\gamma + g(|\gamma|)\tilde{\gamma} \rangle = 0$$

$$\text{Pf } A: \gamma' = A\gamma \quad \varphi_t^A: \mathbb{S}^d \rightarrow \mathbb{S}^d$$

$$\varphi_t^A(\gamma) = e^{tA}\gamma$$

$$\underline{\text{Pf } B: \gamma' = g(|\gamma|) J \gamma} \quad \varphi_t^B: \mathbb{S}^d \rightarrow \mathbb{S}^d$$

$$\varphi_t^B(\gamma) = e^{t g(|\gamma|) J} \gamma$$

E<sup>1</sup>: manifold case

$$\varphi_t^A \in \mathcal{X}(M), \varphi_t^B \in \mathcal{X}(N)$$

then the composition  $\in \mathcal{X}(M)$

# 1) Taylor expansion of the flow (1st time)

Let  $\gamma' = f(\gamma)$  with  $\gamma(0) = \gamma_0$ .

Q: what is the expansion of  $\gamma(t)$ ? (assuming  $f^{(n)}$ )

Notation:  $f^{(n)}: \mathbb{R}^d \rightarrow \mathcal{L}(\underbrace{\mathbb{R}^d \times \mathbb{R}^d \times \dots \times \mathbb{R}^d}_{n \text{ linear}}, \mathbb{R}^d)$

We write  $f^{(n)}(\gamma)(a^1, \dots, a^n) = \sum_{i_1, \dots, i_n} \frac{\partial^n f}{\partial y_{i_1} \dots \partial y_{i_n}} a_1^{i_1} \dots a_n^{i_n}$

Ex: in the linear case  $f(\lambda) = A\gamma$ ,

we find  $\varphi_t(\gamma) = e^{tA}\gamma = \gamma + tA\gamma + \frac{t^2}{2}A^2\gamma + \dots$

Prop: the flow satisfies

$$\varphi_t(\gamma) = \sum_{n=0}^{+\infty} \frac{t^n}{n!} (f(\gamma))^{\triangleright n} = \exp^{\triangleright}(tf)(\gamma)$$

$$= \gamma + t f(\gamma) + \frac{t^2}{2} (f \triangleright f)(\gamma)$$

$$+ \frac{t^3}{6} (f \triangleright (f \triangleright f))(\gamma) + \frac{t^4}{24} f \triangleright (f \triangleright f \triangleright f) + \dots$$

where  $f \triangleright g = g'(f) (\approx \langle \nabla g, f \rangle = \nabla_f g)$ .

The product  $\triangleright : \mathcal{F}(\mathbb{R}^d) \times \mathcal{F}(\mathbb{R}^d) \rightarrow \mathcal{F}(\mathbb{R}^d)$  is non commutative and non associative. (A)

Manifold case:

Moreover for  $\phi \in C^\infty(M, \mathbb{R})$  and  $f \in \mathcal{F}(M)$ , we have

$$\begin{aligned}\phi(f_t(\gamma)) &= \text{exp}(f \triangleright)[\phi] \\ &= \phi(\gamma) + t f \triangleright \phi(\gamma) + \frac{t^2}{2} f \triangleright (f \triangleright \phi)(\gamma) + \dots\end{aligned}$$

Rb: the series in the expansion are formal power series induced by h. One needs to assume analyticity of f typically to obtain CV.

Proof: by induction

- $\gamma^{(0)} = \gamma_0$
- $\gamma^{(1)}(c) = f(\gamma_0)$
- $\gamma^{(1)}(t) = f'(\gamma^{(1)}(1))(\gamma^{(1)}(1)) = (f \triangleright f)(\gamma^{(1)}(1))$
- $\gamma^{(1)}(t) = (f \triangleright f)'(\gamma^{(1)}(1))(\gamma^{(1)}(1))$

$$= (f \triangleright (f \triangleright f))(\gamma(x))$$

,  
,

□

### 3) Order theory of splitting methods

Denote  $A = f^A \triangleright = \sum f^{A,i} \frac{\partial}{\partial x^i}$  ) lie operators  
 $B = f^B \triangleright = \sum f^{B,i} \frac{\partial}{\partial x^i}$

with the identification  $\frac{\partial}{\partial x^i} \approx e_i$  basis of  $\mathbb{R}^d$

$$\text{diff on } \begin{matrix} \text{order } 1 \\ \text{of } f \end{matrix} \cong v.f.$$

Given 2 linear operators  $X, Y$ , the lie algebra

$L(X, Y)$  is the smallest vector space stable by  $[-, -]$  ad containing  
 where  $[-, -]$  is a lie bracket:  $X, Y$

- $[-, -]$  is bilinear

- $[x, x] = 0$

- Jacobi  $[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0$

Rk: other relations could be satisfied. Co

Next that, we work in a general setting  
 with a free lie algebra.

Thm (BCH formula): There exists a map

$$\text{BCH}(x, y) \in \mathcal{L}(x, y) \circ K$$

$$e^x e^y = e^{\text{BCH}(x, y)}, \quad [x, y] = XY - YX$$

and the first terms are:

$$\text{BCH}(x, y) = \overbrace{x + y}^{(1)} + \frac{1}{2} \overbrace{[x, y]}^{(2)}$$

$$+ \frac{1}{12} ([x, [x, y]] + [y, [y, x]]) \quad (3)$$

$$- \frac{1}{24} [y, [x, [x, y]]] \quad (4)$$

+ ...

The complete combinatorial formula is called  
 the Dynkin formula.

$$\begin{aligned}
 \text{then } \phi(\Psi_h(y_0)) &= \phi(\varphi_{b,h,k}^B \circ \dots \circ \varphi_{a,h,k}^A(y_0)) \\
 &= (\phi \circ \dots \circ \varphi_{b,h,k}^B)(\varphi_{a,h,k}^A(y_0)) \\
 &= e^{a_1 h A} [\phi \circ \dots \circ \varphi_{b,h,k}^B](y_0) \\
 &= e^{a_1 h A} e^{b_1 h B} \dots e^{b_N h B} [\phi](y_0)
 \end{aligned}$$

Def: an operator has (local) order p for

$$\left\{
 \begin{array}{l}
 \text{solving } y'(t) = f(y(t)) \text{ if } \exists \delta_0 > 0, \\
 \forall h \leq \delta_0, |y_h(y_0) - y_h(y_0)| \leq C(y_0) h^{p+1}
 \end{array}
 \right.$$

Rq: with stability points, we can go from local to global order:

$$|\varphi_T(y_0) - \Psi_h^N(y_0)| \leq C(T, y_0) h^p$$

Thm: if  $e^{A+hB} = e^A \cdot e^{hB}$  then  $\|e^A - e^{A+hB}\| = O(h^{p+1})$

the splitting method  $\Psi_h$  has (at least) order  $p$ .  
Proof:  $e^{X+\Theta(h^{p+1})} = e^X + \Theta(h^{p+1})$  by Taylor.

Application:

Lie-Trotter:  $\Psi_h = e^{hB} e^{hA}$  order 1  
 and  $e^{hA} e^{hB} = e^{h(A+B)} + \frac{h^2}{2} [A, B] + \dots$

Strang:  $\Psi_h = e^{h_2 A} e^{hB} e^{h_2 A}$   
 $e^{h_2 A} e^{hB} e^{h_2 A} = e^{h(A_2 + B)} + \frac{h^2}{4} [B, A] + \dots$   
 $= e^{h(A_2 + B)} + \frac{h^2}{4} [B, A] + h_2 A + \frac{h^2}{2} [A, B] + \dots$   
 $= e^{h(A+B)} + O(h^3)$  order 2

For higher orders, we need a basis of  $\mathcal{L}(X, Y)$ .

Lyndon words:  $\{a, b, ab, abb, aab, aabb, \dots\}$   
based on the alphabet  $A = \{a, b\}$

$$\text{and } F_a = A, F_b = B,$$

$$F_{ab} = [A, B], F_{abb} = [F_{ab}, F_b],$$

$$F_{aab} = [F_a, F_{ab}], \quad (\text{see Reutenauer, '93})$$

and (was said, '24)

$$\text{the log}(e^{a_1 \lambda A} \cdots e^{a_n \lambda A} \cdots e^{b_1 \lambda B} \cdots e^{b_m \lambda B}) = \sum_{w \in \text{Lynd}(a, b)}^{|w|} p(w) F_w$$

where  $p(w)$  is a polynomial in the  $a_i, b_i$ .

$$p(a) = \sum a_i, \quad p(b) = \sum b_i,$$

$$p(ab) = \frac{1}{2} p(a)p(b) - \sum_{i < j} b_i a_j,$$

$$p(abb) = \frac{1}{12} p(a)p(b)^2 - \frac{1}{2} \sum_{i \leq j \leq k} b_i a_j b_k,$$

$$p(aa'b) = \frac{1}{12} p(a)^2 p(b) - \frac{1}{2} \sum_{i \leq j \leq k} a_i b_j a_k,$$

Rb: more details on the calculation of  $p(w)$  in  
the exercises. and the algebraic structure  $\heartsuit$ .

Then, a splitting method has

$$\text{order 1} \Leftrightarrow \sum a_i = 1 = \sum b_i$$

$$\text{order 2} \Leftrightarrow p(ab) = 0 + \text{order 1}$$

$$\text{order 3} \Leftrightarrow p(abf) = p(aab) = 0 \\ + \text{order 2}$$

etc.

Prop: if a splitting method has order three,

then  $\exists i_0, j_0$  s.t.  $a_{i_0} < 0$  and  $b_{j_0} < 0$ . (Blas, Cor 05)  
 $\equiv$  & Sheng, pg

Proof: see exercises.

