A splitting approach for the KP and the magnetic Schrödinger equation

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Outline

Korteweg–de Vries equation

Kadomtsev–Petviashvili equation

Magnetic Schrödinger equation

Korteweg–de Vries equation

KdV models waves on shallow water surfaces

$$u_t + u_{xxx} + 6uu_x = 0$$

water waves in channels; solitons

(J. Scott Russel, 1834; J. Boussinesq, 1877;
D. Korteweg and G. de Vries, 1895)

space discretization: finite differences

time discretization:
explicit – CFL requires prohibitively small time steps
implicit – possible in 1d; geometric properties?
Split KdV equation

$$u_t = Au + B(u)$$

into linear part $Au = -u_{xxx}$ and nonlinearity $B(u) = -6uu_x$

Korteweg–de Vries equation, splitting

Split KdV equation

$$u_t = -u_{xxx} - 6uu_x$$

Solve the linear dispersion equation

$$u_t = -u_{xxx}$$

in Fourier space (FFT techniques) and Burgers equation

$$u_t = -6uu_x$$

in physical space, e.g., by the method of characteristics

$$w(\tau, x) = \widetilde{w} = w_0(x - 6\tau\widetilde{w})$$

Abstract convergence analysis for Strang splitting:
smooth initial data, exact flows, periodic b.c.
(H. Holden, C. Lubich, and N. Risebro, *Math. Comp.*, 2013)

Burgers type nonlinearities

Many interesting equations in physics are of the form

$$u_t = P(\partial_x)u + \alpha u u_x,$$

where P is a polynomial of $\deg P \geq 2$ and with $\operatorname{Re} P(\mathrm{i}\xi) \leq 0$:

$u_t = u_{xx} + uu_x$ viscous Burgers equation

$u_t = -u_{xxx} - 6uu_x$ Korteweg–de Vries equation

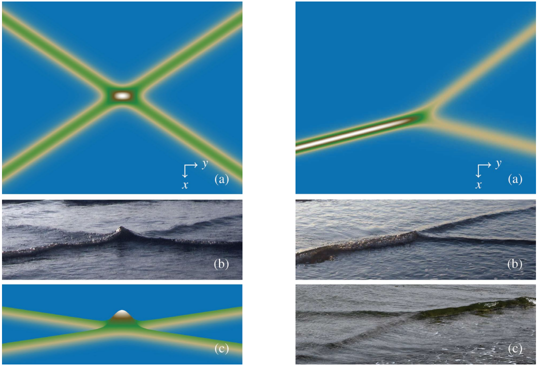
$u_t = u_{xxxxx} - u_{xxx} + uu_x$ Kawahara equation

Splitting: linear part $Au = P(\partial_x)u$
Burgers nonlinearity $B(u) = \alpha u u_x$

(H. Holden, C. Lubich, and N. Risebro, *Math. Comp.*, 2013)

Kadomtsev–Petviashvili equation

KP models the evolution of nonlinear, long waves of small amplitude with slow dependence on the transverse coordinate.
(B. Kadomtsev and V. Petviashvili, *Sov. Phys. Dokl.*, 1970)



Solitary waves for KP; X-type and Y-type interactions
Source: M. Ablowitz and D. Baldwin, *SIAM News 46*, June 2013.

Kadomtsev–Petviashvili equation

KP is a 2d model for nonlinear wave propagation

$$\left(\partial_t u + 6uu_x + \varepsilon^2 u_{xxx}\right)_x + \lambda u_{yy} = 0$$

Description of long wavelength waves, where

$\lambda = 1$	(weak surface tension)	KP II model
$\lambda = -1$	(strong surface tension)	KP I model

In evolution form

$$\partial_t u + 6uu_x + \varepsilon^2 u_{xxx} + \lambda \partial_x^{-1} u_{yy} = 0$$

Soliton solutions; appearance of small scale oscillations.

Numerical comparisons (exponential integrators).
(C. Klein and K. Roidot, *SIAM J. Sci. Comput.*, 2011)

KP equation, splitting

We split the KP equation into

$$v_t = Av = -\varepsilon^2 v_{xxx} - \lambda \partial_x^{-1} v_{yy}$$
$$w_t = B(w) = -6ww_x$$

and use Strang splitting on a regular spatial grid.

For the linear part, we use FFT (with regularized Fourier multiplier).

For the nonlinear advection part, we use the method of characteristics

$$w(\tau, x, y) = w_1(x, y) = w_0(x - 6\tau w_1(x, y), y)$$

This equation is solved by a few fixed-point iterations; requires interpolation of $w_0(\cdot, y)$.

