Geometric integration of Hamiltonian systems

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I. NUMERICAL METHODS FOR INITIAL VALUE PROBLEMS

I. A. PRELIMINARIES

I. A. (i) INITIAL VALUE PROBLEMS

Concerned with *initial value problems*

$$\frac{dy}{dt} = f(y), \quad y(0) = \alpha \in \mathbb{R}^D,$$

where f is a *sufficiently smooth* mapping $f : \Omega \to \mathbb{R}^D$ (Ω is a domain $\subset \mathbb{R}^D$) and α is a point in Ω. (Manifolds not considered.)

Think of f as a *vector field* in Ω. Solution of DE is a curve described by moving point $y(t)$ in such a way that for each t the velocity vector $\dot{y}(t)$ coincides with the value of the vector field at $y(t)$.

I. A. (ii) FLOWS

For fixed t, the *flow* ϕ_t of the differential system (vector field) is a transformation $\phi_t : \Omega \to \Omega$ that maps each $\alpha \in \Omega$ into the value at time t of the solution of the IVP.

Semigroup property: $\phi_t \circ \phi_s = \phi_{t+s}$, $\phi_0 = Id$.

Example: $\Omega = \mathbb{R}^2$, $(d/dt)y_1 = -y_2$, $(d/dt)y_2 = y_1$.

Soln. of IVP is (α fixed, variable t)

$$\begin{bmatrix} y_1(t) \\ y_2(t) \end{bmatrix} = \begin{bmatrix} \alpha_1 \cos t - \alpha_2 \sin t \\ \alpha_1 \sin t + \alpha_2 \cos t \end{bmatrix},$$

so that ϕ_t (α variable, t fixed) is rotation by t radians.

I. B. EULER'S METHOD

I. B. (i) FORMULATION 1 *Institutionum Calculi Integralis 1768*

Given initial value problem and $T > 0$, wanted $y(T)$.

Introduce *grid or step points* $t_n = nh$, $n = 0, 1, \ldots N$, ($N > 0$ an integer), where $h = T/N$ is the *step-length*.

Approximations y_n to $y(t_n)$ are obtained by setting $y_0 = \alpha$ and, for $n = 0, \ldots, N-1$, performing the *steps*

$$y_{n+1} = y_n + hf(y_n).$$

I. B. (ii) FORMULATION 2

Introduce mapping $\psi_h : \Omega \to \mathbb{R}^D$ such that $y \mapsto y + hf(y)$.

Then, one step of Euler's method is $y_{n+1} = \psi_h(y_n)$, cf. with true $y(t_{n+1}) = \phi_h(y(t_n))$.

After N steps:

$$y_N = (\psi_h \circ \psi_h \circ \cdots \circ \psi_h)(\alpha) \neq \psi_{Nh}(\alpha)$$

cf.

$$y(t_N) = (\phi_h \circ \phi_h \circ \cdots \circ \phi_h)(\alpha) = \phi_{Nh}(\alpha).$$

I. B. (iii) ANALYSIS: LOCAL ERROR

Local error at a point y: $\phi_h(y) - \psi_h(y)$

If $z(t)$ is solution of DE with $z(0) = y$ *(local solution at* y*)*

$$\phi_h(y) - \psi_h(y) = \left[z(0) + h\dot{z}(0) + \frac{h^2}{2}\ddot{z}(0) + \cdots\right] + \left[y + hf(y)\right]$$

so that: $\phi_h(y) - \psi_h(y) = O(h^2)$.

Consistency of the first order.

I. B. (iiii) ANALYSIS: GLOBAL ERROR

As $h \to 0$, the *global error* $y_N - y(T)$ is $O(h)$: *convergence of the first order*. Global error is built up of $N = T/h$ contrbtns, each of size $O(h^2)$. For other one-step methods, $y_{n+1} = \psi_h(y_n)$, local errors of size $O(h^{p+1})$ produce global errors of size $O(h^p)$.

I. C. TAYLOR EXPANSION METHODS *Euler 1768*

Differentiation in $dy/dt = f(y)$ leads to $(d^2y/dt^2) = f'(y)dy/dt = f'(y)f(y)$ and to method consistent of the *second-order:*

$$y_{n+1} = y_n + hf(y_n) + \frac{h^2}{2}f'(y_n)f(y_n) = \psi_h(y_n).$$

with global errors $O(h^2)$ (convergence of order 2).

Similarly, incorporate $d^3y/dt^3 = f''(y)[f(y), f(y)] + f'(y)f'(y)f(y)$ for *3rd order;* $f'''[f,f,f] + 3f''[f'f,f] + f'f''[f,f] + f'f'f'f$, etc.

Euler's method only requires evaluation of f at any given point y. Now higher derivatives of the (components of) f required. Conventional wisdom: methods not suited for general purpose algorithm. But...

I. D. MULTISTEP METHODS

I. D. (i) ADAMS METHODS *circa 1855, Bashforth 1883*

Integrate DE

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_{n+1}} y'(\tau)\, d\tau = \int_{t_n}^{t_{n+1}} f(y(\tau))\, d\tau$$

and, for fixed integer k, use *quadrature rule*

$$\int_{t_n}^{t_{n+1}} f(y(\tau))\, d\tau \approx h\left[\beta_{k-1} f(y(t_n)) + \cdots + \beta_0 f(y(t_{n-k+1}))\right],$$

(where β_j chosen for no error if integrand $f(y(t))$ polynomial in t of degree $\leq k-1$), to get order method consistent of order k

$$y_{n+1} - y_n = h\left[\beta_{k-1} f(y_n) + \cdots + \beta_0 f(y_{n-k+1})\right].$$

Note: no ψ_h. Convergence not implied by consistency.

I. D. (ii) IMPLICIT ADAMS METHODS

Alternatively, quadrature rule

$$\int_{t_n}^{t_{n+1}} f(y(\tau))\, d\tau \approx h\left[\tilde{\beta}_k f(y(t_{n+1})) + \cdots + \tilde{\beta}_0 f(y(t_{n-k+1}))\right]$$

may be rendered exact for integrand of degree k and leads to method of order of consistency $k+1$

$$y_{n+1} - y_n = h\left[\tilde{\beta}_k f(y_{n+1}) + \cdots + \tilde{\beta}_0 f(y_{n-k+1})\right].$$

Implicit method: To effect a step, solve a system of D real equations for the D components of y_{n+1}.

Predictor-corrector: take y_{n+1} given by explicit method as first guess for solution of implicit equations *Moulton 1926*.

I. D. (iii) GENERAL LINEAR MULTISTEP METHODS

With number of steps k,

$$\alpha_k y_{n+1} + \cdots + \alpha_0 y_{n-k+1} = h\left[\beta_k f(y_{n+1}) + \cdots + \beta_0 f(y_{n-k+1})\right]$$

where α_j, β_j are free parameters.

Consistency of order of order $2k$ attained by right choice of parameters (or $2k-1$ if method is required to be explicit).

