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

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Consider

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

\(A\) \ldots linear differential operator,
\(B(u)\) \ldots nonlinear operator, generally unbounded.

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

\[ \varphi_{F}^t(\psi_0) \ldots \text{flow of} \quad \dot{\psi} = F(\psi), \quad \psi(0) = \psi_0. \]

**Lie derivative** \( D_F \)

\[
(D_F G)(\psi) := \left. \frac{d}{dt} \right|_{t=0} G(\varphi_{F}^t(\psi)) = G'(\psi)F(\psi).
\]

\[
(\exp(tD_F)G)(\psi) := G(\varphi_{F}^t(\psi)).
\]

**Commutator**

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

Define recursively iterated commutators

\[
ad^0_{D_A}(D_B)u := D_B u, \quad ad^j_{D_A}(D_B)u := [D_A, ad^{j-1}_{D_A}(D_B)](u).
\]
Higher-Order Splittings

\[ u_{n+1} = S(h, u_n) := \prod_{j=1}^{s} e^{a_{s+1-j} hD_A} e^{b_{s+1-j} hD_B} u_n, \quad n = 0, 1, \ldots \]

**Theorem:** The defect of the splitting operator admits the expansion

\[
e^{hD_{A+B}} v - S(h, v) \sim \sum_{k=1}^{p} \sum_{\mu \in \mathbb{N}^k} \frac{1}{\mu!} h^{k+|\mu|} C_{k\mu} \prod_{\ell=1}^{k} \text{ad}_{D_A(D_B)}^{\mu_\ell} e^{hD_A} v.
\]

\(C_{k\mu} \ldots\) computable constants.

The remainder term can be proven separately to be of higher order.
Time-dependent Schrödinger equation (TDSE)

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

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

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

\( \Delta^{(k)} \) \ldots Laplace operator w. r. t. \( k \)-th particle.
Pauli principle implies antisymmetry in \( \psi \! \).  
Fermions indistinguishable!
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

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

Additional constraints for uniqueness

\[ \left\langle \phi_j \left| \phi_k \right. \right\rangle = \delta_{j,k}, \quad \left\langle \phi_j \left| \frac{\partial \phi_k}{\partial t} \right. \right\rangle = -i \left\langle \phi_j \left| T \right| \phi_k \right. \right\rangle. \]
This yields the equations of motion

\[
\begin{align*}
    i \frac{da_J}{dt} &= \sum_K \langle \Phi_J | V | \Phi_K \rangle a_K =: A_V(\phi)a, \\
    i \frac{\partial \phi_j}{\partial t} &= T \phi_j + (1 - P) \sum_k \sum_l \rho_{j,l}^{-1} V_{l,k} \phi_k =: T \phi + B_V(a, \phi),
\end{align*}
\]

where

\[
\begin{align*}
    \psi_j &:= \langle \phi_j | u \rangle, \quad \text{“single-hole functions”}, \\
    \rho_{j,l} &:= \langle \psi_j | \psi_l \rangle, \quad \text{“density matrix”}, \\
    \overline{V}_{l,k} &:= \langle \psi_l | V | \psi_k \rangle, \quad \text{“mean-field operator matrix”}, \\
    P &:= \sum_j |\phi_j\rangle \langle \phi_j|, \quad \text{(orthogonal projector)}.
\end{align*}
\]
Variational Splitting

Time propagation by high-order splitting method

\[
    u_{n+1} = \prod_{j=1}^{s} e^{a_{s+1-j} D_T} e^{b_{s+1-j} D_V} u_n, \quad 0 \leq n \leq N - 1.
\]

1. **\( e^{a_j D_T} u_0 \):** Compute the solution at time \( t_0 + a_j h \) of

\[
    \left\langle \delta u \left| i \frac{\partial}{\partial t} - T \right| u \right\rangle = 0 \quad \forall \delta u \in T_u M, \quad u(t_0) = u_0.
\]

2. **\( e^{b_j D_V} u_0 \):** Compute the solution at time \( t_0 + b_j h \) of

\[
    \left\langle \delta u \left| i \frac{\partial}{\partial t} - V \right| u \right\rangle = 0 \quad \forall \delta u \in T_u M, \quad u(t_0) = u_0.
\]
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

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

$C = C(M_m)$, $m = p = 2$ or $m = 2p - 3, \quad p \geq 3$,

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

$C = C(M_m)$, $m = p = 2, 3$ or $m = 2p - 4, \quad p \geq 4$. 
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 $H^1$ ⇒ 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 $L^2$. 
We use *embedded pairs* of splitting formulae for estimating the local error:

$$j \quad a_j$$  $$j \quad b_j$$

<table>
<thead>
<tr>
<th>$j$</th>
<th>$a_j$</th>
<th>$j$</th>
<th>$b_j$</th>
</tr>
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<tbody>
<tr>
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<td>0.0829844064174052</td>
</tr>
<tr>
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<tr>
<td>3,6</td>
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<td>3,5</td>
<td>$-0.0390563049223486$</td>
</tr>
<tr>
<td>4,5</td>
<td>$1/2 - (a_2 + a_3)$</td>
<td>4</td>
<td>$1 - 2(b_1 + b_2 + b_3)$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$j$</th>
<th>$\hat{a}_j$</th>
<th>$j$</th>
<th>$\hat{b}_j$</th>
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<td>1</td>
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</tr>
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<td>$a_4$</td>
<td>4</td>
<td>$b_4$</td>
</tr>
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<td>6</td>
<td>1.4878666594737946</td>
<td>6</td>
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<tr>
<td>7</td>
<td>$-1.3630829287974774$</td>
<td>7</td>
<td>0</td>
</tr>
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</table>
Cubic NLS with blow-up solution:

