Abstract

We present a MATLAB toolbox for five different classes of exponential integrators for solving (mildly) stiff ordinary differential equations or time-dependent partial differential equations. For the efficiency of such exponential integrators it is essential to approximate the products of the matrix functions arising in these integrators with vectors in a stable, reliable and efficient way. The toolbox contains options for computing the matrix functions directly by diagonalization or by Padé approximation. For large scale problems, Krylov subspace methods are implemented as well.

The main motivation for this toolbox was to provide general tools which on one hand allows one to easily run experiments with different exponential integrators and on the other hand to make it easily extensible by making it simple to include other methods or other options to compute the matrix functions. Thus we implemented the toolbox to be compatible with the ODE solvers included in MATLAB. Most of the methods can be used with adaptive stepping.

1 Introduction

In this paper we present our new MATLAB toolbox EXPODE for exponential integrators containing some of the most prominent integrators developed recently. Our code is based on the implementations provided in [10] and [8].

We strongly recommend the reader to consult the recent and well-written review on exponential integrators by Hochbruck and Ostermann [11]. Historical remarks can be found in [10].

Exponential integrators are usually applied to stiff ordinary differential equations where the stiffness is generated by a linear term. The non-linearity is usually assumed to be well approximated by polynomials. Typical applications are abstract or discretized parabolic or hyperbolic partial differential equations. The unprecedented memory capacity of modern computers can handle correspondingly fine spatial discretizations. Implicit time integration schemes need to solve non-linear systems of equations with a dimension which is a multiple of the dimension of the underlying differential equation. As a consequence, the solution of these systems becomes very costly. Classical explicit schemes, while generally less costly per time step, offer a different problem. They often have interdependent time step and spatial element size requirements for stability. Explicit exponential methods can often avoid or at least weaken these conditions to allow a more efficient use of the memory capacity.

Target equations of our toolbox are very high-dimensional systems where management costs for smart memory management and arithmetics are justified by the high computational costs.

We allow direct computation of actions of the arising matrix functions with vectors or approximation of those with a Krylov method. We have adaptive step size control for some of the methods and support both autonomous and non-autonomous equations.

For an easy entry we are as compatible as possible with MATLAB’s ODE toolbox. We also give fine grained control over the integration process and have a focus on extensibility such that new functionality can be added with only minimal changes to EXPODE’s code.

In some numerical experiments we benchmark EXPODE’s performance. First we use the well known van der Pol equation to test our adaptive step size choices and then use problems typical
for studying exponential integrators [7, 10]. In a more extensive experiment in the end we investigate EXPoDE’s potential when applied to the hyperbolic Maxwell’s equations with the spatial discretization provided by another specialized and well written MATLAB package, the discontinuous Galerkin finite elements provided by [6].

2 Exponential Integrators

In this section we briefly describe the class of problems which can be solved by using our toolbox and the methods which are implemented.

2.1 Problem class

We consider nonlinear initial value problems

\[ u'(t) = F(t, u(t)), \quad u(t_0) = u_0 \]  

(1)

where \( u : \mathbb{R} \to \mathbb{C}^d \) and \( F : \mathbb{R} \times \mathbb{C}^d \to \mathbb{C}^d \).

Exponential integrators are based on linearization of \( F \). One can usually distinguish two different types. The first one uses a fixed linearization,

\[ u'(t) = J u(t) + g(t, u(t)), \quad u(t_0) = u_0, \]  

(2)

where \( J \in \mathbb{C}^{d \times d} \) is an approximation to the Jacobian of \( F \). Roughly speaking, an exponential integrator can be expected to be efficient, if \( J \) contains the stiff part of \( F \) and if \( g \) is nice in the sense that \( g(t, u(t)) \) is a smooth function in \( t \), where \( u \) is the solution of (1).

The second option is to linearize in each time step,

\[ u'(t) = F(t, u(t)) = J_n u(t) + d_n t + g_n(t, u(t)), \quad u(t_n) = u_n, \]  

(3a)

where

\[ J_n = \frac{\partial F}{\partial u} (t_n, u_n), \quad d_n = \frac{\partial F}{\partial t} (t_n, u_n), \quad g_n(t, u(t)) = F(t, u(t)) - J_n u(t) - d_n t. \]  

(3b)

For details on the construction and on the analysis of exponential integrators for time-dependent partial differential equations we refer to the review [11] and the references therein.

2.2 One-step methods

2.2.1 Exponential Runge-Kutta methods

A general exponential Runge-Kutta scheme applied to (2) is of the form

\[ Y_{ni} = e^{c_i h_n J} u_n + h_n \sum_{j=1}^{s} a_{ij} (h_n J) G_{nj}, \quad 1 \leq i \leq s \]  

(4a)

\[ u_{n+1} = e^{h_n J} u_n + h_n \sum_{i=1}^{s} b_i (h_n J) G_{ni}, \]  

(4b)

where

\[ G_{ni} := g(t_n + c_i h_n, Y_{ni}). \]  

(5)

The coefficient functions \( b_i(z) \) are linear combinations of the entire functions

\[ \varphi_k(z) = \int_0^1 e^{(1-\tau)z} \frac{\tau^{k-1}}{(k-1)!} d\tau \]  

and \( a_{ij}(z) \) of \( \varphi_k(c_i z) \) respectively. The following recurrence formula is satisfied

\[ \varphi_{k+1}(z) = \frac{\varphi_k(z) - \varphi_k(0)}{z}, \quad \varphi_0(z) = e^z. \]  

(7)
These functions play a very important role in exponential integrators, and the efficient computation or approximation of $\varphi_k(\gamma h_n J)u$ for $\gamma \in [0, 1]$ is essential, see section 3.2 below.