Unlike one-step methods, consistency of order $p \geq 1$ does not in general imply small global errors *(Dahlquist 1956–1959, zero-instability)*.

Adams still preferred choice.

I. E. RUNGE-KUTTA METHODS

I. E. (i) RUNGE *1895*

As before

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_{n+1}} y'(\tau)\, d\tau = \int_{t_n}^{t_{n+1}} f(y(\tau))\, d\tau.$$

Euler based on rectangle quadrature. More accuracy expected if midpoint rule used alternatively:

$$y_{n+1} = y_n + h_n f(Y), \quad Y = y_n + \frac{h_n}{2} f(y_n).$$

f is evaluated twice in step $n \to n+1$. There are two *stages* per step, but method still follows *one-step* format $y_{n+1} = \psi_h(y_n)$.

I. E. (ii) HEUN *1900*

Aim: replicate Simpson's rule (order 4 with 3 fnctn evaluations). Consider general format with s stages

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i f(Y_i),$$

Y_i are approximations to $y(t_n + c_i h)$ obtained in Euler-like way:

$$\begin{aligned} Y_1 &= y_n \\ Y_2 &= y_n + c_2 h f(Y_1) \\ &\dots \\ Y_s &= y_n + c_s h f(Y_{s-1}). \end{aligned}$$

The *weights* b_i and the *abscissae* c_i are free parameters. Order 3 achieved with 3 stages and order 4 with 8.

I. E. (iii) KUTTA *1901*

Bring all already found stages $Y_1, \ldots, Y_j$ into the computation of Y_{j+1}:

$$\begin{aligned} Y_1 &= y_n, \\ Y_2 &= y_n + a_{2,1} h f(Y_1), \\ Y_3 &= y_n + a_{3,1} h f(Y_1) + a_{3,2} h f(Y_2), \\ &\cdots \\ Y_s &= y_n + a_{s,1} h f(Y_1) + \cdots + a_{s,s-1} h f(Y_{s-1}). \end{aligned}$$

Constructs methods with 4 stages and order 4. Among them the wrongly named THE Runge-Kutta method (weights 1/6, 2/6, 2/6 1/6, which should NEVER be used by ANYBODY.

Also 6 stages and order 5.

Conditions on a_{ij} and b_i to ensure order p cumbersome to write and not well understood.

1 equation for order 1, 2 for order 2, 8 for order 4, 17 for order 5.

A method of order 6 with 8 stages constructed by Huta in 1956, by solving 37 order conditions for 36 unknowns?

I. E. (iiii) BUTCHER *1963*

Butcher considers general format $y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(Y_i) = \psi_h(y_n)$, with the stage vectors Y_i defined (recursively or implicitly) $Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f(Y_j)$.

An s-stage method has $s^2 + s$ free parameters, presented in the *Butcher tableau*

$$\begin{array}{cccc} a_{11} & a_{12} & \dots & a_{1s} \\ a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline b_1 & b_2 & \dots & b_s \end{array}$$

B. provides easy, systematic way to expand in powers of ψ_h and true flow ϕ_h. (Graphs used.)

Thoroughly analyzes order conditions (i.e. conditions that impose that $\psi_h = \phi_h + O(h^{p+1})$):

$$\begin{aligned}
\sum_i b_i &= 1, \\
\sum_{ij} b_i a_{ij} &= 1/2, \\
\sum_{ijk} b_i a_{ij} a_{ik} &= 1/3, \\
\sum_{ijk} b_i a_{ij} a_{jk} &= 1/6, \\
&\dots \quad \dots \quad \dots
\end{aligned}$$

With s stages order $2s$ can be achieved with a unique choice of free parameters (Gauss method).

II. FROM THE CLASSICAL PARADIGM TO GEOMETRIC INTEGRATION

II. A. TOWARDS THE CLASSICAL PARADIGM

II. A. (i) DEVELOPMENT

Methods Euler 1768, Adams 1855, Runge/Kutta 1895 bring computers.

Computers 1945 extend exponentially use of methods which spawns mathematical interest in methods Dahlquist 1956, Butcher 1963, Henrici 1962. Stability, order conditions, convergence.

Computers and mathematics lead to software packages 1965.

II. A. (ii) PACKAGES

(1) user supplies tolerance, initial condition and f through a subroutine $y \mapsto f(y)$,

(2) use a battery of Adams or Runge-Kutta formulae,

(3) adapt order of method and steplength h along the simulation,

(4) fine-tuned for efficiency and robustness.

II. A. (iii) THE CLASSICAL PARADIGM

The elements above describe a harmonious body of knowledge, ranging from mathematical analysis to software engineering (see e.g. books by Hairer, Nørsett & Wanner, first edition), that can be referred to as 'the classical paradigm' (SS 1996).

N.B. Also within the classical paradigm:

• Stiff problems (Dahlquist 1963). Require ad hoc methods and special packages.

• DAE: Differential equations coupled to algebraic constraints.

II. B. LIMITATIONS OF THE CLASSICAL PARADIGM

(1) One-size-fits-all? Can specific features of differential system of interest be taken into account by the method?

(2) Practical useful simulations exist outside the CP:

• Really wish (is it possible) to accurately find $y(T)$? Or rather wish to derive qualitative dynamic information? Or statistical properties of flow?

• Is a package the best choice?

• Are there other mathematical elements (beyond consistency, stability, etc.) that could help in analyzing/designing methods?

Examples: molecular dynamics, astrophysics.

II. C. GEOMETRIC INTEGRATION

A new way of doing numerical initial value problems (SS 1996) characterized by:

(1) Methods for specific classes of problems.

(2) Methods conceived and analyzed by means of geometric properties of flow being simulated.

Examples include: (canonical) Hamiltonian problems/symplecticness, noncanonical Hamiltonian problems, Poisson systems, systems with a symmetry (involution), volume preserving flows, equations on manifolds/Lie groups, etc.

II. D. (CANONICAL) HAMILTONIAN PROBLEMS

II. D. (i) FORMULATION *Hamilton 1834*

Our IVP is *Hamiltonian* if $D = 2d$ and, with $y = (p, q)$ (p, q d-dimensional), there exists $H : \Omega \to \mathbb{R}$, such that

$$f^i = -\frac{\partial H}{\partial q_i}, \qquad f^{i+d} = +\frac{\partial H}{\partial p_i}, \qquad i = 1, \ldots, d.$$

- H is the *Hamiltonian* function.
- d is the *number of degrees of freedom.*
- Ω is the *phase space.*

DE

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \qquad \frac{dq_i}{dt} = +\frac{\partial H}{\partial p_i}, \qquad i = 1, \ldots, d,$$

may be compactly rewritten as

$$\frac{dy}{dt} = J^{-1}\nabla H, \quad J = \begin{bmatrix} O_d & +I_d \\ -I_d & O_d \end{bmatrix} = J^{-T},$$

leading to *conservation of energy*

$$\frac{d}{dt}H(y(t)) = \nabla H(y(t))^T \frac{dy}{dt} = \nabla H(y(t))^T \, J^{-1} \, \nabla H(y(t)) = 0.$$

Model many/most situations where dissipation is absent/may be ignored.