Problem: for non-reversible problems such as the heat equation:

$$\partial_t u = \underbrace{\Delta u}_A + \underbrace{F(u)}_B$$

$\varphi_{-k}^A$  is not defined!

Thus, a splitting method has max order of 2!

Possible solutions: splitting methods with commutators

Eg: Tabataishi-Tanda splitting (1984)

$$\varphi_h = e^{\frac{h^2}{24}[A,B]} e^{\frac{h}{2}A} e^{\frac{h}{2}B} - e^{-\frac{h^3}{24}[B,[B,A]]} e^{\frac{h}{2}B} e^{\frac{h}{2}A} - e^{\frac{h^2}{24}[A,B]}$$

of order 4.

or splitting methods with complex coefficients  
 (Castillo, Thalvi, Descombes, Vilma & Haase, Oettemann; 2009)

## 4) Composition methods

Thm: let  $\Psi_L = \chi_{0, h} \circ \dots \circ \chi_{f, h}$  a composition method  
 with  $\chi$  of order  $\lambda$ , then if  $\begin{cases} \delta_1 + \dots + \delta_\lambda = 1 \\ \delta_1^{\lambda+1} + \dots + \delta_\lambda^{\lambda+1} = 0 \end{cases}$ ,  
 then  $\Psi_L$  has order at least  $\lambda+1$ .

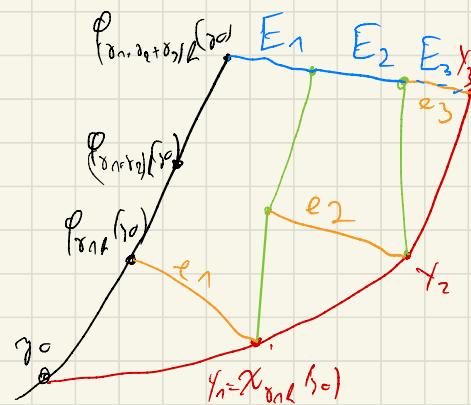
Proof:  $\chi_{\gamma, h}(\gamma) = \varphi_{\gamma, h}(\gamma) + C(\gamma)(h)^{\lambda+1} + \dots$

$$\begin{aligned} Y_0 &= \gamma_0, \quad Y_{i+1} = \chi_{\gamma_i, h}(Y_i), \quad Y_\lambda = \Psi_L(\gamma_0) \\ e_i &:= \chi_{\gamma_i, h}(Y_i) - \varphi_{\gamma_i, h}(Y_i) = C(Y_i)(Y_i, h)^{\lambda+1} + O(h^{\lambda+2}) \\ &\quad = C(\gamma_0)(\gamma_i, h)^{\lambda+1} + O(h^{\lambda+2}) \end{aligned}$$

$$\begin{aligned} E_i &= \varphi_{(\gamma_{i+1}, \dots, \gamma_\lambda), h}(e_i) = (1 + O(h))e_i \text{ as } \varphi_h = \text{id} + O(h) \\ &= C(\gamma_0)(\gamma_i, h)^{\lambda+1} + O(h^{\lambda+2}) \end{aligned}$$

We observe that if  $\sum \delta_i = 1$

$$\begin{aligned} \Psi_L(\gamma_0) - \varphi_{\gamma_0, h}(\gamma_0) &= E_1 + \dots + E_\lambda \\ &= (\text{id} + O(h)) \sum e_i \end{aligned}$$



$$= ((\gamma_0) (\gamma_1^{k+1} + \dots + \gamma_0^{k+1}) h^{k+1} + \mathcal{O}(h^{k+2}))$$

□

def: the adjoint of a method  $\Psi_h$  is  $\Psi_h^* = \Psi_{-h}^{-1}$ ,

that is,  $\Psi_h^* \circ \Psi_h = \text{id}$

if  $\Psi_h^* = \Psi_h$ , the method is symmetric.

Ex: the exact flow satisfies  $\varphi_h^* = \varphi_{-h}^{-1} = \varphi_{-(h)} = \varphi_h$ .

Explicit Euler:  $\Psi_h(\gamma) = \gamma + h f(\gamma)$

$$\gamma_{n+1} = \gamma_n + h f(\gamma_n)$$

$$h \leftrightarrow -h: \quad \gamma_{n+1} = \gamma_n - h f(\gamma_n)$$

$$n+1 \leftrightarrow n: \quad \gamma_n = \gamma_{n+1} - h f(\gamma_{n+1})$$

$$\boxed{\gamma_{n+1} = \gamma_n + h f(\gamma_{n+1})}$$

The adjoint of Exp. Euler is Imp. Euler.

Ex:  $\gamma_{n+1} = \gamma_n + h f\left(\frac{\gamma_n + \gamma_{n+1}}{2}\right)$  is symmetric.

Ex: if  $\tilde{\Psi}_h = \Psi_{h/2}^* \circ \Psi_{h/2}$ , the  $\tilde{\Psi}_h$  is symmetric

↳ try with EE, IE.

Prop: if  $\Psi_L$  is of order  $p$ ,  $\Psi_L^*$  is of order  $p$ .

Moreover, if  $\Psi_L(\gamma) = \varphi_L(\gamma) + C(\gamma) h^{p+1} + O(h^{p+2})$

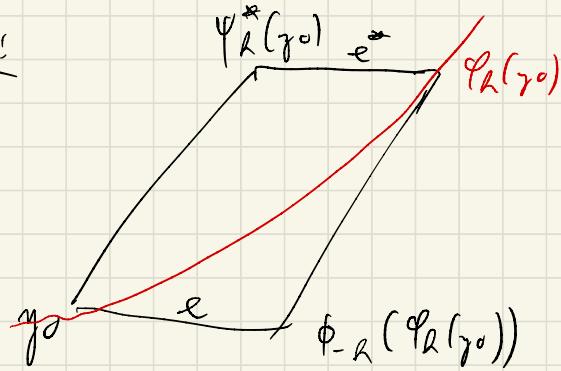
then  $\Psi_L^*(\gamma) = \varphi_L(\gamma) + (-1)^p C(\gamma) h^{p+1} + O(h^{p+2})$

In particular, if  $\Psi_L$  is symmetric, then

$$C(\gamma) = (-1)^p C(\gamma)$$

so that if  $p$  odd, then  $C(\gamma) = 0$  and the method is of order  $p+1$ .

Proof:



$$\text{let } e^* = \Psi_L^*(y_0) - \varphi_L(y_0)$$

$$e = y_0 - \Psi_{-L}(\varphi_L(y_0))$$

$$e = \varphi_{-L}(\varphi_L(y_0)) - \varphi_{-L}(\varphi_L(y_0))$$

$$= -C(\varphi_L(y_0))(-h)^{p+1} + O(h^{p+2})$$

$$= (-1)^p C(\gamma_0) h^{p+1} + O(h^{p+2}) \text{ as } \varphi_L(y_0) = y_0 + O(h)$$

On the other hand,  $y_0 = \Psi_{-L}(\Psi_L^*(y_0))$ ,

$$\begin{aligned} \infty \quad e &= \psi_{-\lambda}(\psi_{\lambda}^*(\gamma_0)) - \psi_{-\lambda}(\phi_{\lambda}(\gamma_0)) \\ &= (\text{id} + O(\lambda)) e^* \quad \text{as } \psi_{\lambda} = \text{id} + O(\lambda) \end{aligned}$$

$$\infty \quad e^* = (\text{id} + O(\lambda)) e = (-1)^p C(\gamma_0) \lambda^{p+1} + O(\lambda^{p+2})$$

□

Application: • there is no real solution to

$$\begin{aligned} \gamma_1 + \dots + \gamma_s &= 1 \\ \gamma_1^{k+1} + \dots + \gamma_s^{k+1} &= 0 \quad \text{for } k \text{ odd.} \end{aligned}$$

• let  $\chi_{\lambda}$  symmetric, let  $\gamma_1 = \gamma_3 = \frac{1}{2 - 2 \overline{\chi_{\lambda}}}$ ,  $\gamma_2 = 1 - 2 \gamma_1$   
of order even

then  $\psi_{\lambda} = \chi_{\gamma_3 \lambda} \circ \dots \circ \chi_{\gamma_1 \lambda}$  is of order  $k+2$ .

This procedure can be repeated: we start with a symmetric method of order 2, apply (4.4) with  $p = 2$  to obtain order 3; due to the symmetry of the  $\gamma$ 's this new method is in fact of order 4 (see Theorem 3.2). With this new method we repeat (4.4) with  $p = 4$  and obtain a symmetric 9-stage composition method of order 6, then with  $p = 6$  a 27-stage symmetric composition method of order 8, and so on. One obtains in this way *any* order, however, at the price of a terrible zig-zag of the step points (see Fig. 4.2).

