High-order Structure-Preserving Discretization Methods for Nonlinear Evolution Equations

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Nonlin. Evolution Equations

Consider

$$\dot{u} = F(u), \quad F(u) = Au + B(u),$$

A . . . linear differential operator,

$B(u)$ . . . nonlinear operator, generally unbounded.

- MCTDHF equations.
- Cubic NLS.
- Dissipative parabolic problem.
- Incompressible Navier–Stokes equations (fully nonlinear).

Lie Derivatives

$\varphi_F^t(\psi_0)$ ... flow of $\qquad \dot{\psi} = F(\psi), \quad \psi(0) = \psi_0.$

Lie derivative D_F

$$(D_F G)(\psi) := \frac{d}{dt}\bigg|_{t=0} G(\varphi_F^t(\psi)) = G'(\psi)F(\psi).$$

$$\Big(\exp(tD_F)G\Big)(\psi) := G(\varphi_F^t(\psi)).$$

Commutator

$$[D_A, D_B] := D_A D_B - D_B D_A = D_{[B,A]}.$$

Define recursively iterated commutators

$$\mathrm{ad}^0_{D_A}(D_B)u := D_B u, \qquad \mathrm{ad}^j_{D_A}(D_B)u := [D_A, \mathrm{ad}^{j-1}_{D_A}(D_B)](u).$$

Higher-Order Splittings

$$u_{n+1} = \mathcal{S}(h, u_n) := \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, h D_A}\, \mathrm{e}^{b_{s+1-j}\, h D_B}\, u_n, \qquad n = 0, 1, \ldots$$

Theorem: The defect of the splitting operator admits the expansion

$$\mathrm{e}^{h D_{A+B}} v - \mathcal{S}(h, v) \sim \sum_{k=1}^{p} \sum_{\substack{\mu \in \mathbb{N}^k \\ |\mu| \le p-k}} \frac{1}{\mu!}\, h^{k+|\mu|}\, C_{k\mu} \prod_{\ell=1}^{k} \mathrm{ad}_{D_A}^{\mu_\ell}(D_B)\, \mathrm{e}^{h D_A}\, v.$$

$C_{k\mu}$ ... computable constants.

The remainder term can be proven separately to be of higher order.

TDSE

Time-dependent Schrödinger equation (TDSE)

$$\mathrm{i}\frac{\partial\psi}{\partial t}(x_1,\ldots,x_f,t) = H\psi(x_1,\ldots,x_f,t), \quad \psi(0)=\psi_0.$$

Hamiltonian for a system of f free electrons interacting by Coulomb force,

$$H := \sum_{k=1}^{f}\left(-\frac{1}{2}\Delta^{(k)} + \sum_{l<k}\frac{1}{|x_k - x_l|}\right) = T + V.$$

$\Delta^{(k)}$ ... Laplace operator w. r. t. k-th particle.

Pauli principle implies antisymmetry in ψ!

Fermions indistinguishable!

MCTDHF

MCTDHF ansatz: Model reduction of TDSE by

$$\psi(x_1,\ldots,x_f,t) \approx u := \sum_J a_J(t)\Phi_J(x,t)$$

$$= \sum_{j_1,\ldots,j_f} a_{j_1,\ldots,j_f}(t)\phi_{j_1}(x_1,t)\cdots\phi_{j_f}(x_f,t) \in \mathcal{M}.$$

Dirac–Frenkel variational principle

$$\left\langle \delta u \,\middle|\, \mathrm{i}\frac{\partial u}{\partial t} - Hu \right\rangle = 0 \quad \forall \text{ variations } \delta u \in \mathcal{T}_u\mathcal{M}.$$

Additional constraints for uniqueness

$$\langle \phi_j | \phi_k \rangle = \delta_{j,k}, \qquad \left\langle \phi_j \,\middle|\, \frac{\partial \phi_k}{\partial t} \right\rangle = -\mathrm{i}\langle \phi_j | T | \phi_k \rangle.$$