II. D. (ii) HAMILTONIAN DYNAMICS

Example: Next slide shows the *phase space* of Ham. ($d = 1$)

$$H(p, q) = \frac{1}{2}p^2 + (1 - \cos q)$$

that describes the motion of a (planar, frictionless) pendulum.

Note:

- Stable equilibrium at $q = 0$ has eigenvalues $\pm i$.
- Stable equilibrium surrounded by closed orbits (periodic solutions).
- Unstable equilibrium at $q = \pi$ has eigenvalues ± 1.

How is the phase plane of nearby systems?

II. D. (iii) THE SYMPLECTIC FORM

In vector space $V = \mathbb{R}^{2d}$ of vectors $y = [p, q]$, consider bilinear form $(\xi, \eta) \in V \times V \mapsto \omega(\xi, \eta) = \xi^T J \eta \in \mathbb{R}$.

If $d = 1$, then $\omega(\xi, \eta) = \xi^p \eta^q - \xi^q \eta^p$ is the *oriented area* of the parallelogram with sides ξ and η.

If $d > 1$, then $\omega(\xi, \eta) = \sum_i (\xi^{p_i} \eta^{q_i} - \xi^{q_i} \eta^{p_i})$ is the *sum of the oriented areas* of the d parallelograms obtained by projecting ξ and η onto the 2-dimensional planes (p_i, q_i).

II. D. (iiii) THE SYMPLECTIC GROUP *Weyl 1939*

A linear transformation A in V (matrix) is *symplectic* if $\omega(A\xi, A\eta) \equiv \omega(\xi, \eta)$, i.e. $A^T J A = J$.

A symplectic linear transformtn. preserves the *exterior powers* ω^2,. . . ,ω^d that have interpretations as higher-dimensional measures. In particular ω^d is the oriented 'volume' of parallelepipeds.

II. D. (v) SYMPLECTIC TRANSFORMATIONS

By using integration, the symplectic form ω can be extended from measuring 2-dimensional parallelograms to measure 2-dimensional surfaces.

A diffeomorphism F in Ω is symplectic if, for each 2-dimensional surface $M \subset \Omega$, $\omega(F(M)) = \omega(M)$.

F is symplectic if and only if, at each $y \in \Omega$, the Jacobian $F'(y)$ is a symplectic matrix.

II. D. (vi) SYMPLECTIC GEOMETRY AND HAMILTONIAN SYSTEMS

For each t, the flow ϕ_t of a Hamiltonian system is a symplectic transformation in Ω *Poincaré 1899, integral invariants*.

Proof. Enough to show that $(d/dt)[\phi_t'(y)^T J \phi_t'(y)] = 0$.

But $(d/dt)\phi_t'(y) = f'(\phi_t(y))\phi_t'(y) = J^{-1}H''(\phi_t(y))\phi_t'(y)$.

So that $(d/dt)[\,] = \phi_t'^T H'' J^{-T} J \phi_t' + \phi_t'^T J J^{-1} H'' \phi_t' = 0$.

Conversely, if a flow preserves $[\phi_t'(y)^T J \phi_t'(y)]$, then $Jf'(y)$ is a symmetric matrix and hence locally exists H such that $Jf = \nabla H$, or $f = J^{-1}\nabla H$.

II. D. (vii) NUMERICAL METHODS AND THE SYMPLECTIC FORM

Integrate pendulum equations by:

• Euler: $y_{n+1} = y_n + hf(y_n)$.

• Implicit Euler: $y_{n+1} = y_n + hf(y_{n+1})$. (Adjoint of Euler $\psi_{-h}^{IE} \circ \psi_h^E = Id$).

• Midpoint rule: $y_{n+1} = y_n + hf(Y)$, $Y = y_n + (h/2)f(Y)$ (unique one-stage RK of order 2, lowest Gauss method).

III. SYMPLECTIC RK AND RELATED METHODS

III. A. SYMPLECTIC RUNGE-KUTTA METHODS

III. A. (i) SYMPLECTICNESS CONDITION

RK method defined by coefficient matrix (a_{ij}) and weights b_i is:

$$\begin{aligned} y_{n+1} &= \psi_h(y_n), \\ y_{n+1} &= y_n + h\sum_{i=1}^{s} b_i f(Y_i), \\ Y_i &= y_n + h\sum_{j=1}^{s} a_{ij} f(Y_j). \end{aligned}$$

Th. (Lasagni 1988/SS 1988/Suris 1988) Relations

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad 1 \le i, j \le s,$$

guarantee symplectiness of ψ_h if DE are Hamiltonian.

III. A. (ii) GAUSS METHODS

Th. (SS 1988) For each s, the s-stage Gauss method (order $2s$ is symplectic.

Examples:

- $s = 1$, *Trapezoidal rule*, order two:

$$\begin{aligned} y_{n+1} &= y_n + hf(Y_1), \\ Y_1 &= y_n + \frac{1}{2}hf(Y_1). \end{aligned}$$

(Note that, eliminating f, $Y_1 = (1/2)(y_n + y_{n+1})$, so that

$$y_{n+1} - y_n = hf(\frac{1}{2}(y_n + y_{n+1})).)$$

To implement, find Y_1 and extrapolate: $y_{n+1} = 2Y_1 - y_n$.

- $s = 2$, order four:

$$\begin{aligned} y_{n+1} &= y_n + \frac{1}{2} h f(Y_1) + \frac{1}{2} h f(Y_2), \\ Y_1 &= y_n + \frac{1}{4} h f(Y_1) + \left(\frac{1}{4} - \frac{\sqrt{3}}{6} \right) h f(Y_2), \\ Y_2 &= y_n + \left(\frac{1}{4} + \frac{\sqrt{3}}{6} \right) h f(Y_1) + \frac{1}{4} h f(Y_2). \end{aligned}$$

System of dimension $2D = 4d$ per step.

- With s stages, order is $2s$ and system has dimension $sD = 2sd$.

III. A. (iii) DIAGONALLY IMPLICIT RK METHODS

Symplecticness condition precludes explicit methods.

Diagonally implicit: $a_{ij} = 0$, whenever $j > i$. Leads to s D-dimensional systems (rather than an sD-system) per step.

Symplecticness conditions leads to $a_{ij} = b_i$ for $i < j$ and $a_{ii} = b_i/2$, leaving s free parameters. Tableau is:

$$\begin{array}{cccc} b_1/2 & 0 & \dots & 0 \\ b_1 & b_2/2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ b_1 & b_2 & \dots & b_s/2 \\ \hline b_1 & b_2 & \dots & b_s \end{array}$$

Note Y_{j+1} coincides with result of performing a step of midpoint rule of length $hb_{j+1}/2$ from $y_n + h(b_1 f(Y_1) + \cdots + b_j f(Y_j))$ and then

$$\psi_h = \psi^{MP}_{b_s h} \circ \cdots \circ \psi^{MP}_{b_1 h}.$$

One step of method is a *concatenation* of s substeps of midpoint rule with steplengths $b_1 h$, . . . , $b_s h$.