If the following simplifying assumptions on the coefficient functions $a_{ij}$ and $b_i$ are satisfied

$$
\sum_{i=1}^{s} b_i(z) = \varphi_1(z), \quad \sum_{j=1}^{s} a_{ij}(z) = c_i \varphi_1(c_i z), \quad 1 \leq i \leq s,
$$

(cf. [7], the scheme (4) can be reformulated as

$$
Y_{ni} = u_n + c_i h_n \varphi_1(c_i h_n J) F(t_n, u_n) + h_n \sum_{j=1}^{s} a_{ij}(h_n J) D_{nj}, \quad 1 \leq i \leq s
$$

(9a)

and

$$
u_{n+1} = u_n + h_n \varphi_1(h_n J) F(t_n, u_n) + h_n \sum_{i=1}^{s} b_i(h_n J) D_{ni},
$$

(9b)

where

$$
D_{nj} = g(t_n + c_j h_n, Y_{nj}) - g(t_n, u_n).
$$

(10)

Thus, all (internal) stages can be interpreted as corrected exponential Euler steps.

In our package, we restrict ourselves to explicit schemes ($a_{ij}(z) = 0$ for $j \geq i$) satisfying (5). Note that this implies $D_{n1} = 0$, and the sum over the inner stages in (9) actually starts with two.

The package includes implementations of the exponential Euler method ($s = 1$), two two-stage schemes proposed by Streinhel and Weiner [21] Example 4.2.2 (cf. (2.39) and (2.40) in [11]) and two three-stage methods by Hochbruck and Ostermann (cf. (5.8) and (5.9) in [7]), two methods with four stages, namely the ETD4RK method by Cox and Matthews in [3] and the ETD4RK-B method by Krogstad in [14] and a method with five stages (cf. (5.19) by Hochbruck and Ostermann in [7]).

For details on the convergence properties of these methods in a framework of parabolic partial differential equations we refer to [7].

Our implementation allows one to easily add other explicit Runge-Kutta schemes, see section 4.3 below. We implemented these methods for constant step sizes only.

### 2.2.2 Exponential Rosenbrock-type methods

If we apply an exponential Runge-Kutta scheme to the linearized equation (3) we obtain exponential Rosenbrock-type methods [8]. For an efficient implementation, these methods should also be reformulated such that most of the matrix functions are multiplied with vectors of small norm:

$$
D_{nj} = g_n(t_n + c_j h_n, Y_{nj}) - g_n(t_n, u_n),
$$

(11)

where

$$
g_n(t, u) = F(t, u) - J_n u - d_n t.
$$

This yields

$$
Y_{ni} = u_n + h_n c_i \varphi_1(c_i h_n J_n) F(t_n, u_n)
$$

$$
+ h_n^2 \varphi_2(c_i h_n J_n) d_n + h_n \sum_{j=2}^{i-1} a_{ij}(h_n J_n) D_{nj},
$$

(12a)

and

$$
u_{n+1} = u_n + h_n \varphi_1(h_n J_n) F(t_n, u_n) + h_n^2 \varphi_2(h_n J_n) d_n + h_n \sum_{i=2}^{s} b_i(h_n J_n) D_{ni}.
$$

(12b)

For autonomous problems, we have $d_n = 0$.

The toolbox contains the exponential Rosenbrock-Euler method, where $s = 1$, and the methods exprb3 and exprb4 that are proposed in section 5.1 in [8]. For all three methods an error estimator is available, which makes it possible to use variable step sizes. The latter two methods use an embedded scheme for the estimation of the local error. For the exponential Rosenbrock-Euler method we used the error estimator described in [2].
2.2.3 exp4

The exp4 scheme proposed in [10] was the seed for many activities on exponential integrators and matrix functions. With the paper, the authors provided MATLAB and C-codes of exp4, which can be used easily. The exp4 scheme has two different error estimators and also features a dense output formula to evaluate the numerical solution at arbitrary times. Our EXPODE package is actually inspired by the original exp4 codes. In particular a lot of fine tuning for the Krylov method for the approximation of the matrix functions (see section 3.2) was motivated by this integrator.

exp4 can be interpreted as a special case of an exponential Rosenbrock-type method, which uses the \( \varphi_1 \) function only.

2.3 Multistep Methods

2.3.1 Exponential Adams methods

Motivated by classical Adams methods [5, 17] their exponential counterpart, exponential Adams methods, were constructed for the solution of semilinear problems \( (2) \) in [18]. In contrast to classical methods, the interpolation is done for the nonlinearity \( g \) instead of the full right hand side \( F \).

For a constant step size \( h \), an exponential \( k \)-step Adams method has the form

\[
\begin{align*}
  u_{n+1} &= e^{-hJ} u_n + h \sum_{j=0}^{k-1} \gamma_j (-hJ) \nabla^j G_n \\
  &= u_n + h \varphi_1 (-hJ)(G_n - Ju_n) + h \sum_{j=1}^{k-1} \gamma_j (-hJ) \nabla^j G_n 
\end{align*}
\]

with coefficient functions

\[
\gamma_j(z) = (-1)^j \int_0^1 e^{(-1-\tau)z} \left( -\tau \choose j \right) d\tau, \quad \text{where} \quad \left( -\tau \choose j \right) = \frac{1}{j!} \prod_{k=0}^{j-1} (-\tau - k).
\]

Here,

\[
\nabla^0 G_n = G_n, \quad \nabla^{j+1} G_n = \nabla^j G_n - \nabla^j G_{n-1}, \quad j \geq 1
\]

denote the backward differences for \( G_j = g(t_j, u_j), \ j = 1, \ldots, n \). The coefficient functions are linear combinations of the \( \varphi \) functions [19]. An analysis of these methods is given in [11]. To start the \( k \)-step methods, we used the fixed point iteration proposed in [12]. Alternatively, we also provide the option to use an exponential Runge-Kutta method to compute the starting values.