Equations of Motion

This yields the equations of motion

$$\mathrm{i}\frac{da_J}{dt} = \sum_K \langle \Phi_J | V | \Phi_K \rangle a_K =: \mathcal{A}_V(\phi) a,$$

$$\mathrm{i}\frac{\partial \phi_j}{\partial t} = T\phi_j + (1-P)\sum_k \sum_l \rho_{j,l}^{-1} \overline{V}_{l,k} \phi_k =: T\phi + \mathcal{B}_V(a,\phi),$$

where

$\psi_j := \langle \phi_j | u \rangle$, "single-hole functions",

$\rho_{j,l} := \langle \psi_j | \psi_l \rangle$, "density matrix",

$\overline{V}_{l,k} := \langle \psi_l | V | \psi_k \rangle$, "mean-field operator matrix",

$P := \sum_j |\phi_j\rangle \langle \phi_j|$, (orthogonal projector).

Variational Splitting

Time propagation by high-order splitting method

$$u_{n+1} = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, h D_T}\, \mathrm{e}^{b_{s+1-j}\, h D_V} u_n\,, \qquad 0 \le n \le N-1\,.$$

- $\mathrm{e}^{a_j h D_T} u_0$: Compute the solution at time $t_0 + a_j h$ of

$$\left\langle \delta u \,\middle|\, \mathrm{i}\frac{\partial}{\partial t} - T \,\middle|\, u \right\rangle = 0 \quad \forall \delta u \in \mathcal{T}_u\mathcal{M}, \qquad u(t_0) = u_0.$$

- $\mathrm{e}^{b_j h D_V} u_0$: Compute the solution at time $t_0 + b_j h$ of

$$\left\langle \delta u \,\middle|\, \mathrm{i}\frac{\partial}{\partial t} - V \,\middle|\, u \right\rangle = 0 \quad \forall \delta u \in \mathcal{T}_u\mathcal{M}, \qquad u(t_0) = u_0.$$

Convergence of Splitting

Theorem (Koch, Lubich 2010;
Koch, Neuhauser, Thalhammer 2010):
Consider the numerical approximation of the MCTDHF equations for a free electron gas given by time semidiscretization based on an order p splitting.

Assume that $\| u(t)\|_{H^m} \leq M_m$ for $0 \leq t \leq T$. Then

$$\left\| u_n - u(t) \right\|_{L^2} \leq C\, h^p\,, \quad C = C(M_m),$$

$$m = p = 2 \;\text{ or }\; m = 2\,p - 3,\; p \geq 3,$$

$$\left\| u_n - u(t) \right\|_{H^1} \leq C\, h^{p-1}\,, \quad C = C(M_m),$$

$$m = p = 2, 3 \;\text{ or }\; m = 2\,p - 4,\; p \geq 4.$$

Outline of Proof

- Stability in the H^1-norm.
- Local error in H^1: $O(h^p)$, constant depends on the H^m-norm of u
  (m as specified; commutator bounds!).
- Stability $+$ consistency in $H^1 \Rightarrow$
  convergence order $p-1$ in H^1.
- Boundedness of the numerical solution in H^1.
- Stability in L^2: Constant depends on H^1-norm.
- Local error in L^2: $O(h^{p+1})$, constant depends on the H^m-norm of u (m as specified).
- Since $\|u_n\|_{H^1}$ is bounded, we conclude convergence order p in L^2.

Embedded Splittings

We use *embedded pairs* of splitting formulae for estimating the local error:

j	a_j
1	0
2,7	0.245298957184271
3,6	0.604872665711080
4,5	$1/2 - (a_2 + a_3)$

j	b_j
1,7	0.0829844064174052
2,6	0.3963098014983680
3,5	-0.0390563049223486
4	$1 - 2\,(b_1 + b_2 + b_3)$

j	$\hat{a}_j$
1	a_1
2	a_2
3	a_3
4	a_4
5	0.3752162693236828
6	1.4878666594737946
7	-1.3630829287974774

