

Exponential Time Integrators for Unsteady Advection–Diffusion Problems on Refined Meshes



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Abstract Time integration of advection dominated advection–diffusion problems on refined meshes can be a challenging task, since local refinement can lead to a severe time step restriction, whereas standard implicit time stepping is usually hardly suitable for treating advection terms. We show that exponential time integrators can be an efficient, yet conceptually simple, option in this case. Our comparison includes three exponential integrators and one conventional scheme, the two-stage Rosenbrock method ROS2 which has been a popular alternative to splitting methods for solving advection–diffusion problems.

1 Introduction

Time integration of unsteady advection–diffusion problems discretized in space on locally refined meshes can be a challenging problem. This is especially the case for advection dominated problems. On the one hand, requirements of accuracy, monotonicity and total variation diminishing (TVD) usually rule out the use of implicit time integration for advection terms [23, Chapter III.1.3] (for a notable exception see [31]). On the other hand, locally refined meshes can impose a severe CFL stability restriction on the time step, thus making explicit schemes very inefficient.

Within the method of lines framework, i.e., when discretization in space is followed by time integration, different approaches exist to cope with this problem. A straightforward and widely used approach is operator splitting [23, Chapter IV],[43, Chapter 3], when advection is usually treated explicitly in time and diffusion implicitly. Though being conceptually simple and easy to apply in practice, splitting

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methods unavoidably lead to splitting errors, see, e.g., [10, 27]. Moreover, a proper use of boundary conditions within the splitting is sometimes not trivial and may lead to error order reduction [15, 38]. To reduce splitting errors many various approaches have been proposed, with none being fully successful. Here we mention source splitting techniques [42] and Rosenbrock schemes [23, Chapter IV.5].

Other possible approaches to integrate advection–diffusion problems efficiently include implicit-explicit (IMEX) methods [23, Chapter IV.4] and multirate schemes [9, 34, 35].

In this paper we show that in some cases exponential time integration schemes can serve as an efficient yet simple way to integrate advection–diffusion problems in time on locally refined meshes. Similar to implicit schemes, exponential schemes have attractive stability properties. However, exponential schemes have also excellent accuracy properties and in some cases, especially for linear ODE (ordinary differential equation) systems, are able to produce exact solution to initial-value problem (IVP) being solved. This is the property we exploit in this work. An example of an IVP that can be solved exactly by an exponential solver is

$$y'(t) = -Ay(t) + g, \quad y(0) = v, \quad t \in [0, T], \quad (1)$$

where $v, g \in \mathbb{R}^N$ are given and $A \in \mathbb{R}^{N \times N}$ represents the advection–diffusion operator discretized in space. Exponential solvers involve matrix-vector products with the matrix exponential and related, the so-called φ functions. More specifically, the exact solution $y(t)$ of (1) can be written as

$$y(t) = v + t\varphi(-tA)(g - Av), \quad t \geq 0, \quad (2)$$

where a matrix-vector product of the matrix function $\varphi(-tA)$ and the vector $g - Av$ has to be computed. Here the function φ is defined as [21]

$$\varphi(z) = \begin{cases} \frac{e^z - 1}{z}, & \text{for } z \neq 0, \quad z \in \mathbb{C}, \\ 1, & \text{for } z = 0. \end{cases}$$

In case $g \equiv 0$ expression (2) reduces to a familiar relation $y(t) = \exp(-tA)v, t \geq 0$. Note that such an “all-at-once” exact solution of systems (1) is also possible if g is a given vector function $g(t)$ of time t , see [1]. Furthermore, to solve general nonlinear IVPs within this approach, across-time iterations of the waveform relaxation type can successfully be employed [25]. Then, at each waveform relaxation iteration, a linear IVP of the type (1) is solved by an exponential scheme. Such an approach is attractive because no time stepping is involved and solution can often be obtained for the whole time interval $t \in [0, T]$.

Exponential time integration is a rapidly developing research area [21]. Two classes of exponential schemes can be distinguished: (1) time-stepping schemes having a certain accuracy order where the matrix exponential or related matrix functions are evaluated *within* each time step and (2) schemes which, formally

speaking, deliver an exact solution to the IVP, where the actions of the matrix exponential or related matrix functions are employed *across* a certain time interval. The former class includes extrapolated second order exponential Euler method (EE2, discussed and tested below), exponential Rosenbrock schemes [22], and predictor-corrector exponential schemes [30]. Examples of the latter class are the scheme (2) applied to IVP (1), exponential waveform relaxation schemes [5] where solution to (3) is sought by replacing A with a preconditioner $M \approx A$ and iterating, and the exponential block Krylov (EBK) method discussed and tested below. Note that exponential schemes of the both classes can handle nonlinear problems, in particular, compressible [28, 29] and incompressible [26] Navier-Stokes equations.

