Splitting methods: analysis and applications — April/May 2017

Project 1. Korteweg–de Vries equation and solitons

1. Show that
$$u(t,x) = 3c\,\mathrm{sech}^2\Big(\tfrac{\sqrt{c}}{2}(x - x_0 - ct)\Big), \qquad \mathrm{sech}\,x = \frac{1}{\cosh x}$$
is a solution of the Korteweg–de Vries (KdV) equation
$$u_t + u_{xxx} + uu_x = 0, \qquad x \in \mathbb{R}.$$
Give an interpretation of the real parameters $c > 0$ and x_0. The above solution is called a *soliton* (solitary wave). What happens for $c \le 0$?

2. Construct the above soliton in the following way.

   (a) Let $\xi = x - ct$ and determine a function $u(t,x) = w(\xi)$ that solves the KdV equation. You will find $w_{\xi\xi\xi} + ww_\xi - cw_\xi = 0$.

   (b) Integrate this equation twice und use that w, w_ξ and $w_{\xi\xi}$ vanish for $x \to \infty$. (After the first integration, you should multiply the resulting equation by the integrating factor w_ξ.) This gives $w_\xi^2 + w^3/3 - cw^2 = 0$.

   (c) The last equation can be integrated by a separation of variables.

3. Solve the KdV equation with periodic boundary conditions on the interval $[0, 2\pi]$ for $0 \le t \le 1$. Use as initial value a soliton with appropriately chosen $c > 0$ and x_0. Employ a spectral discretization (based on FFT) for the linear part and the method of characteristics for the Burgers' nonlinearity. (A similar approach was used for the more complicated Kadomtsev–Petviashvili equation in [1].) Study the error as a function of the time step size τ, the spatial resolution $h = \Delta x$ and the employed interpolation procedure in the method of characteristics.

4. Repeat the above experiment with two solitions and study their interaction. (The initial values of the two solitons must not overlap - why?)

References

[1] L. Einkemmer and A. Ostermann. A splitting approach for the Kadomtsev–Petviashvili equation. *J. Comput. Phys.* 299, 716–730 (2015). `https://arxiv.org/abs/1407.8154`

Project 2. The magnetic Schrödinger equation

Consider Lie splitting for the numerical solution of the initial value problem

$$u_t = (A + B + C)u, \quad u(0) = u_0$$

Split the right-hand side into three terms, for instance in the order BAC, to get

$$u_{n+1} = \mathrm{e}^{\tau C}\mathrm{e}^{\tau A}\mathrm{e}^{\tau B}u_n. \tag{1}$$

1. Summarize the error analysis of this scheme, given in [1].
2. Apply the three-term splitting (1) to the magnetic Schrödinger equation

$$\mathrm{i}\varepsilon u_t = -\frac{\varepsilon^2}{2}\Delta u + \mathrm{i}\varepsilon\mathbf{a}\cdot\nabla u + \frac{1}{2}|\mathbf{a}|^2 u + Vu, \quad u(0) = u_0$$

   with a scalar potential V and divergence-free vector potential $\mathbf{a}$ (both depending on space and time). You will get

$$\begin{aligned} u_t &= Bu = -\frac{\mathrm{i}}{\varepsilon}\left(\frac{1}{2}|\mathbf{a}|^2 + V\right)u, \\ u_t &= Au = \frac{\mathrm{i}\varepsilon}{2}\Delta u, \\ u_t &= Cu = \mathbf{a}\cdot\nabla u, \qquad \nabla\cdot\mathbf{a} = 0. \end{aligned}$$

   Propose efficient numerical schemes for the solution of these subproblems (equidistant discretization in space, periodic boundary conditions). Make a distinction between time invariant and time dependent potentials. In particular, explain how to solve the advection problem with the method of characteristics.
3. In order to use standard FFT techniques, the method of characteristics requires an interpolation procedure, in general. Under which (very restrictive) assumptions, interpolation is not required?

References

[1] M. Caliari, A. Ostermann, and C. Piazzola. A splitting approach for the magnetic Schrödinger equation. To appear in *J. Comput. Appl. Math.* (2016). `https://arxiv.org/abs/1604.08044`

[2] S. Jin and Z. Zhou. A semi-Lagrangian time splitting method for the Schrödinger equation with vector potentials. *Commun. Inf. Syst.*, 13(3):247–289, 2013.

Project 3. Reaction-diffusion splitting

Consider the one-dimensional heat equation

$$u_t(t,x) = u_{xx}(t,x) + f(u(t,x)), \quad u(0,x) = u_0(x),$$

subject to Dirichlet boundary conditions $u(t,0) = b_0(t)$ and $u(t,1) = b_1(t)$.