The package contains exponential \( k \)-step Adams methods for \( k = 1, \ldots, 6 \).

2.3.2 Linearized exponential multistep methods

The same idea of interpolation is now applied to the linearized equation [19]. An additional order of accuracy is gained by exploiting

\[
\frac{\partial g_n}{\partial u}(t_n, u_n) = 0, \quad \frac{\partial g_n}{\partial t}(t_n, u_n) = 0.
\]

See [12] for details. The interpolation polynomial \( \tilde{p}_n \) now additionally satisfies \( \tilde{p}_n(t_n) = 0 \) accordingly. These linearized exponential multistep methods are defined as

\[
\begin{align*}
  u_{n+1} &= u_n + h \varphi_1 (hJ_n)F(t_n, u_n) + h^2 \varphi_2 (hJ_n)d_n + h \sum_{j=1}^{k-1} \tilde{\gamma}_{j+1} (hJ_n) \sum_{\ell=1}^{j} \nabla^\ell G_{n,n}, \\
\end{align*}
\]

with weights

\[
\tilde{\gamma}_{j+1}(z) = (-1)^{j+1} \int_0^1 e^{(-1-\tau)z} \left( -\tau \choose j \right) d\tau
\]

(15b)
and backwards differences now based on $G_{n,m} = g_{n}(t_{m},u_{m})$ keeping the first index fixed. In addition to this general scheme, an implementation of the scheme proposed in [21, formula (39)] is contained in our toolbox. Again using the fixed point iteration proposed in [12], we implemented integrators for $k = 1, \ldots, 5$. Using an exponential Rosenbrock scheme for the initial steps instead, we can obtain exponential linearized multistep methods up to $k = 4$ due to the accuracy of the onestep methods.

## 3 Implementation Issues

In this section we discuss some details of our implementation.

### 3.1 Step Size Control

Step size control is provided for exponential Rosenbrock-type methods and exp4 via a standard Gustafsson approach [5, pp. 31–35 and pp. 550ff] together with different norms of the scaled error vector

$$
\hat{e}_{n} = \left( \frac{e_{n}(i)}{sc(i)} \right)_{i=1}^{d}, \quad sc = ATol + \max \{|u_{n}|,|u_{n-1}|\} \cdot RTol, 
$$

where $(i)$ denotes the $i$-th component and $e_{n}$ is the estimated error in the $n$th time step. By default we use the maximum-norm (complying to MATLAB’s defaults), but can easily switch to other norms like the Euclidian norm or user defined norms defined in a MATLAB function or by an inner product defined via its Gramian matrix. This is implemented in the options NormControl and NormFunction.

The desired accuracy is determined by the absolute ($ATol$) and relative ($RTol$) tolerance and the chosen norms. An implementation using an iterative process for the evaluation of the matrix functions also has an impact on the step size selection. We will discuss this in the following section.

### 3.2 Matrix Functions

We now turn our attention to the matrix functions arising in exponential integrators.

Since the $\varphi$ functions are analytic, $\varphi(hJ)$ can be computed via diagonalization if $J$ is diagonalizable. The evaluation of $\varphi$ at the eigenvalues can be computed directly from (6) via

$$
\varphi_{k}(z) = \begin{cases} 
e{z} - \left(1+z+\frac{z^{2}}{2!}+\ldots+\frac{z^{k-1}}{(k-1)!}\right), & z \neq 0, \\ \frac{1}{z^k}, & z = 0. \end{cases} 
$$

(16)

In finite precision arithmetic, we use a sufficiently high-order Padé approximation in a neighborhood of zero. Alternatively, one could break down recursion formula (7) to the evaluation of the exponential function $\varphi_{0}(z) = e^{z}$ or use contour integration [13, 19, 15, 22].

Diagonalization is inefficient for large matrices, but fortunately, exponential integrators do not require the complete matrix function but $\varphi_{k}(h_{n}J)v$ for a vector $v$ only. This can be approximated within a Krylov subspace with respect to $J$ and $v$, see [4, 9].

Krylov methods have the advantage that they require the evaluation of the matrix-vector products $Jv$ only. It is not necessary to compute the full Matrix $J$ explicitly. The error is controlled via the error estimators proposed in [10, 18].

We implemented configurable maximal Krylov subspace dimensions (cf. KrylovMaxDim option). If the Krylov approximation fails to converge within the maximum allowed dimension of the Krylov space, the step size $h$ has to be reduced such that with the reduced step size, the error estimator fulfills the accuracy requirements. If we cannot reduce the step size (e. g. if we run a code for constant step sizes), a warning is triggered. Note that all products of $\varphi$ functions with the same vector $v$ can be approximated in one Krylov subspace. The dimension of this subspace is chosen such that all $\varphi$ functions are approximated sufficiently well.