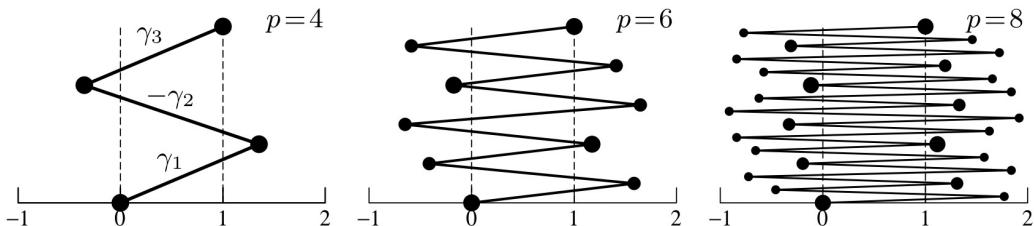
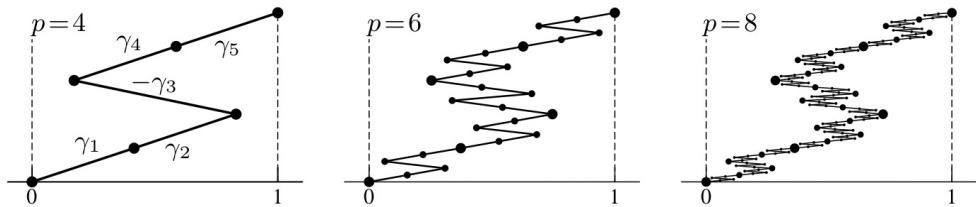


Fig. 4.2. The Triple Jump of order 4 and its iterates of orders 6 and 8

**Example 4.3 (Suzuki's Fractals).** If one desires methods with smaller values of  $\gamma_i$ , one has to increase  $s$  even more. For example, for  $s = 5$  the best solution of (4.2) has the sign structure  $++-++$  with  $\gamma_1 = \gamma_2$  (see Exercise 7). This leads to (Suzuki 1990)

$$\gamma_1 = \gamma_2 = \gamma_4 = \gamma_5 = \frac{1}{4 - 4^{1/(p+1)}}, \quad \gamma_3 = -\frac{4^{1/(p+1)}}{4 - 4^{1/(p+1)}}. \quad (4.5)$$

The repetition of this algorithm for  $p = 2, 4, 6, \dots$  leads to a fractal structure of the step points (see Fig. 4.3).



**Fig. 4.3.** Suzuki's "fractal" composition methods

Pb: lots of evaluations to reach high order, need for back flows . . .

Can we resolve geometry with | simpler  
methods? | cheaper

# Chapter 3: The Runge-Kutta approach

## 1) Definition, examples

Def: a Runge-Kutta method for  $y' = f(y)$   
is of the form

$$\begin{cases} Y_i^n = y_{n+1} + h \sum_{j=1}^i a_{ij} f(Y_j^n) \\ y^{n+1} = y_n + h \sum_{i=1}^s b_i f(Y_i^n) \end{cases}$$

for given coefficients  $b_i$ ,  $a_{ij}$  stored in  
a Butcher tableau

$$\begin{array}{c|ccccc} c & A & & & & \\ \hline & b_1 & \dots & b_s & & \end{array} \quad A = (a_{ij})_{s \times s} \quad c_i = \sum_{j=1}^s a_{ij}$$

If  $A$  is lower triangular strictly, the method  
is explicit (implicit else).

If  $A$  is lower triangular, the method is  
diagonally implicit.

Ex: ~~0|0~~<sub>1</sub> explicit Euler

~~1|1~~<sub>1</sub> Implicit Euler:  $y_{n+1} = y_n + h f(y_{n+1})$

~~1/2 | 1/2~~<sub>1</sub> Midpoint

~~0 | 0 0  
1/2 | 1/2 0  
-----  
0 1~~ explicit midpoint

~~0 | 0 0  
1 | 1/2 1/2  
-----  
1/2 1/2~~ trapezoidal rule

~~0 | 0 0 0 0  
1/2 | 1/2 0 0 0  
1/2 | 0 1/2 0 0  
1 | 0 0 1 0  
-----  
1/6 1/3 1/3 1/6~~ RK 4

Rk: for implicit methods, the system  
has a unique solution for  $L$  small enough  
as  $f$  is Lipschitz (Picard's theorem).

def: partitioned RK method:

for  $\begin{pmatrix} \gamma \\ z \end{pmatrix}' = \begin{pmatrix} f(\gamma, z) \\ g(\gamma, z) \end{pmatrix}$ , we have the method

$$Y_i = y_n + h \sum a_{ij} f(Y_j, Z_j)$$

$$Z_i = z_n + h \sum \hat{a}_{ij} g(Y_j, Z_j)$$

$$y_{n+1} = y_n + h \sum b_i f(Y_i, Z_i)$$

$$z_{n+1} = z_n + h \sum \hat{b}_i g(Y_i, Z_i)$$

Tableaux	$c \mid A$	$\hat{c} \mid \hat{A}$
	$\hline b$	$\hline \hat{b}$

E<sub>7L</sub>:  $\begin{array}{|c|c|} \hline 0 & 0 \\ \hline 1 & 1 \\ \hline \end{array}$  Symplectic Embed

$$\left\{ \begin{array}{l} y_{n+1} = y_n + h f(y_n, z_{n+1}) \\ z_{n+1} = z_n + h g(y_n, z_{n+1}) \end{array} \right.$$

## 2) Taylor expansion of the exact flow (2<sup>nd</sup> time)

In practice, we did not present the full expansion before. We need it now

$$\begin{aligned} \text{We find } \Phi_t(\gamma) &= \gamma + t f + \frac{t^2}{2} f \triangleright f + \frac{t^3}{6} f \triangleright (f \triangleright f) + \dots \\ &= \gamma + t f + \frac{t^2}{2} f' f + \frac{t^3}{6} (f' f' f + f'' (f, f)) \\ &\quad + \frac{t^4}{24} (f' f' f' f + f' f'' (f, f) \cancel{+ 3 f''' (f, f, f)}^{W+H?} \\ &\quad \quad \quad + f''' (f, f, f)) + \dots \end{aligned}$$

It looks a bit more involved. This is why we introduce  
Patch series! 

Def: The set of trees  $\mathcal{T}$  is defined by induction.

$$\rightarrow \bullet \in \mathcal{T}$$

$$\rightarrow \text{if } \tau_1, \dots, \tau_n \in \mathcal{T}, [\tau_1, \dots, \tau_n] \in \mathcal{T}$$



def:  $F: \mathcal{C} \rightarrow J^\infty$  is the elementary differential  
 $\hookrightarrow$  infinite jet bundle  
 $" = "$  polynomial in  $f, f^1, f^2, \dots$

$$\rightarrow F_f(\cdot) = f$$

$$\rightarrow F_f([\tau_1, \dots, \tau_n]) = f^{(n)}(F_f(\tau_1), \dots, F_f(\tau_n))$$

$F$  is extended by linearity on  $S_{\text{can}}(\mathcal{C})$ .

Prop: let  $\curvearrowright: \mathcal{C} \times \mathcal{C} \rightarrow \mathcal{C}$  be the grafting of  
 trees, then  $F_f(\tau_2) \curvearrowright F_f(\tau_1) = F_f(\tau_2 \curvearrowright \tau_1)$

$$\underline{\text{Ex:}} \quad f \triangleright (f'f) = (f'f)'f = f''(f, f) + f'f'f$$

$$F_f(\bullet \curvearrowright \bullet) = \begin{array}{c} \swarrow \searrow \\ \text{---} \end{array} + \begin{array}{c} \nearrow \\ \text{---} \end{array}$$

def: \* the order of  $\tau \in \mathcal{C}$  is  $|\tau| = \text{nb of nodes}$ .

\* the factorial of  $\tau \in \mathcal{C}$  is

$$\{ \gamma(\bullet) = 1$$

$$\gamma([\tau_1, \dots, \tau_n]) = |\tau| \gamma(\tau_1) \dots \gamma(\tau_n)$$

\* the symmetry of  $\tau \in \mathcal{E}$  is

$$\sigma(\tau) = 1$$

$$\sigma([\underbrace{\tau_1, \dots, \tau_1}_{\lambda_1}, \dots, \underbrace{\tau_m, \dots, \tau_m}_{\lambda_m}]) = \prod_{i=1}^m r_i! \sigma(\tau_i)^{\lambda_i}$$

graph

Rq:  $\sigma(\tau)$  is also the number of automorphisms of  $\tau$ .

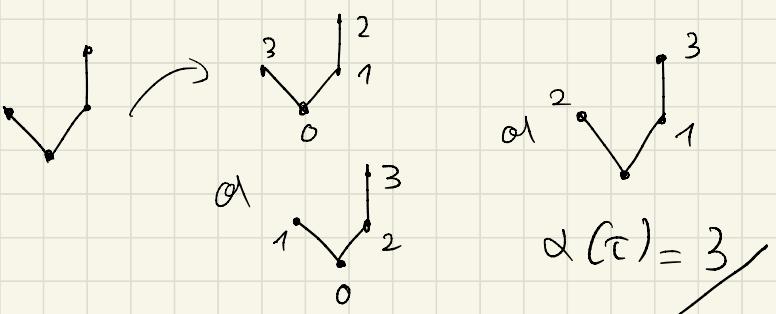
**Table 1.1.** Trees, elementary differentials, and coefficients

$ \tau $	$\tau$	graph	$\alpha(\tau)$	$F(\tau)$	$\gamma(\tau)$	$\phi(\tau)$	$\sigma(\tau)$
1	•	•	1	$f$	1	$\sum_i b_i$	1
2	[•]		1	$f'f$	2	$\sum_{ij} b_i a_{ij}$	1
3	[•, •]		1	$f''(f, f)$	3	$\sum_{ijk} b_i a_{ij} a_{ik}$	2
3	[[•]]		1	$f'f'f$	6	$\sum_{ijk} b_i a_{ij} a_{jk}$	1
4	[•, •, •]		1	$f'''(f, f, f)$	4	$\sum_{ijkl} b_i a_{ij} a_{ik} a_{il}$	6
4	[[•], •]		3	$f''(f'f, f)$	8	$\sum_{ijkl} b_i a_{ij} a_{ik} a_{jl}$	1
4	[[•, •]]		1	$f'f''(f, f)$	12	$\sum_{ijkl} b_i a_{ij} a_{jk} a_{jl}$	2
4	[[[•]]]		1	$f'f'f'f$	24	$\sum_{ijkl} b_i a_{ij} a_{jk} a_{kl}$	1

Rq: 
$$\frac{\alpha(\tau)}{|\tau|!} = \frac{1}{\sigma(\tau) \gamma(\tau)}$$

where  $\alpha$  is the number of ways to obtain  $\tau$

from grafting:



(Butcher)

