Overview of time-propagators for Schrödinger-type equations with expensive-to-evaluate nonlinear part

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Problem setting

We consider *Schrödinger-like* equations of the form

$$\partial_t u(t) = Au(t) + B(t, u(t))$$

where

- A linear, built from (discretized versions of) Laplacians $\frac{1}{2}\mathrm{i}\Delta$, imaginary eigenvalues of large modulus
- B nonlinear in general, smooth but expensive to evaluate

Example: MCTDHF equations

By the standard technique of adding the trivial equation $\partial_t s = 1$ we can transform our equation to *autonomous* form $\partial_t \tilde{u}(t) = \tilde{A}(\tilde{u}(t)) + \tilde{B}(\tilde{u}(t))$ where

$$\tilde{u} = \begin{pmatrix} u \\ s \end{pmatrix}, \quad \tilde{A}(\tilde{u}) = \begin{pmatrix} Au \\ 1 \end{pmatrix}, \quad \tilde{B}(\tilde{u}) = \begin{pmatrix} B(s,u) \\ 0 \end{pmatrix}$$

Goal: to find time-propagation methods for such equations which are

- accurate
- stable (for medium- to long-term integrations)
- require few evaluations of B per time-step

MCTDHF equations

Structure of MCTDHF equations for *coefficients* $a = (a_J)$ and *orbitals* $\phi = (\phi_j)$:

$$
\begin{aligned}
\mathrm{i}\partial_t a_J &= \sum_L \langle \Phi_J | \mathbf{V} | \Phi_L \rangle a_L \\
\mathrm{i}\partial_t \phi_j &= -\frac{1}{2}\Delta\phi_j + (I - P)\sum_{l=1}^{N}\sum_{m=1}^{N}(\rho^{-1})_{j,m}\langle \psi_m | \mathbf{V} | \psi_l \rangle \phi_l, \quad j = 1, \dots, N
\end{aligned}
$$

With

$$
u = \begin{pmatrix} a_J \\ \phi_1 \\ \vdots \\ \phi_N \end{pmatrix}
$$

and

$$
A = \mathrm{blockdiag}(0, \tfrac{1}{2}\mathrm{i}\Delta, \dots, \tfrac{1}{2}\mathrm{i}\Delta), \quad B = \text{"the remaining parts"}
$$

the MCTDHF equations are *Schrödinger-type* equations of the form

$$
\partial_t u(t) = Au(t) + B(t, u(t))
$$

Time propagations methods

We consider

- Splitting methods
- Composition methods (solve B-part with implicit midpoint rule)
- Exponential Runge-Kutta methods
- Exponential multistep methods

These methods are extensively studied in the literature, but

- Exponential Runge-Kutta and multistep methods mainly for parabolic problems
- not under the aspect of stability of medium- to long-term integrations
- not under the aspect of the expensive B-part

Splitting methods

Requirement: The flows of the subproblems

$$\partial_t u(t) = Au(t),\ u(t_0) = u_0 \quad \text{and} \quad \partial_t u(t) = B(u(t)),\ u(t_0) = u_0$$

must be efficiently computable.

For the B-part this is usually *not* the case for problems here considered.

For linear problems one step $u_n \mapsto u_{n+1}$ of stepsize h can be written as

$$u_{n+1} = \mathrm{e}^{b_s hB}\mathrm{e}^{a_s hA} \cdots \mathrm{e}^{b_1 hB}\mathrm{e}^{a_1 hA} u_n$$

with suitable coefficients a_i, b_i

Example (Suzuki composition, A-steps combined, order 4):

a_i	b_i
0.20724538589718786857	0.41449077179437573714
0.41449077179437573714	0.41449077179437573714
-0.12173615769156360571	-0.65796308717750294857
-0.12173615769156360571	0.41449077179437573714
0.41449077179437573714	0.41449077179437573714
0.20724538589718786857	0.00000000000000000000

Composition methods (1)

Let a *symmetric* 2nd order time-propagator Φ_h for

$$\partial_t u(t) = Au(t) + B(u(t))$$

be given such that for one step $u_n \mapsto u_{n+1}$ of stepsize h it holds

$$u_{n+1} = \Phi_h(u_n) \quad \text{and} \quad u_n = \Phi_{-h}(u_{n+1})$$

Higher order time-propagation methods can be obtained by compositions of Φ_h:

$$u_{n+1} = \Phi_{c_s h} \circ \cdots \circ \Phi_{c_1 h}(u_n)$$

with suitable coefficients c_i.
Example (Suzuki composition of order 4):

$$c = \left(\frac{1}{4-4^{\frac{1}{3}}}, \frac{1}{4-4^{\frac{1}{3}}}, \frac{-4}{4-4^{\frac{1}{3}}}, \frac{1}{4-4^{\frac{1}{3}}}, \frac{1}{4-4^{\frac{1}{3}}} \right)$$