In addition, we reuse data from previous steps if possible. For instance, if we compute matrix functions via diagonalization, solving semilinearized ODEs [2], and use the same step size in the
next time step, we do not have to recompute $\varphi_k(h_nJ)$. We also reuse the Krylov subspace for $\varphi_k(h_nJ_n)F(t_n,u_n)$ if we have to reduce the step size to to a step rejection.

For statistical purposes, we provide data about the Krylov process. This data is displayed at the end of the integration process by default. A typical output looks like this:

\begin{verbatim}
statistics:
[ ... ]
number of matrix function evaluation times vector: 331
number of Krylov subspaces: 147
total number of Krylov steps: 1455
number of step size reductions due to Krylov: 0
number of recycled subspaces: 10
maximal dimensions of subspaces: F1: 15, v: 15, D2: 15, D3: 11
\end{verbatim}

The first line reports the number of products of a $\varphi$-function with a vector, the second line contains the number of Krylov subspaces that have been built for different vectors. The third line counts the sum of all Krylov subspace dimensions in the whole integration process. Next we have the number of step size reductions which are necessary to fulfill the error tolerances, followed by the number of reused subspaces. Those can arise after a step rejection – either by the error estimator of the integrator or by the Krylov process. The maximal dimensions in the last line correspond to the maximal dimension of a subspace for a specific vector. Their meanings can be looked up in table 1. Note that the multistep methods require initial steps, such that – depending on the choice of their computation – some of the labels for Runge-Kutta and Rosenbrock-type methods may appear in their statistics as well.

\begin{table}[h]
\centering
\begin{tabular}{lll}
\hline
name & vector & integrator type(s) \\
\hline
F1 & $F(t_n,u_n)$ & linearized \\
v & $\frac{\partial F}{\partial t}(t_n,u_n)$ & linearized \\
D_i, $i = 2, 3$ & $D_{n_i}$ & Rosenbrock-type \\
Y_{plusA}, $i = 1, \ldots, 5$ & $G_{n_i} - Ju_n$ & Runge-Kutta \\
d_i, $i = 4, 7$ & $d_n$ & exp4 \\
GDiff_i, $i = 1, \ldots, 6$ & $\nabla G_n$ & both multistep \\
GDiffInit_i, $i = 1, \ldots, 6$ & $\Delta G_n$ & both multistep \\
\hline
\end{tabular}
\caption{Meaning of the labels in the Krylov statistics output}
\end{table}

4 Usage

In this section we give a brief introduction to the MATLAB package EXPODE. A more extensive documentation is contained in the EXPODE package (manual.pdf).

4.1 Installation and Requirements

We will now describe the minimal requirements and the installation of the EXPODE toolbox. EXPODE runs on all recent and middle-aged computers. The performance strongly depends on the problem and on the available hardware. The toolbox was tested on MATLAB versions down to MATLAB 7.2 (R2006a), released in 2006. It is not compatible to versions prior to 7.0 due to the lack of proper function handles. You can download the package from the author’s web pages. Two different versions are available, a package for users and an extended one for developers. The latter contains some additional tools helpful for extending EXPODE. Usually the user package should be sufficient.

To install, just unpack the archive. This will create a new expode subdirectory. To make it available in MATLAB, just add the package’s root to MATLAB’s path and run the initPaths function with
To make a permanent installation for the current user, put the above line into your `startup.m` file. See MATLAB’s help for more information.

### 4.2 Quick Start

To get a first impression of EXPODE we start with running some of the examples included. To access the examples we add the examples directory to the MATLAB path. Run the following commands

```matlab
>> addpath mydownloadpath/expode/examples;
>> [t, y] = Heat1D([], [], 'run');
```

to solve a heat equation with a time-dependent source term in one dimension. Use

```matlab
>> help Heat1D;
```

to obtain information on the example. The solution will be visualized in a mesh plot. All examples contained in the package can be run by simply calling them without arguments. Short information on the problems is available via `help`. To work with the solver, it is convenient to run the example manually.

```matlab
>> % parameters
>> N = 100; epsilon = 0.1; gamma = 0.1;
>> % get initial conditions
>> [tspan, y0, options] = Heat1D([], [], 'init', N, epsilon, gamma);
>> % run the example
>> [t, y] = expode(@Heat1D, tspan, y0, options);
```

Now we can start playing with options and parameters. Switching to the direct solver for the matrix functions, we use

```matlab
>> options = expset(options, 'MatrixFunctions', 'direct');
```

Other options are set similarly. Some checks on the values set for an option are applied automatically. An overview of the available options for an integrator is provided by calling the integrator `info` without arguments. More detailed information on a specific option can be shown with this command as well:

```matlab
>> exprbinfo % prints all available options for exprb
>> exprbinfo MinStep % prints help text for MinStep option
```

A common task is to create order plots, where the problem is solved on a fixed time interval with a number of different time steps and the error is plotted over these time steps. Computing the error or an approximation to it requires one to evaluate the exact solution or a very accurate reference solution first. If an exact solution is available, this can be done by calling `ode(t, [], 'exact')`. As an example to show how simply this can be done with the package, we consider the `semi1` example. We refer to its help text for detailed information. An order plot for a finite difference spatial discretization with \( N = 50 \) grid points for all Rosenbrock-type methods is created via

```matlab
>> allMethods(@semi1, 'exprb', '', [], 50);
```

The input argument `''` chooses the direct solver for the evaluation of the matrix functions. The chosen step sizes depend on the problem’s `tspan` data and are chosen uniformly logarithmically. This choice and other parameters can be manipulated with options to `allMethods`.