1. Find the solution of $z_{xx} = 0$ that satisfies the boundary conditions b_0 and b_1 and transform the above problem to homogeneous Dirichlet boundary conditions $\widetilde{u} = u - z$

$$\widetilde{u}_t = \widetilde{u}_{xx} + f(\widetilde{u} + z) - z_t. \tag{1}$$

   Henceforth, we consider
   (i) the *standard splitting* of (1) into

$$\widetilde{v}_t = \widetilde{v}_{xx} - z_t, \quad \widetilde{v}(t,0) = \widetilde{v}(t,1) = 0 \tag{2}$$

   and

$$\widetilde{w}_t = f(\widetilde{w} + z); \tag{3}$$

   (ii) the *modified splitting* of (1) into

$$\widetilde{v}_t = \widetilde{v}_{xx} + f(z) - z_t, \quad \widetilde{v}(t,0) = \widetilde{v}(t,1) = 0 \tag{4}$$

   and

$$\widetilde{w}_t = f(\widetilde{w} + z) - f(z). \tag{5}$$

   The first step of the standard [resp. modified] Stang splitting takes the form:

   (a) Compute the initial value $\widetilde{v}(0) = u_0 - z_0$.
   (b) Compute the solution of (2) [resp. (4)] with initial value $\widetilde{v}(0)$ to obtain $\widetilde{v}(\frac{\tau}{2})$.
   (c) Compute the solution of (3) [resp. (5)] with initial value $\widetilde{w}(0) = \widetilde{v}(\frac{\tau}{2})$ to obtain $\widetilde{w}(\tau)$.
   (d) Compute the solution of (2) [resp. (4)] with initial value $\widetilde{v}(0) = \widetilde{w}(\tau)$ to obtain $\widetilde{v}(\frac{\tau}{2})$.
   (e) Set $u_1 = \widetilde{v}(\frac{\tau}{2}) + z(\tau)$, where $\widetilde{v}(\frac{\tau}{2})$ is taken from step (d).

   Write down the general step of the standard and the modified Strang splitting, respectively. That is, given an approximation u_n to the exact solution at time t_n, find the approximation u_{n+1} to the solution at time $t_{n+1} = t_n + \tau$.

2. Solve the one-dimensional heat equation

$$u_t(t,x) = u_{xx}(t,x) + u(t,x)^2, \qquad 0 \le x \le 1$$

   with initial value $u(0,x) = 1 + \sin^2(\pi x)$ and boundary conditions $b_0(t) = b_1(t) = 1$. For the spatial discretization, choose 500 grid points. Study the order of convergence of the standard and the modified Strang splitting at $t = 0.1$ in different norms (e.g., 1-norm, Euclidian norm and maximum norm).

3. Repeat the above experiment with time dependent $b_0(t) = b_1(t) = 1 + \sin 5t$.

4. Repeat the above experiments for Lie and modified Lie splitting.

References

[1] L. Einkemmer and A. Ostermann. Overcoming order reduction in diffusion-reaction splitting. Part 1: Dirichlet boundary conditions. *SIAM J. Sci. Comput.* 37, A1577–A1592 (2015). https://arxiv.org/abs/1411.0465

Project 4. The Baker–Campbell–Hausdorff formula

For non-commuting matrices A and B the Lie splitting method has a splitting error, i.e., $\mathrm{e}^{A}\mathrm{e}^{B} \neq \mathrm{e}^{A+B}$. The Baker–Campbell–Hausdorff formula (BCH for short) provides a matrix $C(t)$ such that

$$\mathrm{e}^{tA}\mathrm{e}^{tB} = \mathrm{e}^{tC(t)}$$

for sufficiently small t. This is useful for deriving order conditions.

1. Study the BCH formula in [1, Section III.4] and derive the explicit representation of $C(t)$ in terms of A and B up to order three, that is, find matrices C_1, C_2, and C_3 such that

$$C(t) = C_1 + C_2 t + C_3 t^2 + \mathcal{O}(t^3).$$

2. Use this representation to derive the (non-stiff) order conditions for the three-stage splitting

$$S = \mathrm{e}^{\alpha_3 \tau A}\, \mathrm{e}^{\beta_2 \tau B}\, \mathrm{e}^{\alpha_2 \tau A}\, \mathrm{e}^{\beta_1 \tau B}\, \mathrm{e}^{\alpha_1 \tau A},$$

   that is, find conditions on the coefficients α and β such that the splitting error satisfies

$$Su - \mathrm{e}^{\tau(A+B)}u = \mathcal{O}(\tau^{p+1})$$

   for all u. What is the maximal order p of this three-stage splitting?

