Minimally implicit Runge-Kutta (MIRK) methods and astrophysical applications

New Frontiers in Strong Gravity
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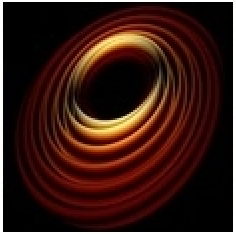

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Strong hyperbolic systems of PDEs:

$$\partial_t U + \partial_i F^i(U) = S(U),$$

If we definde $A^i = \partial F^i / \partial x_j$, for any arbitrary spatial vector ξ_i ,

we request that the combination $\xi_i \cdot A^i$ has real eigenvalues and a complete set of eigenvectors.

The eigenvalues are the local velocities of the propagation of the information in the evolution system of equations.
The eigenvectors indicate the different directions of propagation.
Strong hyperbolic systems of equations are well-posed.

The source term (linear or non-linear) can contain parts that lead to the development of numerical instabilities if explicit methods are used.
The time step required for stable simulations is much smaller than the desirable / allowed for accuracy: stiff source term → e.g., dealing with very different scales.

Goal: Application of the Minimally-Implicit Runge-Kutta (MIRK) methods
in some hyperbolic systems of PDEs with stiff source terms.
Succesfully applied in some astrophysical scenarios.

Contents:

→ MIRK methods for the RRMHD equations.
[I. Cordero-Carrión, S. Santos-Pérez, C. Martínez-Vidallach. AMC 443, 127774 (2023)]

→ MIRK methods for the neutrino transport equations (M1 scheme) in supernovae simulations.
[S. Santos-Pérez, M. Obergaulinger, I. Cordero-Carrión. Arxiv:2302.12089 ++]

→ General idea and potential future applications.

MIRK methods for the RRMHD equations

·· Magnetic fields are key in accretion disks, AGN, relativistic jets, compact objects.

·· A consistent treatment is necessary to avoid numerical resistivity.

·· Hyperbolic equations + constraints (divergence of magnetic and electric fields) → augmented system of hyperbolic equations [Komissarov 2007] (velocity, density, electric and magnetic fields, two additional scalar equations).

·· Structure of the equations:

$$\partial_t E^j = S_E^j - \sigma W[E^j + (v \times B)^j - (v_l E^l) v^j] = \tilde{S}_E^j,$$

$$\partial_t B^j = S_B^j,$$

$$\partial_t Y = S_Y,$$

·· Avoid numerical instabilities due to stiff source term in the evolution equation for the electric field for high conductivities.

MIRK methods for the RRMHD equations

·· PIRK methods to deal with wave-like equations (electric and magnetic fields) for low-order methods.
[I. C.-C. and P. Cerdá-Durán, arXiv:1211.5930 (2012)]
[I. C.-C. and P. Cerdá-Durán, SEMA SIMAI Springer Series Vol. 4 (2014)]

$$\begin{cases} u_t = \mathcal{L}_1(u,v), \\ v_t = \mathcal{L}_2(u) + \boxed{\mathcal{L}_3(u,v)}, \end{cases}$$

linearization: $$\begin{cases} u_t = \bar{\alpha}_1 u + \bar{\alpha}_2 v, \\ v_t = \bar{\gamma}_1 u + \bar{\gamma}_2 v + \boxed{\bar{\lambda} u}, \end{cases}$$

wave-like eq.: $$(\bar{\alpha}_1 - \bar{\gamma}_2)^2 + 4\bar{\alpha}_2(\bar{\gamma}_1 + \bar{\lambda}) < 0.$$

·· Ideal limit: infinite conductivity and $E^i = -(\boldsymbol{v} \times \boldsymbol{B})^i$.

·· Implicit / Semi-implicit methods include additional recoveries of primitive variables from conserved ones [Palenzuela et al. 2009] → potential convergence problems, additional computational cost.