In this work we present comparison results for three different exponential solvers. All these methods are based on the Krylov subspace techniques discussed in [1, 6, 36]. Krylov subspace methods have been successfully used for evaluating matrix exponential and related matrix functions since the eighties, see in chronological order [11, 12, 20, 24, 32, 33, 39]. An attractive property of the Krylov subspace methods, which distinguishes them from the other methods used for large matrix function evaluations $f(A)v$, is their adaptivity with respect to the spectral properties of A and the particular vector v , see [40]. To work efficiently, Krylov subspace methods often need a restarting [14, 18], a mechanism allowing to keep Krylov subspace dimension restricted while preserving convergence of the unrestarted method.

The structure of this paper is as follows. In Sect. 2 the problem and methods used for its solution are presented. Section 3 is devoted to numerical experiments, here the methods are compared and comparison results are discussed. Finally, some conclusions are drawn in Sect. 4.

2 Problem Formulation and Methods

In this paper we assume that a linear PDE of the advection–diffusion type is solved by the method of lines and, after a suitable space discretization, the following IVP has to be solved

$$y'(t) = -Ay(t) + g(t), \quad y(0) = v, \quad t \in [0, T]. \quad (3)$$

Here $A \in \mathbb{R}^{N \times N}$ represents the discretized advection–diffusion operator and the given vector function $g(t)$ accounts for time dependent sources or boundary conditions.

2.1 Exponential Time Integrators

Perhaps the simplest exponential integrator is exponential Euler method which, applied to problem (3), reads

$$y_{n+1} = y_n + \Delta t \varphi(-\Delta t A)(g_n - Ay_n), \quad (4)$$

where Δt is the time step size, y_n is numerical solution at time $t = \Delta t n$ and $g_n = g(\Delta t n)$. The method is inspired by relation (2) and for constant source term g is exact. It is not difficult to check that it is first order accurate.

Using extrapolation [3, 44], i.e., by combining solutions obtained with different time steps, higher order methods can be obtained. Globally extrapolated second order exponential Euler method (EE2) is considered in [1],

- (1) carry out $T/\Delta t$ steps of (4) with Δt , set result to $y_{\Delta t}(T)$,
- (2) carry out $2T/\Delta t$ steps of (4) with $\Delta t/2$, set result to $y_{\Delta t/2}(T)$,
- (3) obtain solution by extrapolation: $y_{EE2}(T) := 2y_{\Delta t/2}(T) - y_{\Delta t}(T)$,

where its combination with EXPOKIT [36], used to evaluate the φ matrix vector products, is argued to be a competitive integrator. The `phiv` function of EXPOKIT is able to efficiently compute actions of the φ matrix functions by a restarted Arnoldi process, where the restarting is done by time stepping based on an error estimation. In experiments presented below we show that EE2/EXPOKIT can be significantly improved by introducing residual-based error control [4, 8, 13] and replacing the restarting procedure by the residual-time (RT) restarting presented in [6, 7].

EE2 is an exponential integrator which evaluates matrix functions *within* a time stepping procedure: at each time step φ is computed by a Krylov subspace method. It is often more efficient [2, 5], if possible, to organize work in such a way that numerical linear algebra work for matrix function evaluations is done *across* time stepping, for a certain time interval. For instance, as shown in [1], if for a certain time range $g(t)$ allows an approximation

$$g(t) \approx Up(t), \quad U \in \mathbb{R}^{N \times m}, \quad p: \mathbb{R} \rightarrow \mathbb{R}^m, \quad m \ll N, \quad (6)$$

then (3) can be solved for this time range by a single projection on a block Krylov subspace. The matrix U and function p in (6) can be easily constructed by truncated singular value decomposition (SVD) of the vectors $g(t_i)$, at a small additional cost [1]. This procedure simultaneously provides an error estimation in (6), so that a proper value for m can be chosen.

To be more specific, consider problem (1), where for simplicity and without loss of generality assume $v = 0$. A usual Krylov subspace solution of (1) constructs a matrix $V_k \in \mathbb{R}^{N \times k}$, whose orthonormal columns span the Krylov subspace [40]

$$\text{span}(g, Ag, \dots, A^{k-1}g),$$

and, searching for an approximate solution $y_k(t) = V_k u(t) \approx y(t)$, reduces (1) to its Galerkin projection

$$V_k^T V_k u'(t) = -V_k^T A V_k u(t) + V_k^T g \quad \Leftrightarrow \quad u'(t) = -H_k u(t) + \beta e_1, \quad (7)$$

where $H_k = V_k^T A V_k$, $e_1 = (1, 0, \dots, 0)^T \in \mathbb{R}^k$ is the first canonical basis vector and $\beta = \|g\|$. We have $V_k^T g = V_k^T V_k(\beta e_1) = \beta e_1$ because, by construction, the first column of V_k is $g/\|g\|$. The small projected IVP (7) can be solved by relation (2), evaluating $\varphi(-tH_k)$ with well developed matrix function techniques for small matrices (see, e.g., [19]).

