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Composition schemes for the guiding-center model

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Abstract. We present composition schemes for solving non-linear transport equations, like the guiding-center model. This is based on direct and adjoint transport steps. The adjoint steps being implicit, they are replaced by explicit approximated adjoint steps using a given number of fixed point iterations. This does not modify the order of accuracy. Several numerical tests assess the performance of the method.

Keywords: composition scheme, splitting, semi-Lagrangian, guiding-center model

1 Introduction

The guiding-center model is a non-linear two-dimensional transport equation that describes a specific drift undergone by charged particles confined in a Tokamak by a strong magnetic field. More precisely, denoting $f = f(t,x,y)$ the density of the charged particles and $\Phi = \Phi(t,x,y)$ the electrostatic potential, the guiding-center model writes:

$$\begin{cases} \partial_t f + \partial_y \Phi \, \partial_x f - \partial_x \Phi \, \partial_y f = 0, \\ -\partial_{xx}\Phi - \partial_{yy}\Phi = f, \end{cases} \tag{1}$$

with $t \in [0,T]$, $x \in [0,L_1]$, $y \in [0,L_2]$ and $T > 0$, $L_1 > 0$, $L_2 > 0$. This is simplified model for turbulence in Tokamak. In order to make accurate predictions, high-order methods are essential.

In this work, we focus on the time discretization. Different schemes have been used in the litterature, especially in the context of semi-Lagrangian methods [10, 2, 6, 4, 9, 7, 11]. We propose here to use a composition scheme in the spirit of [7]. Composition schemes consist in chaining direct and adjoint steps. These methods are interesting because they only need to store one or two copies of the density f. In contrast, high-order Runge-Kutta methods require more storage.

Direct steps are explicit and can be either a 2d transport scheme or a splitting scheme, which is the composition of two 1d transport along the two directions. For these two kind of direct steps, we can identify their associated adjoint steps.

Since the adjoint steps are actually implicit, we propose to replace them by a fixed point algorithm as in [3]. Note that it is sufficient to take the number

of iterations equal to the desired order of accuracy. Contrary to [7], we consider composition schemes with non-symmetric coefficients. Indeed, taking benefit from the equivalence from composition and splitting schemes [5], we use the coefficients obtained from the second order O2 and the fourth order O4 splitting schemes. This enables to optimize the number of steps at a given accuracy.

The rest of the article is as follows. In Section 2, we first detail the direct and adjoint steps, before describing the composition scheme in Section 3. Numerical results are given in Section 4, before concluding in Section 5.

2 Direct and adjoint steps

In this section, we first define the elementary steps involved in the time discretization of the guiding center equation (1).

First, we define the transport operator over a time interval Δt starting from the initial condition g_2 and with advection potential obtained from g_1:

$$\mathcal{T}_{\Delta t}^{\alpha\beta}[g_1]g_2 = g(\Delta t, \cdot, \cdot),$$

where g is the solution to:

$$\begin{cases} \partial_t g + \alpha\, \partial_y \Phi\, \partial_x g - \beta\, \partial_x \Phi\, \partial_y g = 0, \\ -\partial_{xx}\Phi - \partial_{yy}\Phi = g_1, \\ g_{|t=0} = g_2. \end{cases}$$

Let now consider $t_0 = 0 < t_1 < \cdots < t_N = T$ and $f^n \simeq f(t_n, ., .)$. Then, at iteration $n \in \mathbb{N}$, denoting $\Delta t = t_{n+1} - t_n$, the first order direct $2d$ step writes

$$f^{n+1} = \mathcal{S}_{\Delta t}^{2d} f^n = \mathcal{T}_{\Delta t}^{11}[f^n] f^n, \tag{2}$$

while the direct splitting step is given by

$$f^{n+1} = \mathcal{S}_{\Delta t}^{xy} f^n = \mathcal{T}_{\Delta t}^{01}[f^n]\mathcal{T}_{\Delta t}^{10}[f^n] f^n, \tag{3}$$

which corresponds to first make the advection in x and then in y. This splitting version is more adapted to parallelization. The two schemes can be written:

$$f^{n+1} = \mathcal{R}_{\Delta t}[f^n] f^n,$$

with $\mathcal{R}_{\Delta t}[g] = \mathcal{T}_{\Delta t}^{11}[g]$ for the 2d scheme and $\mathcal{R}_{\Delta t}[g] = \mathcal{T}_{\Delta t}^{01}[g]\mathcal{T}_{\Delta t}^{10}[g]$ for the splitting scheme.

