Splitting methods in geometric numerical integration of differential equations

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Based on the paper

Splitting and composition methods in the numerical integration of differential equations

by

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What is *splitting*?

Given the initial value problem

$$x' = f(x), \qquad x_0 = x(0) \in \mathbb{R}^D \tag{1}$$

with $f : \mathbb{R}^D \longrightarrow \mathbb{R}^D$ and solution $\varphi_t(x_0)$, suppose that

$$f = \sum_{i=1}^{m} f^{[i]}, \qquad f^{[i]} : \mathbb{R}^D \longrightarrow \mathbb{R}^D$$

such that

$$x' = f^{[i]}(x), \qquad x_0 = x(0) \in \mathbb{R}^D, \qquad i = 1, \ldots, m \tag{2}$$

can be integrated exactly, with solutions $x(h) = \varphi_h^{[i]}(x_0)$ at $t = h$. Then

$$\chi_h = \varphi_h^{[m]} \circ \cdots \circ \varphi_h^{[2]} \circ \varphi_h^{[1]} \tag{3}$$

verifies $\chi_h(x_0) = \varphi_h(x_0) + \mathcal{O}(h^2)$. First order approximation

What is *splitting*?

- Three steps in splitting:
  1. choosing the set of functions $f^{[i]}$ such that $f = \sum_i f^{[i]}$
  2. solving either exactly or approximately each equation $x' = f^{[i]}(x)$
  3. combining these solutions to construct an approximation for $x' = f(x)$
- Remark: equations $x' = f^{[i]}(x)$ should be simpler to integrate than the original system.

Some advantages of splitting methods

- Simple to implement.
- They are, in general, explicit.
- Their storage requirements are quite modest.
- They preserve structural properties of the exact solution: symplecticity, volume preservation, time-symmetry and conservation of first integrals

Splitting methods constitute an important class of *geometric numerical integrators*

Aim of geometric numerical integration: reproduce the qualitative features of the solution of the differential equation being discretised, in particular its geometric properties.

More on geometric integration

- Properties of the system are built into the numerical method.
- This gives the method an improved qualitative behaviour, but also allows for a significantly more accurate long-time integration than with general-purpose methods.
- Important aspect: theoretical explanation of the relationship between preservation of the geometric properties and the observed favourable error propagation in long-time integration (backward error analysis).

Example 1: symplectic Euler and leapfrog

- Hamiltonian $H(q,p) = T(p) + V(q), \qquad q, p \in \mathbb{R}^d.$
- Equations of motion: $q' = T_p(p), \qquad p' = -V_q(q)$
- Euler method:

$$\begin{aligned} q_{n+1} &= q_n + hT_p(p_n) \\ p_{n+1} &= p_n - hV_q(q_n). \end{aligned} \tag{4}$$

- H is the sum of two Hamiltonians, the first one depending only on p and the second only on q with equations

$$\begin{aligned} q' &= T_p(p) \\ p' &= 0 \end{aligned} \quad \text{and} \quad \begin{aligned} q' &= 0 \\ p' &= -V_q(q) \end{aligned} \tag{5}$$

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Example 1: symplectic Euler and leapfrog

- Solution:

$$\varphi_t^{[T]}: \begin{aligned} q(t) &= q_0 + t\, T_p(p_0) \\ p(t) &= p_0 \end{aligned} \qquad (6)$$

$$\varphi_t^{[V]}: \begin{aligned} q(t) &= q_0 \\ p(t) &= p_0 - t\, V_q(q_0) \end{aligned}$$

- Composing the $t = h$ flows gives the scheme

$$\chi_h \equiv \varphi_h^{[T]} \circ \varphi_h^{[V]}: \begin{aligned} p_{n+1} &= p_n - h\, V_q(q_n) \\ q_{n+1} &= q_n + h\, T_p(p_{n+1}). \end{aligned} \qquad (7)$$

- χ_h is a symplectic integrator, since it is the composition of flows of two Hamiltonians: symplectic Euler method

Example 1: symplectic Euler and leapfrog

- By composing in the opposite order, $\varphi_h^{[V]} \circ \varphi_h^{[T]}$, another first order symplectic Euler scheme:

$$\chi_h^* \equiv \varphi_h^{[V]} \circ \varphi_h^{[T]} : \quad \begin{aligned} q_{n+1} &= q_n + h\, T_p(p_n) \\ p_{n+1} &= p_n - h\, V_q(q_{n+1}). \end{aligned} \tag{8}$$

  (8) is the *adjoint* of χ_h.

- Another possibility: 'symmetric' version

$$\mathcal{S}_h^{[2]} \equiv \varphi_{h/2}^{[V]} \circ \varphi_h^{[T]} \circ \varphi_{h/2}^{[V]}, \tag{9}$$

  Strang splitting, leapfrog or Störmer–Verlet method

- Observe that $\mathcal{S}_h^{[2]} = \chi_{h/2} \circ \chi_{h/2}^*$ and it is also symplectic and second order.

Example 2: Simple harmonic oscillator

- $H(q,p) = \frac{1}{2}(p^2 + q^2)$, where now $q, p \in \mathbb{R}$.
- Equations:

$$x' \equiv \begin{pmatrix} q' \\ p' \end{pmatrix} = \Big[\underbrace{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}}_{A} + \underbrace{\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}}_{B} \Big] \begin{pmatrix} q \\ p \end{pmatrix} = (A+B)\, x.$$

- Euler scheme:

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} 1 & h \\ -h & 1 \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix},$$

- Symplectic Euler method:

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} 1 & h \\ -h & 1-h^2 \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix} = \mathrm{e}^{hB} \mathrm{e}^{hA} \begin{pmatrix} q_n \\ p_n \end{pmatrix}.$$

Example 2: Simple harmonic oscillator

- Both render first order approximations to the exact solution $x(t) = \mathrm{e}^{h(A+B)}x_0$, but there are important differences
- Symplectic Euler is area preserving and

$$\frac{1}{2}(p_{n+1}^2 + hp_{n+1}q_{n+1} + q_{n+1}^2) = \frac{1}{2}(p_n^2 + hp_nq_n + q_n^2).$$

- Symplectic Euler *is* the exact solution at $t = h$ of the *perturbed* Hamiltonian system