Composition methods (2)

A suitable symmetric 2nd order time-propagator Φ_h for

$$\partial_t u(t) = Au(t) + B(u(t))$$

is given by

$$\Phi_h(u) = \mathrm{e}^{\frac{h}{2}A}\phi_h^{(B)}(\mathrm{e}^{\frac{h}{2}A}u)$$

where $\phi_h^{(B)}$ is a *symmetric* method for the subproblem $\partial_t u(t) = B(u(t))$

Note: Such a *symmetric* method $\phi_h^{(B)}$ is necessarily *implicit*!

We propose to use the *implicit midpoint rule* where one step $u_n \mapsto u_{n+1} = \phi_h^{(B)}(u_n)$ of stepsize h is given by

$$u_{n+1} = u_n + hB\Big(\frac{1}{2}(u_n + u_{n+1})\Big)$$

Here the implicit equation for u_{n+1} is approximately solved by a fixed number of fixed point iterations.

Suzuki composition with 4 fixed point iterations for each evaluation of $\phi_h^{(B)}$ yields a method of order 4

But: $5 \times 4 = 20$ evaluations of B per time-step!

Exponential Runge-Kutta methods (1)

Example (Krogstad method of order 4):

$$\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,2} & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,1} - \varphi_{2,3} & \varphi_{2,3} & & \\
1 & \varphi_{1,4} - 2\varphi_{2,4} & 0 & 2\varphi_{2,4} & \\
\hline
 & \varphi_1 - 3\varphi_2 + 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & -\varphi_2 + 4\varphi_3
\end{array}$$

$\varphi_{j,k} = \varphi_j(c_k hA)$, $\varphi_j = \varphi(hA)$ must be efficiently computable

4 evaluations of B per time-step

φ-functions defined by

$$\varphi_k(z) = \int_0^1 \mathrm{e}^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} \mathrm{d}\theta, \quad k \geq 1$$

They satisfy $\varphi_k(0) = \frac{1}{k!}$ and the recurrence relation

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

Cancellation effects for z of small modulus!

Exponential Runge-Kutta methods (2)

Runge-Kutta-Lawson

Lawson transformation: In

$$\partial_t u(t) = Au(t) + B(u(t))$$

substitute

$$v(t) = e^{(t_n - t)A} u(t)$$

Then $v(t)$ satisfies a differential equation of the form

$$\partial_t v(t) = e^{(t_n - t)A} B(e^{(t - t_n)A} v(t))$$

To this differential equation apply the classical explicit 4th order Runge-Kutta method
$\rightsquigarrow$ k-th order Runge-Kutta-Lawson method

No φ-functions required
4 evaluations of B per time-step

Exponential multistep methods (1)

Adams-Bashforth

Solution $u(t)$ of $\partial_t u(t) = Au(t) + B(u(t))$ with $u(t_n) = u_n$ satisfies variation-of-constants formula

$$u(t_n + h) = e^{hA}u_n + \int_0^h e^{(h-\tau)A}B(u(t_n+\tau))\mathrm{d}\tau$$

Idea: To get an approximation $u_{n+1} \approx u(t_n + h)$ replace $B(u(t_n + \tau))$ in the integrand by an interpolation polynomial $p_n(\tau)$ at the points

$$(-(k-1)h, B(u_{n-k+1}), \dots, (-h, B(u_{n-1})), (0, B(u_n))$$

Using the φ-functions the integral in

$$u_{n+1} = e^{hA}u_n + \int_0^h e^{(h-\tau)A}p_n(\tau)\mathrm{d}\tau$$

can then be evaluated exactly

$\rightsquigarrow$ k-th order exponential multistep method of *Adams-Bashforth* type

1 evaluation of B per time-step!

Exponential multistep methods (2)

Predictor-Corrector

Compute an approximation $\tilde{u}_{n+1} \approx u(t_n + h)$ as above (now denoted $\tilde{u}_{n+1}$)

Replace $B(u(t_n + \tau))$ in the integrand of the variation-of-constants formula by an interpolation polynomial $\tilde{p}_n(\tau)$ at the points

$$(-(k-1)h, B(u_{n-k+1}), \dots, (-h, B(u_{n-1})), (0, B(u_n)), (h, B(\tilde{u}_{n+1}))$$

Define

$$u_{n+1} = e^{hA}u_n + \int_0^h e^{(h-\tau)A}\tilde{p}_n(\tau)\mathrm{d}\tau$$

$\tilde{u}_{n+1}$ ... *predictor*, u_{n+1} ... *corrector*

$\rightsquigarrow$ $(k+1)$-th order exponential multistep method with one corrector step

