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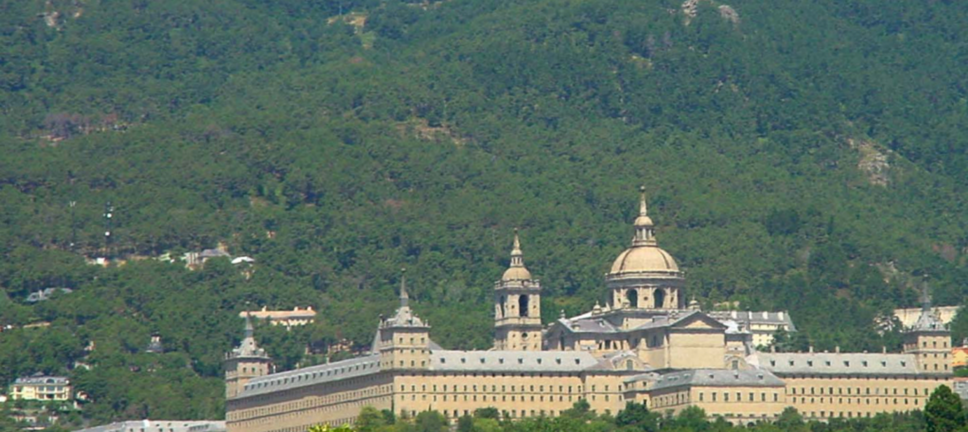

Splitting and composition methods in the numerical integration of differential equations

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... On a paper (to be published in the B. of the SEMA) in collaboration with

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Outline

Basic idea of 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

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

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

Basic idea of splitting

- Problem: how to increase the order of approximation?
- 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 $x' = f(x)$
- Obviously, equations $x' = f^{[i]}(x)$ should be simpler to integrate than the original system.

Basic idea of splitting

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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: explanation of the relationship between preservation of the geometric properties and the observed favourable error propagation in long-time integration

Example 1: symplectic Euler and leapfrog

- Hamiltonian $H(q,p) = T(p) + V(q)$.
- 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

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

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Example 1: symplectic Euler and leapfrog

- Solution:

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

$$\varphi_t^{[V]}: \begin{array}{rcl} q(t) & = & 0 \\ p(t) & = & p_0 - t\,V_q(q_0) \end{array}$$

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

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

- 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:

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

  (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:

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

- 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

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

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

$$\tilde{H}(q, p, h) = \tilde{f}(h) \frac{1}{2}(p^2 + hpq + q^2) \qquad (10)$$

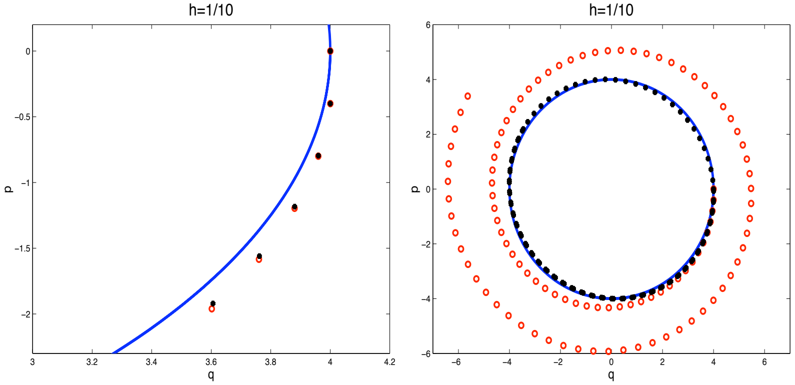
for a certain function $\tilde{f}$.