To implement a new differential equation, we recommend modifying one of the example files in the `examples` directory. You should start in `examples/Hello_World`, where we put some introductory files. `MinEx.m` is a very simple example while `Template.m` uses more advanced features. Both files contain many helpful comments.
4.3 Running Specific Integrators

Here we briefly describe how the specific exponential integrators can be invoked. The calling sequence of all EXPODE integrators is

$$\texttt{>> [t, y] = integrator(@ode, {@jac}, {tspan, y0}, {opts}, {varargin});}$$

where \texttt{integrator} has to be substituted by either \texttt{expode} or one of the specific integrators below. Arguments in braces (\{\}) are optional. The at sign (@) represents either a function handle, a function name as string or an \texttt{inline} object. The function \texttt{@ode} has to evaluate data of the differential equation required for the solution. It follows MATLAB's standard syntax, though it should be callable with

$$\texttt{res = ode(t, y, flag, varargin);}$$

where the flag controls what the function returns. The \texttt{ode} function has to return the evaluation of the right hand side of the differential equation, when the empty string ('') is given as flag. This is needed for all solvers. In addition other flags have to be handled depending on the integrator, see table 2.

| flag   | meaning                        | integrator type(s) |
|--------|--------------------------------|--------------------|
| 'F'    | $F(t, u)$                      | all                |
| jacobian| $J_n = \frac{\partial F}{\partial u}(t, u)$ | linearized         |
| linop  | $J$ from [2]                   | semilinear (req.) and linearized (opt.) |
| gfun   | $g(t, u)$ from [2]             | semilinear (req.) and linearized (opt.) |
| df_dt  | $d_n = \frac{\partial F}{\partial t}(t, u)$ | linearized (opt.) |
| dg_dy  | $\frac{\partial g}{\partial u}(t, u)$ | semilinear (req.) and linearized (opt.) |
| init   | return default [ tspan, y0, opts ] for the equation | all (opt.) |

Flags for \texttt{mabode} file for the different integrators

The \texttt{@jac} argument is only available for the linearized integrators and is a handle to a function evaluating the Jacobian. Alternatively the \texttt{ode} will be queried with the 'jacobian' flag. \texttt{tspan = [ t_0, T ]} is the integration interval, \texttt{y0} the initial condition. \texttt{opts} is an options structure, set with one of the set commands and \texttt{varargin} will be passed to \texttt{ode} to configure parameters of the differential equation.

The command to use an \textit{exponential Runge-Kutta integrator} is \texttt{exprk}. To select one of the schemes described in section 2.2 use the \texttt{Scheme} option. The default scheme is 'Krogstad'. To set the parameters appearing in some of the methods, use the \texttt{Parameters} option. For a detailed overview of the available schemes we refer to the integrator documentation.

The command to use an \textit{exponential Rosenbrock-type integrator} is \texttt{exprb}. To select one of the three available schemes, use the \texttt{Order} option with value 'two', 'three' or 'four', where the latter is the default. To control the parameters for the error estimator for the order four integrator use \texttt{ErrorEstimate}. We refer to the documentation for details on the schemes.

The \texttt{exp4} method is called with the \texttt{exp4} command. It has a built in dense output generator, that allows one to evaluate the numerical solutions at arbitrary times. Specify \texttt{t = [ t_0, \ldots, t_m ]} to use this feature, where the sequence \texttt{\{t_j\}_{j=0}^m} is either strictly increasing or strictly decreasing.

The \textit{semilinear k-step methods} are available via \texttt{expmssemi}, where \texttt{k} is set with the \texttt{kStep} option. Our implementation allows constant step sizes only.

The \textit{linearized k-step methods} are called with \texttt{expms}, where \texttt{k} is defined as for \texttt{expmssemi}. You can also select 'Tokman' to use the scheme suggested in [21] eq. (39)].
| ODEproperty                  | option       | choices                        | integrators |
|------------------------------|--------------|--------------------------------|-------------|
| autonomous/nonautonomous     | NonAutonomous| {'off'}, 'on'                   | linearized  |
| semilinear equation          | Semilin      | {'off'}, 'on'                   | linearized  |
| constant/nonconstant Jacobian| JConstant    | {'off'}, 'on'                   | linearized  |
| complex/real valued solution | Complex      | 'off', {'on'}                   | all         |
| structure of the Jacobian    | Structure    | {'none'}, {normal', 'symmetric', 'skewsymmetric', 'diagonal'} | all         |

Options corresponding to properties of differential equations. Default values are set in braces.

### 4.4 Properties of Equations

Some problems allow one to exploit certain properties to improve the efficiency of the integrator. In Table 3 we collected some properties together with information on how to exploit them in EXPODE. Note that for non autonomous equations you might get wrong results, when the appropriate option is not set.

### 4.5 Matrix Functions

As mentioned before, the evaluation of the matrix functions is a crucial point in the implementation of exponential integrators.

The default setting for the matrix function evaluator is to compute and store the full matrix functions. This is suitable for small or medium sized problems. It requires one to evaluate the full Jacobian or its linear part. For linearized problems, the Jacobian has to be computed in each time step while for methods based on a fixed linearization, it has to be computed only once.

We also provide an implementation of the Arnoldi process to approximate the matrix functions, which can be used for large scale problems. It should not be used for very small problems, where the direct evaluation is more efficient and more reliable.