3. Show that the complex coefficients

$$\alpha_1 = \tfrac{1}{4} + \mathrm{i}\tfrac{\sqrt{3}}{12}, \quad \alpha_2 = \tfrac{1}{2}, \quad \alpha_3 = \tfrac{1}{4} - \mathrm{i}\tfrac{\sqrt{3}}{12}, \quad \beta_1 = \tfrac{1}{2} + \mathrm{i}\tfrac{\sqrt{3}}{6}, \quad \beta_2 = \tfrac{1}{2} - \mathrm{i}\tfrac{\sqrt{3}}{6}$$

   lead to an order three method. This method can be used to solve parabolic problems.

References

[1] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations.* Springer, Berlin, second edition, 2006.

Project 5. Stiff order conditions

Consider the semilinear evolution equation

$$u_t = Au + g(u), \quad u(0) = u_0,$$

where A is a linear unbounded operator that generates a semigroup e^{tA} and g is a sufficiently regular nonlinear map. For this problem, we consider the exponential splitting scheme $u_{n+1} = Su_n$, where the nonlinear propagator is given by

$$S = \mathrm{e}^{\alpha_q \tau A}\, \psi_{\beta_{q-1}\tau}\, \mathrm{e}^{\alpha_{q-1}\tau A} \ldots \psi_{\beta_1 \tau}\, \mathrm{e}^{\alpha_1 \tau A}.$$

The idea behind this splitting is that the actions of the nonlinear flow ψ_t, generated by g, and the linear flow e^{tA} can commonly be computed in a much more efficient manner compared to the flow of the full vector field $A + g$.

1. Rewrite the nonlinear wave equation

$$v_{tt} + v_t = c\Delta v + f(v)$$

as a first-order system with the vector field

$$Au + g(u) = \begin{bmatrix} 0 & I \\ c\Delta & -I \end{bmatrix} u + \begin{bmatrix} 0 \\ f(v) \end{bmatrix}.$$

What is u? Explain how the action of the linear flow e^{tA} can be efficiently approximated by a FFT-based scheme (assuming periodic boundary conditions). How does the nonlinear flow look like?

2. Show that a three-stage scheme ($q = 3$) satisfying the following conditions on the coefficients

$$\begin{aligned} \alpha_1 + \alpha_2 + \alpha_3 &= 1, \\ \beta_1 + \beta_2 &= 1, \\ \beta_1\alpha_1 + \beta_2(\alpha_1 + \alpha_2) &= \tfrac{1}{2}, \\ \beta_1\alpha_1^2 + \beta_2(\alpha_1 + \alpha_2)^2 &= \tfrac{1}{3}, \\ \beta_1^2\alpha_1 + 2\beta_1\beta_2(\alpha_1 + \alpha_2) + \beta_2^2(\alpha_1 + \alpha_2) &= \tfrac{2}{3}, \\ \beta_1^2\alpha_1 + 2\beta_1\beta_2\alpha_1 + \beta_2^2(\alpha_1 + \alpha_2) &= \tfrac{1}{3} \end{aligned} \tag{1}$$

has a local error of size $\mathcal{O}(\tau^4)$, if the exact solution is sufficiently smooth; see [2, Section 4]. The conditions (1) are called stiff order conditions (why?) of order 3.

3. Show that the stiff order conditions (1) coincide with the non-stiff order conditions that result from the Baker–Campbell–Hausdorff formula for a linear problem $u_t = Au + Bu$ with bounded operators (matrices) A and B; see [1].

4. Implement the above scheme for $q = 2$ (choose Strang splitting) and solve the nonlinear wave equation described in [2, Section 1].

References

[1] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations.* Springer, Berlin, second edition, 2006.

[2] E. Hansen and A. Ostermann. High-order splitting schemes for semilinear evolution equations. To appear in *BIT Numer. Math.* (2016). `http://link.springer.com/article/10.1007/s10543-016-0604-2`

Project 6. An almost symmetric Strang splitting scheme

Consider the differential equation

$$y' = A(y) + B(y)y + d, \tag{1}$$

where we assume that the partial problem $y' = A(y)$ can be solved in an efficient way with flow φ_t^A. However, no such assumption is made about the second partial problem $y' = B(y)y + d$. Instead, we assume that for any fixed value, say $y_\star$, the flow corresponding to

$$y' = B(y_\star)y + d$$

can be computed efficiently. This flow, denoted by $\varphi_t^{B(y_\star)}$, is actually given by

$$\varphi_t^{B(y_\star)}(z) = \mathrm{e}^{tB(y_\star)}z + t\phi_1\bigl(tB(y_\star)\bigr)d, \qquad \phi_1(z) = \frac{\mathrm{e}^z - 1}{z}.$$

Show the following statements.