MIRK methods for the RRMHD equations

·· First-order MIRK method (stability criteria to select coefficients):

$$E^j|_{n+1} = E^j|_n + \Delta t\, S_E^j|_n - \Delta t\, \overline{\sigma}|_n \left[c_1 E^j|_n + (1-c_1) E^j|_{n+1} + c_2 (v \times B)^j|_n \right.$$
$$\left. + (1-c_2)(v|_n \times B|_{n+1})^j - c_3 v^j|_n v_l|_n E^l|_n - (1-c_3) v^j|_n v_l|_n E^l|_{n+1}\right],$$
$$B^j|_{n+1} = B^j|_n + \Delta t\, S_B^j|_n,$$
$$Y|_{n+1} = Y|_n + \Delta t\, S_Y|_n.$$

→ Pure explicit method with an effective time step:

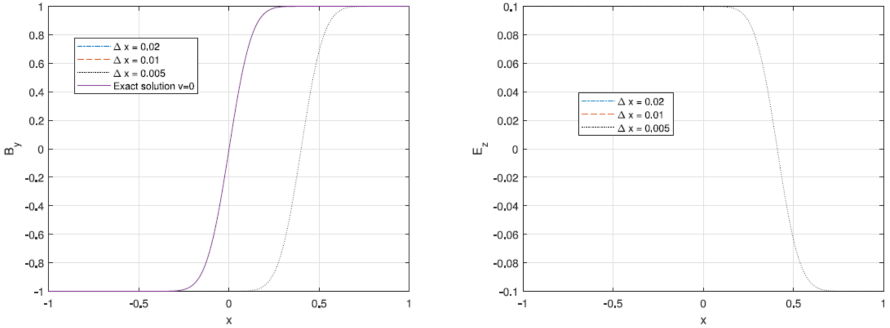
$$E^i|_{n+1} = E^i|_n + \frac{\Delta t}{1 + \Delta t\, \overline{\sigma}|_n}\left[S_E^i|_n + \overline{\sigma}|_n E^l|_n \left(v^i|_n v_l|_n - \delta_l^i\right) - \overline{\sigma}|_n (v|_n \times B|_{n+1})^i\right]$$

·· Analogous derivation for the two-stage second-order MIRK method.

MIRK methods for the RRMHD equations

·· Applications: Self-similar current sheet: 1D problem; CFL=0.8; initial data at t=1:

$$\boldsymbol{v} = (v^x, 0, 0),\ \boldsymbol{E} = (0, 0, 0),\ \boldsymbol{B} = (0, B^y(x, t=1), 0),\quad B^y_e(x,t) = \mathrm{erf}\left(\frac{x}{2}\sqrt{\frac{\sigma}{t}}\right) \qquad \sigma = 10^3$$



Stable simulations with zero and non-zero velocities ($v_x = 0.1$),
first and second-order methods.

MIRK methods for the RRMHD equations

·· Applications: Circular Polarized Alfvén waves: 1D; full system (including matter); EoS for an ideal fluid, $\Gamma = 4/3$; $\rho(x,0) = p(x,0) = 1$; CFL=0.3 → 0.7; $\sigma = 10^8$; KO term;

$$\boldsymbol{B}(x,0) = B_0\,(1, \cos(kx), \sin(kx)),$$

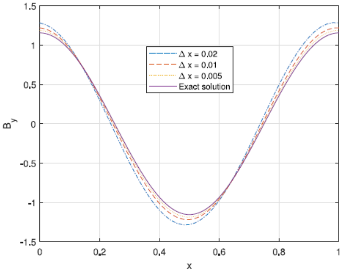
with $k = 2\pi$ and $B_0 = 1.1547$, and

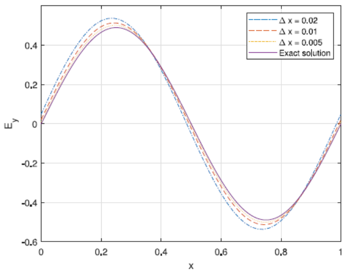
$$\boldsymbol{E}(x,0) = -\boldsymbol{v}(x,0) \times \boldsymbol{B}(x,0),$$

with $\boldsymbol{v}(x,0) = \frac{v_A}{B_0}(0, B^y(x,0), B^z(x,0))$ and $v_A = 0.423695$

Stable simulations, with first and second-order methods.