Can be done in parallel (y is a parameter).

KP equation, exponential integrator

Alternative discretization by an exponential integrator (relying on the above splitting)

$$u_{n+1} = \mathrm{e}^{\tau A} u_n + \tau \varphi_1(\tau A) B(u_n) + \tau \varphi_2(\tau A) \left(B(U) - B(u_n) \right),$$

where

$$U = \mathrm{e}^{\tau A} u_n + \tau \varphi_1(\tau A) B(u_n)$$

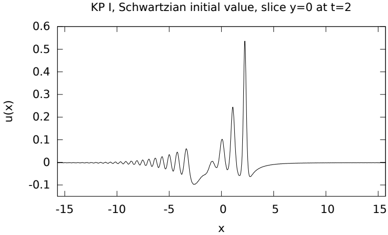
The φ_i functions are given by the recurrence relation

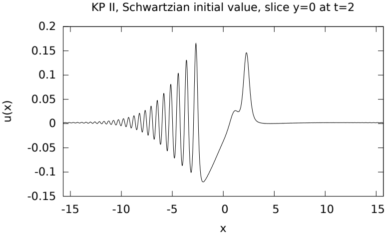
$$z \varphi_{k+1}(z) = \varphi_k(z) - \varphi_k(0), \qquad \varphi_0(z) = \mathrm{e}^z$$

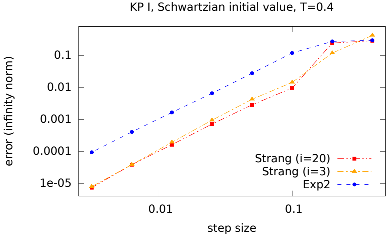
Exponential integrators treat the advection explicitly and require a CFL condition.

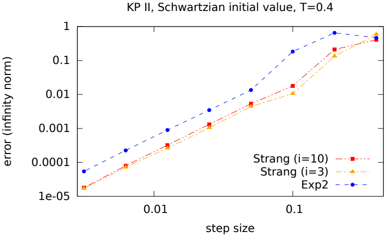
A. Kassam and L. Trefethen, *SISC*, 2005
M. Hochbruck and A.O., *Acta Numerica*, 2010

Initial value $u_0(x,y) = -\frac{1}{2}\partial_x \mathrm{sech}^2\left(\sqrt{x^2+y^2}\right)$







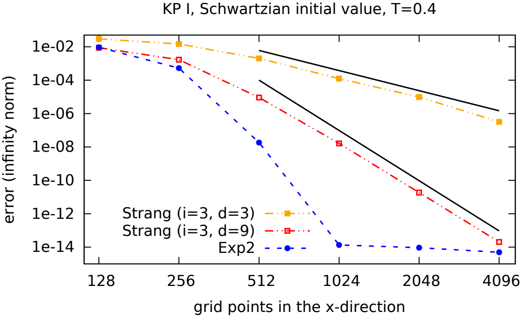


$\Omega = [-5\pi, 5\pi]^2, \quad \varepsilon = 0.1, \quad 2^{11} \times 2^9$ grid points for (x, y)

Loss of exponential convergence

The ninth degree polynomial interpolation is approximately three times as costly as the cubic interpolation.

Nevertheless, Strang splitting is still twice as fast compared to the exponential integrator of order 2.

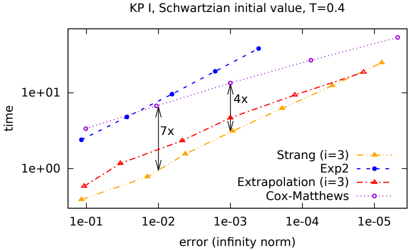


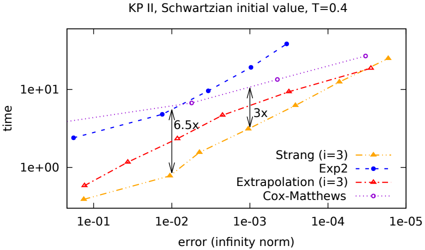
$\Omega = [-5\pi, 5\pi]^2, \quad \varepsilon = 0.1, \quad 2^9$ grid points for y, $\quad \tau = 0.01$

Performance

Compare performance of splitting methods (order 2 and 4) with two exponential integrators.

(S. Cox and P. Matthews, *J. Comput. Phys.*, 2002)





$\Omega = [-5\pi, 5\pi]^2, \quad \varepsilon = 0.1, \quad 2^{11} \times 2^9$ grid points

For $d = 9$ the fourth-order methods behave almost identically.