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

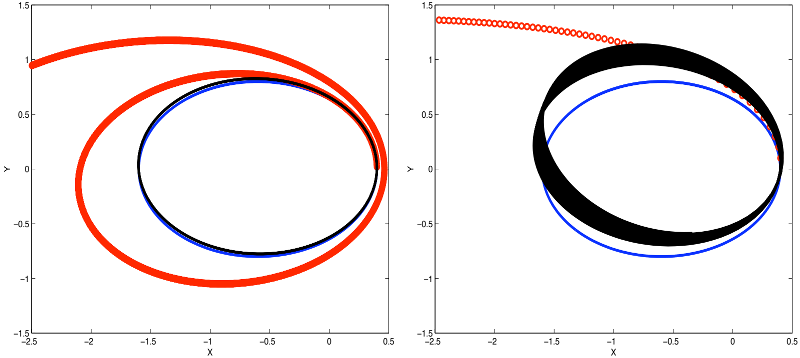
$$H(q,p) = T(p)+V(q) = \frac{1}{2}(p_1^2+p_2^2)-\frac{1}{r}, \qquad r = \sqrt{q_1^2+q_2^2}.$$

- Initial condition:

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

  where $0 \le e < 1$ is the eccentricity of the orbit.
- Total energy is $H = H_0 = -1/2$, the 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

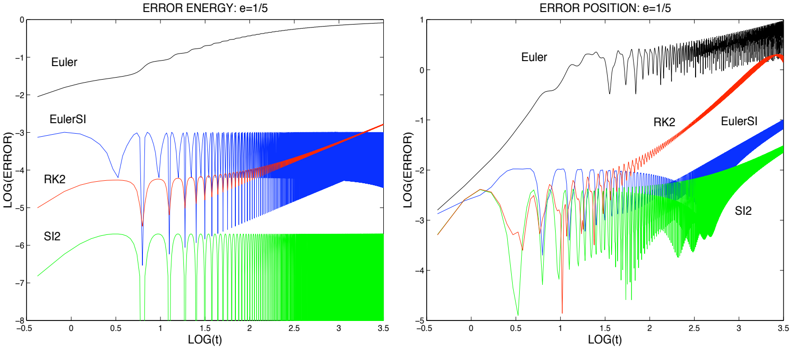


The left panel shows the results for $h = \frac{1}{10}$ and the first 3 periods and the right panel shows the results for $h = \frac{1}{2}$ and the first 15 periods.

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
- More general dynamical systems (Lorenz equations, Lotka–Volterra, ABC-flow)
- PDEs discretized in space (Schrödinger eq., Maxwell equations)

coming from

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

Integrators

- Given the ODE $x' = f(x)$ with vector field
$$F = \sum_{i=1}^{D} f_i(x)\, \frac{\partial}{\partial x_i}, \qquad (11)$$
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
$$\psi_h = \varphi_h + \mathcal{O}(h^{r+1}) \qquad (12)$$
as $h \to 0$, where φ_h is the h-flow of the ODE.
- For each function g
$$g(\varphi_h(x)) = \exp(hF)[g](x) = g(x) + \sum_{k\geq 1} \frac{h^k}{k!} F^k[g](x), \qquad x \in \mathbb{R}^D,$$
where F is the vector field (11).

Series of vector fields

- Assume that

$$g(\psi_h(x)) = g(x) + h\Psi_1[g](x) + h^2\Psi_2[g](x) + \cdots,$$

where each Ψ_k is a linear differential operator and

$$\Psi_h = I + \sum_{k\geq 1} h^k \Psi_k$$

so that formally $g \circ \psi_h = \Psi_h[g]$

- Alternatively, let us consider the series of vector fields $\Psi_h = \exp(F_h)$ with

$$F_h = \sum_{k\geq 1} h^k F_k, \quad \text{with} \quad F_k = \sum_{m\geq 1} \frac{(-1)^{m+1}}{m} \sum_{j_1+\cdots+j_m=k} \Psi_{j_1}\cdots\Psi_{j_m}. \tag{13}$$

Series of vector fields

- The integrator ψ_h can be formally interpreted as the exact 1-flow of the modified vector field F_h.
- Integrator ψ_h is of order r iff

$$F_1 = F, \qquad F_k = 0 \quad \text{for} \quad 2 \leq k \leq r. \tag{14}$$

- These are the order conditions to be verified by ψ_h
- Lie algebra structure inherited from the he Lie algebra structure of the set of vector fields