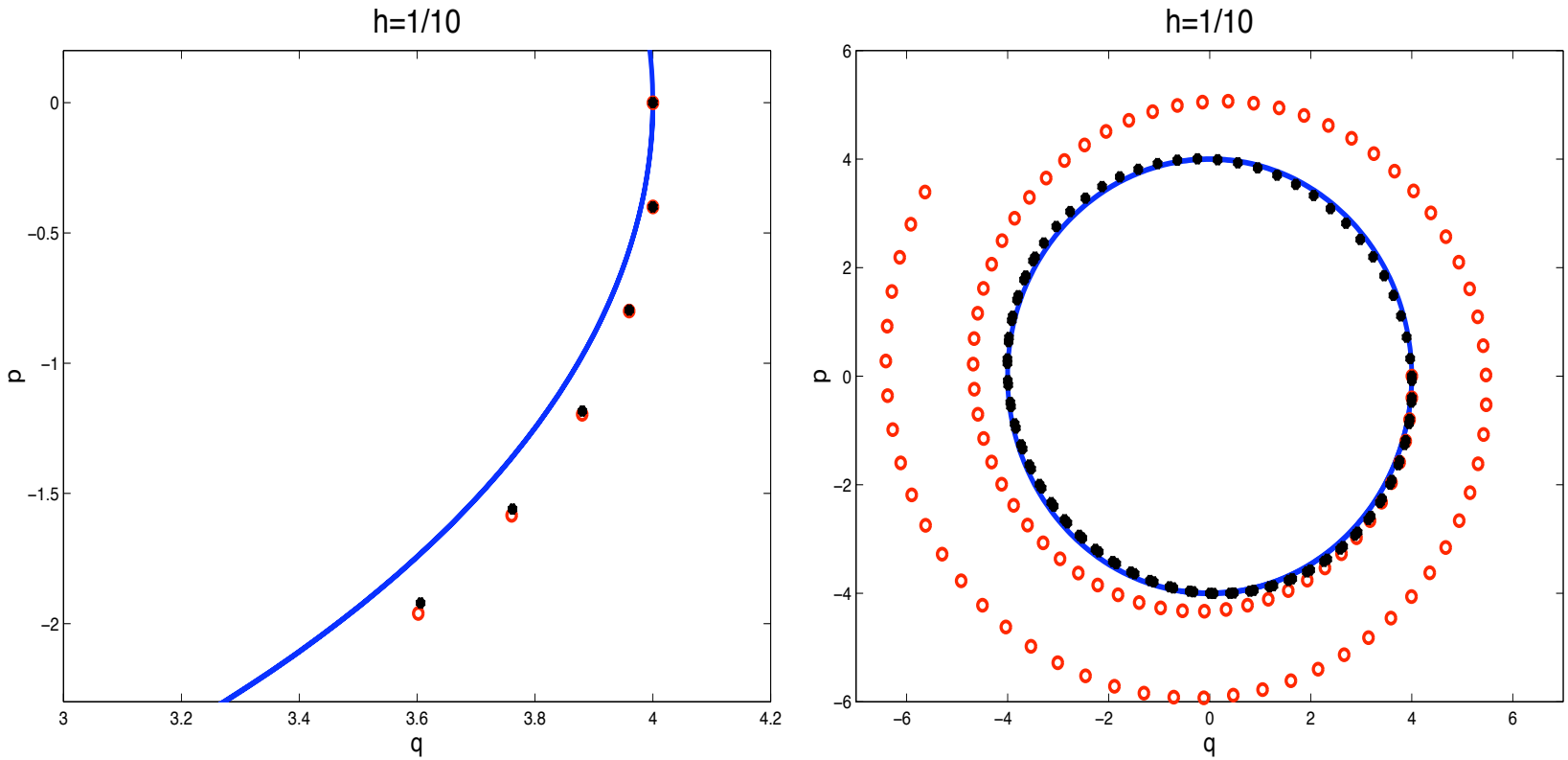
$$\begin{aligned} \tilde{H}(q,p,h) &= \frac{2\arcsin(h/2)}{h\sqrt{4-h^2}}(p^2 + h\,p\,q + q^2) \qquad (10) \\ &= \frac{1}{2}(p^2+q^2) + h\left(\frac{1}{2}\,p\,q + \frac{1}{12}h(p^2+q^2) + \cdots\right). \end{aligned}$$

Example 2: Simple harmonic oscillator

How these features manifest in practice?

- Initial conditions $(q_0, p_0) = (4, 0)$ and integrate with a time step $h = 0.1$ (same computational cost) with Euler and symplectic Euler
- Two experiments:
  1. Represent the first 5 numerical approximations
  2. Represent the first 100 points in the trajectory

Example 2: Simple harmonic oscillator



Euler method (white circles) and the symplectic Euler method (black circles) with initial condition $(q_0, p_0) = (4, 0)$ and $h = 0.1$.

Example 3: The 2-body (Kepler) problem

- Hamiltonian

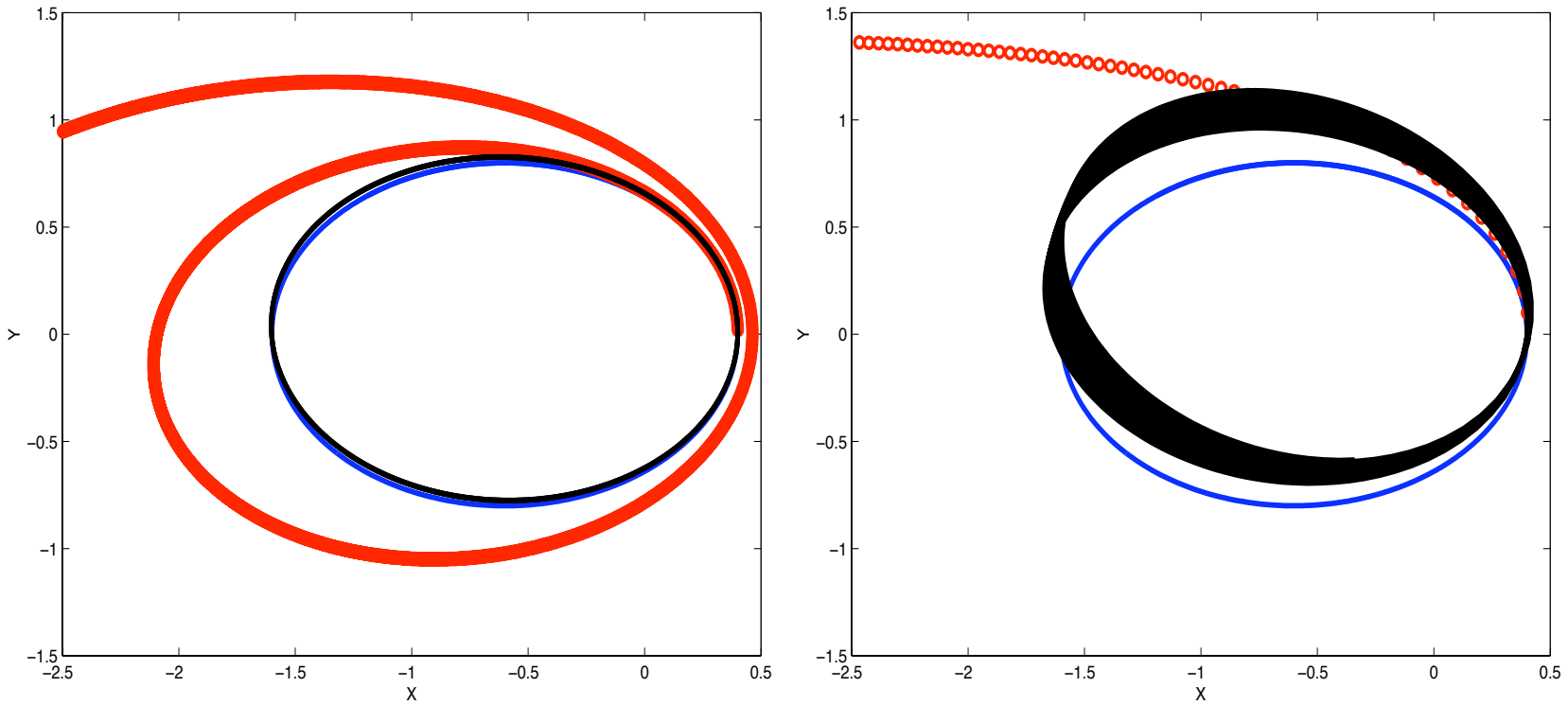
$$H(q,p) = T(p) + V(q) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{r}, \qquad r = \sqrt{q_1^2 + q_2^2}.$$

- Initial condition:

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}},$$

  $0 \leq e < 1$ is the eccentricity of the orbit.
- Total energy $H = H_0 = -1/2$, period of the solution is 2π.
- Two experiments with $e = 0.6$. We compare Euler and symplectic Euler

Example 3: The 2-body (Kepler) problem



The left panel shows the results for $h = \frac{1}{100}$ and the first 3 periods and the right panel shows the results for $h = \frac{1}{20}$ and the first 15 periods.