III. B. SYMPLECTIC PARTITIONED RK METHODS

III. B. (i) SYMPLECTICNESS CONDITION

IVP of special format

$$\frac{dp}{dt} = f(q), \quad \frac{dq}{dt} = g(p).$$

Hamiltonian system has this format if Hamiltonian function has the separated form $H(p,q) = T(p)+V(q)$. Then $f(q) = -\nabla_q V(q)$.

Use different tableaux for each block:

$$p_{n+1} = p_n + h\sum_{i=1}^{s} b_i f(Q_i), \quad q_{n+1} = q_n + h\sum_{i=1}^{s} B_i g(P_i),$$

$$P_i = p_n + h\sum_{j=1}^{s} a_{ij} f(Q_j), \quad Q_i = q_n + h\sum_{j=1}^{s} A_{ij} g(P_j).$$

In shorthand:

$$\begin{array}{cccc} a_{11} & a_{12} & \dots & a_{1s} \\ a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline b_1 & b_2 & \dots & b_s \end{array}, \qquad \begin{array}{cccc} A_{11} & A_{12} & \dots & A_{1s} \\ A_{21} & A_{22} & \dots & A_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ A_{s1} & A_{s2} & \dots & A_{ss} \\ \hline B_1 & B_2 & \dots & B_s \end{array}.$$

Th. (SS 1989/Suris 1990) Method is symplectic (for separated Hamiltonian functions) if

$$b_i A_{ij} + B_j a_{ji} - a_i a_j = 0, \quad 1 \le i, j \le s.$$

III. B. (ii) EXPLICIT SYMPLECTIC PRK METHODS

Given by:

$$\begin{array}{ccccc} 0 & 0 & 0 & \dots & 0 \\ b_1 & 0 & 0 & \dots & 0 \\ b_1 & b_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_1 & b_2 & b_3 & \dots & 0 \\ \hline b_1 & b_2 & b_3 & \dots & b_s \end{array}, \qquad \begin{array}{ccccc} B_1 & 0 & 0 & \dots & 0 \\ B_1 & B_2 & 0 & \dots & 0 \\ B_1 & B_2 & B_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_1 & B_2 & B_3 & \dots & B_s \\ \hline B_1 & B_2 & B_3 & \dots & B_s \end{array},$$

so that:

$$\begin{array}{cc} P_1 = p_n & Q_1 = q_n + hB_1 g(P_1), \\ P_2 = p_n + hb_1 f(Q_1) & Q_2 = q_n + hB_1 g(P_1) + hB_2 g(P_2), \\ \dots & \dots \end{array}$$

Possible to switch tableaux of p and q.

Examples:

- *Symplectic Euler method (Asymmetrical Euler-B)*, 1st order:

$$p_{n+1} = p_n + hf(q_n) \quad q_{n+1} = q_n + hg(p_{n+1}).$$

- *Also (Asymmetrical Euler-A)*, 1st order:

$$p_{n+1} = p_n + hf(q_{n+1}) \quad q_{n+1} = q_n + hg(p_n).$$

- *Störmer 1907 Verlet 1967*, 2nd order, kick-glide-kick:

$$\begin{aligned} p_{n+1/2} &= p_n + (h/2)f(q_n), \\ q_{n+1} &= q_n + hg(p_{n+1/2}), \\ p_{n+1} &= p_{n+1/2} + (h/2)f(q_{n+1}). \end{aligned}$$

• *Leapfrog implementation* of Störmer-Verlet. Eliminate p at integer time levels:

$$\begin{aligned} q_{n+1} &= q_n + hg(p_{n+1/2}), \\ p_{n+1/2} &= p_{n+1/2} + hf(q_{n+1}). \end{aligned}$$

One evaluation of the force per step.

• The PRK class contains symplectic methods of arbitrarily high orders.

III. C. SYMPLECTIC RK-NYSTRÖM METHODS

III. C. (i) SYMPLECTICNESS CONDITION

IVP of special format

$$\frac{dp}{dt} = f(q), \quad \frac{dq}{dt} = M^{-1}p,$$

or, equivalently,

$$M\frac{d^2}{dt^2}q = f(q).$$

Hamiltonian system has this format if Hamiltonian function has the separated form $H(p,q) = \frac{1}{2}p^T M^{-1}p + V(q)$.

RKN method *(Nyström 1925)*: stages Q_i are defined by

$$MQ_i = Mq_n + h\gamma_i p_i + h^2 \sum_j \alpha_{ij} f(Q_j)$$

and solution at next time level is

$$\begin{aligned} p_{n+1} &= p_n + h \sum_i b_i f(Q_i), \\ Mq_{n+1} &= Mq_n + hp_n + h^2 \sum_i \beta_i f(Q_i). \end{aligned}$$

Each RK or PRK method applied to $\dot{p} = f(q)$, $\dot{q} = M^{-1}p$ generates an RKN method. (But properties as RKN may not be the same when seen as RK/PRK.)

In shorthand:

γ_1	α_{11}	α_{12}	$\ldots$	α_{1s}
γ_2	α_{21}	α_{22}	$\ldots$	α_{2s}
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
γ_s	α_{s1}	α_{s2}	$\ldots$	α_{ss}
	β_1	β_2	$\ldots$	β_s
	b_1	b_2	$\ldots$	b_s

Th. Suris 1988/1989. RKN is symplectic for $H = \frac{1}{2}p^T M^{-1} p + V(q)$ if

$$\begin{aligned} \beta_i &= b_i(1-\gamma_i), \\ b_i(\beta_j - \alpha_{ij}) &= b_j(\beta_i - \alpha_{ji}). \end{aligned}$$

III. C. (ii) EXPLICIT SYMPLECTIC RKN METHODS

Have the format:

γ_1	0	0	$\dots$	0
γ_2	$b_1(\gamma_2-\gamma_1)$	0	$\dots$	0
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
γ_s	$b_1(\gamma_s-\gamma_1)$	$b_1(\gamma_s-\gamma_2)$	$\dots$	0
	$b_1(1-\gamma_1)$	$b_2(1-\gamma_2)$	$\dots$	$b_s(\gamma_s-\gamma_s)$
	b_1	b_2	$\dots$	b_s

• Methods of order 4, 5 stages, 4 force evaluation per step, with minimized error constant constructed by M.P. Calvo 1992.

• She also constructed optimized methods of order 8.

IIII. ANALYSIS OF SYMPLECTIC RK METHODS

IIII. A. THE ORDER OF RK METHODS

IIII. A. (i) TAYLOR EXPANSION OF RK SOLUTION

Perform one step of length h from y to $\psi_h(y)$.