Improved stability to be expected compared to method without corrector step

Corrector can be used as error estimator for predictor $\rightsquigarrow$ automatic step-size selection

2 evaluations of B per time-step

Exponential multistep methods (3)

Adams-Lawson

In the integrand of the variation-of-constants formula

$$u(t_n + h) = e^{hA}\left(u_n + \int_0^h e^{-\tau A} B(u(t_n+\tau))\mathrm{d}\tau\right)$$

replace $e^{-\tau A}B(u(t_n+\tau))$ by an interpolation polynomial $p_n(\tau)$ at the points

$$(-(k-1)h, e^{(k-1)hA}B(u_{n-k+1}), \dots, (-h, e^{hA}B(u_{n-1})), (0, B(u_n))$$

Define

$$u_{n+1} = e^{hA}\left(u_n + \int_0^h p_n(\tau)\mathrm{d}\tau\right)$$

Here the integral can be evaluated exactly using the same coefficients as for the classical explicit Adams-Bashforth method

$\rightsquigarrow$ k-th order exponential multistep method of *Adams-Lawson* type

Exponential multistep methods (4)

Adams-Lawson, alternative derivation

Same idea as for Runge-Kutta-Lawson (Lawson transformation): In

$$\partial_t u(t) = Au(t) + B(u(t))$$

substitute

$$v(t) = e^{(t_n - t)A} u(t)$$

Then $v(t)$ satisfies a differential equation of the form

$$\partial_t v(t) = e^{(t_n - t)A} B(e^{(t - t_n)A} v(t))$$

To this differential equation apply a classical explicit Adams-Bashforth method

$\rightsquigarrow$ k-th order exponential multistep method of *Adams-Lawson* type

No φ-functions required

1 evaluation of B per time-step

Again the precictor-corrector idea can be utilized, $\rightsquigarrow$ order $k+1$,

2 evaluations of B per time-step

Test Problem

Nonlinear Schrödinger equation with time dependent potential

The soliton

$$\psi_{\mathrm{ex}}(x,t) = \frac{a\mathrm{e}^{\frac{1}{2}\mathrm{i}((a^2-b^2)t-bx)}}{\cosh(a(bt+x-c))},$$

where $a, b, c \in \mathbb{R}$ are arbitrarily chosen parameters, is the exact solution of the cubic nonlinear Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = -\frac{1}{2}\Delta\psi(x,t)+V_\alpha(x,t)\psi(x,t)+\alpha\kappa|\psi(x,t)|^2\psi(x,t), \quad \psi(x,0) =$$

with $\kappa = -1$, $\alpha = \frac{1}{2}$, and time dependent potential

$$V_\alpha(x,t) = (1-\alpha)\kappa|\psi_{\mathrm{ex}}(x,t)|^2 = \frac{(1-\alpha)\kappa a^2}{\cosh(a(bt+x-c))^2}$$

We use this time-dependent problem to verify the correct implementation and the accuracy of the here considered time propagation methods

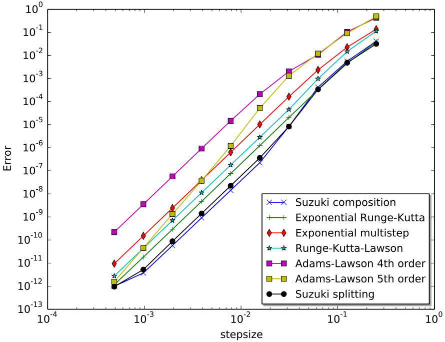
Numerical results

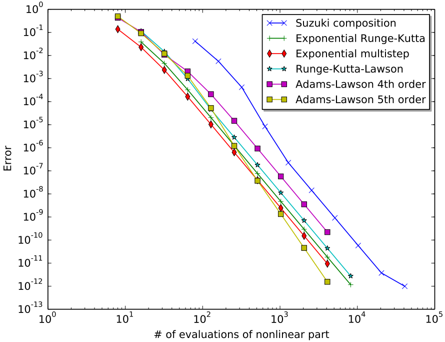
Test problem: nonlinear Schrödinger equation with time dependent potential

We solve this problem on $[x_{min}, x_{max}] = [-16, +16]$ with periodic boundary conditions for $t \in [t_0, t_{end}] = [0, 1]$

Initial value $\psi(0) = \psi_{ex}(0)$, reference solution at $t = 1$: $\psi_{ex}(1)$

Space discretization: spectral method using 1024 basis functions $\rightsquigarrow$ 1024 equidistant grid points in $[x_{min}, x_{max}]$