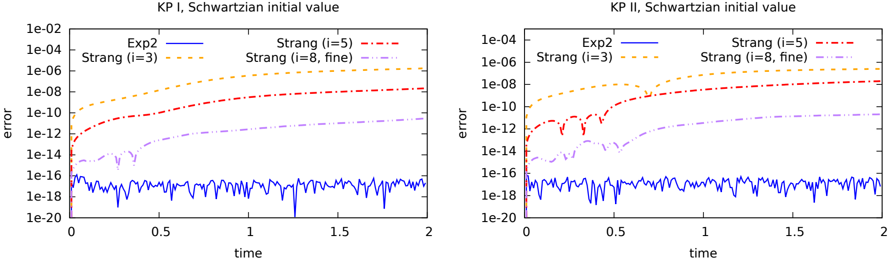
Conservation of mass: $|m(t) - m(0)|$

Total mass

$$m(t) = \int_\Omega u(t,x,y)\,\mathrm{d}(x,y)$$

is conserved by exponential integrators.

(L. Einkemmer and A.O., *J. Comput. Phys.*, 2015)

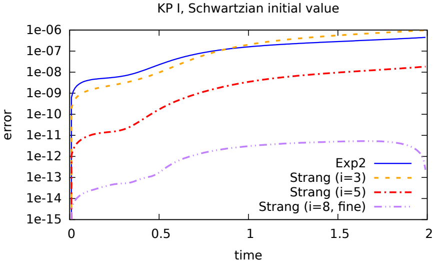


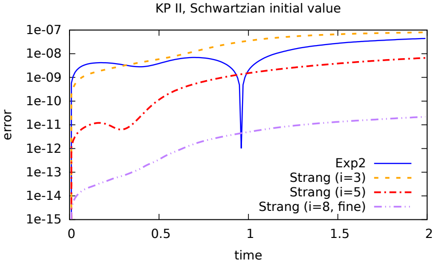
$\Omega = [-5\pi, 5\pi]^2$, $\varepsilon = 0.1$, $2^{11} \times 2^9$ grid points, $\tau = 0.01$

fine grid: $2^{13} \times 2^9$

Conservation of momentum

KP has quadratic invariant $\displaystyle\int_\Omega u(t,x,y)^2 \,\mathrm{d}(x,y)$





$\Omega = [-5\pi, 5\pi]^2, \quad \varepsilon = 0.1, \quad 2^{11} \times 2^9$ grid points, $\quad \tau = 0.01$

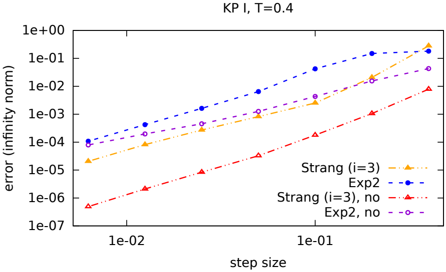
fine grid: $2^{13} \times 2^9$

A last constraint

KP also satisfies the constraint $\int_{-\infty}^{\infty} \partial_{yy} u(t,x,y)\,\mathrm{d}x = 0$ for all $t > 0$, even if the initial value does not.

Numerical methods regularize, but may react with order reduction (C. Klein, C. Sparber, P. Markowich, J. Nonlinear Sci., 2007).

$$u_{\mathrm{no}}(0,x,y) = \tfrac{1}{3}\mathrm{e}^{-(x^2+y^2)/2}, \qquad u(0,x,y) = \tfrac{3}{5}x\mathrm{e}^{-(x^2+y^2)/2}$$



$\Omega = [-5\pi, 5\pi]^2, \quad \varepsilon = 0.1, \quad 2^{11} \times 2^9$ grid points

A three-term splitting

Linear Schrödinger equation in the presence of an electromagnetic field

$$\mathrm{i}\varepsilon\partial_t u = \tfrac{1}{2}(\mathrm{i}\varepsilon\nabla + A)^2 u + Vu, \quad u(0,x) = u_0(x).$$

After transformation with a Coulomb gauge

$$\mathrm{i}\varepsilon\partial_t u = -\tfrac{\varepsilon^2}{2}\Delta u + \mathrm{i}\varepsilon A\cdot\nabla u + \tfrac{1}{2}|A|^2 u + Vu, \quad u(0,x) = u_0(x).$$

Motivates a three-term splitting

$$\partial_t u = (\mathcal{A} + \mathcal{B} + \mathcal{C})u, \quad u(0) = u_0$$

with bounded operator $\mathcal{B}$ and unbounded operators $\mathcal{A}$ and $\mathcal{C}$.

