Exponential Time Integration for Stiff Systems in Rust

Scientific Computing in Rust 2025

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June 4, 2025

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Overview

`https://github.com/ORNL/ORMATEX`. USDOE. 24 Jan. 2025. Web.
doi:10.11578/dc.20250124.7.

ORMATEX provides a Rust-based implementation of the **matrix exponential**, φ-vector products and **exponential integrators** (EI).

- EI are applicable to stiff, linear-dominant systems.
- Utilizes faer for dense and sparse matrix operations[1].
- Provides a python interface to rust-based exponential integrators via **PyO3**.

[1] `https://github.com/sarah-quinones/faer-rs`

Exponential Time Integration

Exponential integrators are expected to be profitable when the linear term is the primary contributor to the system stiffness.

$$\frac{d\mathbf{u}}{dt} = L\mathbf{u} + N(\mathbf{u}, t)$$

$$\mathbf{u}_{t+1} = e^{L\Delta t}\mathbf{u}_{t_0} + \int_0^{\Delta t} e^{L(\Delta t - \tau)} N(t_0 + \tau, \mathbf{u}_{t_0+\tau}) d\tau$$

Approximating the integral via box rule at the left yields Exponential Euler:

$$\mathbf{u}_{t+1} = e^{L\Delta t}\mathbf{u}_{t_0} + \Delta t \varphi_1(L\Delta t) N(t_0, \mathbf{u}_{t_0})$$

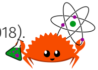
$$\varphi_0(Z) = e^Z, \ \varphi_1(Z) = Z^{-1}(e^Z - 1)$$

EI methods do not employ Newton iterations, but instead require φ-vector products and matrix exp. evaluations.

ORMATEX Capabilities Matrix

Method	Rust Status	Py Bindings	Notes
expm	✓	-	-
Rational function $\varphi(A)$ eval.	✓	✓	CRAM, Padè, Dense A
Krylov based $\varphi(A)$ eval.	✓	-	Sparse A (faer LinOp)
Exp. Rosenbrock (ExpRB)2	✓	✓	Krylov
ExpRB3	✓	✓	Krylov
EPI3	✓	✓	Krylov, KIOPS[2]
EPIRK4	in progress	-	Krylov, KIOPS
Leja ExpRB2,3	in progress	-	-
Leja EPI3	in progress	-	-

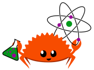
[2] S. Gaudreault, G. Rainwater, and M. Tokman. "KIOPS: A fast adaptive Krylov subspace solver for exponential integrators." J. of Comp. Phys. 372 (2018).



Example Use

```rust
use faer::prelude::*;
use ormatex::matexp_pade;
use ormatex::matexp_cauchy;

pub fn main() {
    // example matrix
    let lmat = faer::mat![
        [-1.0e-3,    1.0e1,      0.],
        [      0., -1.0e1,  1.0e-1],
        [      0.,     0., -1.0e-1],
    ];

    // expm(dt*L) with pade approx
    let dt = 1.0;
    let exp_lmat_pade = matexp_pade::matexp(lmat.as_ref(), dt);

    // expm(dt*L) with partial fraction decomposition method
    let order = 24;
    let matexp_eval = matexp_cauchy::gen_parabolic_expm(order);
    let exp_lmat_pdf =
        matexp_eval.matexp_dense_cauchy(lmat.as_ref(), dt);

    // A simple integration procedure for a pure-linear system
    // Step system u_t+1 = expm(dt*lmat)*u_t
    let mut y = faer::mat![[0.001], [0.1], [1.0]];
    let mut t = 0.0;
    for _i in 0..10000 {
        y = matexp_eval.matexp_dense_cauchy(lmat.as_ref(), dt)
            * y.as_ref();
        t += dt;
    }
```

Figure 1: $\frac{d\mathbf{u}}{dt} = L\mathbf{u}$; $\mathbf{u}_{t+1} = e^{\Delta t L}\mathbf{u}_t$. See: examples/ex_matexp_1.rs