If DE/vector field is smooth,

$$\begin{aligned}\psi_h(y) \;=\; & y \\ & +h\Big(\sum_i b_i\Big)\Big[f\Big] \\ & +h^2\Big(\sum_{ij} b_i a_{ij}\Big)\Big[f'(y)\cdot f(y)\Big] \\ & +\frac{h^3}{2}\Big(\sum_{ijk} b_i a_{ij} a_{ik}\Big)\Big[f''(y)\cdot[f(y),f(y)]\Big] \\ & +h^3\Big(\sum_{ijk} b_i a_{ij} a_{jk}\Big)\Big[f'(y)\cdot f'(y)\cdot f(y)\Big]+\cdots\end{aligned}$$

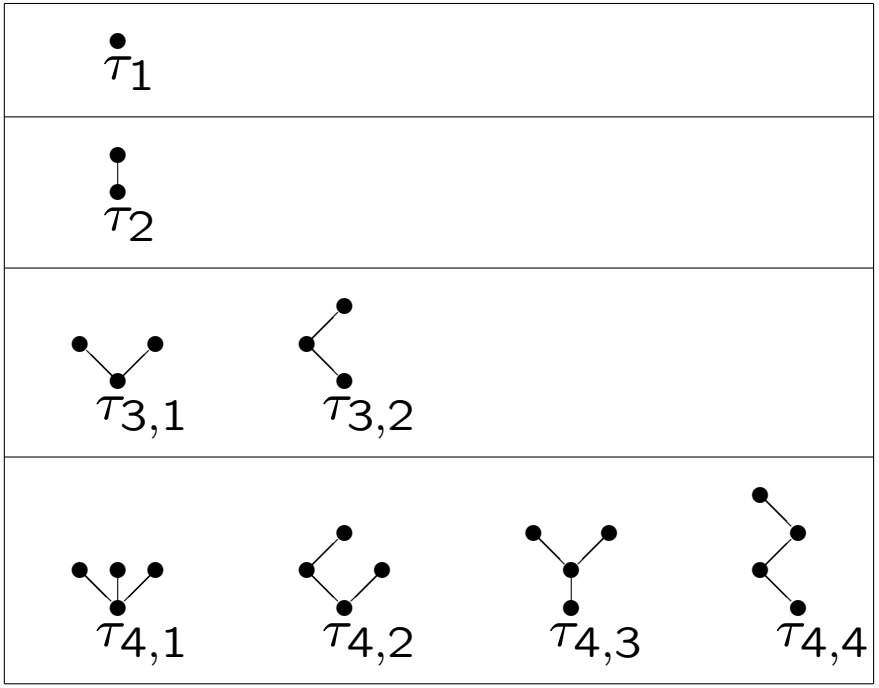
+ We encounter a sum of terms of the form $\frac{h^\ell}{\sigma}\Big(\cdot \Big) \Big[\cdot \Big]$, where

• σ is a positive integer. Does not depend on system or method.

• $\Big(\cdot \Big)$ is an homogenous polynomial of degree ℓ in the tableau elements: *elementary weight.* Depends on method.

• $\Big[\cdot \Big]$ is a combination of (Fréchet) derivatives of the vector field f: *elementary differential.* Depends on system.

+ All these elements easily written in terms of *rooted trees*.


τ_1
τ_2
$\tau_{3,1}$
$\tau_{3,2}$
$\tau_{4,1}$
$\tau_{4,2}$
$\tau_{4,3}$
$\tau_{4,4}$

IIII. A. (ii) ORDER CONDITIONS

RK solution:

$$\psi_h(y) = y + \sum_{\ell=1}^{\infty} h^\ell \sum_{\tau \in RT_\ell} \frac{1}{\sigma(\tau)}\, c(\tau) F(\tau)(y).$$

True flow:

$$\psi_h(y) = y + \sum_{\ell=1}^{\infty} h^\ell \sum_{\tau \in RT_\ell} \frac{1}{\sigma(\tau)}\, \frac{1}{\gamma(\tau)} F(\tau)(y).$$

where $\gamma(\tau)$ is the so-called *density* of τ.

Hence order $\geq p$ iff for each tree of order $\leq p$, $c(\tau) = 1/\gamma(\tau)$.

Note. Size of $c(\tau) - 1/\gamma(\tau)$ for trees of order $p+1$ important!

The first order conditions are:

$$\begin{aligned}
\sum_i b_i &= 1, \\
\sum_{ij} b_i a_{ij} &= 1/2, \\
\sum_{ijk} b_i a_{ij} a_{ik} &= 1/3, \\
\sum_{ijk} b_i a_{ij} a_{jk} &= 1/6, \\
&\ldots \quad \ldots \quad \ldots
\end{aligned}$$

Butcher showed that these order conditions are mutually independent if the number of stages s and the tableau elements a_{ij}, b_i are free. However . . .

IIII. A. (iii) SIMPLIFYING ASSUMPTIONS

Essential in construction of high-order methods.

Constraints in tableau ($c_i = a_{i1} + \cdots + a_{is}$)

$$B(p): \quad \sum_i b_i c_i^{q-1} = \frac{1}{q}, \quad q = 1, \ldots, p,$$

$$C(\eta): \quad \sum_j a_{ij} c_j^{q-1} = \frac{c_i^q}{q}, \quad q = 1, \ldots, p,$$

$$D(\zeta): \quad \sum_i b_i c_i^{q-1} a_{ij}^{q-1} = \frac{b_j}{q}(1 - c_j^q), \quad q = 1, \ldots, \zeta.$$

Th. (Butcher 1964) $B(p)$, $C(\eta)$, $D(\zeta)$, where $p \leq 2\eta + 2$ and $p \leq \zeta + \eta + 1$, guarantee order $\geq p$.

IIII. B. THE RK GROUP

IIII. B. (i) COMPOSING RK METHODS (Butcher 1969)

A step $y \mapsto z = \psi_h^{[1]}(y)$ with an RK method, followed by a step $z \mapsto w = \psi_h^{[2]}(z)$ with a 2nd RK method is a single step of an RK method $\psi_h^{[3]}$, product of $\psi^{[1]}$ and $\psi^{[2]}$.

Example 1: (Forward) Euler $z = y + hf(y)$ followed by backward Euler $w = z + hf(w)$ yields

$$w = y + (2h)\Big[\frac{1}{2}f(y) + \frac{1}{2}f(w)\Big],$$

trapezoidal rule over an interval of length $2h$.

Example 2: Backward Euler $z = y + hf(z)$ followed by (forward) $w = z + hf(z)$ Euler gives:

$$w = y + (2h)f(z), \quad z = y + hf(z),$$

midpoint rule over an interval of length $2h$.

Example 3: A diagonally implicit symplectic RK method with weights b_i is the product of midpoint rule with steplenght $b_1 h$, followed by midpoint rule with steplength $b_2 h$, ...

Butcher derived formulae for the elementary weights of the product in terms of the elementary weights of the factors: $c^{[3]}(\tau_1) = c^{[1]}(\tau_1) + c^{[2]}(\tau_1)$, $c^{[3]}(\tau_2) = c^{[1]}(\tau_2) + c^{[2]}(\tau_1)c^{[1]}(\tau_1) + c^{[2]}(\tau_2)$, ...