1. Standard Strang splitting applied to (1)

$$y_1 = \varphi_{\frac{\tau}{2}}^A \circ \varphi_\tau^{B(y_0)} \circ \varphi_{\frac{\tau}{2}}^A(y_0)$$

is first order only.

2. The modified Strang splitting

$$\begin{aligned} y_{1/2} &= \varphi_{\frac{\tau}{2}}^{B(y_0)} \circ \varphi_{\frac{\tau}{2}}^A(y_0) \\ y_1 = M_\tau(y_0) &= \varphi_{\frac{\tau}{2}}^A \circ \varphi_\tau^{B(y_{1/2})} \circ \varphi_{\frac{\tau}{2}}^A(y_0). \end{aligned}$$

is second-order accurate. However, it is not symmetric.

3. Let $L_{\frac{\tau}{2}}(y_0) = y_{1/2} = \varphi_{\frac{\tau}{2}}^{B(y_0)} \circ \varphi_{\frac{\tau}{2}}^A(y_0)$ denote a Lie step with half the step size. Compute its adjoint method (i.e. the inverse with negative step size).

4. Combining $L_{\frac{\tau}{2}}$ with its adjoint gives the (implicit) Strang splitting

$$y_1 = S_\tau(y_0) = L_{\frac{\tau}{2}}^* \circ L_{\frac{\tau}{2}}(y_0) = \varphi_{\frac{\tau}{2}}^A \circ \varphi_{\frac{\tau}{2}}^{B(y_1)}(y_{1/2}).$$

This method is of second order and symmetric (why?).

5. Employing fixed-point iteration

$$y_1^{(k+1)} = \varphi_{\frac{\tau}{2}}^A \circ \varphi_{\frac{\tau}{2}}^{B\left(y_1^{(k)}\right)}(y_{1/2}), \qquad y_1^{(0)} = y_{1/2}$$

yields a scheme which is symmetric of order $k+1$. (A one-step method Φ_τ is called *symmetric of order q* if

$$\Phi_\tau^* = \Phi_\tau + \mathcal{O}\left(\tau^{q+1}\right),$$

where Φ_τ^* is the adjoint method of Φ_τ.)

The resulting scheme can again be used for composition methods (see project 7).

6. Implement the scheme and one of its compositions for a problem chosen from [1].

References

[1] L. Einkemmer and A. Ostermann. An almost symmetric Strang splitting scheme for the construction of high order composition methods. *J. Comput. Appl. Math.* 271, 307-318 (2014). `https://arxiv.org/abs/1306.1169`

Project 7. High-order splitting

It can be a tedious task to construct splitting methods of high order directly from the order conditions. A much simpler approach is through composition. Let Φ_τ be a basic one-step method (i.e., $u_{n+1} = \Phi_\tau(u_n)$) and $\gamma_1, \ldots, \gamma_s$ (real) numbers. The method

$$\Psi_\tau = \Phi_{\gamma_s \tau} \circ \cdots \circ \Phi_{\gamma_1 \tau} \tag{1}$$

is called composition method (based on the step sizes $\gamma_1 \tau, \ldots, \gamma_s \tau$), see [1, Section II.4]

1. Show the following result (e.g. by Taylor expansion). Let the basic method be of order p. If

$$\begin{aligned} \gamma_1 + \ldots + \gamma_s &= 1 \\ \gamma_1^{p+1} + \ldots + \gamma_s^{p+1} &= 0, \end{aligned}$$

   then the composition method (1) is at least of order $p+1$.

   Taking Ψ_τ as the new basic method, this construction can be repeated if the order of Ψ_τ is even (why?).

2. Find explicit formulas for the triple jump ($s = 3$, $\gamma_1 = \gamma_3$) and compute, starting off from Strang splitting as the basic method, methods of order 4, 6, and 8. Why does this construction automatically give methods of even order?

3. Solve the linear Schrödinger equation

$$u_t = \mathrm{i}\left(\tfrac{1}{2}\Delta - V\right) u, \qquad 0 \le t \le 1, \qquad u(0,x) = \mathrm{e}^{-10x^2}$$

   on the one-dimensional torus (i.e., with periodic boundary conditions) and potential $V(x) = \cos(2\pi x)$. Plot the error of the above methods of order 2 to 8 as a function of the step size in a double logarithmic scale and comment the obtained results.

References

[1] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations.* Springer, Berlin, second edition, 2006.