Def: a B-series is a formal power series: given  
a:  $\mathcal{C} \rightarrow \mathbb{R}$  a one-form / the coefficient map,

$$B_R^f(a) = \sum_{\tau \in \mathcal{C}} \frac{\lambda^{|\tau|}}{\sigma(\tau)} a(\tau) F_f(\tau).$$

Thm: the exact flow of  $\gamma' = f(\gamma)$  is given by

$$\varphi_t = \text{id} + B_t^f \left( \frac{1}{t} \right)$$

Proof:  $f(\gamma_0 + B_t^f(\gamma^{-1})(\gamma_0))$

$$= \sum_{k=0}^{+\infty} f^{(k)}(\gamma_0) (B_t^f(\gamma^{-1})^{(0)}, \dots, B_t^f(\gamma^{-1})^{(k)})$$

$$= \sum_{k=0}^{+\infty} \sum_{\tau_1, \dots, \tau_k \in \mathcal{C}} \frac{t^{|\tau_1|} \dots t^{|\tau_k|}}{k! \sigma(\tau_1) \dots \sigma(\tau_k) \delta(\tau_1) \dots \delta(\tau_k)} f^{(k)}(F_f(\tau_1), \dots, F_f(\tau_k))$$

$$= \sum_{k=0}^{+\infty} \sum_{\tau_1, \dots, \tau_k \in \mathcal{C}} \frac{\tau^{|c|-1}}{\sigma(c) \delta(c)} |\tau| F_f(\tau)(\gamma_0)$$

$$= \sum_{k=0}^{+\infty} \sum_{\tau = [\tau_1, \dots, \tau_k] \in \mathcal{C}} \frac{|\tau| \tau^{|c|-1}}{\sigma(c) \delta(c)} F_f(\tau)(\gamma_0)$$

as going from the sum  $\sum_{\tau_1, \dots, \tau_k \in \mathcal{C}}$  to  $\sum_{\tau = [\tau_1, \dots, \tau_k] \in \mathcal{C}}$

yields the coefficient  $\frac{k!}{n_1! \dots n_m!} \binom{k}{n_1, \dots, n_m}$  as we go from ordered subtrees  $\tau_1 \dots \tau_k$  to non-ordered subtrees.

$$\text{then } \frac{d}{dt} (\gamma_0 + P_f(\gamma^{-1})(\gamma_0))$$

$$= \frac{d}{dt} \left( \sum_{c \in \mathcal{C}} \frac{\tau^{|c|}}{\sigma(c) \delta(c)} F_f(\tau)(\gamma_0) \right)$$

$$= \sum_{c \in \mathcal{C}} \frac{|\tau| \tau^{|c|-1}}{\sigma(c) \delta(c)} F_f(\tau)(\gamma_0)$$

□

### 3) Order theory of RK methods

Lemma:  $b f(\gamma_0 + \beta_L^f(\alpha)(\gamma_0)) = \beta_L^f(b)(\gamma_0)$

where  $\begin{cases} b([\tau_1, \dots, \tau_n]) = \alpha(\tau_1) \dots \alpha(\tau_n) \\ b(\cdot) = 1 \end{cases}$

proof: similar as last proof with  $\frac{1}{\gamma}$  replaced by  $\alpha$ .

Thm: a RK method  $\gamma_{n+1} = \Psi_L(\gamma_n)$  satisfies

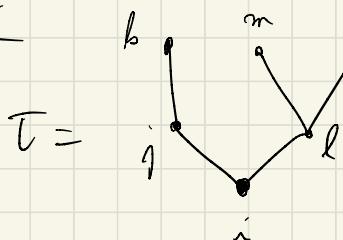
$$\Psi_L(\gamma_0) = \gamma_0 + \beta_L^f(\alpha) \text{ where}$$

$$\alpha(\tau) = b^T \beta(\tau) \text{ and } \alpha(\cdot) = 1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

and  $\begin{cases} \beta(\cdot) = 1 \\ \beta([\tau_1, \dots, \tau_n]) = \alpha(\tau_1) \dots \alpha(\tau_n). \end{cases}$   $\left( \alpha([\tau_1, \dots, \tau_n]) = A(\alpha(\tau_1) \dots \alpha(\tau_n)) \right)$

$$m \diamond v = \begin{pmatrix} m_1 v_1 \\ \vdots \\ m_d v_d \end{pmatrix}$$

SL:



$$\begin{aligned} \alpha(\tau) &= \sum b_i \alpha_{ij} \alpha_{ik} \alpha_{il} \alpha_{lm} \alpha_{ln} \\ &= \sum b_i \alpha_{ij} \alpha_{kl} \alpha_{il} \alpha_{lm}^2 \end{aligned}$$

proof: if  $Y_i = \gamma_0 + B_k^f(\alpha_i)(\gamma_0)$

$$\text{then } Y_i = \gamma_0 + \sum a_{ij} \lambda f(\gamma_0 + B_k^f(\alpha_j)(\gamma_0)) \\ \stackrel{\text{(lemal)}}{=} \gamma_0 + \sum a_{ij} B_k^f(\beta_j)(\gamma_0)$$

$$\text{where } \begin{cases} \beta_j([\epsilon_1, \dots, \epsilon_n]) = \alpha(\epsilon_1) \dots \alpha(\epsilon_n) \\ \beta_j(\cdot) = 1 \end{cases}$$

$$= \gamma_0 + B_k^f \left( \sum a_{ij} \beta_j \right) (\gamma_0)$$

then by identification  $\alpha_i(\epsilon) = \sum a_{ij} \beta_j(\epsilon) \in (A \beta)$ .

$$\text{that is } \alpha([\epsilon_1, \dots, \epsilon_n]) = A(\alpha(\epsilon_1) \circ \dots \circ \alpha(\epsilon_n))$$

$$\text{then } y_1 = \gamma_0 + h \sum b_i f(Y_i)$$

$$= \gamma_0 + h \sum b_i f(\gamma_0 + B_k^f(\alpha_i)(\gamma_0))$$

$$= \gamma_0 + \sum b_i B_k^f(\beta_i)(\gamma_0)$$

$$= \gamma_0 + B_k^f(B^T \beta)(\gamma_0)$$

□

Thm: a RK method has order p if

$$\forall \tau \in \mathbb{C}, |\tau| \leq p, \frac{1}{\gamma(\tau)} = a(\tau).$$

$\mathcal{C}$	condition	order
•	$\sum b_i = 1$	1
↓	$\sum b_i c_i = \frac{1}{2}$	2
↙	$\sum b_i a_{ij} q_j = \frac{1}{6}$	3
↙	$\sum b_i c_i^2 = \frac{1}{3}$	
↖	$\sum b_i a_{ij} a_{jk} c_k = \frac{1}{24}$	
↖	$\sum b_i a_{ij} q_j^2 = \frac{1}{12}$	4
↙	$\sum b_i c_i a_{ij} q_j^2 = \frac{1}{8}$	
↙	$\sum b_i c_i^3 = \frac{1}{4}$	

A000081  
OEIS

order	1	2	3	4	5	6	7	8	9	10
Nb conditions	1	1	2	4	9	20	48	115	286	719

- Rk:
- degeneracy may appear  
for  $d=1$ ,  $F_f(\mathbb{J}) = F_f(Y)$
  - $\forall \tau_0 \in \mathbb{C}, \exists f \in \mathbb{E}(R^d)$  st  

$$\begin{cases} F_f(\tau_0) \neq 0 \\ F_f(\tau)(0) = 0, \tau \neq 0 \end{cases}$$
  - A  $\overset{RK}{\text{method}}$  is of order  $p$  for all ODE  $\dot{y}(t) = f(t, y(t))$  iff  $\forall n \leq p, \sum_{|\pi|=n} = a(\pi)$

Extension to S-series: we consider forests  $\mathcal{F}$   
as concatenation of trees.  
↑  
with empty  
forest 1

a S-series is a differential operator

$$S_d^f(a) [\phi] = \sum_{\pi \in \mathcal{P}} \frac{a^{|\pi|} a(\pi)}{\sigma(\pi)} F^f(\pi) [\phi]$$

where  $a(\tau_1 \dots \tau_n) = a(\tau_1) \dots a(\tau_n)$  character

$$F^f(\pi) = \phi^{f^{m_i}}(F^f(\tau_1), \dots, F^f(\tau_r))$$

## 4) Algebraic structures of composition

② Deshuffle Hopf algebra: primitive elements and universal flavor

Let  $\cdot$  be the commutative, associative concatenation of trees:

$\vee \mid$  is a forest with 2 trees.

Let  $\mathbb{P}$  be the algebra of forests ( $+$ ,  $\times$ ,  $\cdot$ ) with the unit 1 and counit  $\delta_1$ .

Define the deshuffle coproduct  $\Delta_{\text{sh}}: \mathbb{P} \rightarrow \mathbb{P} \otimes \mathbb{P}$

$$\Delta_{\text{sh}} 1 = 1 \otimes 1$$

$$\Delta_{\text{sh}} \tau = \tau \otimes 1 + 1 \otimes \tau, \tau \in \mathcal{E}$$

$$\Delta_{\text{sh}} (w_1 \cdot w_2) = (\Delta_{\text{sh}} w_1) \cdot (\Delta_{\text{sh}} w_2)$$

Recall that  $(a \otimes b) \cdot (a' \otimes b') = (a \cdot a') \otimes (b \cdot b')$ .