IIII. B. (ii) ADJOINTS OF GENERAL ONE-STEP METHODS

For the true flow ϕ_h, the inverse mapping ϕ_h^{-1} coincides with ϕ_{-h} (stepping backwards in time).

For a numerical method, if $z = \psi_h(y)$, then y retreived from z by applying, with steplength $-h$, *another* numerical method ψ^*, *the adjoint* of ψ.

Example 1: The adjoint of (forward) Euler is backward Euler:

$$z = y + hf(y), \Rightarrow y = z - hf(z).$$

- The adjoint of the adjoint of ψ is ψ.

- A method is *symmetric or selfadjoint* if $\psi = \psi^*$.

- Symmetric methods are necessarily of even order.

- The adjoint of a product is the product (in reverse order) of the adjoints of the factors.

- The product of a method and its adjoint is symmetric.

Example 2: Symplectic Euler A and B are mutually adjoint. Their product is the (symmetric, 2nd order) Störmer-Verlet.

IIII. B. (iii) EFFECTIVE ORDER (Butcher 1969)

A method ψ is of *effective order* p is a method χ_h exists such that $\Psi = \chi \circ \phi \circ \chi^{-1}$ is of standard order p. The interest lies in cases where the effective order of ψ is $>$ than its (standard) order.

Since $\Psi_h \circ \cdots \circ \Psi_h$ can be written as

$$(\chi_h \circ \phi_h \circ \chi_h^{-1}) \circ \cdots \circ (\chi_h \circ \phi_h \circ \chi_h^{-1}) = \chi_h \circ (\psi_h \circ \cdots \circ \psi_h) \circ \chi_h^{-1},$$

n steps with Ψ are implemented by n steps of ψ, except for a pre/postprocessing applied only once. Hence we obtain effectively order p by implementing a lower order (cheaper) method.

IIII. B. (iiii) B-series (Hairer-Wanner 1974)

Given a real-valued mapping defined in $\emptyset \cup RT$, the corresponding B-series is the formal series

$$c(\emptyset)y + \sum_{\ell=1}^{\infty} h^{\ell} \sum_{\tau \in RT_{\ell}} \frac{1}{\sigma(\tau)} c(\tau) F(\tau)(y).$$

• Each RK methods corresponds to a B-series, whose coefficients are $c(\emptyset) = 1$ and the elementary weights.

• The true flow is a B-series with $c(\emptyset) = 1$ and $c(\tau) = 1/\gamma(\tau)$.

• Other numerical methods, such as Taylor expansion methods, also correspond to B-series.

B-series with $c(\emptyset) = 1$ form a group wrt. composition.

IIII. C. SYMPLECTIC RK ANALYSIS

IIII. C. (i) SYMPLECTICNESS CONDITION

Th. (Lasagni 1988/SS 1988/Suris 1988) Relations

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad 1 \leq i, j \leq s,$$

guarantee symplectiness of ψ_h if DE are Hamiltonian.

Proof. Originally by explicitly checking that Jacobian of ψ is a symplectic matrix $A^T J A = J$.

The condition is essentially also necessary (Lasagni).

A better approach (Calvo-SS 1994) is first to investigate when a general B-series is formally symplectic. It turns out that this happens if and only if for all pairs of rooted trees u, v,

$$c(u \circ v) + c(v \circ u) = c(u)c(v).$$

If the B-series stems from an RK method then this condition holds if and only if

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad 1 \leq i, j \leq s, .$$

Result applicable to methods, other than RK, that originate B-series.

IIII. C. (ii) SYMPLECTICNESS CONDITIONS ARE SIMPLIFYING ASSUMPTIONS (SS-Abia 1991)

A B-series if of order $\geq p$ if and only if for all rooted trees with $\leq p$ vertices, $c(\tau) = 1/\gamma(\tau)$. Now

$$\frac{1}{\gamma(u \circ v)} + \frac{1}{\gamma(v \circ u)} = \frac{1}{\gamma(u)} \frac{1}{\gamma(v)}.$$

because true solution flow is symplectic. If B-series is also symplectic

$$c(u \circ v) + c(v \circ u) = c(u)c(v),$$

and order condition for $u \circ v$ and $v \circ u$ are equivalent if order conditions for smaller trees u and v hold.

Hence for symplectic RK methods there is one order condition for *nonsuperflous free tree*:

IIII. D. BACKWARD ERROR ANALYSIS

IIII. D. (i) CONCEPT

What is the error when 1.4 is given as an answer for $\sqrt{2}$?

• $-0.0142 \simeq 1.4 - \sqrt{2}$ measures the difference between our answer and the true answer. *Forward error analysis.*

• $-0.040 \simeq 1.4^2 - 2$ measures the difference between the problem we have solved and the one we would have liked solved. *Bacward error analysis.*

IIII. D. (ii) MODIFIED EQUATIONS

(Warming-Hyett 1974, Griffiths-SS 1986)

Example: $dy/dt = f(y) = \lambda y$, $y(0) = \alpha \in \mathbb{R}$, solved by Euler's $y_{n+1} = (1 + h\lambda)y_n$.

- First order:

$$\psi_{h,f}(y) - \phi_{h,f}(y) = (1 + h\lambda)y - \exp(h\lambda) = -\frac{(h\lambda)^2}{2}y + O(h^3).$$

- But, wrt. $dy/dt = \tilde{f}_h(y) = (\lambda - (h\lambda^2)/2)y$:

$$\psi_{h,f}(y) - \phi_{h,\tilde{f}_h}(y) = O(h^3),$$

with consistency of the second order.

Graphic of preceding one

• In general, given numerical method and DE $dy/dt = f(y)$, it is possible, for each $N = 1, 2, \ldots$, to construct vector fields $\tilde{f}_h^N$ such that $\psi_{h,f} - \phi_{h,\tilde{f}_h^N} = O(h^{N+1})$.

• $\tilde{f}_h^N$ can be chosen to be of the form $\tilde{f}_h^N(y) = f^0 + hf^1(y) + \cdots + h^N f^N(y)$.

• The series $\tilde{f}_h^N(y) = f^0 + hf^1(y) + \cdots$, does not (in general) converge. (Maps are not flows.)

• By suitably truncating the series, one may achieve $\psi_{h,f} - \phi_{h,\tilde{f}_h}$ to be exponentially small, under assumptions of analyticity (Neishtadt 1984).

• For B-series methods, $\tilde{f}_h^N(y) = f^0 + hf^1(y) + \cdots$ is a B-series, whose coefficients can be systematically found (Hairer 1994, Murua 1995).

IIII. D. (iii) THE CASE OF SYMPLECTIC INTEGRATORS

For a Hamiltonian problem, symplectic (resp. non-symplectic) integrators have modified equations that are (resp. are not) Hamiltonian.

Thus, broadly speaking, the effect of using a symplectic method is to perturb the differential equation *within* the class of Hamiltonian problems. For nonsymplectic methods, the perturbation may be small, but is 'unHamiltonian'.