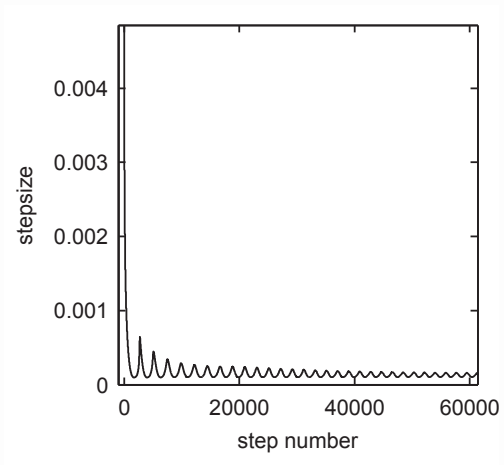
j	$\hat{b}_j$
1	b_1
2	b_2
3	b_3
4	b_4
5	0.4463374354420499
6	-0.0060995324486253
7	0

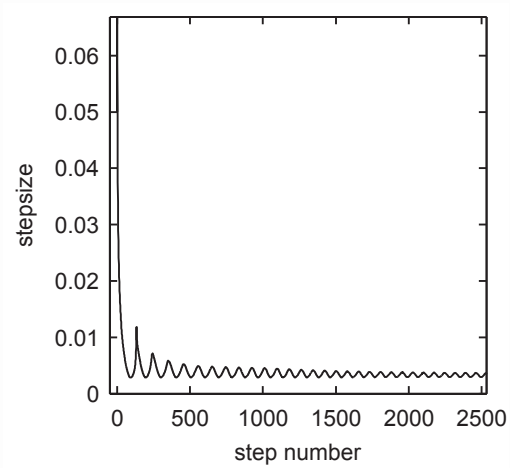
Embedded Splittings (2)

Cubic NLS with blow-up solution:

$$\mathrm{i}\frac{\partial\psi}{\partial t}(x,t) = -\frac{1}{2}\Delta\psi(x,t) - 2|\psi(x,t)|^2\psi(x,t), \quad x \in \mathbb{R}^2, \quad t \geq 0.$$

Time-stepping for pairs 2(1) (left) and 4(3) (right):



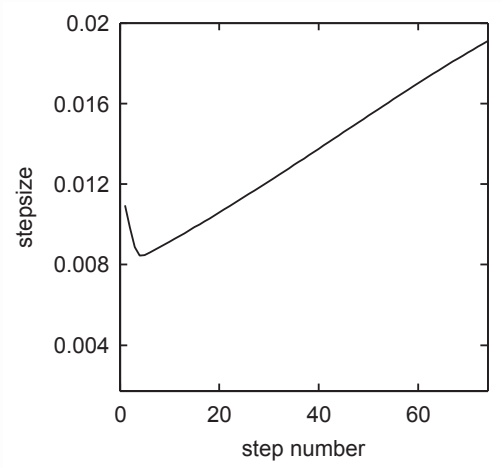


Embedded Splittings (3)

Dissipative parabolic problem:

$$\frac{\partial u}{\partial t}(x,t) = \frac{1}{2}\Delta u(x,t) + u(x,t)(1-u(x,t)), \quad x \in [-8,8]^3,\ t \geq 0.$$

Time-stepping for a complex 4(3) pair:



ANTARES

- Model of stellar convection and pulsation $\rightsquigarrow$ photometric and spectroscopic properties of stars.
- Convection/diffusion evolutionary PDE, singularly perturbed, integral constraints.
- ANTARES code —
  A Numerical Tool for Astrophysical RESearch.
- (W)ENO method for convective part.
- Dissipative FD approximation for diffusive part.
- TVD Runge–Kutta time integrator.

Model Problem

Idealized model in 2D:

- Incompressible mixture of two fluids.
- Heated from below $\rightsquigarrow$ convection.
- Mass concentration (salinity) gradient $\rightsquigarrow$ counteracting convection.
- Radiative transport $\leftarrow$ diffusion approximation.
- Boussinesq approximation: Density variations only in buoyancy term of vertical velocity equation.
- Feature: Layer formation.