Composition methods

- Closely related to splitting integrators are composition methods.
- Idea: given a numerical integrator ψ_h (explicit or implicit) of order q, consider a new method $\tilde{\psi}_h$ of the form

$$\tilde{\psi}_h = \psi_{\alpha_s h} \circ \psi_{\alpha_{s-1} h} \circ \cdots \circ \psi_{\alpha_1 h}, \tag{15}$$

with coefficients α_i such that $\tilde{\psi}_h$ has a higher order of accuracy.

Example: Yoshida–Suzuki technique

- ψ_h is a symmetric method of order $2k > 0$. Then

$$\psi^p_{\alpha_1 h} \circ \psi_{\alpha_0 h} \circ \psi^p_{\alpha_1 h} \tag{16}$$

is a symmetric method of order $2k+2$ if

$$\alpha_1 = \frac{1}{2p - (2p)^{1/(2k+1)}}, \qquad \alpha_0 = 1 - 2p\alpha_1. \tag{17}$$

- If $\mathcal{S}_h^{[2]} : \mathbb{R}^D \longrightarrow \mathbb{R}^D$ is the Störmer–Verlet integrator, then

$$\mathcal{S}^{[2]}_{\alpha_1 h} \circ \mathcal{S}^{[2]}_{\alpha_0 h} \circ \mathcal{S}^{[2]}_{\alpha_1 h}, \qquad \text{with} \qquad \alpha_1 = \frac{1}{2 - 2^{1/3}}, \qquad \alpha_0 = 1 - 2\alpha_1 < 0$$

is a 4th-order method with 3 evaluations of $\mathcal{S}_h^{[2]}$. With $p = 2$ $\longrightarrow$ method of order 6 with 9 $\mathcal{S}_h^{[2]}$, and so on.
- Methods of arbitrary order, but with large truncation errors

Example: Yoshida–Suzuki technique

- ψ_h is a symmetric method of order $2k > 0$. Then
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is a symmetric method of order $2k + 2$ if
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- If $\mathcal{S}^{[2]}_h : \mathbb{R}^D \longrightarrow \mathbb{R}^D$ is the Störmer–Verlet integrator, then
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- Methods of arbitrary order, but with large truncation errors

More general compositions

- How to build more efficient schemes by composition?
- By composing

$$\chi_h = \varphi_h^{[m]} \circ \cdots \circ \varphi_h^{[2]} \circ \varphi_h^{[1]} \tag{18}$$

with its adjoint

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

one gets a second order method $\psi_h = \chi_{h/2} \circ \chi_{h/2}^*$

- Idea: find appropriate coefficients $(\alpha_1, \ldots, \alpha_{2s}) \in \mathbb{R}^{2s}$ such that

$$\psi_h = \chi_{\alpha_{2s}h} \circ \chi_{\alpha_{2s-1}h}^* \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi_{\alpha_1 h}^* \tag{19}$$

is of a prescribed order r.

Associated vector field

- For χ_h one has $g(\chi_h(x)) = e^{Y_h}[g](x)$ with $Y_h = \sum_{k\geq 1} h^k Y_k$, so that for $\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h}$

  $$\Psi_h = \exp(-Y_{-h\alpha_1})\exp(Y_{h\alpha_2}) \cdots \exp(-Y_{-h\alpha_{2s-1}})\exp(Y_{h\alpha_{2s}}),$$

  $h^k F_k \in \mathcal{L}_k$ for each $k \geq 1$ and $\mathcal{L} = \bigoplus_{k\geq 1} \mathcal{L}_k$ is the graded Lie algebra generated by the vector fields $\{hY_1, h^2 Y_2, h^3 Y_3, \ldots\}$
- If Ψ_h is of order r when $f = f^{[1]} + f^{[2]}$, then it is also of order r when f is arbitrarily split as $f = f^{[1]} + \cdots + f^{[m]}$ with $m > 2$.
- Ψ_h is also of order r for arbitrary integrators χ_h consistent with the ODE