Explanation

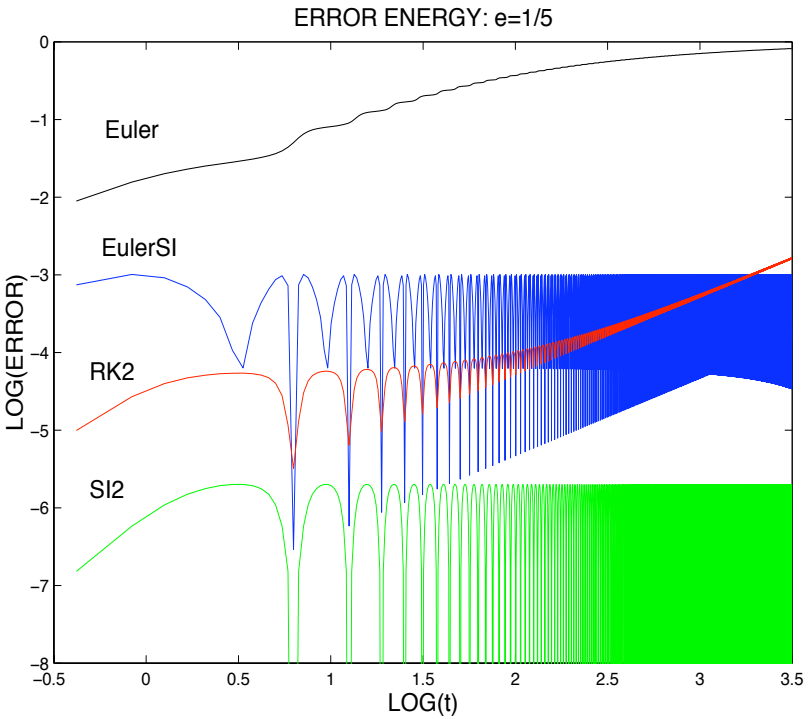
- Several symmetries: H, $L = q_1 p_2 - q_2 p_1$, etc. integrals of motion.
- Symmetry group: $\mathrm{SO}(4)$ (Laplace–Runge–Lenz vector preserved).
- Symplectic Euler method exactly conserves the angular momentum.
- Numerical solution is the exact solution of a slightly perturbed Kepler problem, $\mathrm{SO}(4)$ is no longer the symmetry group and the trajectories are not closed.

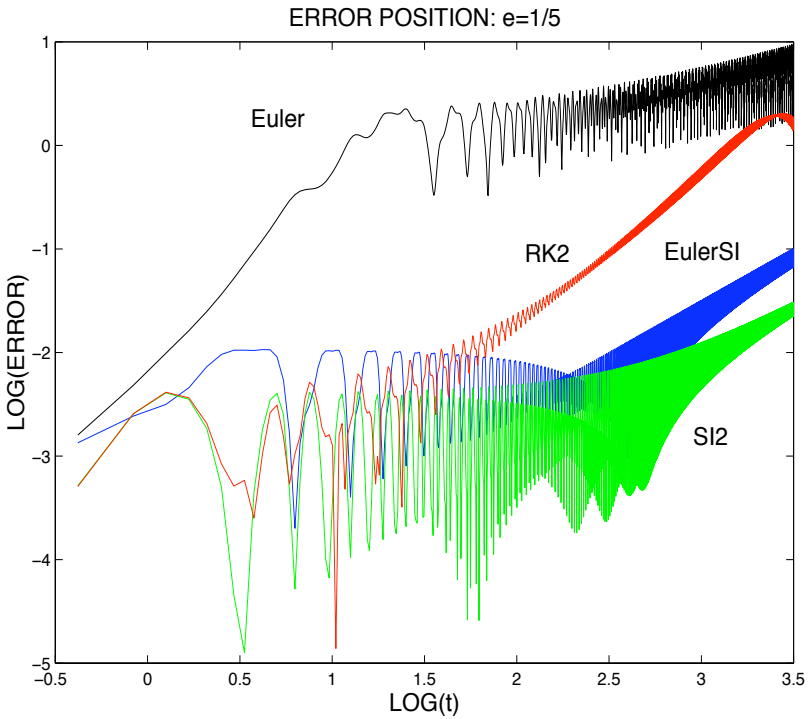
Again, backward error analysis.

Example 3: The 2-body (Kepler) problem

- Next we check how the error in the preservation of energy and the global error in position propagates with time.
- Methods: Euler, symplectic Euler, Heun (RK2), leapfrog (SI2)
- Step size chosen so that all the methods require the same number of force evaluations
- $e = 1/5$ and integrate for 500 periods

Example 3: The 2-body (Kepler) problem





Average error in energy does not grow for symplectic methods and the error in positions grows only linearly with time, in contrast with Euler and Heun schemes.

More examples

- Hamiltonian systems
- Poisson systems
- Lotka–Volterra eqs., ABC-flow, Duffing oscillator (‘conformal Hamiltonian’)
- PDEs discretized in space (Schrödinger eq., Maxwell equations)

coming from

- Celestial Mechanics
- Molecular dynamics
- Quantum physics
- Electromagnetism
- Particle accelerators

Conclusions (until now)

- Symplectic Euler and leapfrog provide a good qualitative description including preservation of invariants and structures in phase space.
- Favourable error propagation in long-time integration
- ... although the order of accuracy is very low
- Examples of geometric numerical integrators

Question: is it possible to build higher order schemes within this class?
YES!

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Yoshida–Suzuki technique

From leapfrog $\mathcal{S}^{[2]} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ (2nd order) one gets a 4th order integrator $\mathcal{S}^{[4]} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ as

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]}, \quad \text{with} \quad \alpha = \frac{1}{2 - 2^{1/3}}, \qquad \beta = 1 - 2\alpha. \tag{11}$$

In general,

$$\mathcal{S}_h^{[2k+2]} = \mathcal{S}_{\alpha h}^{[2k]} \circ \mathcal{S}_{\beta h}^{[2k]} \circ \mathcal{S}_{\alpha h}^{[2k]}, \tag{12}$$

with

$$\alpha = \frac{1}{2 - 2^{1/(2k+1)}}, \qquad \beta = 1 - 2\alpha, \tag{13}$$

gives a method $\mathcal{S}_h^{[2k]}$ of order $2k$ ($k \geq 1$).

Yoshida–Suzuki technique

This technique can be applied to

$$x' = f(x) \quad \text{with} \quad f(x) = \sum_{i=1}^{m} f^{[i]}(x)$$

starting from the basic first order integrator

$$\chi_h = \varphi_h^{[m]} \circ \cdots \circ \varphi_h^{[2]} \circ \varphi_h^{[1]}, \tag{14}$$

its adjoint

$$\chi_h^* = \chi_{-h}^{-1} = \varphi_h^{[1]} \circ \varphi_h^{[2]} \circ \cdots \circ \varphi_h^{[m]}$$

and finally

$$\mathcal{S}_h^{[2]} = \chi_{h/2} \circ \chi_{h/2}^* \tag{15}$$

More general compositions

- More efficient schemes:

$$\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h} \tag{16}$$

with appropriately chosen coefficients $(\alpha_1, \ldots, \alpha_{2s}) \in \mathbb{R}^{2s}$.