Exact solution refers to the one in the stiff limit (close enough for very high conductivities).





MIRK methods for the M1 neutrino transport equations

·· The explosion mechanism of CCSNe cannot be understood without a detailed account of the generation and transport of neutrinos.

·· Boltzmann equation (7D problem) → momentum-space integration of the distribution function. Truncation: n=0 or diffusion; n=1, quite used – M1 scheme.

·· Optically thick regime → very different timescales of different interactions and stiff source term for very high opacities.

·· Structure of the equations: (emission, absorption, scattering... potentially stiff)

$$\partial_t E = S_E + C^{(0)}, \qquad C^{(0)} = c\,\kappa_a (E_{\rm eq} - E),$$
$$\partial_t F^i = S_F^i + C^{(1),i}, \qquad C^{(1),i} = -c\,\kappa_{\rm tra} F^i.$$

Failing in the optically thick regime where $c\kappa\Delta t \gg 1$

·· IMEX-like method [Just et al. 2015]. Complexity of applying IMEX methods: opacities, equilibrium profile.

MIRK methods for the M1 neutrino transport equations

·· Similar derivation of MIRK methods, taking into account stability and limit at the stiff limit: effective time-step when written similar to explicit methods.

→ First-order:

$$E^{n+1} = E^n + \frac{\Delta t}{1+\Delta t\,\kappa^n}\left[S_E^n + \kappa^n(E^n_{\rm eq} - E^n)\right]$$

$$(F^i)^{n+1} = (F^i)^n + \frac{\Delta t}{1+\Delta t\,\kappa'^n}\left[(S_F^i)^n - \kappa'^n(F^i)^n\right]$$

→ Second-order: (similar expressions for F)

$$E^{(1)} = E^n + \Delta t\left[S_E^n + a\,\kappa^n(E^n_{\rm eq} - E^n) + (1-a)\,\kappa^n(E^n_{\rm eq} - E^{(1)})\right],$$

$$E^{n+1} = \frac{1}{2}[E^{(1)} + E^n] + \Delta t\left[\frac{1}{2}S_E^{(1)} + a'\,\kappa^{(1)}(E^{(1)}_{\rm eq} - E^{(1)}) + \frac{1-a}{2}\kappa^{(1)}(E^{(1)}_{\rm eq} - E^n) + \left(\frac{a}{2} - a'\right)\kappa^{(1)}(E^{(1)}_{\rm eq} - E^{n+1})\right],$$

Opt 1) Second order at the stiff limit for smooth variables:

$a' = \frac{a-1}{2}$ (similar for b').

Opt 2) Guarantee of stiff limit even if non-smooth variables:

$b' = \frac{(1-b)^2}{2b}$, $b \in (-\infty, 0) \cup (1/2, 1)$ (similar for a').

MIRK methods for the M1 neutrino transport equations

·· Applications: Simple test: test 1 from [J.A. Pons, J.M. Ibáñez, J.A. Miralles, MNRAS 317, 550-562 (2000)]:

Difussion limit (P = p E = E/3) in spherical symmetry (1D problem) and $\kappa_{\rm a} = 0$:

$$\partial_t E + \partial_r F + \frac{F}{r} = -c\,\kappa_{\rm a}\left(E_{\rm eq} - E\right) \quad (\kappa_{\rm a} \rightarrow 0)$$

$$\partial_t F + \partial_r P + \frac{3P - E}{r} = -c\,\kappa_{\rm tra} F \quad \left(\frac{3P-E}{r} \rightarrow 0\right)$$

Analytical solution, c=1 (geometrical units):

$$E(t,r) = \left(\frac{\kappa_{\rm tra}}{t}\right)^{3/2} \exp\left(-\frac{3\kappa_{\rm tra} r^2}{4t}\right), \qquad F(t,r) = \frac{r}{2t} E(t,r)$$