To switch on the Krylov method, set

```matlab
>> options = exprbset('MatrixFunctions', 'arnoldi');
```

Krylov subspace methods can be implemented by using the matrices $J_n$ or $J$ explicitly (saved as sparse matrices) or in a matrix-free fashion, where subroutines for the evaluation of the matrix-vector products $J_n v$ or $J v$, respectively, are provided. The options for these matrix-free versions are activated by setting

```matlab
>> options = exprbset(options, 'JacobianV', 'on');
>> options = exprbset(options, 'LinOpV', 'on');
```

respectively. If one of these options is 'on', then the corresponding ODEfile should provide flags 'jacobian_v' or 'linop_v' respectively. Alternatively a function handle to a function defined as function res = evalFun(t, y) can be provided instead of 'on' to evaluate the required parts in its own routine.

To add more flexibility we also enabled the user to provide his or her own implementation to compute the matrix functions. This is especially interesting for situations where the matrix functions can be computed more cheaply, more easily, or in a structure-preserving way due to special properties of the matrix. Then, instead of the 'direct' or 'arnoldi' settings a function handle has to be given

```matlab
function [ hOut, varargout ] = ...
matFun(job, t, y, h, flag, v, reusable, reuse, facs).
```
We refer to the documentation contained in the package for detailed instruction. Here we will only give a short introduction.

Due to the possible complexity of this task, a number of stages have to be incorporated into the process: in addition to the evaluation itself there is an 'init', a 'registerjobs' and an 'initstep' phase to precompute data – indicated by the corresponding value for flag. It might happen that the evaluator requires to reduce the step size to guarantee the prescribed accuracy. Therefore it is possible to return a different value for hOut than the input step size h to indicate such a time step reduction.

Details of the implementation can be found in the manual. We suggest taking the two EXPODE internal evaluators – matFun/matFunDirect.m and matFun/matFunKrylov.m – as a guideline.

4.6 Custom Integrators

The EXPODE package was implemented such that it is open for user specified extensions in many different ways. An example was pointed out in the previous section for the evaluation of the matrix functions. It is also possible to add new time integrators to the package. To do so, one should use the developer package of EXPODE, which contains some useful tools for this purpose. The integration steps for the integrators are written as plugins to the expode routine. The developer does not need to worry about things like direct user interaction syntactical options checking, output control and other management tasks.

We provide scripts to generate an integrator stub and for deployment. For a rudimentary integrator only three files have to be edited after running the generation script: a setup routine which gives some information to the expode, a routine that provides the options for the user and the integration step itself. Detailed information on the development process are available in the documentation contained in the EXPODE package.

5 Examples

In this section we want to discuss some numerical examples.

5.1 van der Pol equation

To benchmark the adaptive step size implementation, let us consider the well-known van der Pol equation [23]. It describes a non-linearly damped oscillator. Written as a second order ODE it reads

\[ u''(t) - \mu(1 - u(t)^2)u'(t) + u(t) = 0. \]

With large \( \mu \) the equation becomes very stiff. A plot of the solution with \( u(0) = [2, -0.6]^T \) and \( \mu = 1000 \) can be found in figure 1. At the vertical edges the first derivative of the solution becomes very large so that small step sizes have to be chosen. We plotted the step sizes selected by the step size control of exprb4, exprb3 and exp4. Due to their larger (classical) order, exprb4 and exp4 can choose larger step sizes.

5.2 Semilinear Problem

Another MATLAB package implementing exponential Runge-Kutta methods and exponential multistep methods, is EXPINT [1]. Note that the evaluation of matrix functions in EXPINT corresponds to the "direct" option in our package. This favors our package for large scale problems. We compare the efficiency of both packages on the semilinear problem

\[ u'(x) = \Delta u + \frac{1}{1 + u^2} + \Phi, \quad u(0, x, y) = x(1-x)y(1-y) \quad (17) \]

with homogeneous Dirichlet conditions on \( \Omega = [0, 1]^2 \). \( \Phi \) is chosen such that the exact solution is given by \( u(t, x, y) = x(1-x)y(1-y)\exp(t) \), see e.g. [1] or [7]. The space discretization was done with finite differences with \( N = 50 \) inner grid points in each dimension. This yields a system of ODEs of medium size dimension \( N^2 = 2500 \). We compared EXPINT’s and our implementation of the Hochbruck-Ostermann exponential Runge-Kutta scheme [7] and our implementation of
the three stage exponential Rosenbrock method. Additionally we solved the one-dimensional version of this problem with \( N = 100 \) grid points to retrieve a low-dimensional ODE of \( N = 100 \) degrees of freedom. The results are shown in figure 2.

Figure 2: Left: Time vs. error plots for the one-dimensional version, middle: step size vs. error and right: time vs. error plots for the two-dimensional version of the semilinear problem. Dotted: EXPINT, dashed: EXPODE with diagonalization, dash-dotted: EXPODE with Krylov method for the Matrix functions, solid: exprb, thin dashed in the middle image: slope line of order four.

In the left image we see that for low dimensional systems and small target accuracies, EXPINT is clearly preferable, since it is much faster. Especially the Krylov matrix function evaluator has negative impact on the performance since it has the overhead of building up the Krylov subspaces each time step while EXPINT only computes some matrix exponentials via Padé approximation. For \( 100 \times 100 \) matrices the solution of the linear systems arising there is quite cheap.

In the middle image we see numerical order four of all solvers.

EXPINT uses Padé approximations and a scaling and squaring technique to compute the \( \varphi \) functions. Let \( J \) be the discretized Laplacian operator, then \( hJ \) has to be scaled, such that its norm is smaller than a given bound. This implies that smaller time step sizes lead to fewer scaling and squaring steps. After computing the \( \varphi \) functions of the matrix once only matrix vector products are needed for the time stepping, such that a smaller time step size actually leads to faster computations.