For B-series methods the modified Hamiltonian functions may be explicitly written as a so-called *H-series*, written in terms of free nonsuperfluous trees. (cf. simplifying assumptions).

GRAPHIC OF MOD HAMILTONIAN

78 The interpretation of a step of a symplectic integrator applied to the system with Hamilonian H as (very high order approximation to) the exact flow of a perturbed Hamiltonian $\tilde{H}_h$, leads to many useful results.

- Small errors in energy over exponentially long times.
- Linear error growth for completely integrable and other systems.
- Preservation of KAM tori.
- . . .

IIII. D. (iiii) VARIABLE STEPSIZES

The dependence of $\tilde{H}$ on h, implies that the backward error analysis breaks down whenever h is adjusted along the computation.

Several fixes (Stoffer, Leimkuhler, . . .) of this difficulty have been suggested in the literature.

more variable steps

V. SPLITTING/COMPOSITION METHODS

V. A. SPLITTING METHODS

V. A. (i) THE SIMPLEST SPLITTING METHOD

Consider differential system (not necessarily Hamiltonian)

$$\frac{dy}{dt} = f_1(y) + f_2(y),$$

and assume that each of the systems

$$\frac{dy}{dt} = f_1(y), \quad \frac{dy}{dt} = f_2(y),$$

can be integrated exactly. Then (e.g. Trotter 1959)

$$\psi_h = \phi_{hf_2} \circ \phi_{hf_1}$$

defines a consistent numerical method for the full system.

Example 1. We saw before special systems, $y = (p, q)$,

$$\frac{dy}{dt} = \begin{bmatrix} \frac{dp}{dt} \\ \frac{dq}{dt} \end{bmatrix} = f(y) = \begin{bmatrix} F(q) \\ G(p) \end{bmatrix}.$$

Split

$$f(y) = f_1(y) + f_2(y), \quad f_1(y) = \begin{bmatrix} F(q) \\ 0 \end{bmatrix}, \quad f_2(y) = \begin{bmatrix} 0 \\ G(p) \end{bmatrix}$$

with flows

$$\phi_{h,f_1}(y) = \begin{bmatrix} p + hF(q) \\ q \end{bmatrix}, \quad \phi_{h,f_2}(y) = \begin{bmatrix} p \\ q + hG(p) \end{bmatrix}.$$

Splitting method is Asymmetric Euler (B). If full system is Hamiltonian $H = T(p) + V(q)$, split systems are Hamiltonian for $H_1 = V(q)$, $H_2 = T(p)$, hence symplecticness.

Example 2. Change the roles of p and q, to get Asymmetric Euler A.

Example 3, Three body problem. Three bodies in 3-dimensional space subject to gravitational attraction. Split as:

$$\frac{d}{dt}\begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} = \begin{bmatrix} -Gm_1m_2(q_1-q_2)/r_{12}^3 - Gm_1m_3(q_1-q_3)/r_{12}^3 \\ -Gm_1m_2(q_2-q_1)/r_{12}^3 \\ -Gm_1m_3(q_3-q_1)/r_{12}^3 \\ 0 \\ p_2/m_2 \\ p_3/m_3 \end{bmatrix}$$

(q_1 constant, (p_2, q_2) Kepler, (p_3, q_3) Kepler, p_1 quadrature.)

and

$$\frac{d}{dt}\begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -Gm_1m_2(q_2-q_3)/\|q_2-q_3\|^3 \\ -Gm_1m_3(q_3-q_2)/\|q_3-q_2\|^3 \\ p_1/m_1 \\ 0 \\ 0 \end{bmatrix}$$

(p_1, q_2, q_3 constant, others vary linearly.)

Note this corresponds to splitting $H_1 = T_2 + T_3 + V_{12} + V_{13}$, $H_2 = T_1 + V_{23}$. Hence method is symplectic.

Example 4, Linear/nonlinear splitting. In the Schroedinger problem in one space dimension

$$i\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}u + V(x)u$$

each of the parts

$$i\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}u, \quad i\frac{\partial u}{\partial t} = V(x)u$$

may be exactly solved, the linear part in Fourier space, the nonlinear in physical space.

In general, (simple) splitting:

– Only $p = 1$ (but see later).

+ Cheap to implement.

+ Good geometric properties.

+ Allows numerical use of analytical solutions.

+/– Exploits/requires special structure of problem. (cf. one-size-fits-all).

V. A. (ii) STRANG'S SPLITTING 1963

Given by

$$\psi_h = \phi_{h/2f_2} \circ \phi_{hf_1} \circ \phi_{h/2f_2}.$$

- Now numerical method is selfadjoint and hence second order.

- Can be seen as composition of simple splitting and its adjoint:

$$\begin{aligned} \psi_h &= \left(\phi_{h/2f_2} \circ \phi_{h/2f_1}\right) \circ \left(\phi_{h/2f_1} \circ \phi_{h/2f_2}\right) \\ &= \left(\phi_{h/2f_2} \circ \phi_{h/2f_1}\right) \circ \left(\phi_{h/2f_2} \circ \phi_{h/2f_1}\right)^*. \end{aligned}$$

Example 5. In the context of Example 1 above, Strang splitting yields the Störmer-Verlet method.

V. A. (iii) HIGHER ORDER SPLITTING

More generally consider numerical method

$$\psi_h = \phi_{b_s h f_2} \circ \phi_{a_s h f_1} \circ \cdots \circ \phi_{b_2 h f_2} \circ \phi_{a_2 h f_1} \circ \phi_{b_1 h f_2} \circ \phi_{a_1 h f_1} \circ \phi_{b_0 h f_2}$$

where b_0, . . . , b_2, a_1,. . . , a_s are $2s+1$ free parameters that may be used to boost the order.

No loss of generality in starting and ending with f_2 as choices $b_s = 0$ or $b_0 = 0$ allowed.

- Simple splitting has $b_0 = 0$, $b_1 = a_1 = 1$.

- $b_0 = a_1 = 1$, $b_1 = 0$ gives simple splitting with f_1, f_2 switched.

- Strang has $b_0 = b_1 = 1/2$, $a_1 = 0$ (or $b_0 = b_2 = 0$, $b_1 = 1$, $a_1 = a_2 = 1/2$ if parts are switched).

V. A. (iiii) SPLITTING WITH INEXACT FLOWS

In simple splitting use, rather than exact flows,

$$\psi_h = \psi^{[2]}_{h,f_2} \circ \psi^{[1]}_{h,f_1}$$

where $\psi^{[i]}_{h,f_i}$ is a consistent method for $dy/dt = f_i(y)$.

Example 6, Dimensional splitting. To advance in time, after space discretization, in the twodimensional parabolic problem for $u(x_1, x_2, t)$:

$$\frac{\partial}{\partial t}u = \frac{\partial^2}{\partial x_1^2}\, u + \frac{\partial^2}{\partial x_2^2}\, u \quad + \text{boundary conditions}$$

(or more general) advance first with the problem $\partial u/\partial t = \partial^2 u/\partial x_1^2$, and then with $\partial u/\partial t = \partial^2 u/\partial x_1^2$. Alternating directions.