- When $f = f^{[a]} + f^{[b]}$ and $\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$, then (16) can be rewritten as

$$\psi_h = \varphi^{[b]}_{b_{s+1}h} \circ \varphi^{[a]}_{a_s h} \circ \varphi^{[b]}_{b_s h} \circ \cdots \circ \varphi^{[b]}_{b_2 h} \circ \varphi^{[a]}_{a_1 h} \circ \varphi^{[b]}_{b_1 h}, \tag{17}$$

where $b_1 = \alpha_1$ and for $j = 1, \ldots, s$,

$$a_j = \alpha_{2j-1} + \alpha_{2j}, \qquad b_{j+1} = \alpha_{2j} + \alpha_{2j+1} \tag{18}$$

(with $\alpha_{2s+1} = 0$). Conversely, any integrator of the form (17) satisfying $\sum_{i=1}^{s} a_i = \sum_{i=1}^{s+1} b_i$ can be expressed as (16) with $\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$.

Mathematical formalism

- Given the ODE $x' = f(x)$ one has the vector field F such that, for each function g

$$F[g](x) = \sum_{j=1}^{D} f_j(x) \frac{\partial g}{\partial x_j}(x). \tag{19}$$

- If φ_h is the h-flow of the ODE, then

$$g(\varphi_h(x)) = \exp(hF)[g](x) = g(x) + \sum_{k \geq 1} \frac{h^k}{k!} F^k[g](x), \qquad x \in \mathbb{R}^D,$$

- A one-step numerical integrator for a time step h, $\psi_h : \mathbb{R}^D \longrightarrow \mathbb{R}^D$, is said to be of order r if

$$\psi_h = \varphi_h + \mathcal{O}(h^{r+1}) \quad \text{as} \quad h \to 0.$$

Mathematical formalism

- Analogously, for a basic integrator $\chi_h : \mathbb{R}^D \to \mathbb{R}^D$, we consider the linear differential operators X_n ($n \geq 1$) acting as

$$X_n[g](x) = \frac{1}{n!} \frac{d^n}{dh^n} \, g(\chi_h(x))|_{h=0} \, ,$$

so that formally $g(\chi_h(x)) = X(h)[g](x)$, where

$$X(h) = I + \sum_{n \geq 1} h^n X_n,$$

- Alternatively, one may consider the series of vector fields

$$Y(h) = \sum_{n \geq 1} h^n Y_n = \log(X(h))$$

that is,

$$Y_n = \sum_{m \geq 1}^{n} \frac{(-1)^{m+1}}{m} \sum_{j_1 + \cdots + j_m = n} X_{j_1} \cdots X_{j_m},$$

so that $X(h) = \exp(Y(h))$, and $g(\chi_h(x)) = \exp(Y(h))[g](x)$. The basic integrator is of order r if

$$Y_1 = F, \qquad Y_n = 0 \quad \text{for} \quad 2 \leq n \leq r.$$

- For $\chi_h^* = \chi_{-h}^{-1}$, one gets $g(\chi_h^*(x)) = \mathrm{e}^{-Y(-h)}[g](x)$. Thus, χ_h is time-symmetric if and only if $Y(h) = hY_1 + h^3 Y_3 + \cdots$, and time-symmetric methods are of even order.

Series of differential operators

- In the general case, for the composition method

$$\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h}$$

one has $g(\psi_h(x)) = \Psi(h)[g](x)$, where $\Psi(h) = I + h\Psi_1 + h^2\Psi_2 + \cdots$ is a series of differential operators satisfying

$$\Psi(h) = X(-\alpha_1 h)^{-1} X(\alpha_2 h) \cdots X(-\alpha_{2s-1} h)^{-1} X(\alpha_{2s} h),$$

the series $X(h)$ is associated with χ_h and $X(h)^{-1}$ to χ^*_h.

- Alternatively, we may use

$$\Psi(h) = \mathrm{e}^{-Y(-h\alpha_1)}\, \mathrm{e}^{Y(h\alpha_2)} \cdots \mathrm{e}^{-Y(-h\alpha_{2s-1})}\, \mathrm{e}^{Y(h\alpha_{2s})}, \qquad (20)$$

to obtain $\log(\Psi(h)) = \sum_{n\geq 1} h^n F_n$, so that rth order compositions methods obey the conditions

$$F_1 = F, \qquad F_n = 0 \quad \text{for} \quad 2 \leq n \leq r. \qquad (21)$$

- For the splitting integrator

$$\psi_h = \varphi^{[b]}_{b_{s+1}h} \circ \varphi^{[a]}_{a_s h} \circ \varphi^{[b]}_{b_s h} \circ \cdots \circ \varphi^{[b]}_{b_2 h} \circ \varphi^{[a]}_{a_1 h} \circ \varphi^{[b]}_{b_1 h},$$

when $f(x) = f^{[a]}(x) + f^{[b]}(x)$, the series $\Psi(h)$ of differential operators associated to the integrator ψ_h is

$$\Psi(h) = \mathrm{e}^{b_1 h F^{[b]}} \, \mathrm{e}^{a_1 h F^{[a]}} \cdots \mathrm{e}^{b_s h F^{[b]}} \, \mathrm{e}^{a_s h F^{[a]}} \, \mathrm{e}^{b_{s+1} h F^{[b]}} \tag{22}$$

in terms of the Lie derivatives $F^{[a]}$ and $F^{[b]}$

Order conditions

- Polynomial equations whose solutions provide the coefficients in

$$\begin{aligned}\psi_h &= \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h} \\ \psi_h &= \varphi^{[b]}_{b_{s+1}h} \circ \varphi^{[a]}_{a_s h} \circ \varphi^{[b]}_{b_s h} \circ \cdots \circ \varphi^{[b]}_{b_2 h} \circ \varphi^{[a]}_{a_1 h} \circ \varphi^{[b]}_{b_1 h}\end{aligned}$$

- Several procedures to obtain them (rooted trees, BCH formula, Lyndon words)
- BCH:

$$Z = \log(\mathrm{e}^X \mathrm{e}^Y) = X + Y + \sum_{m=2}^{\infty} Z_m, \qquad (23)$$

Procedure

1. Consider Ψ_h, expressed as a product of exponentials of differential operators, i.e.,

$$\begin{aligned} \Psi(h) &= \mathrm{e}^{-Y(-h\alpha_1)}\,\mathrm{e}^{Y(h\alpha_2)}\cdots\mathrm{e}^{-Y(-h\alpha_{2s-1})}\,\mathrm{e}^{Y(h\alpha_{2s})}, \\ \Psi(h) &= \mathrm{e}^{b_1 hF^{[b]}}\,\mathrm{e}^{a_1 hF^{[a]}}\cdots\mathrm{e}^{b_s hF^{[b]}}\,\mathrm{e}^{a_s hF^{[a]}}\,\mathrm{e}^{b_{s+1} hF^{[b]}} \end{aligned}$$

2. Apply repeatedly the BCH formula to get the series expansion $\log(\Psi(h)) = \sum_{n\geq 1} h^n F_n$
3. Impose conditions $F_1 = F, \quad F_k = 0$ for $2 \leq k \leq r$.