Splitting and composition

- When the ODE is split in two parts (that is, $m = 2$), ψ_h can be rewritten as

$$\psi_h = \varphi^{[2]}_{b_{s+1}h} \circ \varphi^{[1]}_{a_s h} \circ \varphi^{[2]}_{b_s h} \circ \cdots \circ \varphi^{[2]}_{b_2 h} \circ \varphi^{[1]}_{a_1 h} \circ \varphi^{[2]}_{b_1 h} \qquad (20)$$

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

$$a_j = \alpha_{2j-1} + \alpha_{2j}, \qquad b_{j+1} = \alpha_{2j} + \alpha_{2j+1} \qquad (21)$$

(with $\alpha_{2s+1} = 0$).

- Conversely, any integrator of the form (20) satisfying that $\sum_{i=1}^{s} a_i = \sum_{i=1}^{s+1} b_i$ can be expressed in the form (19) with $\chi_h = \varphi^{[2]}_h \circ \varphi^{[1]}_h$.

Order conditions

- Polynomial equations whose solutions provide the coefficients in $\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h}$
- Several procedures to obtain them (rooted trees, BCH formula)
- BCH:

$$Z = \log(\mathrm{e}^X \, \mathrm{e}^Y) = X + Y + \sum_{m=2}^{\infty} Z_m, \qquad (22)$$

Procedure

1. Consider Ψ_h, expressed as a product of exponentials of vector fields
2. Apply repeatedly the BCH formula to get the exponential of the modified vector field F_h
3. Impose conditions $F_1 = F, \qquad F_k = 0$ for $2 \leq k \leq r$.

In particular,

$$\Psi_h = \exp\left(hf_{1,1}Y_1 + h^2 f_{2,1}Y_2 + h^3 f_{3,1}Y_3 + h^3 f_{3,2}[Y_1, Y_2] + \mathcal{O}(h^4)\right) \tag{23}$$

$$f_{1,1} = \sum_{i=1}^{2s} \alpha_i, \qquad f_{2,1} = \sum_{i=1}^{2s} (-1)^{i+1}\alpha_i^2, \qquad f_{3,1} = \sum_{i=1}^{2s} \alpha_i^3, \qquad \text{etc.} \tag{24}$$

order conditions are $f_{1,1} = 1$, $f_{k,j} = 0$, $k = 2, \ldots, r$.

Order conditions

- These order conditions are also valid for the composition

$$\psi_h = \varphi^{[2]}_{b_{s+1}h} \circ \varphi^{[1]}_{a_s h} \circ \varphi^{[2]}_{b_s h} \circ \cdots \circ \varphi^{[2]}_{b_2 h} \circ \varphi^{[1]}_{a_1 h} \circ \varphi^{[2]}_{b_1 h}$$

- Simplifications occur for systems with additional structure, e.g.
  - $H(q,p) = T(p) + V(q)$
  - $H(q,p) = \frac{1}{2}p^T M p + V(q)$
  - $H(q,p) = \frac{1}{2}p^T M p + \frac{1}{2}q^T N q$
  - $x' = f^{[1]}(x) + \varepsilon f^{[2]}(x)$, with $|\varepsilon| \ll 1$

Different families

In consequence, different classes of integrators:

- Near-integrable systems: $x' = f^{[1]}(x) + \varepsilon f^{[2]}(x)$. 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 $H(q,p) = \frac{1}{2}p^T Mp + V(q)$. In this case $[F^{[2]}, [F^{[2]}, [F^{[2]}, F^{[1]}]]] = 0$, which leads to additional simplifications. Reduced number of evaluations (Blanes-Moan)