Strang splitting carries over in the form:

$$\psi_h = \psi^{[2]*}_{h/2,f_2} \circ \psi^{[1]}_{h,f_1} \circ \psi^{[2]}_{h/2,f_2}$$

provided that $\psi^{[1]}_{h,f_1}$ is selfadjoint so as to ensure selfadjointness (and hence second order) of the overall method.

Example 7, Molecular dynamics. Model biomolecule by system of $N >> 1$ classical particles interacting classically with each other. Forces are categorized as (1) those associated with chemical bonds, typically strong, but few, $O(N)$. (2) nonbonded, weaker but many $O(N^2)$.

Split $H_1 = T + V_b$, $H_2 = V_{nb}$. Flow for H_2 available (kick). For H_1 use, e.g. Verlet with small stepsize (multiple time-stepping).

V. B. COMPOSITION METHODS

V. B. (i) COMPOSING A BASIC METHOD WITH ITSELF

Given a method $\psi_h^{[B]}$ (the *basic* method) consider the new method

$$\psi_h = \psi_{\gamma_s h}^{[B]} \circ \cdots \circ \psi_{\gamma_2 h}^{[B]} \circ \psi_{\gamma_1 h}^{[B]}$$

In practice:

• The basic method is of low order, but possesses a geometric property, preserved by compositions.

• One wishes to use the free parameters γ_i so as to boost the order.

Example 8. We saw that symplectic diagonally implicit RK methods are of this form with the midpoint rule as basic method.

Example 9, Creutz/Gocksch 1989, Forest 1989, Suzuki 1990, Yoshida 1900. Assume basic method to be of order p and, choose γ_1, γ_2, γ_3, so as to have

$$\gamma_1 + \gamma_2 + \gamma_3 = 1, \quad \gamma_1^{p+1} + \gamma_2^{p+1} + \gamma_3^{p+1} = 0,$$

(i.e. $\gamma_1 = \gamma_3 = 1 - 2\gamma_2 = 1/[2 - 2^{1/(p+1)}]$). Then new method is of order $p + 1$.

If the basic method is of selfadjoint and of (even) order p, new method is in fact of order $p + 2$.

If the new method is taken as basic for newer one, then order $p + 2$,... Hence methods of arbitrarily high orders exist.

V. B. (ii) COMPOSING A METHOD WITH ITS ADJOINT

If basic method is not selfadjoint the preceding format is not very useful. Rather (McLachlan 1995), consider compositions

$$\psi_h = \psi^{[B]}_{\beta_s h} \circ \psi^{[B]*}_{\alpha_s h} \cdots \circ \psi^{[B]}_{\beta_1 h} \circ \psi^{[B]*}_{\alpha_1 h}$$

of the basic method and its adjoint.

• Clearly this format coincides with that in B. (i) if basic method is selfadjoint.

• High-order splitting methods as in A (iii) also fit in the present format. Just take as basic method here the simplest splitting method.

V. C. ORDER CONDITIONS

V. C. (i) THE APPROACH VIA TREES

Formats of splitting/composition methods contain free parameters. These are to be used to boost the order of the method and optimize the error constants (i.e. the residuals in the order conditions that are not satisfied).

The particular problem envisaged may be important, for instance in the 3 body problem may wish to consider the situation $m_1 >> m_2, m_3$.

A convenient approach based on trees developed by Murua/SS 1999.

V. C. (ii) BCH APPROACH

A more traditional (and more difficult to implement) technique uses the BCH formula. Here presented for composition of a method and its adjoint.

Step 1. Write the modified vector field for the basic method:

$$\tilde{f}_h^{[B]} = f^{(1)}(y) + hf^{(2)}(y) + h^2 f^{(3)}(y) + \cdots$$

(The modified vector field of the adjoint obtained by changing sign of h.) Thus mappings being composed are (formally) replaced by *flows*.

Step 2. Each flow is interpreted as the *exponential* of its Lie operator.

Step 3. The composition of mappings (now turned into a product of exponentials) is written as a single exponential via the BCH formula.

Step 4. The exponential just found is interpreted as a flow of a vector field $\tilde{f}_h$ (i.e. step 2 is undone). Comparison between $\tilde{f}_h$ and the true f yields the order conditions.

V. D. LIE FORMALISM

V. D. (i) LIE OPERATORS

With vector field f we associate the Lie operator L_f acting on real-valued functions F defined on phase space

$$F \mapsto L_f \cdot F, \quad (L_f \cdot F)(y) = f_1(y)\frac{\partial F}{\partial y_1} + \cdots + f_D(y)\frac{\partial F}{\partial y_D}.$$

Thus

$$(L_f \cdot F)(\phi_{t,f}(\alpha) = \frac{d}{dt}F(\phi_{t,f}(\alpha))$$

and

$$(L_f^k \cdot F)(\phi_{t,f}(\alpha) = \frac{d^k}{dt^k}F(\phi_{t,f}(\alpha))$$

Evaluating the derivatives at time $t = 0$, we obtain

$$F(\phi_{t,f}(\alpha)) = \Big(\big(\sum_{k=0}^{\infty} \frac{t^k L_f^k}{k!}\big) \cdot \Big)(\alpha) = (\exp(tL_f) \cdot F)(\alpha).$$

Use with F equal to a coordinate function $y \mapsto y_i$ and find the Taylor expansion of the flow in terms of the Lie operator.

This is the identification between flows and exponentials required in steps 2 and 4.

V. D. (ii) COMMUTATORS

$[L_f, L_g] = L_f L_g - L_g L_f$ *(commutator of* L_f *and* L_g*)* is itself a Lie operator for a third vector field called the Lie bracket $[f, g]$ of the vector fields f and g.

The j-th component of $[f, g]$ is $\sum_i (f_i \partial g_j / \partial y_i - g_i \partial f_j / \partial y_i)$.

If f and g are Hamiltonian (with Ham. functions H and G resp.) so is their Lie bracket. The Hamiltonian function for $[f, g]$ is given by $-\{H, G\}$, with $\{\cdot, \cdot\}$ the Poisson bracket:

$$\{H, G\} = \sum_i \Big(\frac{\partial H}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial G}{\partial q_i} \Big).$$

V. D. (iii) THE BAKER 1898-CAMPBELL 1905-HAUSSDORFF 1906 FORMULA

Combines products of exponentials into a single exponential.

If

$$e^X = I + X + \frac{1}{2}X^2 + \frac{1}{6}X^3 + \cdots, e^Y = I + Y + \frac{1}{2}Y^2 + \frac{1}{6}Y^3 + \cdots$$

$$e^X e^Y = I + X + Y + \frac{1}{2}(X^2 + 2XY + Y^2) + \frac{1}{6}(X^3 + 3X^2Y + \cdots) + \cdots$$

then $\exp(X)\exp(Y) = \exp(Z)$, where

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, [X, Y]] + [Y, [Y, X]]) + \cdots$$