This makes  $\mathbb{P}$  a bialgebra.

morally an inverse

$\mathbb{P}$  becomes a Hopf algebra if there is an antipode  $S: \mathbb{P} \rightarrow \mathbb{P}$

$$\text{s.t. } \mu \circ (S \otimes \text{Id}) \circ \Delta = \mu \circ (\text{Id} \otimes S) \circ \Delta = 1 \delta_1$$

Here  $S_{\text{sh}}(\tau) = -\tau$

$$S_{\text{sh}}(w_1 \cdot w_2) = S_{\text{sh}}(w_2) \cdot S_{\text{sh}}(w_1) \quad (S \text{ is an antimorphism wrt. but as it's commutative, it is just a morphism})$$

→ Note how we are not using the tree structure at all.

$$Ex: \Delta_{\mathbb{W}}(\cdot) = (\Delta_{\mathbb{W}} \cdot) \cdot (\Delta_{\mathbb{W}} \cdot)$$

$$= (\cdot \otimes 1 + 1 \otimes \cdot) \cdot (1 \otimes 1 + 1 \otimes 1)$$

$$= \cdot 1 \otimes 1 + \cdot \otimes 1 + 1 \otimes \cdot + 1 \otimes 1$$

$$\text{and } (S_{\mathbb{W}} \otimes \text{Id}) \circ \Delta_{\mathbb{W}}(\cdot) = \cdot 1 \otimes 1 - \cdot \otimes 1 - 1 \otimes \cdot + 1 \otimes 1$$

$$\mu \text{---} - - = 0 \quad \underline{\text{OK}}$$

def:  $\pi \in \mathcal{P}$  is primitive if  $\Delta \pi = \pi \otimes 1 + 1 \otimes \pi$ , gathered in  $\mathbb{G}$ .  
 $\boxed{\pi \in \mathcal{P} \text{ is group-like if } \Delta \pi = \pi \otimes \pi, \text{ gathered in } G.}$

Prop: ( $\mathbb{G} = \mathcal{C}$  set of trees here)

$$\exp(\tau) = 1 + \tau + \frac{1}{2}\tau \cdot \tau + \dots \text{ formal series}$$

$$\boxed{\exp: \mathbb{G} \rightarrow G \quad \log: G \rightarrow \mathbb{G}}$$

$\mathbb{G}$  represents the vector fields and  $G$  represents the flows

$$\log(\pi) = \sum_{n \geq 1} \frac{(-1)^{n-1}}{n} (\pi - 1)^{-n}$$

Proof:

$$\begin{aligned} \text{Note that } \Delta \exp(\tau) &= \exp(\Delta \tau) \text{ as } \Delta(\alpha \cdot \beta) = (\Delta \alpha) \cdot \beta + \alpha \cdot (\Delta \beta) \\ &= \exp(\tau \otimes 1 + 1 \otimes \tau) \end{aligned}$$

$$\begin{aligned}
 &= \exp(\tau \otimes 1) \cdot \exp(1 \otimes \tau) \text{ as they commute} \\
 &= (\exp(\tau) \otimes 1) \cdot (1 \otimes \exp(\tau)) \\
 &= \exp(\tau) \otimes \exp(\tau)
 \end{aligned}$$

the one checks that  $\log = \exp^{-1}$ .  $\square$

Idea:  $\log^*(\pi)$  is the v� generating the flow  $\pi$  for the law  $\star$ . Here  $\exp$  is the flow generated by the Euler method.

Rk: The dual of a Hopf algebra is a Hopf algebra.

$$(\mathbb{P}, \cdot, \Delta_{\mathbb{W}}) \quad \xleftrightarrow{*} \quad (\mathbb{P}^*, \star, \Delta_{\star})$$

$$\text{so } \langle \Delta_{\star} \alpha, w_1 \otimes w_2 \rangle = \langle \alpha, w_1 \cdot w_2 \rangle$$

$$\langle \alpha \star \beta, w \rangle = \langle \alpha \otimes \beta, \Delta_{\mathbb{W}} w \rangle$$

## (b) Grassmann-Larson Hopf algebra and exact flow

Consider now the composition of flows.

$$\text{We observe } F(\tau_1)[F(\tau_2)[\phi]] = F(\tau_1 \tau_2 + \tau_1 \curvearrowright \tau_2) [\phi]$$

Define the Grassmann-Larson product by

$$\Pi \diamond \tilde{\Pi} = \sum_{\substack{\Delta_W \Pi = \\ \Pi(1) \otimes \Pi(2)}} \Pi_{(1)} \cdot (\Pi_{(2)} \curvearrowright \tilde{\Pi}) \quad (\text{See Guia Orden})$$

This yields a new Hopf algebra called the Grassmann-Larson Hopf algebra  $(\mathcal{F}, \diamond, \Delta_W)$  with some primitive elements  $\boxed{\gamma}$ .

$$\exp^\diamond(c) = 1 + c + \frac{1}{2} c \diamond c + \dots$$

$$\text{Idea: } \exp^\diamond: \boxed{\gamma} \rightarrow G_{GL} \quad \gamma' = f(\gamma)$$

$$\text{which amounts to } \begin{array}{c} \text{h.f.} \\ \downarrow \\ \text{V.f.} \end{array} \longrightarrow \phi(\gamma^{(h)}) = \phi(\gamma_0) + h \phi'(\gamma_0) f(\gamma_0) + \dots$$

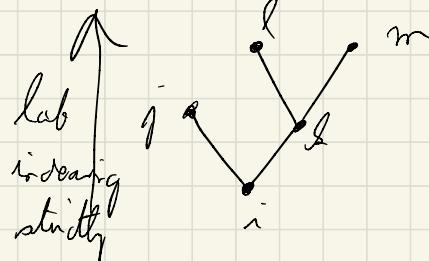
$$\text{while } \exp^\diamond: \boxed{\gamma} \rightarrow G_{\text{End}\alpha}$$

$$\text{gives } h f \rightarrow \phi(\gamma_1) = \phi(\gamma_0 + h f(\gamma_0)) = \phi(\gamma_0) + h \dots$$

Application: We deduce from  $\phi(y(\zeta)) = F^{\text{ff}}(\exp^\diamond(\cdot))[\phi]$

$$\text{that } \frac{1}{(\partial \alpha)^\pi} = \frac{\alpha(\pi)}{|\pi|!}$$

where  $\alpha(\pi)$  is the number of labellings of  $\pi$ :



lab:  $V \rightarrow \{1, \dots, |V|\}$  bijection  
st lab increases strictly from bottom to top.

$$\text{and } \alpha(\tau_1 \dots \tau_n) = \alpha(\tau_1) \dots \alpha(\tau_n).$$

Note that all coefficient ways are characters

$$\alpha(\pi_1, \pi_2) = \alpha(\pi_1) \alpha(\pi_2)$$

so that if  $\alpha = e$  on  $\mathbb{F}_q$ , then

$$\text{as } 1 + g + g \cdot g + g \cdot g \cdot g + \dots =: S^*(g)$$

$$\begin{matrix} \\ \parallel \\ \text{Fl} \end{matrix}$$

then it implies  $\alpha = e$  on  $\mathbb{F}_q$ .

## © Composition and Cones - Kleinsche Hopf algebra

q°: How do we compute  $S_R^f(a)[S_R^f(b)[\phi]]?$

An admissible cut  $c$  is a choice of edges of a tree  $\tau$  such that by removing these edges, any directed path (from bottom to top) meets at most one cutting edge.

The cut  $c$  splits the tree  $\tau$  into a rooted tree (if not the total  <sup>$\tau_c$</sup>  <sub>cut</sub>) and a forest  $\tau \setminus c$ .

$E_R$ : cut	✓	✓	✓	+	✓	✓	✓	total	✓	✓
$\tau_c$	✓	✓	✓	✓	✓	✓	✓	1	not	
$\tau \setminus c$	1	!	.	.	!	.	..	✓	admissible	

The BCK coproduct is

$$\Delta_{BCK}^\tau = \sum_{c \in \text{Adm}} (\tau \setminus c) \otimes \tau_c$$

$$\Delta_{BCK}(\pi_1 \cdot \pi_2) = (\Delta_{BCK} \pi_1) \cdot (\Delta_{BCK} \pi_2)$$

Thm:  $(\mathbb{P}, \cdot, \Delta_{BCK})$  is a Hopf algebra with antipode  $S_{BCK}$ , detailed later.

$$\text{Thm: } S_L^t(a) [S_L^t(t) [\phi]] = S_L^t(a * b) [\phi]$$

where  $a, b \in \mathbb{P}^*$

and the composition law is

$$a * b = \mu(a \otimes b) \circ \Delta_{BCK}, \quad \mu(x \otimes y) = xy$$

$$\begin{aligned} & \& : (a * b)(\langle \rangle) = b(\langle \rangle) + a(1)b(1) + a(\cdot)b(\langle \rangle) \\ & & + a(\cdot)b(\langle \rangle) + a(\cdot)a(1)b(\cdot) + a(\cdot)^2 b(1) + a(\langle \rangle) \end{aligned}$$

Rk: a similar set of algebraic tools exist for Lie-group methods, based on a left grafting operation and ordered planar forests.

Rk: The dual of the BCK Hopf algebra is isomorphic to the GL Hopf algebra.

# Chapter 4: Geometric Numerical Integration

## 1) Preservation of quadratic invariants

Prop: a RK method preserves all linear invariants.

Prop: a RK method cannot preserve all polynomial invariants of fixed degree  $p \geq 3$ ,  
(see exercises).

Thm: a RK method preserves all quadratic invariants  $\checkmark$   
if  $\hat{b}_i \hat{a}_{ij} + \hat{b}_j \hat{a}_{ji} = b_i b_j$ ,  $\forall i, j = 1, \dots, s$ .  $\textcircled{\ast}$

For PRK methods, we have the condition

$$\begin{cases} \hat{b}_i \hat{a}_{ij} + \hat{b}_j \hat{a}_{ji} = \hat{b}_i b_j & \forall i, j \\ \hat{b}_i = b_i \end{cases}$$

for preserving all invariant of the form  $\gamma^T D \gamma$ .