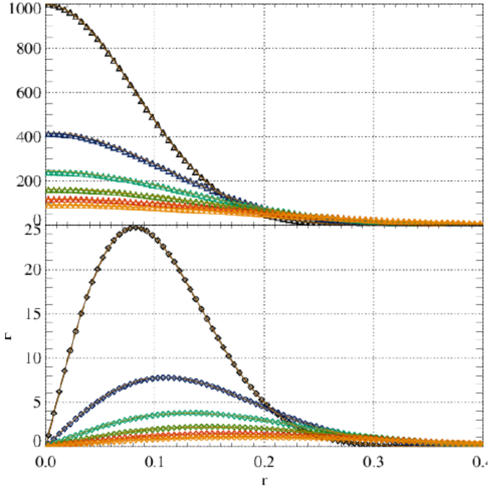
MIRK methods for the M1 neutrino transport equations

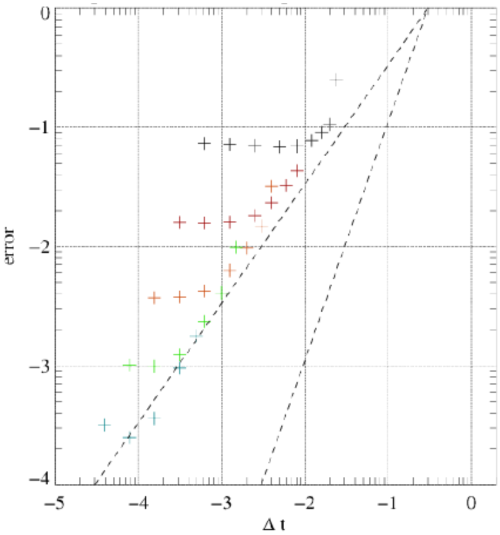
·· Applications: Simple test: kappa=100 (optically thin) and kappa=10^5 (optically thick).

Exact solution used at boundary conditions and initial data at t=1.
Solid lines: exact solution.

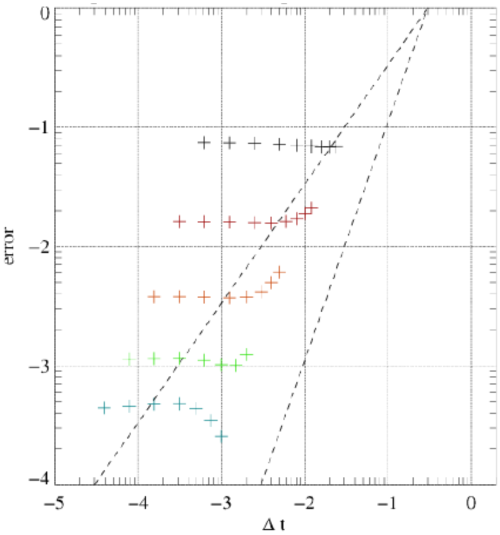
Convergence study with the L2 norm.
Several spatial reconstructions.
Temporal integrator: RK1 / RK2 with MIRK1 / MIRK2 as building block of substeps.

Total error: sum of spatial + temporal errors – each one with own scaling [Rembiasz et al., 2017].