For the direct solver in EXPODE we have an initialization phase, where we diagonalize the operator \( hA \), which takes the same time independent of \( h \). Then we apply \( \varphi_k(hA) \) directly as EXPINT does, so we get only slightly increased costs for higher accuracy by the smaller time step size.

In EXPODE with the Arnoldi method for the matrix functions we build up Krylov subspaces in each timestep and cannot reuse data from previous time steps. Nevertheless, this is much faster than computing the matrix functions themselves.
5.3 Brusselator

As our next example we use the Brusselator example, which was also used to benchmark the original exp\textsuperscript{4} code \cite{10}. It models a reaction-diffusion process with two species $u = u(t,x,y)$ and $v = v(t,x,y)$. The equation reads

$$
\frac{d}{dt} \begin{pmatrix} u \\ v \end{pmatrix} = A \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} \gamma + u^2v \\ u - u^2v \end{pmatrix}, \quad A = \begin{bmatrix} \alpha \Delta - (\beta + 1) & 0 \\ \beta & \alpha \Delta \end{bmatrix}
$$

together with homogeneous Neumann boundary conditions. The initial value for $u$ is taken from MATLAB’s \texttt{peaks} function and $v(0,\cdot,\cdot) \equiv 0$. The stiffness results from the diffusion term $A$. We choose the parameters $\gamma = 1$, $\beta = 3.4$ and the diffusion coefficient $\alpha = 10^{-2}$. Space discretization is done via finite differences with $100^2$ grid points in $\Omega = [0,1]^2$. This results in a system of 20,000 unknowns.

In figure 3 we present time step vs. error and work-precision diagrams for the fourth order representatives of each of our integrator classes. The multistep integrators use the fixed point iteration for their starting values. As matrix function evaluator we choose the Arnoldi Krylov method with a maximal dimension of 36 for the Krylov subspaces for the linearized one-step methods and 100 for the others. We choose to use constant step sizes with matching tolerances for the Arnoldi process, since not all integrators allow adaptive step sizes. The error is measured in the maximum norm against a reference solution computed by MATLAB’s \texttt{ode15s} with sufficiently high accuracy requirements. This means that we only consider the ODE error and not the spatial error. We added dashed lines for slope of order four.

In the time vs. error plot we arranged data for the same runs and additionally gave two curves for the multistep integrators using exprb (linearized) and exprk (exponential Adams) for the initial values.

Figure 3: Step size vs. error and time vs. error plots for different fourth order integrators applied to the Brusselator example. Integrators: 3 stage exprb (solid line), exp4 (dashed line), 5 stage Hochbruck-Ostermann exponential Runge-Kutta-Scheme (dash-dotted line), 3 step expms with initial values computed by fixed point iteration (dotted, plus markers) and with exprb initial values (dotted, square markers) and 4 step expmssemi with Runge-Kutta initial values (dashed, plus markers) and with initial values computed by fixed point iteration (dashed, square markers).

In the first image we observe fourth order convergence for all schemes as $h \to 0$. The two linearized one-step methods have the best error constants (offset on the error-axis) closely followed by the exponential Runge-Kutta scheme.

In the second one we see the linearized one step methods lead to the best accuracy for a given computation time. Here the exponential Runge-Kutta scheme lags a bit further behind, since it is computationally more expensive due to its five internal stages. exp4 has seven of them, but the first three and the second three of them can be computed simultaneously, see \cite{10}, so exprb\textsuperscript{4} and exp4 have approximately the same computational costs. The multistep integrators (with plus sign markers) are much weaker for larger time steps. The reason for this is the fixed point iteration which gets relatively more expensive when the time step size increases. In figure 4 we
Figure 4: Left: number of fixed point steps required to fulfill the accuracy requirement for the different step sizes in the Brusselator Example. \texttt{expms}: dotted, plus markers, \texttt{expmssemi}: dashed, plus markers. Right: approximate costs for the fixed point iterator linestyles and markers as in left picture, approximate costs for the (non-startup) time steps, approximate costs for the whole integration, line styles as left, now square markers.

show the number of fixed point steps required versus the step size chosen and an approximation of the normal time step costs versus the fixed point step costs. Each fixed point step costs approximately as much as the number of backwards steps in use times the cost of one time step. So the \texttt{expms} solver fixed point step costs 3 normal time steps, the \texttt{expmssemi} fixed point step 4 normal time steps. The plot assumes constant time for the matrix function evaluator. We also gave curves for multistep methods with \texttt{exprb/exprk} initial values, which are significantly more efficient, especially for larger step sizes in this case. Note that multistep methods of order higher than four can only be obtained using the fixed point iteration.

5.4 2D Maxwell’s equations with spatial discontinuous Galerkin discretization

As an example for a hyperbolic problem we consider Maxwell’s equations in two space dimensions. For a charge free domain the equations are given by

\[
\begin{align*}
\mu \frac{\partial}{\partial t} \vec{H} &= -\nabla \times \vec{E} \\
\varepsilon \frac{\partial}{\partial t} \vec{E} &= \nabla \times \vec{H}.
\end{align*}
\]

Here \( \vec{E} \) denotes the electric field, \( \vec{H} \) the magnetic field, \( \varepsilon \) the permittivity and \( \mu \) the permeability. Assuming constant \( \mu \) and \( \varepsilon \) and using normalized cartesian coordinates we can eliminate the two material parameters.