Rq: this is quite restrictive! An explicit RK method cannot satisfy  $\textcircled{\ast}$  and have order 1. (Exercise)

(Hint: consider  $f = J \nabla H$ ,  $H = \frac{P^2 - I^2}{2}$ ,  $\gamma^{n+1} = R(CH) \gamma^n$   
 $|R(CH)| = 1$   ~~$\neq 1$~~   
R polynomial)

$$\text{Proof: } \mathcal{I}(\gamma) = \gamma^T C \gamma, \text{ Convex}$$

$$\mathcal{I}'(\gamma) f(\gamma) = 0 \text{ so that } \gamma^T C f(\gamma) = 0$$

$$\gamma_1 = \gamma_0 + h \sum b_i f(Y_i)$$

$$Y_i = y_0 + L \sum a_{ij} f(Y_j)$$

$$\begin{aligned} \gamma_1^T C \gamma_1 &= (\gamma_0 + h \sum b_i f(Y_i))^T C (\gamma_0 + h \sum b_i f(Y_i)) \\ &= \gamma_0^T C \gamma_0 + h^2 \sum b_i b_j f(Y_i)^T C f(Y_j) \\ &\quad + h \sum b_i \underbrace{\gamma_0^T C f(Y_i)}_{=0} + h \sum b_i f(Y_i)^T C \gamma_0 \\ &= Y_i^T C f(Y_i) - h \sum a_{ij} f(Y_i)^T C f(Y_j) \\ &= \gamma_0^T C \gamma_0 + h^2 \sum (b_i b_j - b_i a_{ij} - b_j a_{ji}) f(Y_i)^T C f(Y_j) \end{aligned}$$

□

Euler midpoint  $\frac{1/2}{1/2}$  preserves quadratic invariants.

→ show simulation pendulum.

$$\text{for } H(p, q) = \frac{p^2 + q^2}{2}$$

## 2) Symplectic methods

Thm: a RK method preserving quadratic invariants is symplectic.

Proof:  $y_{n+1} = \phi_h(y_n)$  RK method

We have to show that  $Y_n = \frac{\partial y_n}{\partial y_0}$  satisfies

$$Y_n^T J Y_n = J, \forall n.$$

Recall the variational equation  $\varphi_t(y_0)$  flow of  $\begin{cases} \dot{y} = f(y) \\ y(0) = y_0 \end{cases} \quad (1)$

$$\begin{cases} \dot{y}' = f'(y), & y(0) = y_0 \\ \dot{Y}' = f'(y)Y, & Y(0) = \text{Id} \end{cases} \quad (2) \quad Y_t = \frac{\partial \varphi_t}{\partial y}$$

Claim: the following diagram commutes

$$\begin{cases} \dot{y}' = f(y), & y(0) = y_0 \end{cases}$$

$$\downarrow \quad y_{n+1} = \overset{(d)}{\phi_h}(y_n)$$

$$\xrightarrow{Y_n = \frac{\partial y}{\partial y_0} \quad (1)} \begin{cases} \dot{y}' = f(y), & y(0) = y_0 \\ \dot{Y}' = f'(y)Y, & Y(0) = \text{Id} \end{cases}$$

(5)

$$\downarrow \quad \begin{cases} (y_{n+1}, Y_{n+1}) \\ \overset{(d+1)}{\phi_h}(y_n, Y_n) \end{cases}$$

$$\{y_n\}$$

$$\xrightarrow{Y_n = \frac{\partial y_n}{\partial y_0}} \{y_n, Y_n\}$$

Indeed  $(y_{n+1}, \gamma_{n+1}) = \Phi_R(y_n, \gamma_n)$  gives

$$\left\{ \begin{array}{l} y_{n+1} = y_n + h \sum b_i f(z_i) \\ \gamma_{n+1} = \gamma_n + h \sum b_i f'(z_i) z_i \\ z_i = y_n + h \sum a_{ij} f(z_j) \\ z_i = \gamma_n + h \sum a_{ij} f'(z_j) \gamma_j \end{array} \right.$$

On the other hand,

$$\frac{\partial}{\partial y_0} \begin{pmatrix} y_{n+1} = y_n + h \sum b_i f(z_i) \\ z_i = y_n + h \sum a_{ij} f(z_j) \end{pmatrix} \text{ yields with } Y_n = \frac{\partial y_n}{\partial y_0}$$

$$\left\{ \begin{array}{l} Y_{n+1} = Y_n + h \sum b_i f'(z_i) \frac{\partial z_i}{\partial y_0} \\ \frac{\partial z_i}{\partial y_0} = Y_n + h \sum a_{ij} f'(z_j) \frac{\partial z_j}{\partial y_0} \end{array} \right.$$

with  $Z_i = \frac{\partial z_i}{\partial y_0}$  yields the same thing.  $\checkmark$

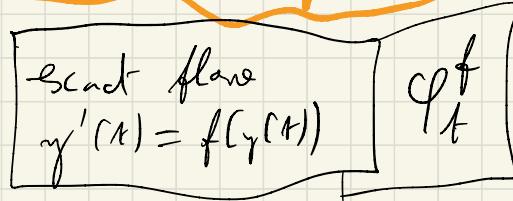
However,  $J(\tilde{Y}) = Y^T J Y$  is a quadratic invariant of the augmented method. The RK method preserves it. As it coincides with the original method,  $J$  is preserved and the method is symplectic.  $\square$

Euler: Midpoint, Trapezoidal rule, Stoermer-Verlet and symplectic Euler are symplectic.

→ Share simulations solar system

### 3) Backward error analysis

idea:



integrated  
 $y_{n+1} = \phi_h^t(y_n)$

modified ODE |  $\phi_t^f$   
 $\tilde{y}'(t) = \tilde{f}(\tilde{y}(t))$

$\phi_h = \phi_{\tilde{h}}$

and that

It is easier to study  $\phi_t$ 's on a continuous problem.

Ex: for  $y' = A y$ , the Euler method

$$\text{is } y_{n+1} = (I + hA) y_n$$

and the exact flow is  $y(t) = e^{R A} y_0$

Then we want  $\gamma_1 = e^{\lambda \tilde{A} h} \gamma_0$

that is  $e^{\lambda \tilde{A} h} = I + \lambda A$

$$\boxed{\tilde{A} h = \frac{1}{h} \log(I + \lambda A)}$$

$$= \sum_{k=1}^{+\infty} \frac{h^{k-1}}{k} (-\gamma)^{k-1} A^k$$

much  
from h  
little.

General case without P-series:

$$\begin{aligned} \text{Assume } & \phi_h^f(r_0) = \gamma_0 + h f(\gamma_0) + h^2 d_2 + h^3 d_3 + \dots \quad (\text{constant}) \\ & \phi_h^f(\gamma_0) = \gamma_0 + \phi_h^f(r^{-1})(\gamma_0) \\ & \qquad \qquad \qquad = \gamma_0 + h f(r_0) + \frac{h^2}{2} f' f + \frac{h^3}{6} (f'' f + f' f'') + \dots \\ & \tilde{h} \tilde{f} = h f + h^2 f_2 + h^3 f_3 + \dots \end{aligned}$$

The condition  $\phi_h^f = \phi_h^{\tilde{f}}$  gives

$$\begin{aligned} \phi_h^{\tilde{f}} &= \text{id} + B_h^{\tilde{f}}(r^{-1}) \\ &= \gamma_0 + (h f + h^2 f_2 + h^3 f_3 + \dots) + \frac{1}{2} (h f + h^2 f_2 + \dots)' (h f + h^2 f_2 + \dots) \\ &\quad + \frac{h^3}{6} (f'' f + f' f'') + \dots \\ &= \gamma_0 + h f + h^2 (f_2 + \frac{1}{2} f' f) \end{aligned}$$

$$+ L^3 \left( f_3 + \frac{1}{2} f_2' f + \frac{1}{2} f' f_2 + \frac{1}{8} f' f' f + \frac{1}{6} f''(f, f) \right) + \dots$$

This yields the conditions:

$$f_2 + \frac{1}{2} f' f = d_2$$

$$f_3 + \frac{1}{2} f_2' f + \frac{1}{2} f' f_2 + \frac{1}{8} f' f' f + \frac{1}{6} f''(f, f) = d_3$$

;

That is  $f_2 = d_2 - \frac{1}{2} f' f$

$$\begin{aligned} f_3 &= d_3 - \frac{1}{2} (d_2 - \frac{1}{2} f' f)' f - \frac{1}{2} f' (d_2 - \frac{1}{2} f' f) \\ &\quad - \frac{1}{8} f' f' f - \frac{1}{6} f''(f, f) \end{aligned}$$

$$\begin{aligned} f_3 &= d_3 - \frac{1}{2} d_2' f - \frac{1}{2} f' d_2 + \frac{1}{4} f' f' f + \frac{1}{4} f''(f, f) \\ &\quad + \frac{1}{4} f' f' f - \frac{1}{8} f' f' f - \frac{1}{6} f''(f, f) \end{aligned}$$

$$f_3 = d_3 - \frac{1}{2} d_2' f - \frac{1}{2} f' d_2 + \frac{1}{3} f' f' f + \frac{1}{12} f''(f, f)$$

The integrator  $\phi_L^f$  satisfies  $|\phi_L^f(\gamma_0) - \tilde{\gamma}^{[3]}(L)| \leq C L^4$

where  $\tilde{\gamma}' = \left( f + L(d_2 - \frac{1}{2} f' f) + L^2 (d_3 - \frac{1}{2} d_2' f - \frac{1}{2} f' d_2 + \frac{1}{3} f' f' f + \frac{1}{12} f''(f, f))(\tilde{\gamma}) \right)$ ,

(under smoothness assumptions on  $f$ )

In particular for the Euler method,  $d_2 = d_3 = \dots = 0$

$$\text{we find } h\tilde{f} = hf - \frac{h^2}{2} f'f + \frac{h^3}{3} (f'f'f + \frac{1}{14} f'''(f,f)) + \dots$$

If  $f(\gamma) = A\gamma$ , we find back  $\tilde{A}_k$ . (by induction)

Chm.: Let  $f_{j+1}(\gamma) = \lim_{L \rightarrow 0} \frac{\phi_h^{f^{[E_j]}}(\gamma) - \phi_h(\gamma)}{h^{j+1}}$ , then

$$|\phi_h^f(\gamma_0) - \phi_h^{f^{[N]}}(\gamma_0)| \leq C_N h^{N+1},$$

$$\text{where } h\tilde{f}^{[N]} = h f_1 + \dots + h^N f_N$$

(under assumptions on  $f$ ).