Now consider, still assuming $v = 0$, problem (3) where $g(t)$ allows (6). Projecting (3) on a block Krylov subspace [40]

$$\text{span}(U, AU, \dots, A^{k-1}U) = \text{colspan}V_k, \quad V_k \in \mathbb{R}^{N \times km},$$

we can reduce (3) to its projected form

$$u'(t) = -H_k u(t) + E_1 p(t), \quad (8)$$

where we now have $H_k \in \mathbb{R}^{km \times km}$ and $E_1 \in \mathbb{R}^{km \times m}$ is a matrix whose columns are the first m columns of the $km \times km$ identity matrix. These observations lead to the exponential block Krylov (EBK) method described in [1].

The EBK solver exploits a stopping criterion and restarting which are based on the exponential residual concept [4, 8, 13]. In particular, EBK iterations stop as soon as for the computed approximate solution $y_k(t)$ holds

$$\|r_k(t)\| \leq \tau_0 1, \quad r_k(t) \equiv -A y_k(t) + g(t) - y_k'(t), \quad t \in [0, T].$$

The EBK method can be summarized as follows (see [1] for details):

- (1) form the approximation (6),
- (2) carry out $k = 1, \dots, k_{\max}$ block Krylov steps, obtaining V_k, H_k , (9)
- (3) solve projected IVP (8), compute solution $y_k(T) = V_k u(T)$.

Comparing the EE2 and EBK schemes, we note that an attractive feature of EE2 is its relative simplicity. On the other hand, a strong point for EBK is its potential efficiency, as a single block Krylov subspace has to be constructed for the whole time interval $t \in [0, T]$.

2.2 ROS2 Method: Beyond Splitting

Rosenbrock schemes [23, Chapter IV.5] have been a popular alternative to splitting methods, as they allow to reduce splitting errors and avoid other negative effects related to splitting, such as order reduction. Let $f(t, y) = -Ay(t) + g(t)$ be the ODE right hand side in (3). The two-stage Rosenbrock method ROS2 reads

$$\begin{aligned} y_{n+1} &= y_n + \frac{3}{2}\Delta tk_1 + \frac{1}{2}\Delta tk_2, \\ (I - \gamma \Delta t \widehat{A})k_1 &= f(t_n, y_n), \\ (I - \gamma \Delta t \widehat{A})k_2 &= f(t_{n+1}, y_n + \Delta tk_1) - 2k_1. \end{aligned} \tag{10}$$

The method is second order consistent for any $\widehat{A} \in \mathbb{R}^{N \times N}$ and, to have good stability properties, one usually takes $\widehat{A} \approx A$. Typically, \widehat{A} corresponds to the terms in A which have to be integrated implicitly in time. For instance in [41], for advection-diffusion-reaction problems, \widehat{A} is taken such that

$$I - \gamma \Delta t \widehat{A} = (I - \gamma \Delta t A_{\text{diff}})(I - \gamma \Delta t A_{\text{react}}),$$

where A_{diff} contains diffusion terms and A_{react} is the reaction Jacobian. In this work we take \widehat{A} to be either A or the diffusion part of A . Following suggestion in [23, Chapter IV.5, Remark 5.2] we set $\gamma = 1$.

3 Numerical Experiments

Numerical experiments described here are carried in Matlab on a Linux PC with 6 Intel Core i5-8400 2.80 GHz CPUs with 16 GB RAM.

3.1 Test 1: Time Dependent Source and Boundary Conditions

In this test we solve (3) where A is a finite-element discretization of the two-dimensional advection–diffusion operator:

$$L[u] = -v \nabla^2 u + \mathbf{v} \cdot \nabla u, \quad u = u(x, y), \quad (x, y) \in [-1, 1] \times [-1, 1], \tag{11}$$

where v is the viscosity parameter and the velocity field is $\mathbf{v} = [v_1(x, y), v_2(x, y)]$,

$$v_1(x, y) = y(1 - x^2), \quad v_2(x, y) = x(y^2 - 1).$$

For this test, the function $g(t)$ in (3) takes the form

$$g(t) \equiv y'_{\text{ex}}(t) + Ay_{\text{ex}}(t),$$

where $y_{\text{ex}}(t)$ is exact solution function chosen as

$$\begin{aligned} y_{\text{ex}}(t) &= \alpha(t)(A^{-1}g_{\text{bc}} + T\varphi(-TA)g_{\text{peak}}), \\ \alpha(t) &= 1 - e^{-t/300} + e^{-t/100}. \end{aligned} \tag{12}$$