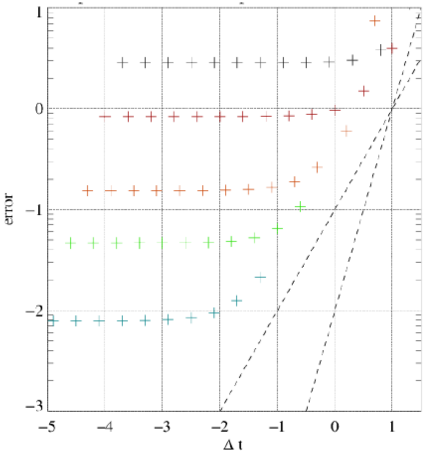




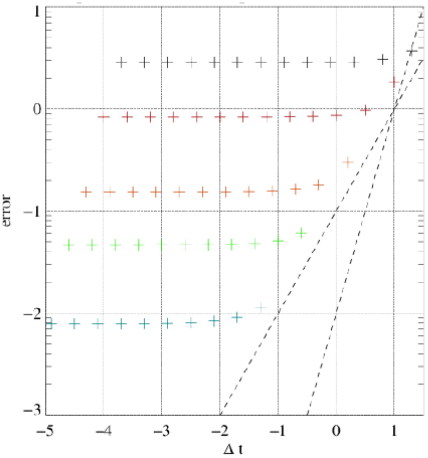
kappa=100, PLM-MIRK1



kappa=100, PLM-MIRK2



kappa=10^5, PLM-MIRK1



kappa=10^5, PLM-MIRK2

- Spatial scaling: 2nd order.
- Temporal scaling: more difficult to measure, looks like 1st to 2nd order.
- MIRK2 seems to show lower error.

MIRK methods for the M1 neutrino transport equations

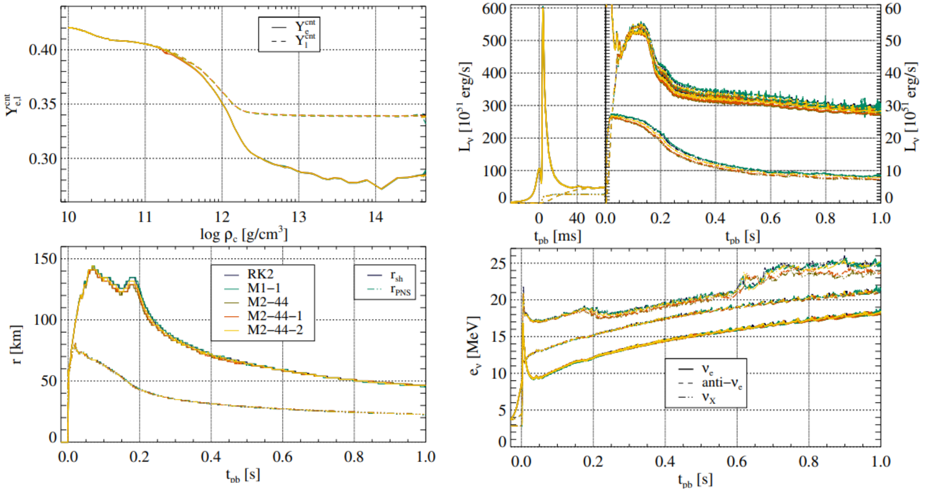
·· Applications: Spherically symmetric core-collapse.
15 solar mass star, SFHo EoS, standard set of reactions (see more details in arXiv reference).

·· Linear stability at stiff limit and recovery of stiff limit:
→ Wrong parameters: unstable simulations.
→ Stability not forcing recovery: stable but wrong simulation.
→ Stability + recovery: expected and stable Results.

·· Slight modifications from pure explicit methods and similar computational cost.