Given a scheme $\mathcal{S}_{\Delta t}$, its adjoint is defined as follows: $\mathcal{S}_{\Delta t}^* = (\mathcal{S}_{-\Delta t})^{-1}$.

Proposition 1. *The adjoints of the first order 2d and splitting steps are:*

$$f^{n+1} = \mathcal{S}_{\Delta t}^{2d,*} f^n = \mathcal{T}_{\Delta t}^{11}[f^{n+1}] f^n,$$
$$f^{n+1} = \mathcal{S}_{\Delta t}^{xy,*} f^n = \mathcal{T}_{\Delta t}^{10}[f^{n+1}]\mathcal{T}_{\Delta t}^{01}[f^{n+1}] f^n.$$

They can be written:

$$f^{n+1} = \mathcal{R}_{\Delta t}^*[f^{n+1}] f^n,$$

with $\mathcal{R}_{\Delta t}^*[g] = \mathcal{T}_{\Delta t}^{11}[g]$ for the 2d adjoint step and $\mathcal{R}_{\Delta t}^*[g] = \mathcal{T}_{\Delta t}^{10}[g]\mathcal{T}_{\Delta t}^{01}[g]$ for the splitting adjoint step.

Proof. For the direct scheme, by defining $\mathcal{I}^{2d}_{\Delta t} g = \mathcal{T}^{11}_{-\Delta t}[(\mathcal{S}^{2d}_{\Delta t})^{-1} g] g$, we have

$$\mathcal{I}^{2d}_{\Delta t}\mathcal{S}^{2d}_{\Delta t} g = \mathcal{T}^{11}_{-\Delta t}[(\mathcal{S}^{2d}_{\Delta t})^{-1}\mathcal{S}^{2d}_{\Delta t} g]\mathcal{S}^{2d}_{\Delta t} g = \mathcal{T}^{11}_{-\Delta t}[g]\mathcal{S}^{2d}_{\Delta t} g = g.$$

This leads to

$$S^{2d,*}_{\Delta t} f^n = \mathcal{I}^{2d}_{-\Delta t} f^n = \mathcal{T}^{11}_{\Delta t}[(\mathcal{S}^{2d}_{-\Delta t})^{-1} f^n] f^n = \mathcal{T}^{11}_{\Delta t}[S^{2d,*}_{\Delta t} f^n] f^n = \mathcal{T}^{11}_{\Delta t}[f^{n+1}] f^n.$$

For the splitting scheme, defining $\mathcal{I}^{xy}_{\Delta t} g = \mathcal{T}^{10}_{-\Delta t}[(\mathcal{S}^{xy}_{\Delta t})^{-1} g]\mathcal{T}^{01}_{-\Delta t}[(\mathcal{S}^{xy}_{\Delta t})^{-1} g] g$, we have

$$\begin{aligned}\mathcal{I}^{xy}_{\Delta t}\mathcal{S}^{xy}_{\Delta t} g &= \mathcal{T}^{10}_{-\Delta t}[(\mathcal{S}^{xy}_{\Delta t})^{-1}\mathcal{S}^{xy}_{\Delta t} g]\mathcal{T}^{01}_{-\Delta t}[(\mathcal{S}^{xy}_{\Delta t})^{-1}\mathcal{S}^{xy}_{\Delta t} g]\mathcal{S}^{xy}_{\Delta t} g \\ &= \mathcal{T}^{10}_{-\Delta t}[g]\mathcal{T}^{01}_{-\Delta t}[g]\mathcal{T}^{xy}_{\Delta t} g = \mathcal{T}^{10}_{-\Delta t}[g]\mathcal{T}^{01}_{-\Delta t}[g]\mathcal{T}^{01}_{\Delta t}[g]\mathcal{T}^{10}_{\Delta t}[g] g = g.\end{aligned}$$