Here $g_{\text{bc}} \in \mathbb{R}^N$ is a vector containing Dirichlet boundary values prescribed below and the vector $g_{\text{peak}} \in \mathbb{R}^N$ consists of the values of function $e^{-10x^2-50y^2}$ on the mesh. The boundary conditions imposing by g_{bc} are

$$u(-1, y) = u(1, y) = u(x, -1) = 5, \quad u(x, 1) = 5 + 5e^{-50x^2}.$$

Note that $A^{-1}g_{\text{bc}}$ is the steady state solution of (3) for $g(t) \equiv g_{\text{bc}}$ and $T\varphi(-TA)g_{\text{peak}}$ is the solution of (3) with $g(t) \equiv g_{\text{peak}}$ at time $t = T$. The final time is $T = 1000$ in this test. In Fig. 1 the exact solution $y_{\text{ex}}(T)$ is plotted.

In this test the IFISS finite element discretization [16, 37] by bilinear quadrilateral (Q_1) finite elements with the streamline upwind Petrov–Galerkin (SUPG) stabilization is employed. We set viscosity to $\nu = 1/6400$ and use nonuniform Cartesian stretched 256×256 and 512×512 grids with default refinement parameters, which get finer near the domain boundaries, see Table 1.

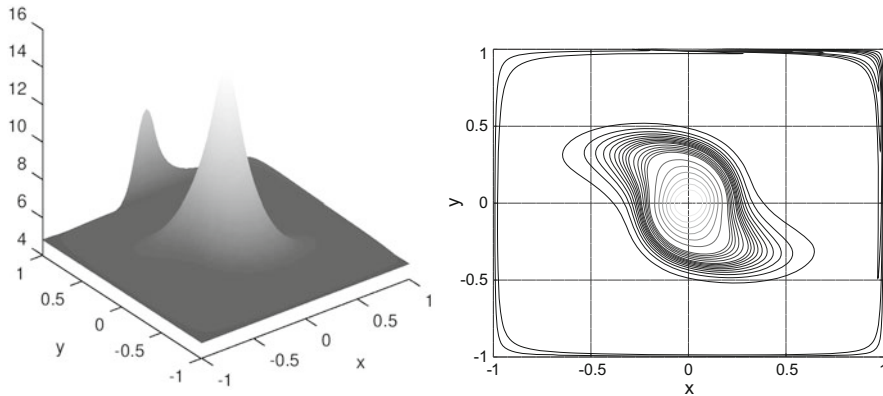


Fig. 1 Solution function (12) on the mesh 256×256 at final time $T = 1000$ as surface (left) and contour (right) plots

Table 1 Parameters of the IFISS stretched meshes

Mesh	$\min h_x = \min h_y$	$\max h_x = \max h_y$	Ratio $\max h_{x,y} / \min h_{x,y}$	max.elem. Peclet for $\nu = 1/6400$
256×256	5.9804×10^{-4}	0.0312	52.17	1.9989×10^2
512×512	2.0102×10^{-4}	0.0176	87.5535	1.1248×10^2

When constructing an advection-diffusion matrix, the IFISS package provides the value the maximum finite element grid Peclet number, evaluated per element as

$$\frac{1}{2\nu} \min \left\{ \frac{h_x}{\cos \alpha}, \frac{h_y}{\sin \alpha} \right\} \|v\|_2, \quad \alpha = \arctan \frac{v_2}{v_1},$$

where $h_{x,y}$ and $v_{1,2}$ are respectively the element sizes and the velocity components. The maximum element Peclet numbers reported for these meshes are given in Table 1. Due to the SUPG stabilization, the resulting matrices for both meshes are weakly nonsymmetric: the ratio $\|A - A^T\|_1 / \|A + A^T\|_1$ amounts approximately to 0.022 (mesh 256×256) and 0.012 (mesh 512×512).