As domain we use a magnetic box \( \Omega = [-1, 1]^3 \). Our initial conditions are chosen, such that

\[
\begin{align*}
\vec{E} &= \begin{bmatrix} 0 \\ 0 \\ \sin(k\pi x) \cdot \sin(k\pi y) \cdot \cos(tk\sqrt{2}\pi) \end{bmatrix} \\
\vec{H} &= \begin{bmatrix} -\frac{1}{\sqrt{2}} \sin(k\pi x) \cdot \cos(k\pi y) \cdot \sin(tk\sqrt{2}\pi) \\ \frac{1}{\sqrt{2}} \cos(k\pi x) \cdot \sin(k\pi y) \cdot \sin(tk\sqrt{2}\pi) \\ 0 \end{bmatrix}
\end{align*}
\]

is the exact solution. We assume the arising quantities to be constant in the \( z \)-direction to reduce to two spatial dimensions. The space discretization is done using the discontinuous Galerkin method (DG-method) from the codes by [6]. We created grids with a tiny triangle in the center to simulate very filigree structures and bad quality grids. We run four different ratios between
maximal area of the outer elements to area of the center triangle, see figure 5 for examples. For grid generation we use [?].

Figure 5: Examples for the grids used in the Maxwell example with ratios 1 (left) and $(\frac{1}{4})^2$ (right).

We were interested how the existence of tiny elements in an otherwise mostly coarse grid would affect the stability requirements by an exponential integrator.

In our numerical experiment we created time vs. error plots. The error was measured in the $L^2$-Norm against the exact solution. The spatial resolution was refined and the time step sizes were chosen such that the solvers are stable and the time and the spatial discretization errors are almost equal.

We compared the explicit space saving order four Runge-Kutta method used in [6] with our three stage exponential Rosenbrock-type (exprb) and the exp4 integrators, both using the Arnoldi method to compute the matrix functions. The time step size in the Runge-Kutta solver is automatically chosen, such that the solver is stable. This automatically leads to a time discretization error in the magnitude of the spatial error. For exprb and exp4 we set the accuracy requirement to the values retrieved by a reference solution and allowed adaptive step size choice. We also used the $L^2$ norm for the step size estimator. This was done providing a custom error norm function using the mass-scalarproduct from the DG-codes via the NormFunction option.

The results are shown in Figure 6. We give plots of spatial step size ($\Delta x$) vs. error (measured against the exact solution, not the reference solution), $\Delta x$ vs. chosen time step sizes ($h$) and a time vs. error plots.

In the first row of images we see, that the accuracy matches the requirements of the spatial discretization.

For the smallest grid ratio we see, that the exponential methods choose larger time steps. Still we get no speed gain, because we have to build an up to 36-dimensional Krylov subspace in each time step.

While both the Runge-Kutta and the exponential methods decrease their time step sizes due the bigger irregularity of the grid for shrinking grid ratios, the gap between the curves grows. This also corresponds to the time vs. error plots, where the exponential methods get relatively faster for more irregular grids. In the following table we present the average quotient of the time step size of the exprb integrator and the Runge-Kutta solver and the average speedup by grid ratio:

| ratio          | 1 | $(\frac{1}{4})^2$ | $(\frac{1}{16})^2$ | $(\frac{1}{64})^2$ |
|----------------|---|------------------|-------------------|-------------------|
| avg. $h$ quotient (exprb vs. Runge-Kutta) | 8.06053 | 15.481 | 26.1532 | 35.5925 |
| avg. speedup (exprb vs. Runge-Kutta) | 1.23683 | 2.23478 | 3.39336 | 4.46899 |

We see that the exponential methods need to decrease their step size much less than the Runge-Kutta solver when decreasing the ratio. such that they become relatively more efficient on the more irregular grids. On the last grid exprb is about five times faster than the conventional integrator.

The step size estimator was tested by manually increasing the time step size. In this case the solver became unstable, so the step size estimator actually detects the stability requirement.
Figure 6: Results for the Maxwell example. Integrators: 3 stage exprb (solid line), exp4 (dashed line) and Runge-Kutta (dash dotted line), Ratios: 1, $(\frac{1}{4})^2$, $(\frac{1}{16})^2$ and $(\frac{1}{64})^2$ of the method.

It should be noted that EXPODE saves the solution in one long vector, while the MATLAB DG-codes use a custom format, where each field component is saved as one rectangular matrix containing the degrees of freedom for each finite element in its columns. For this reason our ODE file has to switch between these two formats in each function evaluation, which slows down the computation.

5.5 Conclusions

We presented a new advanced toolbox for exponential integrators, which implements several exponential integration schemes in recent research and uses modern techniques to approximate the arising matrix functions. We designed the toolbox to solve large systems of differential equations, and we have shown its applicability to those systems here. We also noticed rather weak performance for lower-dimensional systems, but the time cost was relatively small nonetheless. This coincides with the package’s philosophy: develop with small problems to use it with larger ones.

We allow substantial control over the integration process without the need of changing
EXPODE code directly. See for instance the usage of the mass norm in Maxwell example. This makes it easier to combine EXPODE with other MATLAB packages that perform well for other aspects of the equation. For example, one may want to find a spatial discretization using the DG-Codes from [6].

It has been shown that our Krylov matrix function evaluator is able to absorb spatial irregularity to some extent. This lead to some ideas for the extension of the package by an improved Krylov method that can use the problem’s mass matrix and mass scalar product to respect spatial structures. We are currently implementing this idea, and the initial tests are quite promising.

The EXPODE package is flexible, and we expect to implement further exponential schemes in the future.

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