For the composition $\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h}$ we get

$$\begin{aligned}\log(\Psi(h)) &= hw_1 Y_1 + h^2 w_2 Y_2 + h^3(w_3 Y_3 + w_{12}[Y_1, Y_2]) \\ &\quad + h^4(w_4 Y_4 + w_{13}[Y_1, Y_3] + w_{112}[Y_1, [Y_1, Y_2]]) + \mathcal{O}(h^5)\end{aligned}$$

$w_{j_1 \cdots j_m}$ are polynomials of degree $n = j_1 + \cdots + j_m$ in the parameters $\alpha_1, \ldots, \alpha_{2s}$:

$$w_1 = \sum_{i=1}^{2s} \alpha_i, \qquad w_2 = \sum_{i=1}^{2s} (-1)^i \alpha_i^2, \qquad w_3 = \sum_{i=1}^{2s} \alpha_i^3. \tag{24}$$

Order conditions are $w_1 = 1$, and $w_{j_1 \cdots j_m} = 0$ whenever $2 \leq j_1 + \cdots + j_m \leq r$

For the splitting scheme $\psi_h = \varphi^{[b]}_{b_{s+1}h} \circ \varphi^{[a]}_{a_s h} \circ \varphi^{[b]}_{b_s h} \circ \cdots \circ \varphi^{[b]}_{b_2 h} \circ \varphi^{[a]}_{a_1 h} \circ \varphi^{[b]}_{b_1 h}$ one gets analogous results

Order conditions for composition methods with symmetry

- Order conditions for $\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h}$ are simplified if

$$\alpha_{2s-j+1} = \alpha_j, \qquad \text{for all } j.$$

  Then the method is time-symmetric: $\psi^*_h = \psi_h$.
- Also if

$$\alpha_{2j} = \alpha_{2j-1}, \quad \forall\, j,$$

  one gets simplifications. In that case the scheme can be rewritten as

$$\psi_h = \mathcal{S}^{[2]}_{h\beta_s} \circ \cdots \circ \mathcal{S}^{[2]}_{h\beta_1}, \tag{25}$$

  where $\beta_j = 2\alpha_{2j}$ and $\mathcal{S}^{[2]}_h = \chi_{h/2} \circ \chi^*_{h/2}$.

- Compositions satisfying both assumptions:

$$\psi_h = \mathcal{S}^{[2]}_{h\beta_s} \circ \cdots \circ \mathcal{S}^{[2]}_{h\beta_1},$$

with

$$\beta_j = \beta_{s-j+1}, \quad \forall\, j.$$

Symmetric compositions of symmetric schemes

- Number of order conditions

k	1	2	3	4	5	6	7	8	9	10	11
n_k	1	1	2	3	6	9	18	30	56	99	186
m_k	1	0	1	1	2	2	4	5	8	11	17

Simplifications also occur for systems with special structure, e.g.

- Separable Hamiltonians $H(q,p) = T(p) + V(q)$
- RKN methods $H(q,p) = \frac{1}{2}p^T M p + V(q)$
- Generalized Harmonic Oscillator: $H(q,p) = \frac{1}{2}p^T M p + \frac{1}{2}q^T N q$
- Near-integrable systems: $x' = f^{[a]}(x) + \varepsilon f^{[b]}(x)$, with $|\varepsilon| \ll 1$

Different families

In consequence, different classes of integrators:

- Near-integrable systems: $x' = f^{[a]}(x) + \varepsilon f^{[b]}(x)$. Since $\varepsilon \ll h$, one only cancels error terms with small powers of ε and not all the coefficients at an order h^k (Mclachlan, Laskar-Robutel)
- Runge–Kutta–Nyström like methods. Appropriate for $y'' = g(y)$ and $H(q,p) = \frac{1}{2}p^T M p + V(q)$. In this case $[[[F^{[b]}, F^{[a]}], F^{[b]}], F^{[b]}] = 0$, which leads to additional simplifications. Reduced number of evaluations (Blanes-Moan)

Near-integrable systems

For $x' = f^{[a]}(x) + \varepsilon f^{[b]}(x)$, the splitting technique is well adapted. In this case

$$\Psi(h) = \mathrm{e}^{b_1 h\varepsilon F^{[b]}}\, \mathrm{e}^{a_1 h F^{[a]}} \cdots \mathrm{e}^{b_s h\varepsilon F^{[b]}}\, \mathrm{e}^{a_s h F^{[a]}}\, \mathrm{e}^{b_{s+1} h\varepsilon F^{[b]}}.$$

so that,

$$\begin{aligned}\log(\Psi(h)) \;=\; & h v_a F^{[a]} + \varepsilon(h v_b F^{[b]} + h^2 v_{ab} F^{[ab]} + \\ & h^3 v_{aba} F^{[aba]} + h^4 v_{abaa} F^{[abaa]}) \\ & + \varepsilon^2 (h^3 v_{abb} F^{[abb]} + h^4 v_{abba} F^{[abba]}) + \\ & \varepsilon^3 h^4 v_{abbb} F^{[abbb]} + \mathcal{O}(\varepsilon h^5).\end{aligned}$$

In practical applications $\varepsilon \ll h$, so that one eliminates error terms with small powers of ε. If $v_a = 1 = v_b$, $v_{ab} = v_{aba} = v_{abaa} = v_{abb} = 0$,

$$\log(\Psi(h)) - hF = \mathcal{O}(\varepsilon h^5 + \varepsilon^2 h^4),$$

Runge–Kutta–Nyström methods

- Equation

$$y'' = g(y), \tag{26}$$

is equivalent to $x' = f^{[a]}(x) + f^{[b]}(x)$ with

$$f^{[a]}(y, v) = (v, 0), \qquad f^{[b]}(y, v) = (0, g(y)), \tag{27}$$

- Exact flows are computable:

$$\begin{aligned} \varphi_h^{[a]}(y, v) &= (y + hv, v), \\ \varphi_h^{[b]}(y, v) &= (y, v + hg(y)). \end{aligned} \tag{28}$$

- In addition, $[[[F^{[b]}, F^{[a]}], F^{[b]}], F^{[b]}] = F^{[babb]} = 0$ identically.
- Reduction in the number of order conditions:

k	2	3	4	5	6	7	8	9	10	11
n_k	1	2	3	6	9	18	30	56	99	186
l_k	1	2	2	4	5	10	14	25	39	69

- For $H(p,q) = \frac{1}{2}p^T M p + \frac{1}{2}q^T N q$, only one independent condition to increase the order from $r = 2k-1$ to $r = 2k$, and two to increase the order from $r = 2k$ to $r = 2k+1$.
- One can also use modified potentials to get more efficient methods

Processing

- Idea: to enhance an integrator ψ_h (the *kernel*) with $\pi_h : \mathbb{R}^D \longrightarrow \mathbb{R}^D$ (the *post-processor*) as

$$\hat{\psi}_h = \pi_h \circ \psi_h \circ \pi_h^{-1}.$$

- Application of n steps leads to

$$\hat{\psi}_h^n = \pi_h \circ \psi_h^n \circ \pi_h^{-1},$$

- Advantageous if $\hat{\psi}_h$ is more accurate than ψ_h and the cost of π_h is negligible, since it provides the accuracy of $\hat{\psi}_h$ at the cost of (the least accurate) ψ_h.

Example

- Störmer–Verlet method

$$\begin{aligned}\psi_{h,2} &= \varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]} = \varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_h^{[a]} \circ \varphi_{-h}^{[a]} \circ \varphi_{h/2}^{[a]} \\ &= \varphi_{h/2}^{[a]} \circ \psi_{h,1} \circ \varphi_{-h/2}^{[a]} = \pi_h \circ \psi_{h,1} \circ \pi_h^{-1}\end{aligned}$$

  with $\pi_h = \varphi_{h/2}^{[a]}$.

- Applying the first order method $\psi_{h,1} = \varphi_h^{[b]} \circ \varphi_h^{[a]}$ with processing yields a 2nd order of approximation.