In addition to the requested accuracy tolerance, two input parameters have to be provided to EBK: the number of the truncated SVD terms m and the number of time snapshots n_s to construct approximation (6). From the problem description, we see that $y_{\text{ex}}(t)$ is a linear combination of two linearly independent vectors for any t . Hence, $g(t)$ is a linear combination of no more than four vectors and we should take $m \leq 4$. The actual situation is displayed by the singular values available from the thin SVD of the time samples: the largest truncated singular value σ_{m+1} is an upper bound for the truncation error $\|g(t) - Up(t)\|_2$, see, e.g., [17]. In this case it turns out that taking $m = 2$ is sufficient. A proper snapshot number n_s can be estimated from given $\alpha(t)$ or by checking, for constructed U and $p(t)$, the actual error $\|g(t) - Up(t)\|$ a posteriori, see (Table 2). Based on this, we set $n_s = 120$ in all EBK runs in this test. This selection procedure for n_s is computationally very cheap and can be done once, before all the test runs.

As the problem is two-dimensional, linear systems with A can be solved efficiently by sparse direct methods. Therefore to solve the linear systems in ROS2, we use the Matlab standard sparse LU factorization (provided by UMFPACK) computing it once and using at each time step.

Table 2 Error of approximation (6), 256×256 mesh. The EBK errors are obtained for $\text{tol} = 10^{-6}$

n_s	$\max_{s \in [0, T]} \ g(s) - Up(s)\ $	$\frac{\int_0^T \ g(s) - Up(s)\ ds}{\int_0^T \ g(s)\ ds}$	EBK error (13)
30	2.37×10^{-3}	1.82×10^{-5}	2.24×10^{-5}
60	1.27×10^{-4}	9.83×10^{-7}	1.23×10^{-6}
120	7.40×10^{-6}	5.73×10^{-8}	7.90×10^{-8}

The error reported below for the test runs is measured as

$$\text{error} = \frac{\|y(T) - y_{\text{ex}}(T)\|_2}{\|y_{\text{ex}}(T)\|_2}. \tag{13}$$

The results of the test runs are presented in Tables 3 and 4. As we see, EBK turns out to be more efficient than the other solvers. Within the EE2 integrator, the change of the Krylov subspace solver from EXPOKIT’s `phiv` to the RT-restarted algorithm leads to a significant increase in efficiency. Note that this gain is not due to the restarting but due a more reliable residual-based error control. Restarting is usually not done because, due to a sufficiently small Δt , just a couple Krylov steps are carried out in EE2 each time step. In both EE2/EXPOKIT and EE2/RT we should be careful with setting a proper tolerance value, which is used at each time step for stopping the Krylov subspace method evaluating the φ matrix function. Taking a large tolerance value may lead to an accuracy loss. For increasingly small tolerance values the same accuracy will be observed (as it is determined by the time step size) at a higher cost: more matrix-vector multiplications per time step will be needed for the φ matrix function evaluations.

From Tables 3 and 4 we also see that the ROS2 solver becomes less efficient than EE2/RT on the finer mesh as the costs for solving linear systems become more pronounced.

Table 3 Test 1. Results for the 256×256 mesh

Method	CPU time, s	Fevals ^a	l.s.s. ^b	Error
EBK, $\text{tol} = 10^{-4}$	0.36	20	—	8.01×10^{-8}
EBK, $\text{tol} = 10^{-6}$	0.40	24	—	7.90×10^{-8}
EE2/RT, $\Delta t = 20, \text{tol} = 10^{-4}$	1.84	500	—	1.51×10^{-3}
EE2/RT, $\Delta t = 10, \text{tol} = 10^{-4}$	3.52	900	—	3.79×10^{-4}
EE2/RT, $\Delta t = 5, \text{tol} = 10^{-4}$	6.93	1800	—	9.50×10^{-5}
EE2/EXPOKIT, $\Delta t = 20, \text{tol} = 10^{-4}$	17.99	9408	—	1.51×10^{-3}
EE2/EXPOKIT, $\Delta t = 10, \text{tol} = 10^{-4}$	24.53	12,608	—	3.79×10^{-4}
EE2/EXPOKIT, $\Delta t = 5, \text{tol} = 10^{-4}$	37.74	19,200	—	9.50×10^{-5}
ROS2, $\hat{A} = A, \Delta t = 20$	1.95	100	100	3.03×10^{-3}
ROS2, $\hat{A} = A, \Delta t = 10$	3.59	200	200	7.60×10^{-4}
ROS2, $\hat{A} = A, \Delta t = 5$	6.85	400	400	1.91×10^{-4}
ROS2, $\hat{A} = A_{\text{diff}}, \Delta t = 2$	19.55	1000	1000	8.49×10^{-4}
ROS2, $\hat{A} = A_{\text{diff}}, \Delta t = 1$	34.72	2000	2000	7.59×10^{-6}
ROS2, $\hat{A} = A_{\text{diff}}, \Delta t = 0.5$	68.33	4000	4000	1.90×10^{-6}