Chm.: If  $\phi_h$  is of order  $p$ , then  $f_j = 0, 2 \leq j \leq p$ .

• If  $\tilde{f}$  is an invariant of  $\phi_h$  ( $I(\phi_h(\gamma)) = I(\gamma)$ ), then

$$I'(\gamma)(f_1(\gamma)) = 0, \forall \gamma$$

• If  $\phi_h^* = \text{id}$ , then  $\tilde{f}_h = \tilde{f} \circ h$  ( $\Leftrightarrow f_{2j} = 0, \forall j$ )

• If  $\phi_h$  is symplectic, then  $\forall j, \exists j, f_j = J \nabla H_j$ .  
and  $f = J \nabla H$

• If  $\text{div}(f) = 0$  and  $\phi_h$  is volume preserving, then  $\text{div}(\tilde{f}) = 0$

Idea: the optics of  $\phi_L$  are read on  $\tilde{f}_L$ . 

Proof: let us prove the synthetic are by induction

Initialisation:  $\tilde{f}_L^{[1]} = f$  and  $f = J \nabla H$  by assumption. ✓

Assume  $\tilde{f}_L^{[N]} = J \nabla H_L^{[N]}$ ,  $H_L^{[N]} = H + L H_2 + \dots + L^{N-1} H_N$

By definition of  $f_i$ ,

$$\phi_L(\gamma) = \phi_L^{f_L}(\gamma) + L^{N+1} f_{N+1}(\gamma) + O(L^{N+2})$$

We can differentiate :

$$\frac{\partial \phi_L}{\partial \gamma} = \frac{\partial \phi_L^{f_L}}{\partial \gamma} + L^{N+1} \frac{\partial f_{N+1}}{\partial \gamma} + O(L^{N+2})$$

$$\text{We know that } J = \frac{\partial \phi_L}{\partial \gamma}^T \quad \frac{\partial \phi_L}{\partial \gamma} = \frac{\partial \phi_L^x}{\partial \gamma}^T \quad J \frac{\partial \phi_L^x}{\partial \gamma},$$

$$\text{Thus } J = \left( \frac{\partial \phi_L^{f_L}}{\partial \gamma} + L^{N+1} \frac{\partial f_{N+1}}{\partial \gamma} + O(L^{N+2}) \right)^T J \left( \quad \right)$$

) not obvious. We  
can do this as we work  
with smooth maps.

$$= J + L^{N+1} \left( \underbrace{\begin{pmatrix} \frac{\partial f_{N+1}}{\partial \gamma} \end{pmatrix}^T J}_{= J^{-1} \frac{\partial f_{N+1}}{\partial \gamma}} \underbrace{\frac{\partial \varphi_L^{f_L^{CNJ}}}{\partial \gamma}}_{+ \underbrace{\begin{pmatrix} \frac{\partial \varphi_L^{f_L^{CNJ}}}{\partial \gamma} \end{pmatrix}^T J \frac{\partial f_{N+1}}{\partial \gamma}}_{+ O(L^{N+2})}} \right)$$

Thus, we find  $\left( \frac{\partial f_{N+1}}{\partial \gamma} \right)^T J + J \frac{\partial f_{N+1}}{\partial \gamma} = 0$

That is,  $J^{-1} \frac{\partial f_{N+1}}{\partial \gamma}$  is symmetric

We proved that implies that  $\exists H_{N+1}$  (at least locally)

such that  $J^{-1} f_{N+1} = \nabla H_{N+1}$  OK

True globally  
if domain is  
simply connected.

The concept of backward error analysis propagates to global error under analyticity assumption.

Thm: if  $f$  and the  $d_j$  are analytic in  $B_R(y_0)$ , for

$R \leq R_0$  small enough,  $\exists N = \left\lfloor \frac{R_0}{\lambda} \right\rfloor$ ,

$$|\phi_h(y_0) - \varphi_{\ell^+}^{F_N}(y_0)| \leq C_R e^{-\frac{R_0}{\lambda}}$$

Corollary: Consider  $H: D \rightarrow \mathbb{R}$  with  $D$  open set of  $\mathbb{R}^d$  and

$H$  analytic in  $D$ , if  $f = \nabla H$  and the integration step is in the compact  $K \subset D$ , then  $\exists R_0$  s.t.  $\forall R \leq R_0$ ,

$$N = \left\lfloor \frac{R_0}{\lambda} \right\rfloor, \quad \begin{cases} H(y_n) = H(y_0) + \mathcal{O}(h^P) \\ \text{order} \end{cases}$$

$$\hat{H}(y_n) = \tilde{H}(y_0) + \mathcal{O}(e^{-\frac{R_0}{2\lambda}}) /$$

$$h_n \leq e^{\frac{R_0}{2\lambda}}$$

(see GNi, 2006 and references therein)

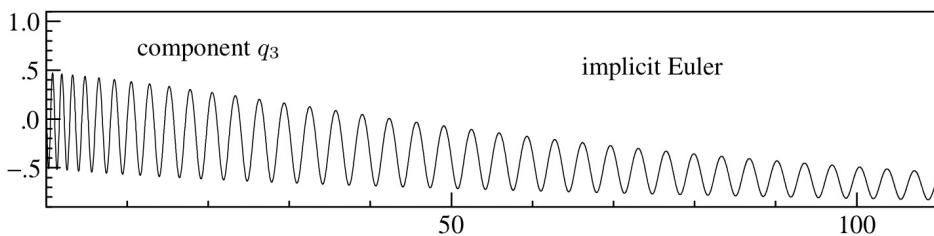
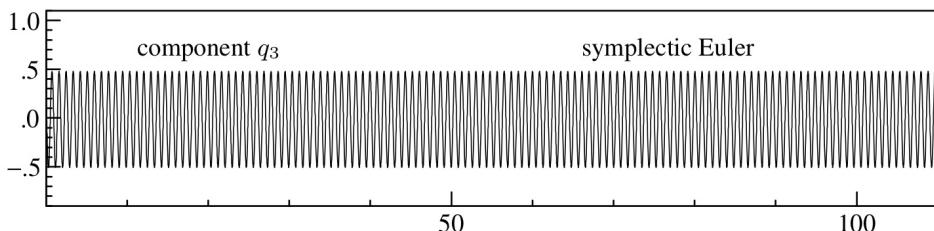
→ Show simulation.

$$\underline{E}:\quad H(q, p) = \frac{p^2}{2} - \cos(q)$$

The midpoint rule is symplectic and satisfies

$$\tilde{f}_L = \int \nabla \tilde{H}_L$$

$$\tilde{H}_L = H + \frac{\hbar^2}{48} \left( \cos(2q) - 2p^2 \cos(q) \right) + O(\hbar^4)$$



**Fig. 1.2.** Spherical pendulum problem solved with the symplectic Euler method (1.19)-(1.20) and with the implicit Euler method; initial value  $q_0 = (\sin(1.3), 0, \cos(1.3))$ ,  $p_0 = (3\cos(1.3), 6.5, -3\sin(1.3))$ , step size  $h = 0.01$

## 4) B-series formulation of BEA

Question: what are  $B^{B^f(C^b)}(\alpha)$  and  $S^{B^f_b(b)}(\alpha)$ ?

$$\text{(where } B^{R^f} = B^{L^f} = B^f \text{)}$$

a partition  $p \in P(T)$  of a tree  $T$  is a subset of the edges of  $T$ .  $T \setminus p$  are the remaining forests.  $T_p$  is the tree obtained by contracting the trees in  $T \setminus p$  to a and putting the edges back.

$P$	<img alt="Tree T with edges (1,2), (1,3), (2,4), (3,5), (4,6), (5,7), (6,8), (7,9), (8,10), (9,11), (10,12), (11,13), (12,14), (13,15), (14,16), (15,17), (16,18), (17,19), (18,20), (19,21), (20,22), (21,23), (22,24), (23,25), (24,26), (25,27), (26,28), (27,29), (28,30), (29,31), (30,32), (31,33), (32,34), (33,35), (34,36), (35,37), (36,38), (37,39), (38,40), (39,41), (40,42), (41,43), (42,44), (43,45), (44,46), (45,47), (46,48), (47,49), (48,50), (49,51), (50,52), (51,53), (52,54), (53,55), (54,56), (55,57), (56,58), (57,59), (58,60), (59,61), (60,62), (61,63), (62,64), (63,65), (64,66), (65,67), (66,68), (67,69), (68,70), (69,71), (70,72), (71,73), (72,74), (73,75), (74,76), (75,77), (76,78), (77,79), (78,80), (79,81), (80,82), (81,83), (82,84), (83,85), (84,86), (85,87), (86,88), (87,89), (88,90), (89,91), (90,92), (91,93), (92,94), (93,95), (94,96), (95,97), (96,98), (97,99), (98,100), (100,101), (101,102), (102,103), (103,104), (104,105), (105,106), (106,107), (107,108), 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Thm:  $(\mathcal{P}, \cdot, \Delta_{CEM})$  is a Hopf algebra with unit  $\bullet$ .