This leads to

$$\mathcal{S}^{xy,*}_{\Delta t} f^n = \mathcal{I}^{xy}_{-\Delta t} f^n = \mathcal{T}^{10}_{\Delta t}[(\mathcal{S}^{xy}_{-\Delta t})^{-1} f^n]\mathcal{T}^{01}_{\Delta t}[(\mathcal{S}^{xy}_{-\Delta t})^{-1} f^n] f^n = \mathcal{T}^{10}_{\Delta t}[f^{n+1}]\mathcal{T}^{01}_{\Delta t}[f^{n+1}] f^n.$$

As proposed in [3], the implicit adjoint steps can be approximated by K iterations of fixed point algorithm:

$$f^{n+1} = f^{n+1,K}, \quad f^{n+1,k} = \mathcal{R}^*_{\Delta t}[f^{n+1,k-1}] f^n, \ k = 1, \dots, K, \quad f^{n+1,0} = f^n.$$

We denote the two corresponding approximated scheme:

$$f^{n+1} = \tilde{\mathcal{S}}^{2d,*}_{\Delta t} f^n, \quad f^{n+1} = \tilde{\mathcal{S}}^{xy,*}_{\Delta t} f^n.$$

Finally, we recall that composing a scheme with its adjoint, $\mathcal{S}^*_{\Delta t}\mathcal{S}_{\Delta t}$, results in a second order accurate scheme [5]. We will consider in the next Section more general composition methods.

3 Composition scheme

Composition schemes aim at constructing high-order time discretizations by composing different elementary steps. Let $s \in \mathbb{N}^*$ and composition coefficients $\alpha_1, \dots, \alpha_s, \beta_1, \dots, \beta_s \in \mathbb{R}$. The n-th iteration of the composition scheme reads:

$$f^{n+1} = \mathcal{S}_{\alpha_s \Delta t}\tilde{\mathcal{S}}^*_{\beta_s \Delta t} \cdots \mathcal{S}_{\alpha_2 \Delta t}\tilde{\mathcal{S}}^*_{\beta_2 \Delta t}\mathcal{S}_{\alpha_1 \Delta t}\tilde{\mathcal{S}}^*_{\beta_1 \Delta t} f^n,$$

where $\mathcal{S}$ and $\tilde{\mathcal{S}}^*$ refer either to the 2d or the splitting direct and approximated adjoint steps defined in the previous section. This can be equivalently written $f^{n+1}_0 = f^n$:

$$\begin{aligned}\text{for } i = 1, \dots, s, \quad f^{n+1}_{2i-1} &= \tilde{\mathcal{S}}^*_{\beta_i \Delta t} f^{n+1}_{2(i-1)} \\ f^{n+1}_{2i} &= \mathcal{S}_{\alpha_i \Delta t} f^{n+1}_{2i-1},\end{aligned}$$

and $f^{n+1} = f^{n+1}_{2s}$. Note that we use the approximated adjoint step with K substeps, as detailed in Section 2, instead of the implicit exact adjoint step.