^aNumber of function evaluations or matvec (matrix-vector) products

^bNumber of linear system solutions

Table 4 Test 1. Results for the 512×512 mesh

Method	CPU time, s	Fevals ^a	l.s.s. ^b	Error
EBK, $\tau_{01} = 10^{-4}$	1.26	4	—	3.08×10^{-8}
EBK, $\tau_{01} = 10^{-6}$	1.31	8	—	2.33×10^{-8}
EE2/RT, $\Delta t = 20, \tau_{01} = 10^{-4}$	9.10	450	—	8.91×10^{-4}
EE2/RT, $\Delta t = 10, \tau_{01} = 10^{-4}$	17.97	900	—	2.40×10^{-4}
EE2/RT, $\Delta t = 5, \tau_{01} = 10^{-4}$	35.90	1800	—	8.07×10^{-5}
ROS2, $\hat{A} = A, \Delta t = 20$	11.82	100	100	1.90×10^{-3}
ROS2, $\hat{A} = A, \Delta t = 10$	22.68	200	200	5.46×10^{-4}
ROS2, $\hat{A} = A, \Delta t = 5$	36.91	400	400	1.85×10^{-4}
ROS2, $\hat{A} = A_{\text{diff}}, \Delta t = 2$	86.55	1000	1000	5.73×10^{-3}
ROS2, $\hat{A} = A_{\text{diff}}, \Delta t = 1$	167.95	2000	2000	4.44×10^{-6}
ROS2, $\hat{A} = A_{\text{diff}}, \Delta t = 0.5$	331.38	4000	4000	1.11×10^{-6}

^aNumber of function evaluations or matvec (matrix-vector) products

^bNumber of linear system solutions

3.2 Test 2: Time Dependent Boundary Conditions

In the previous test we see that the EBK solver apparently profits from the specific source function, exhibiting a very quick convergence. Although this is not an unusual situation, we now consider another test problem which appears more difficult for EBK. We take the same matrix A as in the first test and the following initial value vector v and source function $g(t)$:

$$g(t) = \alpha(t)g_{\text{bc}}, \quad v = -T\varphi(-TA)g_{\text{peak}},$$

where $\alpha(t)$ and g_{bc} are the same as in (12). This test problem does not have a known analytical solution and we compute a reference solution $y_{\text{ref}}(t)$ by running EE2/RT with a tiny time step size. The errors of computed numerical solutions $y(t)$ reported below are

$$\text{error} = \frac{\|y(T) - y_{\text{ref}}(T)\|_2}{\|y_{\text{ref}}(T)\|_2}$$

Note that $y_{\text{ref}}(t)$ is influenced by the same space error as $y(t)$, hence, the error shows solely the time error.

From the problem definition we see that the number of SVD terms m can be at most 2. Therefore, in this test EBK is run with the block size $m = 2$ and $n_s = 80$ time snapshots (the value is determined in the same way as in Test 1). For this test we include in comparisons the two solvers which come out as best in the first test, EBK and EE2/RT. The results presented in Table 5 show that EBK does require more steps for this test but is still significantly more efficient than EE2/RT.

Table 5 Test 2. Results for the 256×256 mesh

Method	CPU time, s	Fevals ^a	l.s.s. ^b	Error
EBK, $\tau_{01} = 10^{-4}$, $n_s = 80$	0.77	36	—	1.83×10^{-5}
EBK, $\tau_{01} = 10^{-6}$, $n_s = 80$	1.32	50	—	1.91×10^{-7}
EE2/RT, $\Delta t = 10$, $\tau_{01} = 10^{-6}$	6.53	1306	—	8.91×10^{-5}
EE2/RT, $\Delta t = 5$, $\tau_{01} = 10^{-6}$	11.54	2406	—	5.58×10^{-5}

^a Number of function evaluations or matvec (matrix-vector) products

^b Number of linear system solutions

4 Conclusions

We show that exponential time integrators can be an attractive option for integrating advection–diffusion problems in time, as they possess good accuracy as well as stability properties. In presented tests, they outperform state-of-the-art implicit-explicit ROS2 solvers. Exponential solvers which are able to exploit their matrix function evaluation machinery for a whole time interval (such as EBK in this paper) appear to be preferable to exponential integrators where matrix functions have to be evaluated at each time step.