Different families

- Methods with modified potentials.
  When $[F^{[2]},[F^{[2]},[F^{[2]},F^{[1]}]]]=0$, in addition to $F^{[1]}$ and $F^{[2]}$, there are other vector fields whose flow is computable, e.g.,

$$F_{3,1}\equiv[F^{[2]},[F^{[1]},F^{[2]}]]=2\sum_{i,j=1}^{l}g_i\frac{\partial g_j}{\partial y_i}\frac{\partial}{\partial v_j}\equiv g^{(3)}(y)\cdot\nabla_v$$

  with flow $\varphi_t^{[3,1]}:\ x(t)=(y_0,v_0+tg^{(3)}(y_0))$
- More:

$$\begin{aligned}F_{5,1}&\equiv[F^{[2]},F^{[2]},F^{[1]},F^{[1]},F^{[2]}],\\F_{7,1}&\equiv[F^{[2]},F^{[1]},F^{[2]},F^{[2]},F^{[1]},F^{[1]},F^{[2]}]\\F_{7,2}&\equiv[F^{[2]},F^{[2]},F^{[2]},F^{[1]},F^{[1]},F^{[1]},F^{[2]}].\end{aligned}$$

Different families

- Idea: to include the flow of

$$C_{b,c,d,e,f} \equiv bF_b + h^2 c\, F_{3,1} + h^4 d\, F_{5,1} + h^6 (eF_{7,1} + fF_{7,2}), \quad (25)$$

instead of $\varphi^{[2]}_{b_i h}$ in the scheme

$$\psi_h = \varphi^{[2]}_{b_{s+1} h} \circ \varphi^{[1]}_{a_s h} \circ \varphi^{[2]}_{b_s h} \circ \cdots \circ \varphi^{[2]}_{b_2 h} \circ \varphi^{[1]}_{a_1 h} \circ \varphi^{[2]}_{b_1 h}$$

- In this way the number of evaluations is much reduced $\Longrightarrow$ more efficient methods

Processing

- Idea: to enhance and 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

$$\begin{aligned}\psi_{h,2} &= \varphi^{[1]}_{h/2} \circ \varphi^{[2]}_{h} \circ \varphi^{[1]}_{h/2} = \varphi^{[1]}_{h/2} \circ \varphi^{[2]}_{h} \circ \varphi^{[1]}_{h} \circ \varphi^{[1]}_{-h} \circ \varphi^{[1]}_{h/2} \\ &= \varphi^{[1]}_{h/2} \circ \psi_{h,1} \circ \varphi^{[1]}_{-h/2} = \pi_h \circ \psi_{h,1} \circ \pi_h^{-1}\end{aligned}$$

  with $\pi_h = \varphi^{[1]}_{h/2}$.

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

Processing

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

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

- The analysis of order conditions of $\hat{\psi}_h$ shows that many of them can be satisfied by π_h, so that ψ_h must fulfill a much reduced set of restrictions
- If

$$\psi_h = \varphi^{[2]}_{b_{s+1}h} \circ \varphi^{[1]}_{a_s h} \circ \varphi^{[2]}_{b_s h} \circ \cdots \circ \varphi^{[2]}_{b_2 h} \circ \varphi^{[1]}_{a_1 h} \circ \varphi^{[2]}_{b_1 h}$$

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

Methods in the literature

- Next we review the literature and collect specific methods of different families
- Number of stages
- Order
- Authors and year

$$\psi_h = \mathcal{S}^{[2]}_{\alpha_k h} \circ \cdots \circ \mathcal{S}^{[2]}_{\alpha_1 h} \circ \mathcal{S}^{[2]}_{\alpha_1 h}$$

Order	4	6	8	10
	3- For-Ru(89)	**7**-Yoshida(90)	**15**-Yoshida(90)	**31**-Suz-Um(93)
	Yos(90),etc.	**9**-McL(95)	Suz-Um(93)	**31-33**-Ka-Li(97)
	5-Suz(90)	Kahan-Li(97)	**15-17**-McL(95)	**33**-Tsitouras(00)
	McL(95)	**11-13**-Sof-Spa(05)	Kahan-Li(97)	**31-35**-Wanner(02)
			19-21-Sof-Spa(05)	**31-35**-Sof-Spa(05)