A possible choice of composition coefficients is to impose $\alpha_i = \beta_i$ for any $i = 1, \dots, s$, which makes the scheme the composition of second-order steps. However, according to [8], the composition coefficients can also be more generally computed from splitting coefficients $a_0, a_1, \dots, a_s$ and $b_1, \dots, b_s$ through the relations $\beta_1 = a_0,\ \alpha_1 = b_1 - \beta_1,\ \beta_i = a_i - \alpha_{i-1},\ \alpha_i = b_i - \beta_i,\ i = 2, \dots, s$. We will focus on a second order scheme $O2$, taking $s = 1$ $a_0 = a_1 = 1/2,\ b_1 = 1$, and a fourth order scheme $O4$ [1], taking $s = 6$ and $a_0 = 0.07920369643119569,\ a_1 = 0.353172906049774,\ a_2 = -0.0420650803577195,\ b_1 = 0.209515106613362,\ b_2 = -0.143851773179818$, completing by symmetry: $a_3 = 1-2(a_0+a_1+a_2),\ a_{6-i} = a_i,\ i = 0, 1, 2,\ b_3 = 1/2 - b_1 - b_2,\ b_{7-i} = b_i,\ i = 1, 2, 3$.

By default, we will take for K the order of the corresponding composition scheme, that is $K = 2$, for $O2$ and $K = 4$ for $O4$, thanks to the following property, due to [3] in the symmetric case.

Proposition 2. *Let $(E, \|\cdot\|)$ a normed space, and $f^0 \in E$. Let $\mathcal{R}^*_{\Delta t}[g], \mathcal{R}_{\Delta t}[g] : E \to E$, Lipschitz and Lipschitz in $\Delta t \in \mathbb{R}$ and $O(\Delta t)$-Lipschitz in $g \in E$, first order approximations of $\mathcal{T}^{exact}_{\Delta t}$. Let $s \in \mathbb{N}^*$ and $\alpha_1, \dots, \alpha_s, \beta_1, \dots, \beta_s \in \mathbb{R}$. We suppose that the composition method is given by $f^1_0 = f^0 \in E$*

$$f^1_{2i-1} = \mathcal{R}^*_{\beta_i \Delta t}[f^1_{2i-1}] f^1_{2(i-1)} \tag{4}$$

$$f^1_{2i} \ = \mathcal{R}_{\alpha_i \Delta t}[f^1_{2i-1}] f^1_{2i-1} \tag{5}$$

for $i = 1, \dots, s$ and $f^1 = f^1_{2s}$. We suppose that the method is of order $\geq p$: $\|f^1 - \mathcal{T}^{exact}_{\Delta t} f^0\| = O(\Delta t^{p+1})$. Then, if the adjoint step (4) is replaced by its K-th fixed point iteration, with $K \geq p$, the modified method is still of order $\geq p$.

Proof. Let us denote $\tilde{f}^1_j$ the solution to the approximated scheme. At the $2i-1$-th iteration, we have $\tilde{f}^{1,k}_{2i-1} = \mathcal{R}^*_{\beta_i \Delta t}[\tilde{f}^{1,k-1}_{2i-1}] \tilde{f}^1_{2(i-1)}$, $k = 1, \dots, K$, and $f^1_{2i-1} = \mathcal{R}^*_{\beta_i \Delta t}[f^1_{2i-1}] f^1_{2(i-1)}$. Using the $O(\Delta t)$-Lipschitz in g_1 and Lipschitz property in g_2 of $\mathcal{R}^*_{\beta_i \Delta t}[g_1] g_2$, we get

$$\begin{aligned}
\|\tilde{f}^{1,K}_{2i-1} - f^1_{2i-1}\| &\leqslant \|\mathcal{R}^*_{\beta_i \Delta t}[\tilde{f}^{1,K-1}_{2i-1}] \tilde{f}^1_{2(i-1)} - \mathcal{R}^*_{\beta_i \Delta t}[f^1_{2i-1}] \tilde{f}^1_{2(i-1)}\| \\
&\quad + \|\mathcal{R}^*_{\beta_i \Delta t}[f^1_{2i-1}] \tilde{f}^1_{2(i-1)} - \mathcal{R}^*_{\beta_i \Delta t}[f^1_{2i-1}] f^1_{2(i-1)}\| \\
&\leqslant C_1 \Delta t \|\tilde{f}^{1,K-1}_{2i-1} - f^1_{2i-1}\| + C_2 \|\tilde{f}^1_{2(i-1)} - f^1_{2(i-1)}\|.
\end{aligned}$$