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References

1. Botchev, M.A.: A block Krylov subspace time-exact solution method for linear ordinary differential equation systems. *Numer. Linear Algebra Appl.* **20**(4), 557–574 (2013) <https://doi.org/10.1002/nla.1865>
2. Botchev, M.A.: Krylov subspace exponential time domain solution of Maxwell’s equations in photonic crystal modeling. *J. Comput. Appl. Math.* **293**, 24–30 (2016) <https://doi.org/10.1016/j.cam.2015.04.022>
3. Botchev, M.A., Verwer, J.G.: Numerical integration of damped Maxwell equations. *SIAM J. Sci. Comput.* **31**(2), 1322–1346 (2009) <https://doi.org/10.1137/08072108X>
4. Botchev, M.A., Grimm, V., Hochbruck, M.: Residual, restarting and Richardson iteration for the matrix exponential. *SIAM J. Sci. Comput.* **35**(3), A1376–A1397 (2013) <https://doi.org/10.1137/110820191>
5. Botchev, M.A., Oseledets, I.V., Tyrtshnikov, E.E.: Iterative across-time solution of linear differential equations: Krylov subspace versus waveform relaxation. *Comput. Math. Appl.* **67**(12), 2088–2098 (2014) <https://doi.org/10.1016/j.camwa.2014.03.002>
6. Botchev, M.A., Knizhnerman, L.A.: ART: Adaptive residual-time restarting for Krylov subspace matrix exponential evaluations. *J. Comput. Appl. Math.* **364**, 112311 (2020) <https://doi.org/10.1016/j.cam.2019.06.027>
7. Botchev, M.A., Knizhnerman, L.A., Tyrtshnikov, E.E.: A residual concept for Krylov subspace evaluation of the φ matrix function (2020). Preprint arXiv:2010.08494. <https://arxiv.org/abs/2010.08494>

8. Celledoni, E., Moret, I.: A Krylov projection method for systems of ODEs. *Appl. Numer. Math.* **24**(2–3), 365–378 (1997) [https://doi.org/10.1016/S0168-9274\(97\)00033-0](https://doi.org/10.1016/S0168-9274(97)00033-0)
9. Constantinescu, E.M., Sandu, A.: Multirate timestepping methods for hyperbolic conservation laws. *J. Sci. Comput.* **33**(3), 239–278 (2007)
10. Csomós, P., Faragó, I., Havasi, Á.: Weighted sequential splittings and their analysis. *Comput. Math. with Appl.* **50**(7), 1017–1031 (2005)
11. Druskin, V.L., Knizhnerman, L.A.: Two polynomial methods of calculating functions of symmetric matrices. *U.S.S.R. Comput. Maths. Math. Phys.* **29**(6), 112–121 (1989)
12. Druskin, V.L., Knizhnerman, L.A.: Krylov subspace approximations of eigenpairs and matrix functions in exact and computer arithmetic. *Numer. Lin. Alg. Appl.* **2**, 205–217 (1995)
13. Druskin, V.L., Greenbaum, A., Knizhnerman, L.A.: Using nonorthogonal Lanczos vectors in the computation of matrix functions. *SIAM J. Sci. Comput.* **19**(1), 38–54 (1998) <https://doi.org/10.1137/S1064827596303661>
14. Eiermann, M., Ernst, O.G.: A restarted Krylov subspace method for the evaluation of matrix functions. *SIAM J. Numer. Anal.* **44**, 2481–2504 (2006)
15. Einkemmer, L., Ostermann, A.: Overcoming order reduction in diffusion-reaction splitting. Part I: Dirichlet boundary conditions. *SIAM J. Sci. Comput.* **37**(3), A1577–A1592 (2015) <https://doi.org/10.1137/140994204>
16. Elman, H.C., Ramage, A., Silvester, D.J.: IFISS: A computational laboratory for investigating incompressible flow problems. *SIAM Rev.* **56**(2), 261–273 (2014)
17. Golub, G.H., Van Loan, C.F.: *Matrix Computations*, 3rd edn. The Johns Hopkins University Press, Baltimore and London (1996)
18. Güttel, S., Frommer, A., Schweitzer, M.: Efficient and stable Arnoldi restarts for matrix functions based on quadrature. *SIAM J. Matrix Anal. Appl.* **35**(2), 661–683 (2014)
19. Higham, N.J.: *Functions of Matrices: Theory and Computation*. Society for Industrial and Applied Mathematics, Philadelphia (2008)
20. Hochbruck, M., Lubich, C.: On Krylov subspace approximations to the matrix exponential operator. *SIAM J. Numer. Anal.* **34**(5), 1911–1925 (1997)
21. Hochbruck, M., Ostermann, A.: Exponential integrators. *Acta Numer.* **19**, 209–286 (2010) <https://doi.org/10.1017/S0962492910000048>
22. Hochbruck, M., Ostermann, A., Schweitzer, J.: Exponential Rosenbrock-type methods. *SIAM J. Numer. Anal.* **47**(1), 786–803 (2008/2009). <https://doi.org/10.1137/080717717>
23. Hundsdorfer, W., Verwer, J.G.: *Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations*. Springer, Berlin (2003)
24. Knizhnerman, L.A.: Calculation of functions of unsymmetric matrices using Arnoldi’s method. *U.S.S.R. Comput. Maths. Math. Phys.* **31**(1), 1–9 (1991)
25. Kooij, G.L., Botchev, M.A., Geurts, B.J.: A block Krylov subspace implementation of the time-parallel Paraexp method and its extension for nonlinear partial differential equations. *J. Comput. Appl. Math.* **316**(Supplement C), 229–246 (2017) <https://doi.org/10.1016/j.cam.2016.09.036>
26. Kooij, G., Botchev, M.A., Geurts, B.J.: An exponential time integrator for the incompressible Navier–Stokes equation. *SIAM J. Sci. Comput.* **40**(3), B684–B705 (2018) <https://doi.org/10.1137/17M1121950>
27. Lanser, D., Verwer, J.G.: Analysis of operator splitting for advection–diffusion–reaction problems from air pollution modelling. *J. Comput. Appl. Math.* **111**(1–2), 201–216 (1999)
28. Li, S.J.: Efficient p -multigrid method based on an exponential time discretization for compressible steady flows (2018). arXiv preprint 1807.01151. <https://arxiv.org/abs/1807.01151>
29. Li, S.J.: Time advancement of the Navier-Stokes equations: p -adaptive exponential methods. *J. Flow Control Measurement Vis.* **8**(2), 63–76 (2020) <https://doi.org/10.4236/jfcmv.2020.82004>
30. Li, S.J., Luo, L.S., Wang, Z.J., Ju, L.: An exponential time-integrator scheme for steady and unsteady inviscid flows. *J. Comput. Phys.* **365**, 206–225 (2018) <https://doi.org/10.1016/j.jcp.2018.03.020>