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

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

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

Time-stepping for a complex 4(3) pair:
Model of stellar convection and pulsation → 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 $\implies$ convection.
- Mass concentration (salinity) gradient $\implies$ counteracting convection.
- Radiative transport $\leftrightarrow$ diffusion approximation.
- Boussinesq approximation: Density variations only in buoyancy term of vertical velocity equation.
- Feature: Layer formation.
**Model Equations**

\[ \nabla \cdot u = 0, \]

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

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

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

\( u : \mathbb{R}^3 \to \mathbb{R}^2 \ldots \text{velocity} \)

\( \rho_0 \ldots \text{(constant) reference density} \)

\( P = \bar{P} + P' \ldots \text{pressure}, \quad S = \bar{S} + S' \ldots \text{concentration} \)

\( \Theta = \bar{\Theta} + \Theta' \ldots \text{temperature}, \quad \Theta_0, S_0 \ldots \text{reference values} \)

\( \kappa_T \ldots \text{thermal diffusion coefficient} \)

\( \kappa_S \ldots \text{mass concentration diffusion coefficient} \)

\( g_z \ldots \text{external source term}, \quad \nu \ldots \text{kinematic viscosity} \)
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

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

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, $p = 2$:

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

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

$A$-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:

\[ f_j := (L^1_h u)_j = \frac{1}{12\Delta x} (-u_{j+2} + 8u_{j+1} - 8u_{j-1} + u_{j-2}), \]

\[ \hat{f}_{j+1/2} = \frac{1}{16} (-f_{j-1} + 9f_j + 9f_{j+1} - f_{j+2}), \]

\[ \hat{f}_{j-1/2} = \frac{1}{16} (-f_{j-2} + 9f_{j-1} + 9f_j - f_{j+1}), \]

\[ (L^2_h f)_j = \frac{\hat{f}_{j+1/2} - \hat{f}_{j-1/2}}{\Delta x} \]
\[ \approx \frac{1}{16\Delta x} (-f_{j+2} + 10f_{j+1} - 10f_{j-1} + f_{j-2}), \]

\[ u''(x_j) \approx (L_h u)_j = (L^2_h L^1_h u)_j. \]
Dissipative FD in Space

‘Old ANTARES 2’, 4\textsuperscript{th} order, compatible with finite volume approach, extrapolation to cell boundaries:

\[ f_j := (L_h^1 u)_j = \frac{1}{12\Delta x} \left( -u_{j+2} + 8u_{j+1} - 8u_{j-1} + u_{j-2} \right), \]

\[ \hat{f}_{j+1/2} = \frac{1}{12} \left( -f_{j-1} + 7f_{j} + 7f_{j+1} - f_{j+2} \right), \]

\[ \hat{f}_{j-1/2} = \frac{1}{12} \left( -f_{j-2} + 7f_{j-1} + 7f_{j} - f_{j+1} \right), \]

\[ (L_h^2 f)_j = \frac{\hat{f}_{j+1/2} - \hat{f}_{j-1/2}}{\Delta x} = (L_h^1 f)_j, \]

\[ u''(x_j) \approx (L_h u)_j = ((L_h^1)^2 u)_j. \]
\textbf{Dissipative FD in Space}

‘New ANTARES’, 4\textsuperscript{th} order, compatible with finite volume approach, direct use of cell centers (corresponds with usual centered five-point stencil):

\[ f_j := (L_h^{[1]} u)_j = \frac{1}{12\Delta x} (u_{j-1} - 15u_j + 15u_{j+1} - u_{j+2}), \]

\[ (L_h^{[2]} f)_j = \frac{1}{\Delta x} (f_j - f_{j-1}), \]

\[ u''(x_j) \approx (L_h u)_j = (L_h^{[2]} L_h^{[1]} u)_j. \]
Consider stability function $R(z)$.

Heat equation $\dot{u} = b\Delta u$.

Associate spatial discretization $u_j \leftrightarrow e^{\pm i\theta k}$.

Compute amplification factor

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

Dissipative discretization:

\[ |g(\theta, \mu)| < 1 \quad \text{(possibly for } \mu \leq C). \]

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

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

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

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

Restrictions on \( \mu \) s.t. \( 0 < g(\pi, \mu) < 1 \):
- **left**: \( g = 0, g' \neq 0 \);
- **middle**: \( g = 0 \);
- **right**: \(|g| = 1\).

<table>
<thead>
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<th>Integrator / space discretization</th>
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<th>New ANTARES</th>
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</thead>
<tbody>
<tr>
<td>SDIRK, ( p = 2, s = 1 )</td>
<td>0.5</td>
<td>0.375</td>
</tr>
<tr>
<td>SDIRK, ( p = 2, s = 2 )</td>
<td>—</td>
<td>0.75</td>
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<tr>
<td>SDIRK, ( p = 2, s = 3 )</td>
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<td>1.125</td>
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<tr>
<td>SDIRK, ( p = 2, s = 4 )</td>
<td>—</td>
<td>1.5</td>
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<tr>
<td>SDIRK, ( p = 3, s = 2 )</td>
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<tr>
<td>SDIRK, ( p = 3, s = 3 )</td>
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<td>SDIRK, ( p = 3, s = 4 )</td>
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<tr>
<td>explicit Euler</td>
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<tr>
<td>Osher/Shu, ( p = 2 )</td>
<td>—</td>
<td>0.375</td>
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<tr>
<td>Osher/Shu, ( p = 3 )</td>
<td>0.399</td>
<td>0.471</td>
</tr>
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</table>
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)!
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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