Model Equations

$$\nabla \cdot u = 0,$$

$$\dot{u} = -\nabla \cdot \left(u \otimes u + \frac{1}{\rho_0} P' I_3 \right) + \nu \Delta u - \left(\frac{\Theta'}{\Theta_0} - \frac{S'}{S_0} \right) g_z,$$

$$\dot{\Theta}' = -\nabla \cdot \left(u(\bar{\Theta} + \Theta') - \kappa_T \nabla \Theta' \right),$$

$$\dot{S}' = -\nabla \cdot \left(u(\bar{S} + S') - \kappa_S \nabla S' \right).$$

$u : \mathbb{R}^3 \to \mathbb{R}^2$ ... velocity

ρ_0 ... (constant) reference density

$P = \bar{P} + P'$ ... pressure, $S = \bar{S} + S'$ ... concentration

$\Theta = \bar{\Theta} + \Theta'$ ... temperature, Θ_0, S_0 ... reference values

κ_T ... thermal diffusion coefficient

κ_S ... mass concentration diffusion coefficient

g_z ... external source term, ν ... kinematic viscosity

Time Integrators

We investigate several TVD RK integrators:

The total variation in the spatial approximation should be reduced during time integration!

Commonly, this property comes with a time-step limitation: Guaranteed, if

$$\Delta t_{RK} \leq R_{CFL}^{(RK)} \Delta t_{FE}.$$

Classical order two: Osher/Shu (Heun's method).

Classical order three: Osher/Shu.

SDIRK methods $p = 2,\ p = 3$ by Ferracina & Spijker.

SDIRK Implementation

SDIRK, $p = 2$:

$$a_{i,j} = \begin{cases} \frac{1}{2s}, & i = j,\ 1 \le i \le s, \\ \frac{1}{s}, & 1 \le j < i \le s, \\ 0, & \text{otherwise}, \end{cases}$$

$$b_j = \frac{1}{s}, \quad j = 1, \ldots, s.$$

A-stable! CFL numbers: $R_{CFL} = 2s$.

Implementation with memory independent of s!

Explicit Euler predictor for free!

Step-size selected adaptively according to fixed point convergence! (Alternative iterators would allow larger time-steps, but considered intractable.)

Dissipative FD in Space

'Old ANTARES 1', 4th order, compatible with finite volume approach, extrapolation to cell boundaries:

$$
\begin{aligned}
f_j &:= (L_h^{[1]}u)_j = \frac{1}{12\Delta x}\left(-u_{j+2} + 8u_{j+1} - 8u_{j-1} + u_{j-2}\right), \\
\hat{f}_{j+1/2} &= \frac{1}{16}(-f_{j-1} + 9f_j + 9f_{j+1} - f_{j+2}), \\
\hat{f}_{j-1/2} &= \frac{1}{16}(-f_{j-2} + 9f_{j-1} + 9f_j - f_{j+1}), \\
(L_h^{[2]}f)_j &= \frac{\hat{f}_{j+1/2} - \hat{f}_{j-1/2}}{\Delta x} \\
&= \frac{1}{16\Delta x}\left(-f_{j+2} + 10f_{j+1} - 10f_{j-1} + f_{j-2}\right), \\
u''(x_j) &\approx (L_h u)_j = (L_h^{[2]} L_h^{[1]} u)_j.
\end{aligned}
$$

Dissipative FD in Space

'Old ANTARES 2', 4th order, compatible with finite volume approach, extrapolation to cell boundaries:

$$
\begin{aligned}
f_j &:= (L_h^{[1]}u)_j = \frac{1}{12\Delta x}\left(-u_{j+2} + 8u_{j+1} - 8u_{j-1} + u_{j-2}\right), \\
\hat{f}_{j+1/2} &= \frac{1}{12}(-f_{j-1} + 7f_j + 7f_{j+1} - f_{j+2}), \\
\hat{f}_{j-1/2} &= \frac{1}{12}(-f_{j-2} + 7f_{j-1} + 7f_j - f_{j+1}), \\
(L_h^{[2]}f)_j &= \frac{\hat{f}_{j+1/2} - \hat{f}_{j-1/2}}{\Delta x} = (L_h^{[1]}f)_j, \\
u''(x_j) &\approx (L_h u)_j = ((L_h^{[1]})^2 u)_j.
\end{aligned}
$$