31. Lie, K.A., Mykkelvedt, T.S., Møyner, O.: A fully implicit WENO scheme on stratigraphic and unstructured polyhedral grids. *Comput. Geosci.* **24**(2), 405–423 (2020)
32. Park, T.J., Light, J.C.: Unitary quantum time evolution by iterative Lanczos reduction. *J. Chem. Phys.* **85**, 5870–5876 (1986)
33. Saad, Y.: Analysis of some Krylov subspace approximations to the matrix exponential operator. *SIAM J. Numer. Anal.* **29**(1), 209–228 (1992)
34. Savcenco, V., Hundsdorfer, W., Verwer, J.G.: A multirate time stepping strategy for stiff ordinary differential equations. *BIT Numer. Math.* **47**(1), 137–155 (2007)
35. Schlegel, M., Knoth, O., Arnold, M., Wolke, R.: Multirate Runge–Kutta schemes for advection equations. *J. Comput. Appl. Math.* **226**(2), 345–357 (2009). <https://doi.org/10.1016/j.cam.2008.08.009>
36. Sidje, R.B.: EXPOKIT. A software package for computing matrix exponentials. *ACM Trans. Math. Softw.* **24**(1), 130–156 (1998) www.maths.uq.edu.au/expokit/
37. Silvester, D.J., Elman, H.C., Ramage, A.: Incompressible flow & iterative solver software (2019). <http://www.manchester.ac.uk/ifiss/>
38. Sommeijer, B.P., van der Houwen, P.J., Verwer, J.G.: On the treatment of time-dependent boundary conditions in splitting methods for parabolic differential equations. *J. Numer. Methods Engrg.* **17**(3), 335–346 (1981). <https://doi.org/10.1002/nme.1620170304>
39. van der Vorst, H.A.: An iterative solution method for solving $f(A)x = b$, using Krylov subspace information obtained for the symmetric positive definite matrix A . *J. Comput. Appl. Math.* **18**, 249–263 (1987)
40. van der Vorst, H.A.: *Iterative Krylov Methods for Large Linear Systems*. Cambridge University Press, Cambridge (2003)
41. Verwer, J.G., Spee, E.J., Blom, J.G., Hundsdorfer, W.: A second order Rosenbrock method applied to photochemical dispersion problems. *SIAM J. Sci. Comput.* **20**, 456–480 (1999)
42. Verwer, J.G., Hundsdorfer, W., Blom, J.G.: Numerical time integration for air pollution models. *Surv. Math. Ind.* **10**, 107–174 (2002) <https://ir.cwi.nl/pub/4620>
43. Zlatev, Z.: *Computer Treatment of Large Air Pollution Models*. Kluwer Academic Publishers, New York (1995)
44. Zlatev, Z., Dimov, I., Faragó, I., Havasi, Á.: *Richardson Extrapolation: Practical Aspects and Applications*. De Gruyter, Berlin (2018)