Consequently, iteratively, we have:

$$\begin{aligned}
\|\tilde{f}^1_{2i-1} - f^1_{2i-1}\| &\leqslant (C_1 \Delta t)^K \|\tilde{f}^1_{2(i-1)} - f^1_{2i-1}\| + \frac{C_2}{1 - C_1 \Delta t} \|\tilde{f}^1_{2(i-1)} - f^1_{2(i-1)}\| \\
&\leq (C_1 \Delta t)^K \|f^1_{2(i-1)} - f^1_{2i-1}\| + (\frac{C_2}{1 - C_1 \Delta t} + (C_1 \Delta t)^K) \|\tilde{f}^1_{2(i-1)} - f^1_{2(i-1)}\|.
\end{aligned}$$

Since, using the Lipschitz property in Δt, $\|f^1_{2(i-1)} - f^1_{2i-1}\| = \|\mathcal{R}^*_0[f^1_{2i-1}] f^1_{2(i-1)} - \mathcal{R}^*_{\beta_i \Delta t}[f^1_{2i-1}] f^1_{2(i-1)}\| = O(\Delta t)$, we obtain that $||\tilde{f}^1_{2i-1} - f^1_{2i-1}|| = O(\Delta t^{p+1})$ as soon as $||\tilde{f}^1_{2(i-1)} - f^1_{2(i-1)}|| = O(\Delta t^{p+1})$. The property is also true at the $2i$-th iteration, and this leads to the result, by using the triangular inequality. □

4 Numerical results

The May model Before considering the guiding center model, we test the composition scheme on the May model [3], which is the following non-linear differential system:

$$\begin{cases} x'(t) = a\,x(t)(1 - x(t)/b) - c\,x(t)y(t)/(x(t) + d) \\ y'(t) = e\,y(t) - y^2(t)/(fx(t)). \end{cases}$$

We consider the following initial condition $x(0) = 100, y(0) = 20$ and the following parameters: $a = 0.6,\ b = 10,\ c = 0.5, d = e = 0.1,\ f = 2$. We compute the error in L^∞ norm on $\mathbb{R}^2$ and consider as reference solution at time $T = 5$ $(x(T), y(T)) = (4.463072920803955, 3.133825837839541)$, obtained with a RK4 scheme using $\Delta t = 1.25 \cdot 10^{-6}$.

Here the equivalent "transport operator" is defined by $\mathcal{T}_{\Delta t}^{\alpha\beta}[(u^*, v^*)](u^0, v^0) = (u(\Delta t), v(\Delta t))$, where u is solution to:

$$\begin{cases} u'(t) = \alpha a u(t)(1 - u(t)/b) - \beta c u(t) v^*/(u^* + d) \\ v'(t) = \alpha e v(t) - \beta v(t) v^*/(f u^*), \\ (u(0), v(0)) = (u^0, v^0). \end{cases}$$

The exact formula is used:

$$v(t) = v^0 \exp((\alpha e - \beta v^*/(f u^*))t),\ u(t) = \frac{b \exp((\alpha a - \frac{\beta c v^*}{u^* + d})t)}{\gamma(\exp((\alpha a - \frac{\beta c v^*}{u^* + d})t) - 1) + \frac{b}{u^0}},$$

with $\gamma = \alpha a/(\alpha a - \frac{\beta c v^*}{u^* + d})$. Numerical results are shown on Figure 1. The functions $0.1\Delta t^2$ and $5 \cdot 10^{-5}\Delta t^4$ are also plotted for comparison, and we can check that the RK4 scheme behaves asymptotically as $3.5\Delta t^4$, meaning that the $O4$ scheme RK4 scheme with a time step $\Delta t/16$ has around the same accuracy as the $O4$ scheme using $K = 4$ and time step Δt.