Dissipative FD in Space

'New ANTARES', 4th order, compatible with finite volume approach, direct use of cell centers (corresponds with usual centered five-point stencil):

$$
\begin{aligned}
f_j &:= (L_h^{[1]} u)_j = \frac{1}{12\Delta x}\left(u_{j-1} - 15u_j + 15u_{j+1} - u_{j+2}\right), \\
(L_h^{[2]} f)_j &= \frac{1}{\Delta x}\left(f_j - f_{j-1}\right), \\
u''(x_j) &\approx (L_h u)_j = (L_h^{[2]} L_h^{[1]} u)_j .
\end{aligned}
$$

Dissipativity Analysis

- Consider stability function $R(z)$.
- Heat equation $\dot{u} = b\Delta u$.
- Associate spatial discretization $u_{j\pm k} \leftrightarrow \mathrm{e}^{\pm \mathrm{i}\theta k}$.
- Compute *amplification factor*

  $$g(\theta,\mu) = R((L_h u)_j), \qquad \mu = b\frac{\Delta t}{(\Delta x)^2}.$$

- Dissipative discretization:

  $|g(\theta,\mu)| < 1$ (possibly for $\mu \le C$).

  No oscillations: $0 < g(\theta,\mu) < 1$.

Amplification factor

For SDIRK with $p = 2,\ s = 1$,

$$g(\theta,\mu) = -\frac{\mu\,(\cos(\theta))^2 + 7\,\mu - 8\,\mu\,\cos(\theta) - 6}{\mu\,(\cos(\theta))^2 + 7\,\mu - 8\,\mu\,\cos(\theta) + 6}.$$

θ	$g(\theta,\mu)$
$-\pi$	$-\frac{-3+8\,\mu}{3+8\,\mu}$
$-\frac{3\pi}{4}$	$-\frac{-12+15\,\mu+8\,\mu\,\sqrt{2}}{12+15\,\mu+8\,\mu\,\sqrt{2}}$
$-\frac{\pi}{2}$	$-\frac{-6+7\,\mu}{6+7\,\mu}$
$-\frac{\pi}{4}$	$-\frac{12-15\,\mu+8\,\mu\,\sqrt{2}}{-12-15\,\mu+8\,\mu\,\sqrt{2}}$
0	1
$\frac{\pi}{4}$	$-\frac{12-15\,\mu+8\,\mu\,\sqrt{2}}{-12-15\,\mu+8\,\mu\,\sqrt{2}}$
$\frac{\pi}{2}$	$-\frac{-6+7\,\mu}{6+7\,\mu}$
$\frac{3\pi}{4}$	$-\frac{-12+15\,\mu+8\,\mu\,\sqrt{2}}{12+15\,\mu+8\,\mu\,\sqrt{2}}$
π	$-\frac{-3+8\,\mu}{3+8\,\mu}$

Step Size Limitations

Old space discretizations: $g(\pi, \mu) \equiv 1 \Rightarrow$ no damping.