Processing

- Very useful in geometric numerical integration
- ψ_h is of *effective order r* if a post-processor π_h exists for which $\hat{\psi}_h$ is of (conventional) order r, that is,

$$\pi_h \circ \psi_h \circ \pi_h^{-1} = \varphi_h + \mathcal{O}(h^{r+1}).$$

- Many of the order conditions can be satisfied by π_h, so that ψ_h must fulfill a much reduced set of restrictions
- If

$$\psi_h = \varphi^{[b]}_{b_{s+1}h} \circ \varphi^{[a]}_{a_s h} \circ \varphi^{[b]}_{b_s h} \circ \cdots \circ \varphi^{[b]}_{b_2 h} \circ \varphi^{[a]}_{a_1 h} \circ \varphi^{[b]}_{b_1 h}$$

  the number and complexity of the conditions to be verified by a_i, b_i is reduced
- Highly efficient processed methods (reduced number of stages in the kernel)

A collection of splitting and composition methods

- More than 100 different integrators
- Symmetric comp. of symmetric methods. Orders 4-10.
- Compositions

$$\begin{aligned}\psi_h &= \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h} \\ \psi_h &= \varphi^{[b]}_{b_{s+1}h} \circ \varphi^{[a]}_{a_s h} \circ \varphi^{[b]}_{b_s h} \circ \cdots \circ \varphi^{[b]}_{b_2 h} \circ \varphi^{[a]}_{a_1 h} \circ \varphi^{[b]}_{b_1 h}\end{aligned}$$

  Orders 3-6.
- RKN splitting integrators. Order 4-8.
- RKN splitting m. with modified potentials. Orders 3-8.
- Splitting methods for near-integrable systems.
- Also with processing

Preserving properties and BEA

- The treatment done for the linear oscillator can be generalized to *any* nonlinear ODE.
- Recall that each integrator ψ_h has associated a series $\Psi(h) = I + h\Psi_1 + h^2\Psi_2 + \cdots$, and
- $\log(\Psi(h)) = hF_1 + h^2F_2 + \cdots$, so that $F_k[g] = g'(x)f_k(x)$.
- Therefore there exists a modified differential equation (formal series in powers of h),

$$\tilde{x}' = f_h(\tilde{x}) \equiv f(\tilde{x}) + hf_2(\tilde{x}) + h^2 f_3(\tilde{x}) + \cdots \qquad (29)$$

  associated to the integrator ψ_h.
- Then, $x_n = \tilde{x}(t_n)$, with $t_n = nh$.

- To study the long-time behaviour of the numerical integrator we analyze the solutions of (29) viewed as a small perturbation of $x' = f(x)$.
- for symmetric methods, the modified differential equation only contains even powers of h;
- for volume-preserving methods applied to a divergence-free dynamical system, the modified equation is also divergence-free;
- for symplectic methods applied to a Hamiltonian system, the modified differential equation is (locally) Hamiltonian.

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- In the particular case of a symplectic integrator, there exist smooth functions $H_j : \mathbb{R}^{2d} \longrightarrow \mathbb{R}$ for $j = 2, 3, \ldots$, such that $f_j(x) = J\nabla H_j(x)$
- In consequence, there exists a modified Hamiltonian

$$\tilde{H}(q,p) = H(q,p) + hH_2(q,p) + h^2 H_3(q,p) + h^3 H_4(q,p) + \cdots$$

such that

$$q' = \nabla_p \tilde{H}(q,p), \qquad p' = -\nabla_q \tilde{H}(q,p).$$

- If the method is order r, say, then $\tilde{H} = H + h^r H_{r+1} + \cdots$.

Remarks

- The series in (29) does not converge in general.
- One has to give bounds on $f_j(x)$ so as to determine an optimal truncation index and estimate the difference $x_n - \tilde{x}(h)$.
- Rigourous proof that a symplectic method of order r with constant h applied to H verifies that $H(x_n) = H(x_0) + \mathcal{O}(h^r)$ for exponentially long time intervals (Nekhorosev like results).
- The modified differential equation of a numerical scheme depends explicitly on h. Then, a different modified equation each time the step size h is changed.
- Poor long time behavior observed in practice when a symplectic scheme is implemented directly with a standard variable step-size strategy.

Some numerical examples

- System: perturbed Kepler problem with Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{r} - \frac{\varepsilon}{2r^3}\left(1 - \alpha\frac{3q_1^2}{r^2}\right), \qquad (30)$$

- (Dynamics of a satellite in the gravitational field produced by an oblate planet)
- Different families of methods can be tested and compared.

- $H = T(p) + V(q)$. We can use symmetric compositions

$$\psi_h = \mathcal{S}^{[2]}_{h\beta_s} \circ \cdots \circ \mathcal{S}^{[2]}_{h\beta_1},$$

with $\mathcal{S}^{[2]}_h$ the Störmer–Verlet method.

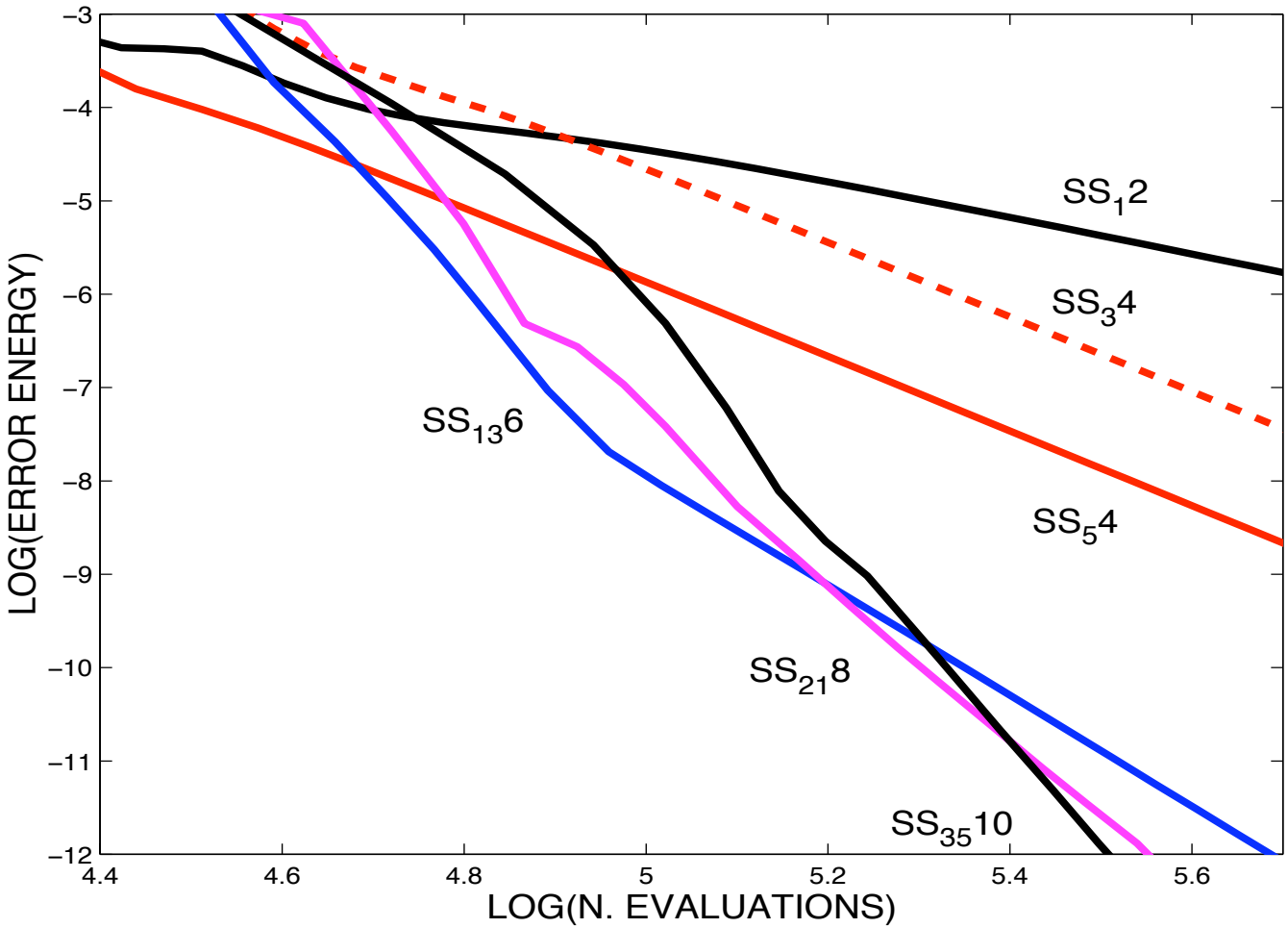
- Also schemes

$$\begin{aligned} \psi_h &= \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h} \\ \psi_h &= \varphi^{[b]}_{b_{s+1}h} \circ \varphi^{[a]}_{a_s h} \circ \varphi^{[b]}_{b_s h} \circ \cdots \circ \varphi^{[b]}_{b_2 h} \circ \varphi^{[a]}_{a_1 h} \circ \varphi^{[b]}_{b_1 h} \end{aligned}$$