As in [3], we see that the number of iterations needed to keep the order of accuracy (that is 4 for $O(4)$ and 2 for $O(2)$) is a sharp bound, both for the splitting and $2d$-scheme. The $O2$ $2d$-scheme (which is in fact the classical predictor-corrector scheme) is more accurate than the $O2$ splitting scheme for a given Δt, and for the $O4$ scheme, the splitting scheme is little more accurate. Concerning the efficiency, the $O4$ $2d$-scheme with $K = 4$ is around 50 (resp. 30) slower than the RK4 scheme, in our python (resp. C) implementation, meaning that it is around 3 (resp. 2) times slower than the classical RK4 scheme for a given accuracy.

The guiding center model We now consider the guiding center model. Centered Lagrange interpolation of degree 17 (ref. [2]) is used for the interpolation and the characteristics (assumed to be exact in the previous analysis) are approximated by the RK4 method, for the $2d$-scheme and by a RK2 method for the splitting scheme (similar results are obtained with a RK4 scheme). Initial condition is $f(t = 0, x, y) = \sin(y) + 0.015\cos(x/2),\ x \in [0, 4\pi],\ y \in [0, 2\pi]$,

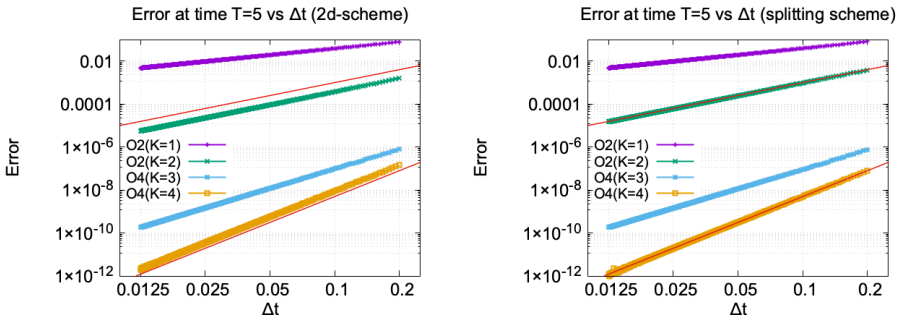

Fig. 1. Error at time $T = 5$ vs Δt for $2d$-scheme (left) and splitting scheme (right) for the May model

periodic boundary conditions are considered for f, Dirichlet boundary conditions for Φ. Numerical results are shown on Figures 2, 3 and 4. We consider only the $O4$ scheme with $K = 4$: the $2d$-scheme and the splitting scheme. The reference solution has been computed with the $O4$ $2d$ scheme with 256×256 spatial discretization points and a time step $\Delta t = 0.0078125$. Both schemes exhibit a convergence order around 4, with enhanced convergence for the $2d$-scheme for large time steps and convergence order around 5. For comparison, we consider also the fourth order time-scheme (RKEI4) developed in [11], whose error is approximated by the function $4 \cdot 10^{-4} \Delta t^4$. The cost of the $O4$ $2d$-scheme is around 6 times slower, while the error is divided by 40. So again, we see that the scheme is around $2-3$ times slower than the RKEI4 scheme for a given accuracy. On the other hand, it seems that the O4 schemes seem to behave well regarding the mass and energy conservation (see Figure 3), and they have both similar accuracy. This is rather unsual for splitting schemes. The L^1 et L^2 norms are on the contrary better conserved by the RKEI4 scheme. Note also that the splitting version, despite the known inherent disadvantage of breaking the conservative/advective form of the equations, is faster (around 6 times faster than the 2d version, in our implementation, in the O4 case), can be easily parallelized, and conservative versions are easier to handle. The fact that it gives quite good results for a high order time discretization (O4 here) may thus enlarge its range of applicability.

5 Conclusion and perspectives

In this paper, we present second and fourth order composition schemes for the guiding-center model. They are based on explicit steps and approximated adjoint steps, which are all composition of 2d or 1d transports. Note that the total number of steps is quite large: for instance, the fourth order method requires 30 steps per iteration (counting all the steps of the fixed point iterations). However, the numerical simulations show that it is only 2-3 slower than the RKEI4 scheme

[11]. Since composition methods reduces the amount of copies of f to be stored, they can still be competitive for some applications.