Processed				
	P**3-17**-McL(02)	P**5-15**	P**9-19**	P**15-25**
			B-Casas-Murua(06)	

Composition method-adjoint / generic splitting

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

Order	3	4	6	8
	3- Ru(84)	**3**-Ru-Yos,etc	**9**-Forest(91)	**27**- ??
		4,5-McL(95)	**10**-B-Moan(02)	
		6-B-Moan(02)		
Processed				
		P**2-7**	P**5-10**	P**14**- ??
		B-Casas-Murua(06)		

$$\psi_h = \varphi^{[2]}_{b_{s+1}h} \circ \varphi^{[1]}_{a_s h} \circ \varphi^{[2]}_{b_s h} \circ \cdots \circ \varphi^{[2]}_{b_2 h} \circ \varphi^{[1]}_{a_1 h} \circ \varphi^{[2]}_{b_1 h}$$

with $[F^{[2]},[F^{[2]},[F^{[2]},F^{[1]}]]] = 0$

Order	4	5	6	8
	3S-Ru-Yos,etc	**5**NABA-Oku-Seel(94)	**7**SABA-For(91)	**16**SABA/BAB-?
	4NAB-McL-At(92)	**6**NAB-McL-At(92)	Oku-Skeel(94)	**17**SABA-Ok-Lu(94)
	4NBAB-Cal-SS(93)	**6**NBAB-Chou-Sha(99)	**7**SBAB-For(91)	**24**SS-Ca-SS(93)
	4,5SABA-McL(95)		**8-15**SABA/BAB	
	5SBAB-B-Moan(01)		**11,14**SBAB-B-M(02)	
	6SABA/BAB-B-Moan(02)			

Processed

P**3,4**	P**4-7**
P**9-11**	B-Casas-Ros(01)

Splitting for linear systems

$$\psi_h = \varphi^{[2]}_{b_{s+1}h} \circ \varphi^{[1]}_{a_s h} \circ \varphi^{[2]}_{b_s h} \circ \cdots \circ \varphi^{[2]}_{b_2 h} \circ \varphi^{[1]}_{a_1 h} \circ \varphi^{[2]}_{b_1 h}$$

with $[F^{[2]},[F^{[2]},[F^{[2]},F^{[1]}]]] = [F^{[1]},[F^{[1]},[F^{[1]},F^{[2]}]]] = 0$

Order	4	6	8	10	12
	4,6	**6**	**8**	**10**	**12**
			Gray-Manolopoulos(96)		
Processed					
	P3,4	P3,4	P4-5	McL-Gray(97)	
	P2-40		**orders: 2-20**		B-Casas-Murua(06)

Specific problem

Numerical solution of the time-dependent Schrödinger eq.:

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{1}{2m}\nabla^2 + V(x,t)\right)\Psi(x,t) \qquad (26)$$

- 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 with

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

Schrödinger equation

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

- $\mathbf{H} \in \mathbb{R}^{N\times N}$
- Solution: $\mathbf{u}(t) = \mathrm{e}^{-it\mathbf{H}}\mathbf{u}_0$
- Exponential is very expensive for large N
- $\mathrm{e}^{-it\mathbf{H}}$ is not only unitary, but also symplectic with $\mathbf{q} = \mathrm{Re}(\mathbf{u})$ and $\mathbf{p} = \mathrm{Im}(\mathbf{u})$
- Equivalent equations: $\mathbf{q}' = \mathbf{H}\,\mathbf{p}, \quad \mathbf{p}' = -\mathbf{H}\,\mathbf{q}$

Schrödinger equation

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

- $\mathbf{H} \in \mathbb{R}^{N\times N}$
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- Equivalent equations: $\mathbf{q}' = \mathbf{H}\,\mathbf{p}, \quad \mathbf{p}' = -\mathbf{H}\,\mathbf{q}$