- $T(p)$ is quadratic in momenta $\Rightarrow$ RKN methods.
- Finally,

$$H = H_0 + \varepsilon H_I,$$

where H_0 corresponds to the Kepler problem, which is exactly solvable $\Rightarrow$ methods for near-integrable systems.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SS12
SS34
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SS54
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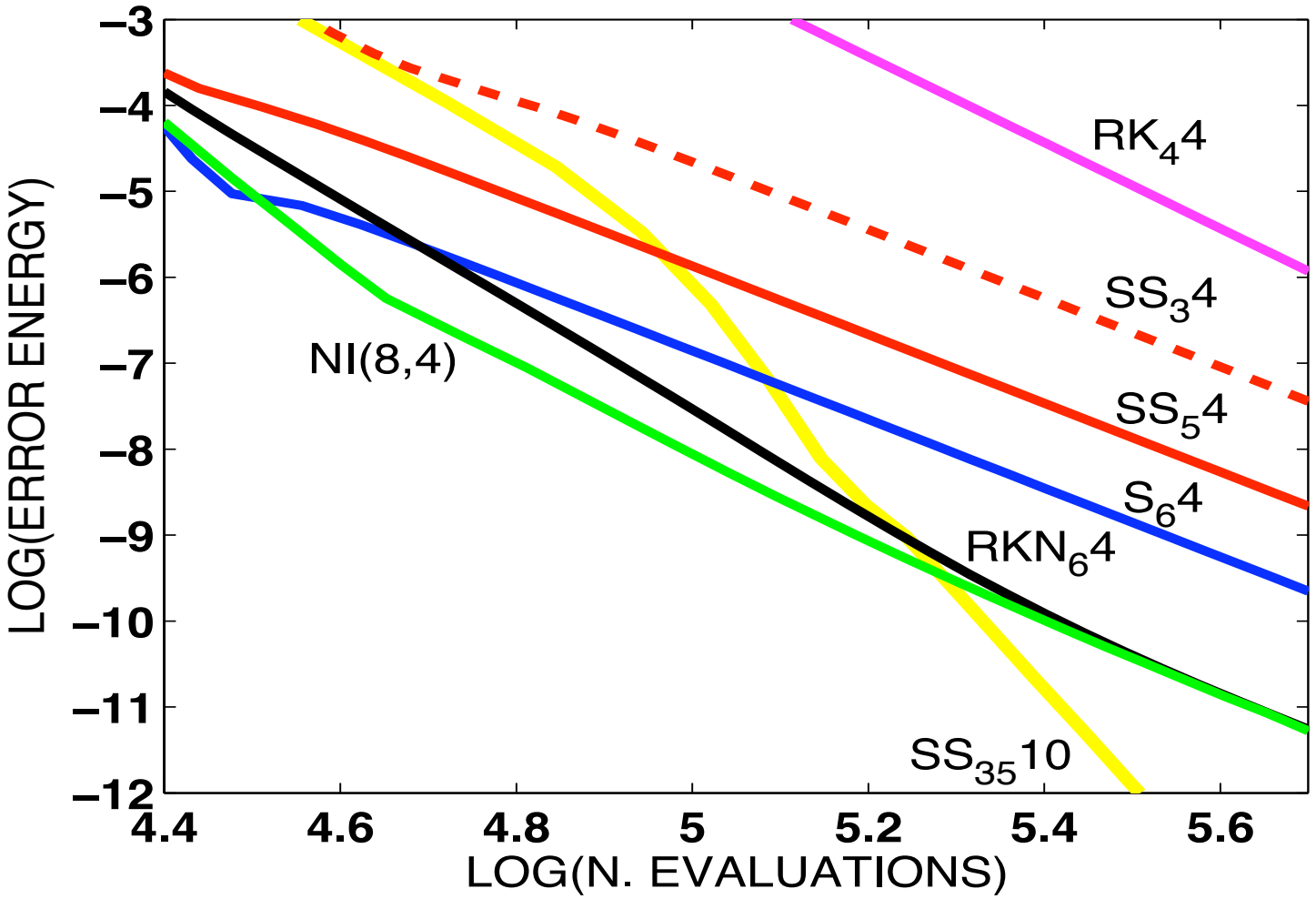
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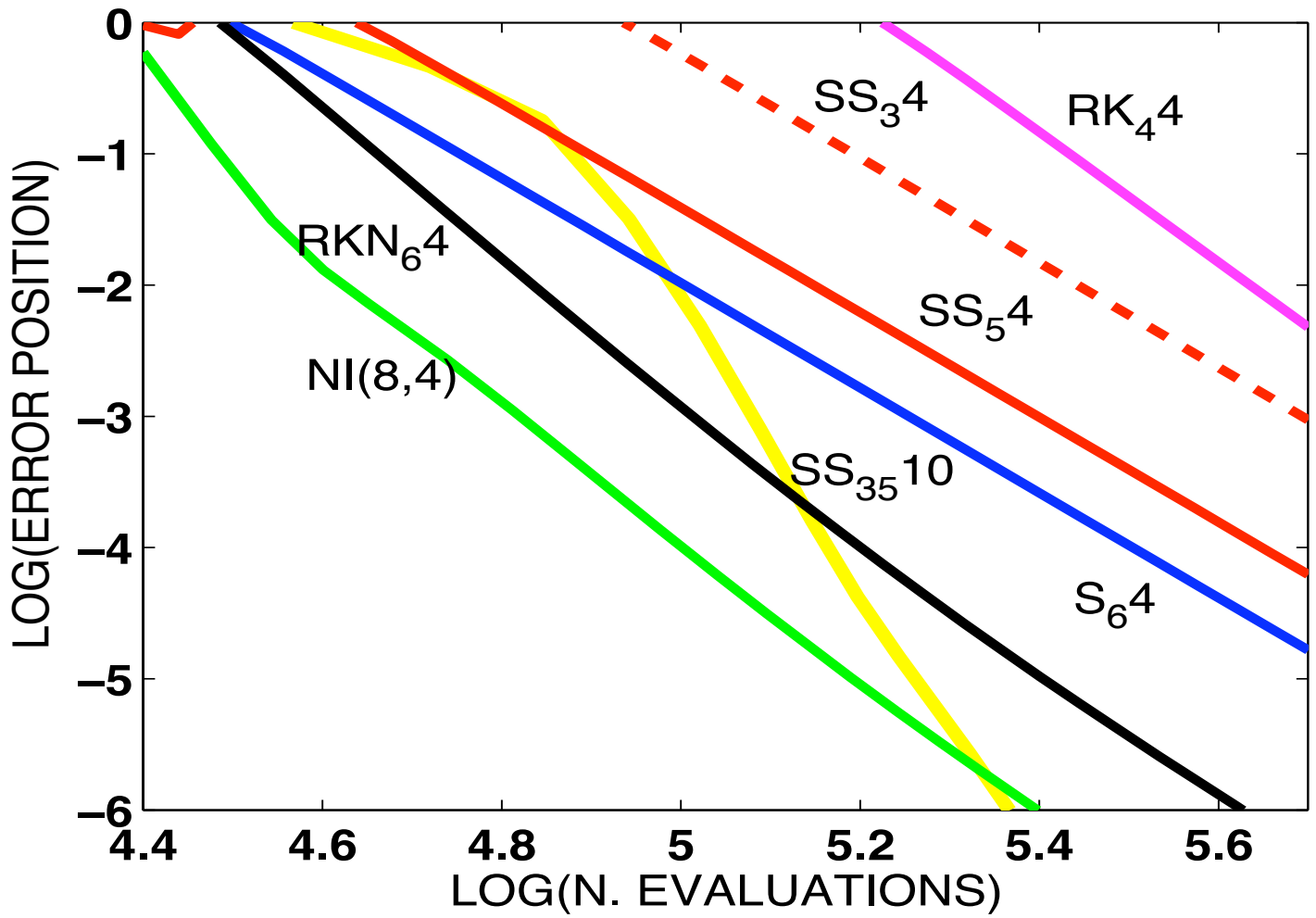
RK4
SS34
SS54
S64
RKN64
NI(8,4)
SS3510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4.6
4.8
5
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5.4
5.6
LOG(ERROR POSITION)
LOG(N. EVALUATIONS)
SS3 4
RK4 4
RKN6 4
SS5 4
NI(8,4)
SS35 10
S6 4