Let  $b \in \mathcal{C}^*$ , extended as a character to  $\mathcal{P}$ , let  $a \in \mathcal{P}^*$ ,  
 then  $S^{B^t(b)}(a) = S^t(b \star a)$  (and similar for  $B$ -series)  
 ↳ substitution

$$\text{and } b \star a = \mu \circ (b \otimes a) \circ \Delta_{CEM}$$

$b$ : modified  $V + R$   
 $a$ : integrator  
 $e$ : exact flavor  $e(\pi) = \frac{1}{\gamma(\pi)}$

) characters over  $\mathcal{P}$

BE A: the goal is to find  $b$  s.t.  $b \star e = a$

We write  $\begin{cases} a = \exp(b) \\ b = \log(a) \end{cases}$ .

Note that  $\exp\left(\sum \frac{b(\pi)}{\sigma(\pi)} \pi\right) = \sum \frac{a(\pi)}{\sigma(\pi)} \pi$ , which is the formula in the dual.

$$\text{scr}: G_{\star} \rightarrow G_{*}$$

$$\text{log}: G_{*} \rightarrow G_{\star}$$

with  $G_{\star} = \{ a \in \mathbb{P}^*, \text{ a character, } a(1) = 0 \}$

$$G_{*} = \{ a \in \mathbb{P}^*, \text{ a character, } a(1) = 1 \}$$

groups

In particular, the inverse of  $a \in G_{*}$  is

$$\begin{aligned} a^{*, -1}(\tau) &= \sum_{p \in P(\tau)} (-1)^{|p|} a(\tau \setminus p) \\ &= (a \circ S_{BCK})(\tau) \end{aligned}$$

(extended as a character)

$$\text{and } b \star e = a$$

$$\Rightarrow b \star (e - s_1) = a - s_1$$

$$\Rightarrow b = (a - s_1) \star \underbrace{(e - s_1)}_{w}^{*, -1}$$

$$\text{where } w \star (e - s_1) = s_1. \Leftrightarrow w \star e = s_1 + s.$$

## 5) Volume preservation and anatomic series

We saw that a method is volume-preserving for  $\gamma' = f(\gamma)$ ,  $\boxed{\operatorname{div}(f) = 0}$  iff  $\boxed{\operatorname{div}(\hat{f}) = 0}$ .

If  $f = J \nabla H$ , a symplectic method preserves volume.

For  $f$  general, this is more difficult.

Q: Can we identify the  $\tilde{f} = B_f^R(b)$  that satisfy  $\operatorname{div}(\tilde{f}) = 0$ ?

def: (anatomic ordered forests)

$V$  set of nodes,  $E$  set of edges,  $(v, w) \in E \Rightarrow$  an edge is going from  $v$  to  $w$ .  
Assume each node is the source of at most one edge.

The nodes that are the source of none are called roots and are numbered from 1 to  $n$ . A connected component with root  $r$  is a tree and without is an atom. We call anatomic forests in  $\mathbb{P}_n$  these graphs (up to equivalence of graphs).

Ex:   $\in \mathbb{P}_0$ ,   $\in \mathbb{P}_1$ ,   $\in \mathbb{P}_2$

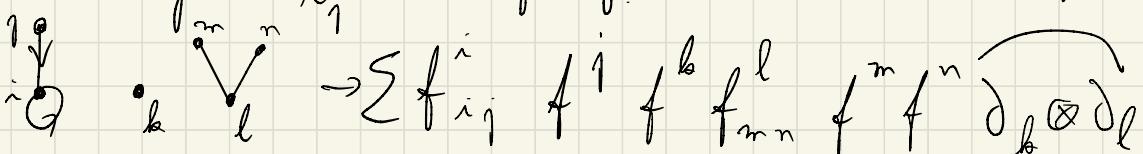
The order is the # of nodes.

def: elem. differential

edge = derivation

node = evaluation

root  $j = \partial_{x_j}$  basis of v.f.



Rq: a tree represents a v.f. = diff operator of order 1

def: let  $\gamma \in \mathcal{P}_n$ , then

$$\wedge \gamma = \frac{1}{n!} \sum_{\sigma \in S_n} E(\sigma) \sigma \cdot \gamma$$

where  $\sigma \cdot \gamma$  permutes the roots following  $\sigma$ .

$\Omega_n = \wedge \mathcal{P}_n$

Ex:  $\wedge \cdot \bullet = \frac{1}{2} (\bullet \circ - \circ \bullet)$

def: let  $d: \Omega_n \rightarrow \Omega_{n-1}$  be

$$d\gamma = \sum_{v \in V} D^{n \rightarrow v} \gamma \text{ where } D^{n \rightarrow v} \text{ grafts}$$

$n$  to  $v$ .

$$\underline{\text{Ex:}} \quad d(\mathbb{Q} \cdot \mathbb{I}) = \mathbb{Q} \cdot + \langle \mathbb{Q} \cdot \mathbb{I} \rangle + \mathbb{Q} \cdot$$

$$+ \mathbb{Q} \cdot \mathbb{I}.$$

Application: consider an acyclic tree  $\gamma$

then  $\boxed{\text{div } F_f(\gamma)} = F_f(\text{div } f).$

$$\underline{\text{Ex:}} \quad \bullet \rightarrow f^i \partial_i = f$$

$$\bullet \rightarrow f^i_i = \sum \frac{\partial f^i}{\partial x^i} = \text{div}(f)$$

Acyclic De Rham complex:

$$\dots \xrightarrow{d} \Omega_3 \xrightarrow{d} \Omega_2 \xrightarrow{d} \Omega_1 \xrightarrow{d} \Omega_0$$

Prop:  $d^2 = 0$  on  $\Omega_n$  (exercise)

$$\underline{\text{Ex:}} \quad d(h \cdot I) = \frac{1}{2} (d \cdot I - d I \cdot)$$

$$= \frac{1}{2} (I + J \cdot + 0 \cdot - I - V - 0 I)$$

$$d^2(h \cdot I) = \frac{1}{2} (d I \cdot + d 0 \cdot - d V - d 0 I)$$

$$\begin{aligned}
 &= \frac{1}{2}((\textcirclearrowleft + \textcirclearrowright + \textcirclearrowuparrow) + (2\textcirclearrowdownarrow + \textcirclearrowleft)) \\
 &\quad - ((\textcirclearrowleft + 2\textcirclearrowdownarrow) - (\textcirclearrowuparrow + \textcirclearrowleft + \textcirclearrowright)) \\
 &= 0 \quad \checkmark
 \end{aligned}$$

Thm: The aromatic De Rham complex is exact,  
 that is,  $\text{Ker}(d|_{\Omega_n}) = \text{Im}(d|_{\Omega_{n+1}})$

Proof: difficult. (see Lauter, McLachlan, MK, Verdier, 2023)

Application: basis of  $\text{Ker}(d|_{\Omega_1})$  is  
 order 3

$$2d_H \wedge \bullet \ddot{\bullet} = \bullet \bullet + \bullet \circ \bullet - \circ \bullet \bullet - \bullet \swarrow \bullet,$$

order 4

$$2d_H \wedge \bullet \ddot{\bullet} = \bullet \bullet \bullet + \bullet \bullet \circ + \Delta \bullet \bullet - \bullet \swarrow \bullet \bullet - \bullet \bullet \swarrow - \circ \bullet \bullet,$$

$$2d_H \wedge \bullet \bullet \swarrow = \bullet \swarrow \bullet \bullet + 2\bullet \bullet \bullet + \bullet \bullet \bullet - 2\bullet \bullet \bullet - \bullet \bullet \bullet - \circ \bullet \bullet \bullet,$$

$$2d_H \wedge \circ \bullet \bullet = \bullet \bullet \circ + \circ \bullet \bullet + \circ \circ \bullet \bullet - \bullet \bullet \circ - \circ \circ \bullet - \circ \bullet \bullet \bullet.$$

Chm (Isaacs, Quigley, Toe, 2007)  
Chartier, Mirela, 2007

No RK method preserves volume.

proof: (idea) assume  $\text{div}(f) = 0$ , that is  $0, 0, \dots \rightarrow 0$

then  $\tilde{f}$  is of the form  $d\pi$ ,  $\pi \in \Omega_2$

We observe that  $d\pi \cdot \frac{1}{0 \rightarrow 0} = \frac{1}{2}(\bullet - \nabla)$

$$d\pi \cdot \bullet = \frac{1}{2}(\bullet + \Delta - \nabla - \square)$$

$$d\pi \cdot \nabla = \bullet + \frac{1}{2}\nabla - \square - \frac{1}{2}\nabla$$

There are quadratic trees everywhere (that won't <sup>overlap</sup> each other)

However, the  $f$  of a RK method is made of Butcher Trees only. Abroad  $\square$

Open problem: does there exist a volume preserving aromatic RK method?

Ex:  $y_{n+1} = y_n + h f(y_n) (1 + \alpha \text{div}(hf)(y_n))$

$\alpha \in \mathbb{R}$

see Bagfjellmo, 2019; Branicio, Larvor, 2026 for Hopf algebra structure.

## 6) Lie group methods

→ see Homework

## References :

- Hairer, Lubich, Warner, Geometric Numerical Integration, 2006
- Sohles, Mørkøe - Kaas, Nørsett, Zanna, Lie group methods, 2000
- McLachlan, Quispel, splitting methods, 2002
- Blanes, Casas, Muñoz, Splitting methods for differential equations, 2024
- Chartier, Hairer, Verlent, Algebraic structure of B-series, 2010
- Lawrent, McLachlan, Mørkøe - Kaas, Verlent, The aromatic bicanon for the description of divergence-free aromatic forms and volume-preserving integrators, 2023
- Foissy, an introduction to Hopf algebras of trees, 2013