Error analysis

Let $\mathcal{C}$ and $\mathcal{A}+\mathcal{C}$ generate C_0 semigroups, and

$$\begin{aligned}
\|[\mathcal{A},\mathcal{C}]\mathrm{e}^{s\mathcal{A}}u(t)\| &\le c_1 \\
\|\mathcal{C}\mathrm{e}^{s\mathcal{A}}\mathcal{B}u(t)\| &\le c_2 \\
\|\mathcal{C}^2\mathrm{e}^{s\mathcal{A}}u(t)\| &\le c_3 \\
\|\mathcal{C}\mathrm{e}^{\sigma\mathcal{A}}\mathcal{C}\mathrm{e}^{s(\mathcal{A}+\mathcal{C})}u(t)\| &\le c_4 \\
\|[\mathcal{A}+\mathcal{C},\mathcal{B}]\mathrm{e}^{s(\mathcal{A}+\mathcal{C})}u(t)\| &\le c_5
\end{aligned}$$

Theorem. (M. Caliari, A.O., C. Piazzola, *Comput. Appl. Math.*, 2016)
The following bound for the local error holds

$$\|\mathrm{e}^{\tau\mathcal{C}}\mathrm{e}^{\tau\mathcal{A}}\mathrm{e}^{\tau\mathcal{B}}u(t)-u(t+\tau)\| \le C\tau^2$$

with a constant C that does not depend on t and τ.

Application to magnetic Schrödinger equation

Space discretization by a uniform grid.

Potential step is easily performed in physical space

$$\partial_t u = \mathcal{B} u = -\tfrac{\mathrm{i}}{\varepsilon}\left(\tfrac{1}{2}|A|^2 + V\right) u$$

Kinetic step can be handled analytically in Fourier space

$$\partial_t u = \mathcal{A} u = \frac{\mathrm{i}\varepsilon}{2}\Delta u$$

Advection step by method of characteristics and either interpolation or nonequispaced FFT

$$\partial_t u = \mathcal{C} u = A \cdot \nabla u, \qquad \nabla \cdot A = 0$$

A one dimensional example

N		interpolation of degree $p-1$				Fourier	
		$p=2$	$p=4$	$p=6$	$p=8$	DFT	NFFT
128	mass	1.4e-01	1.8e-02	2.1e-03	2.8e-04	2.8e-15	8.6e-14
	CPU	0.13	0.12	0.12	0.12	0.10	0.16
256	mass	9.4e-02	2.7e-03	7.2e-05	2.5e-06	2.0e-15	1.0e-14
	CPU	0.13	0.13	0.13	0.14	0.19	0.17
512	mass	5.2e-02	2.9e-04	2.0e-06	1.8e-08	3.6e-15	1.7e-14
	CPU	0.16	0.19	0.17	0.16	0.27	0.19
1024	mass	1.6e-02	1.8e-05	3.0e-08	9.6e-11	4.0e-15	5.5e-14
	CPU	0.22	0.23	0.23	0.24	0.56	0.23
2048	mass	4.2e-03	1.1e-06	4.9e-10	3.8e-12	3.3e-15	1.3e-14
	CPU	0.36	0.37	0.37	0.37	1.42	0.33

Table: Error in mass conservation and CPU time (in seconds).

A two dimensional example

2d example with space dependent vector and scalar potentials, and $\varepsilon = 1$. Final time $T = 50$ and 1000 time steps.

$N_1 = N_2$		interpolation of degree $p-1$		Fourier		
					NFFT	
		$p=4$	$p=6$	DFT	$m=8$	$m=4$
128	mass	1.0e-01	2.5e-03	9.9e-11	1.0e-10	2.2e-07
	CPU	25.2	33.5	174.3	23.7	20.6
256	mass	6.9e-03	3.9e-05	1.3e-08	1.3e-08	2.5e-02
	CPU	101.7	117.9	2254	99.6	87.7
512	mass	4.3e-04	6.2e-07	*	9.7e-11	2.0e-07
	CPU	412.7	506.8	*	435.7	400.4
1024	mass	2.7e-05	9.6e-09	*	9.7e-11	1.9e-07
	CPU	1796	2139	*	1948	1709

Table: Error in mass conservation and CPU time (in seconds).

A three dimensional example with NFFT

3d example with space dependent vector and scalar potentials, and $\varepsilon = 1$. Final time $T = 50$ and 1000 time steps.

Advection step with method of characteristics and nonequispaced FFT (standard parameters).

$N_1 = N_2 = N_3$	mass error	CPU
16	6.1e-13	5.6
32	8.2e-14	37.7
64	7.1e-13	396.5
128	1.3e-12	2986

Table: Error in mass conservation and CPU time (in seconds).

References

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