Schrödinger equation

Numerical solution of the time-dependent Schrödinger eq.:

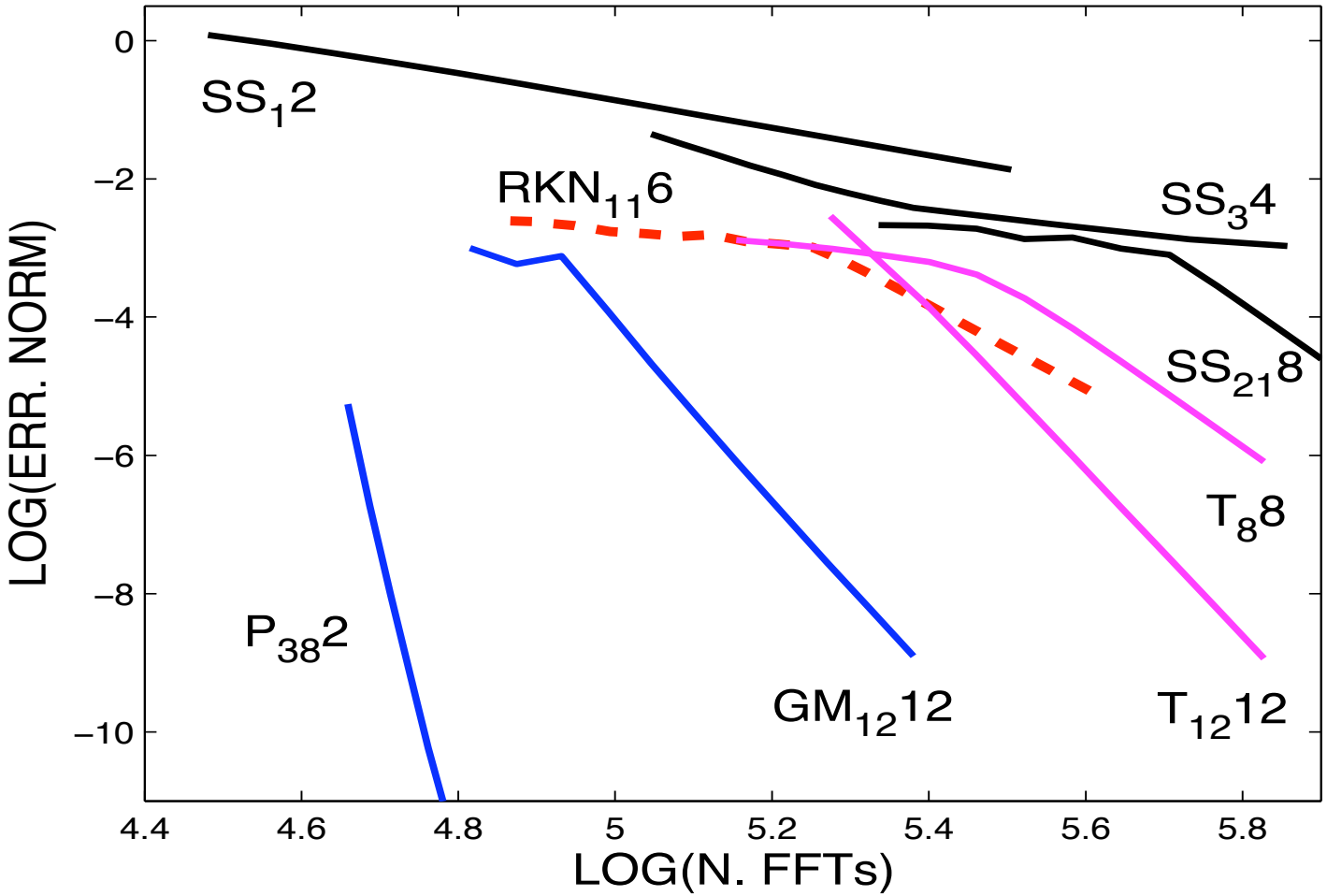
$$i\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{1}{2m}\nabla^2 + V(x,t)\right)\Psi(x,t) \qquad (31)$$

- One-dimensional problem $x \in [x_0, x_N]$ $(\psi(x_0,t) = \psi(x_N,t) = 0$
- Space discretization of $\psi(x,t)$: $[x_0, x_N]$ is split in N parts of length $\Delta x = (x_N - x_0)/N$ and $\mathbf{u} = (u_0, \ldots, u_{N-1})^T \in \mathbb{C}^N$ is formed, with $u_n = \psi(x_n, t)$
- One ends up with a linear problem

$$i\frac{d}{dt}\mathbf{u}(t) = \mathbf{H}\,\mathbf{u}(t), \qquad \mathbf{u}(0) = \mathbf{u}_0 \in \mathbb{C}^N,$$

Morse potential

- $V(x) = D(1 - \mathrm{e}^{-\alpha x})^2$
- $m = 1745$, $D = 0.2251$, $\alpha = 1.1741$
- $\psi_0(x,t) = \rho \exp(-\beta(x - \bar{x})^2)$, $\beta = \sqrt{Dm\alpha^2/2}$, $\bar{x} = -0.1$, ρ: const.
- $t \in [0, 20T]$, $T = 2\pi/(\alpha\sqrt{2D/m})$
- $x \in [-0.8, 4.32]$, split into $N = 128$ parts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P382
GM12 12
T12 12
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−10
4.4
4.6
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5
5.2
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5.8
LOG(ERR. NORM)
LOG(N. FFTs)

Moral of the tale

- Splitting methods are very flexible: different schemes can be used as basic integrator
- Advice: try to incorporate as much information as possible about your DE into your scheme
- Other issues not treated here: stability, negative coefficients, optimization strategies, highly oscillatory problems, variable step size, ...

Basic references

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- B. Leimkuhler and S. Reich, *Simulating Hamiltonian Dynamics*, Cambridge University Press, Cambridge (2004).
- R.I. McLachlan and R. Quispel, Splitting methods, *Acta Numerica* **11** (2002), pp. 341-434.

Basic references

...And, of course,

- S. Blanes, F.C., and A. Murua, Splitting and composition methods in the numerical integration of differential equations, arXiv:0812.0377 (1 December 2008)