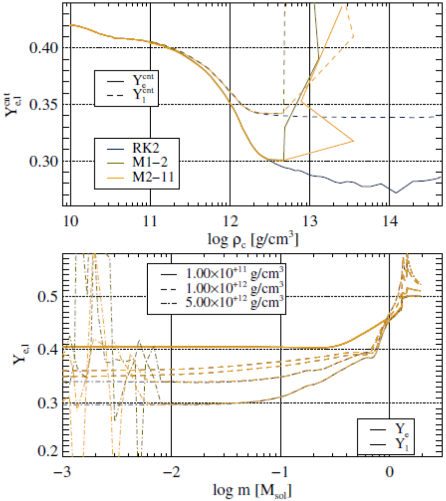
model	a	a'	b	b'	result
M2-11	+1/2	−1/4	+1/2	−1/4	×
M2-12	+1/2	−1/4	+1/2	+1/4	×
M2-13	+1/2	−1/4	−1/2	−3/4	×
M2-14	+1/2	−1/4	−1/2	−9/4	△
M2-21	+1/2	+1/4	+1/2	−1/4	×
M2-22	+1/2	+1/4	+1/2	+1/4	×
M2-23	+1/2	+1/4	−1/2	−3/4	×
M2-24	+1/2	+1/4	−1/2	−9/4	△
M2-31	−1/2	−3/4	+1/2	−1/4	×
M2-32	−1/2	−3/4	+1/2	+1/4	×
M2-33	−1/2	−3/4	−1/2	−3/4	×
M2-34	−1/2	−3/4	−1/2	−9/4	△
M2-41	−1/2	−9/4	+1/2	−1/4	×
M2-42	−1/2	−9/4	+1/2	+1/4	×
M2-43	−1/2	−9/4	−1/2	−3/4	×
M2-44	−1/2	−9/4	−1/2	−9/4	✓
M2-44-1	−1/4	−25/8	−1/4	−25/8	✓
M2-44-2	−1/16	−289/32	−1/16	−289/32	✓
M2-44-3	−1/2	−9/4	−1/4	−25/8	✓
M2-44-4	−1/4	−25/8	−1/2	−9/4	✓
M2-51	−1/2	−9/4	3/4	1/24	×
M2-52	−1/2	−9/4	3/4	−1/8	×
M2-53	3/4	1/24	3/4	1/24	×
M2-54	3/4	−1/8	−1/2	−9/4	△
M2-55	3/4	1/24	−1/2	−9/4	✓

MIRK methods for the M1 neutrino transport equations

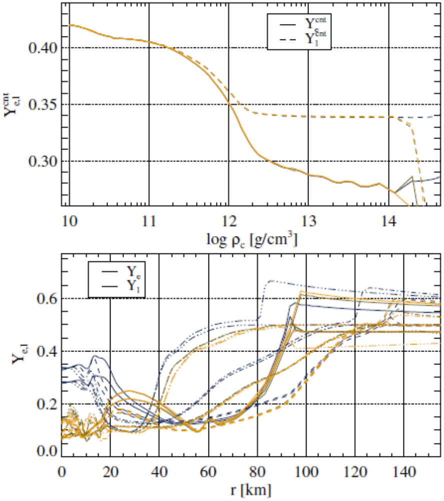


Stability
+
recovery

MIRK methods for the M1 neutrino transport equations



Wrong parameters



Stability not forcing recovery

General idea and potential future applications

·· Hyperbolic equations with stiff source terms which can be somehow linearized with respect to the conserved (evolved) variables:

$$\partial_t U + \partial_i F^i(U) = S(U), \qquad S(U) = S_E(U) + \frac{1}{\epsilon}[S_I(U) - U_0];$$

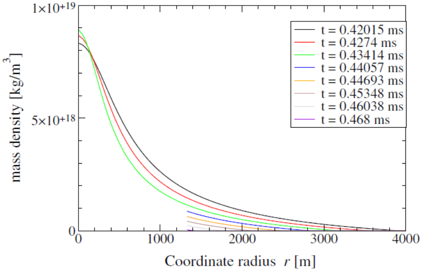
$$S_I(U) = \sum_{i=1}^{n} G_i(U) \boxed{U^i.}$$

Only the conserved variables are evaluated implicitly.
The factors multiplying these conserved variables are always evaluated explicitly.

·· Other potential examples: general relativistic force-free electrodynamics, rarefied gases problems, shallow water equations with friction...

Black hole singularities: infinite cannot be treated numerically

→ Remap somehow your space-time: puncture method commonly used in free evolution schemes (BSSN) and BBH simulations.



→ Excise a topological sphere from your numerical grid containing the black hole singularity:

· Pretorius 2005 simulations used GHG and excision.

· Excision can be combined with the CFC formulation [Cordero-Carrión et al., 2014].

· Small modification recently used in core-collapse simulations [B. Sykes et al., 2023].

More ideas are about to come in the 1D case.
More research needed for 2D / 3D cases.