Schrödinger equation

We may write

$$\frac{d}{dt}\left\{\begin{array}{c}\mathbf{q}\\ \mathbf{p}\end{array}\right\} = \left(\begin{array}{cc}\mathbf{0} & \mathbf{H}\\ -\mathbf{H} & \mathbf{0}\end{array}\right)\left\{\begin{array}{c}\mathbf{q}\\ \mathbf{p}\end{array}\right\} = (\mathbf{A}+\mathbf{B})\left\{\begin{array}{c}\mathbf{q}\\ \mathbf{p}\end{array}\right\},$$

with

$$\mathbf{A} \equiv \left(\begin{array}{cc}\mathbf{0} & \mathbf{H}\\ \mathbf{0} & \mathbf{0}\end{array}\right), \qquad \mathbf{B} \equiv \left(\begin{array}{cc}\mathbf{0} & \mathbf{0}\\ -\mathbf{H} & \mathbf{0}\end{array}\right).$$

Observe that

$$\mathrm{e}^{\mathbf{A}} = \left(\begin{array}{cc}\mathbf{I} & \mathbf{H}\\ \mathbf{0} & \mathbf{I}\end{array}\right), \qquad \mathrm{e}^{\mathbf{B}} = \left(\begin{array}{cc}\mathbf{I} & \mathbf{0}\\ -\mathbf{H} & \mathbf{I}\end{array}\right)$$

Schrödinger equation

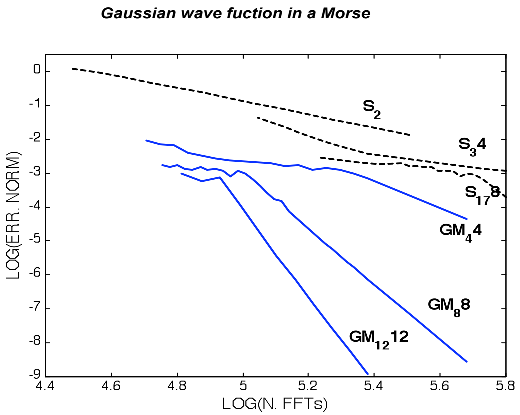
- Spliltting methods of the form

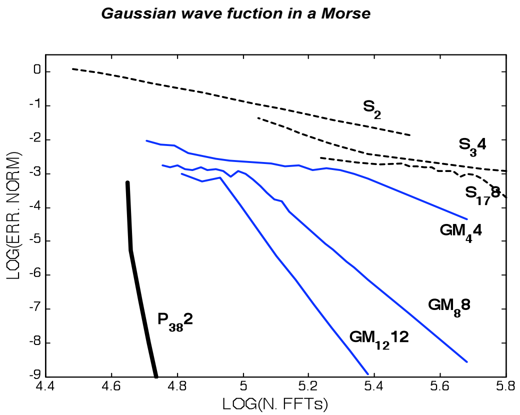
$$\mathbf{O}_n(h) = \mathrm{e}^{hb_{s+1}\mathbf{B}}\,\mathrm{e}^{ha_s\mathbf{A}}\ \cdots\ \mathrm{e}^{hb_2\mathbf{B}}\,\mathrm{e}^{ha_1\mathbf{A}}\,\mathrm{e}^{hb_1\mathbf{B}}. \qquad (27)$$

- Processed methods $\mathbf{S}(h) = \mathbf{P}(h)\,\mathbf{K}(h)\,\mathbf{P}^{-1}(h)$ with $\mathbf{K}(h)$ of type (27) and enlarged stability intervals

Example: 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


Gaussian wave fuction in a Morse
LOG(ERR. NORM)
LOG(N. FFTs)
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
4.4
4.6
4.8
5
5.2
5.4
5.6
5.8
S2
S34
S178
GM44
GM88
GM1212


Gaussian wave fuction in a Morse
LOG(ERR. NORM)
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0
-1
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-9
4.4
4.6
4.8
5
5.2
5.4
5.6
5.8
S2
S34
S178
GM44
GM88
GM1212
P382

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