Moreover, the method is quite generic. Here a semi-Lagrangian scheme has been used for the spatial discretization but conservative schemes, like finite-volume or discontinuous Galerkin schemes, could be considered instead. The method could then be tested to more complex models.

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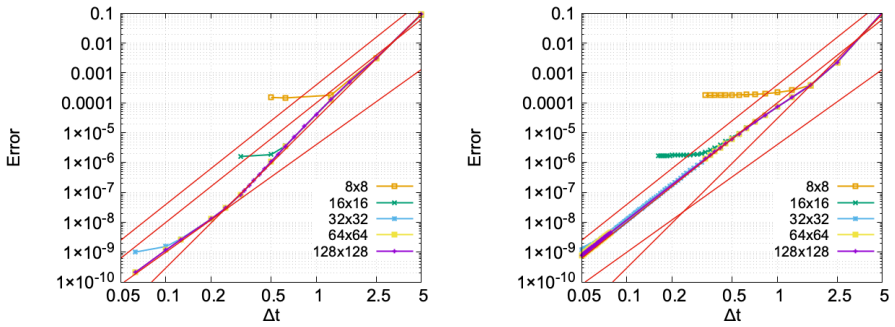

Fig. 2. L^∞ error at time $T = 5$ vs Δt for $2d$-scheme (left) and splitting scheme (right) for the guiding center model for different spatial discretizations. The functions $3 \cdot 10^{-5}\Delta t^5$, $4 \cdot 10^{-4}\Delta t^4$,$10^{-4}\Delta t^4$ and $4 \cdot 10^{-6}\Delta t^{3.6}$ are also plotted for comparison.

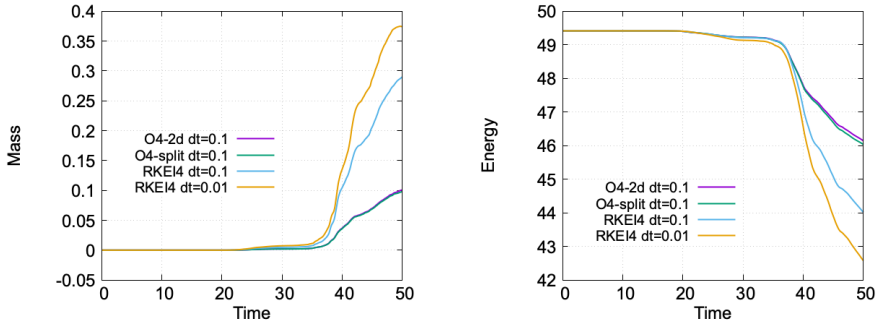

Fig. 3. Time evolution of mass (left) and energy (right). Spatial discretization: 128×128.

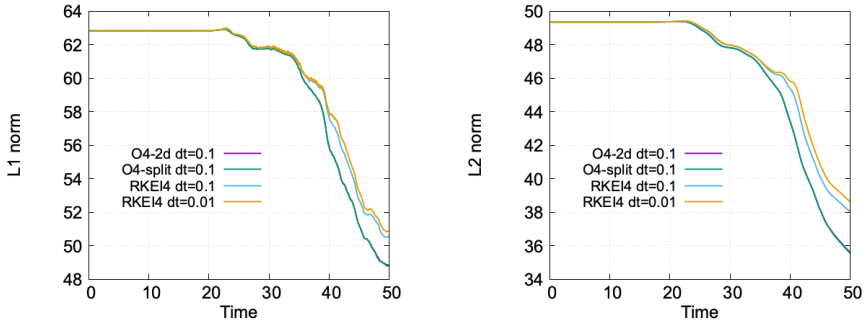

Fig. 4. Time evolution of L^1 norm (left) and L^2 norm (right). Spatial discretization: 128×128.