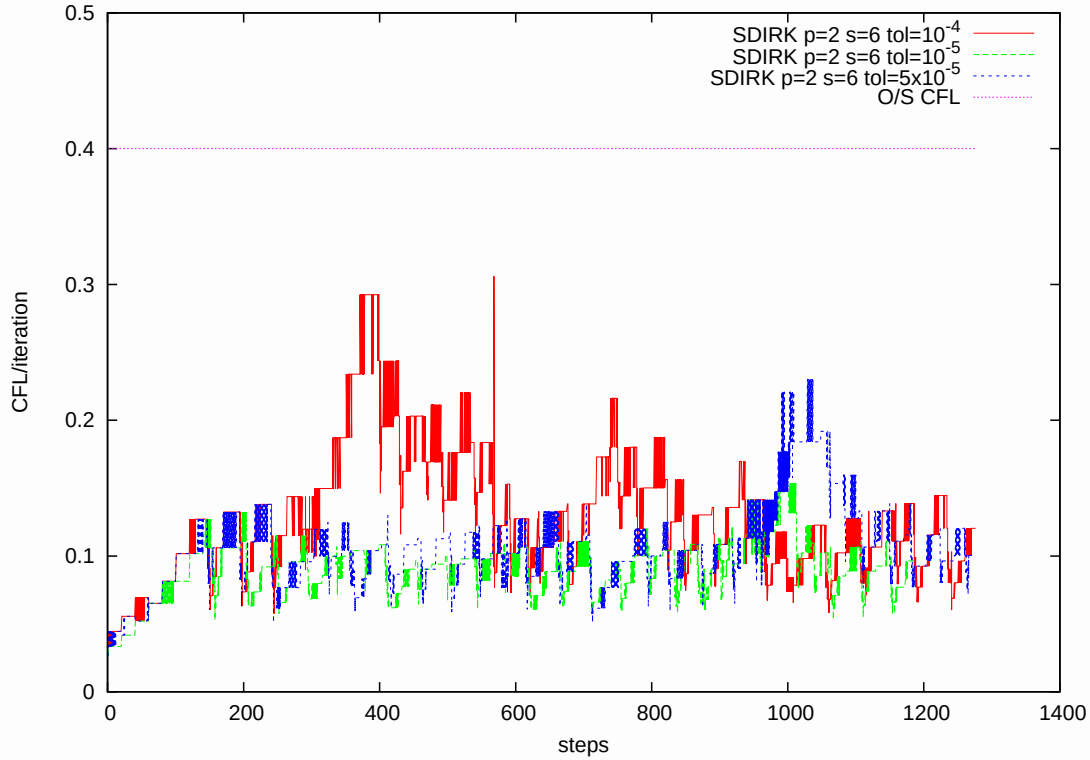
Restrictions on μ s.t. $0 < g(\pi, \mu) < 1$:

left: $g = 0, g' \neq 0$; middle: $g = 0$; right: $|g| = 1$.

Integrator / space discretization	3pt			New ANTARES		
SDIRK, $p = 2,\ s = 1$	0.5	0.5	—	0.375	0.375	—
SDIRK, $p = 2,\ s = 2$	—	1	—	—	0.75	—
SDIRK, $p = 2,\ s = 3$	1.5	1.5	—	1.125	1.125	—
SDIRK, $p = 2,\ s = 4$	—	2.0	—	—	1.5	—
SDIRK, $p = 3,\ s = 2$	—	—	3.232	—	—	2.424
SDIRK, $p = 3,\ s = 3$	2.328	2.328	9.273	1.746	1.746	6.955
SDIRK, $p = 3,\ s = 4$	—	—	15.25	—	—	11.44
explicit Euler	0.25	0.25	0.5	0.187	0.187	0.375
Osher/Shu, $p = 2$	—	—	0.5	—	—	0.375
Osher/Shu, $p = 3$	0.399	0.399	0.628	0.299	0.299	0.471

Numerical Results

Comparison of O/S ($p = 2$) and SDIRK ($p = 2,\ s = 6$):



Performance needs further tuning!

We expect higher efficiency for other models (A-stars)!

Results

The movie shows two runs:

O/S ($p = 2$) (left) and SDIRK ($p = 2,\ s = 6$) (right).

Differences explained by:

- Turbulence.
- Random initial perturbations.

[Plot of mass concentration (salinity)]

(. . . start movie . . .)

Conclusions and Outlook

- Convergence of high-order splitting methods. ✓
- Embedded splitting — efficient local error estimate, adaptive time-stepping. ✓
- Dissipative FD space discretization for flow problems. ✓
- TVD Runge–Kutta methods for astrophysics. ✓
- SDIRK methods have less strict step-size restrictions for dissipativity. ✓
- SDIRK $p = 3$: smaller error constant, fewer fixed point iterations, same memory demand.

  TODO: Implementation in ANTARES code.

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