MCTDHF test problem

1D helium atom

$$i\partial_t \Psi(t) = H_0 \Psi(t)$$

$$H_0 = -\frac{1}{2}(\partial_x^2 + \partial_y^2) - \frac{2}{\sqrt{x^2+b^2}} - \frac{2}{\sqrt{y^2+b^2}} + \frac{2}{\sqrt{(x-y)^2+b^2}}$$

Smoothed Coulomb potential, shielding parameter $b = 0.7408$

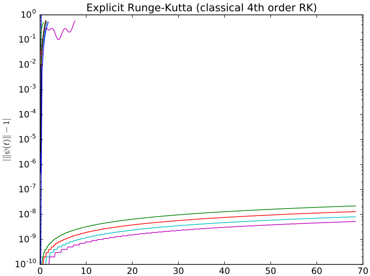
1D MCTDHF: $f = 2$ particles, $N = 6$ orbitals,
$[x_{min}, x_{max}] = [-240, +240]$, 4096 equidistant grid points

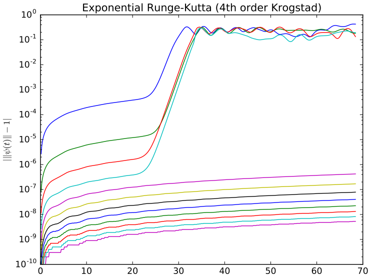
Initial data: groundstate (energy $E_0 = -2.89924$), computed using imaginary time propagation

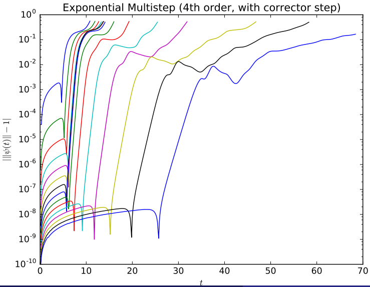
Benchmark test: follow stationary groundstate solution on $[t_0, t_{end}] = [0, 4\pi/0.1837] = [0, 68.41]$ using $1000, 2000, 3000, \ldots, 12000$ time-steps
monitor $|\|\psi(t)\| - 1|$ (conservation of norm)

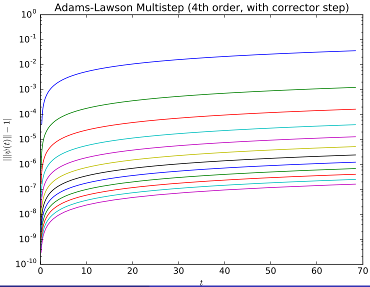
Numerical results

MCTDHF following stationary solution (groundstate)









MCTDHF test problem

1D helium atom irradiated by laser field

$$i\partial_t \Psi(t) = H(t)\Psi(t) = H_0\Psi(t) + (x+y)\mathcal{E}(t)\Psi(t)$$

with H_0 from above and laser field

$$\mathcal{E}(t) = \mathcal{E}_0 f(t) \sin(\omega t)$$

Peak amplitude $\mathcal{E}_0 = 0.1894$, frequency $\omega = 0.1837$

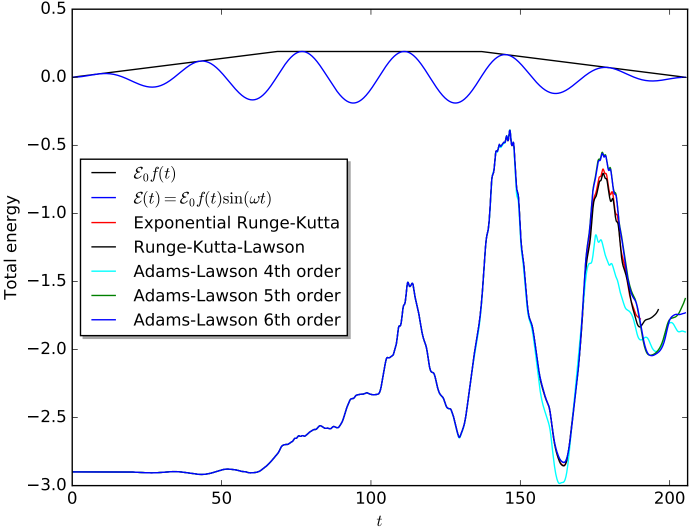
Trapezoidal envelope $f(t)$ with 2-cycle turn-on, 2-cycle flat top, and 2-cycle turn-off (cycle duration of laser $= 2\pi/\omega = 34.20$)

Initial data (groundstate) and MCTDHF parameters as in the previous test problem

60000 time-steps on $[t_0, t_{end}] = [0, 6\pi/\omega] = [0, 205.22]$

Numerical results

1D helium atom irradiated by laser field



Numerical results

1D helium atom irradiated by laser field