Case Study: Bateman

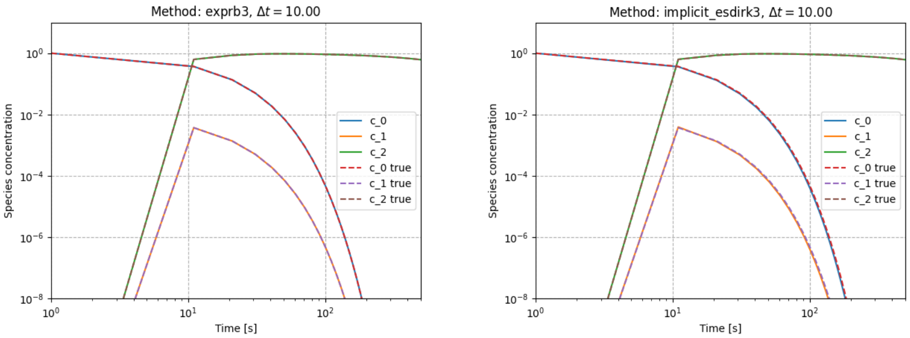


Figure 2: Exp. Rosenbrock3 (Left) vs ESDIRK3 (Right), $\Delta t = 10(s)$

$$\frac{du}{dt} = \mathbf{L}u$$

$$L = \begin{bmatrix} -0.1 & 0 & 0 \\ 0.1 & -1 \times 10^{1} & 0 \\ 0 & 1 \times 10^{1} & -1 \times 10^{-3} \end{bmatrix}$$

- 3 species: c_0, c_1, c_2.
- ICs: $c_0(t = 0) = 1$
- $c_{1,2}(t = 0) = 0$

Case Study: Bateman

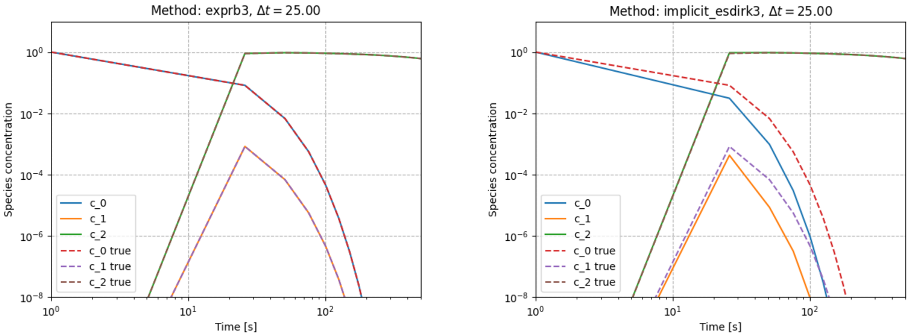


Figure 3: Exp. Rosenbrock3 (Left) vs ESDIRK3 (Right), $\Delta t = 25(s)$

$$\frac{du}{dt} = \mathbf{L}\mathbf{u}$$

$$L = \begin{bmatrix} -0.1 & 0 & 0 \\ 0.1 & -1 \times 10^{1} & 0 \\ 0 & 1 \times 10^{1} & -1 \times 10^{-3} \end{bmatrix}$$

- 3 species: c_0, c_1, c_2.
- ICs: $c_0(t = 0) = 1$
- $c_{1,2}(t = 0) = 0$

Case Study: Bateman

$$\frac{d\mathbf{u}}{dt} = \mathbf{L}\mathbf{u}$$

$$L = \begin{bmatrix} -0.1 & 0 & 0 \\ 0.1 & -1 \times 10^{1} & 0 \\ 0 & 1 \times 10^{1} & -1 \times 10^{-3} \end{bmatrix}$$

- 3 species: c_0, c_1, c_2.
- ICs: $c_0(t=0) = 1$
- $t_{final} = 100\text{s}$

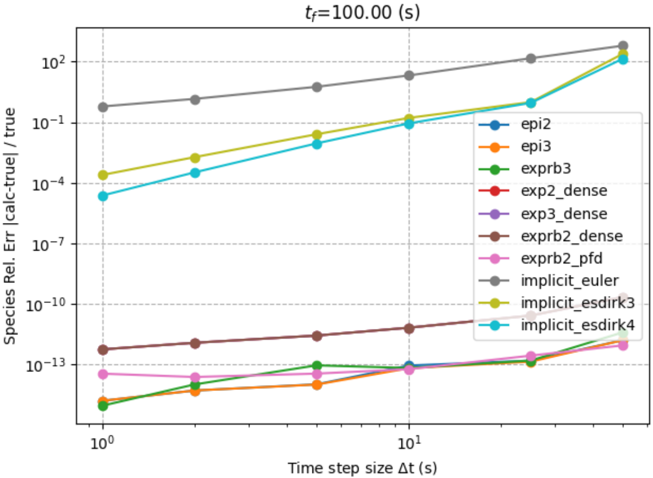


Figure 4: Error vs. Time Step Size

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Case Study: Bateman+Advection

$$\frac{\partial u}{\partial t} = \color{red}{Lu} - \color{blue}{v\nabla u}$$

$$L = \begin{bmatrix} -1 & 0 & 0 \\ 1 & -1\times 10^2 & 0 \\ 0 & 1\times 10^2 & -1\times 10^{-2} \end{bmatrix}$$

- BCs: Periodic.
- ICs: Smooth wave 0^{th} species.
- 2^{nd} order CG FEM. $\Delta x = 0.0156$(m).
- $t_{final} = 2$s. v=0.5m/s.

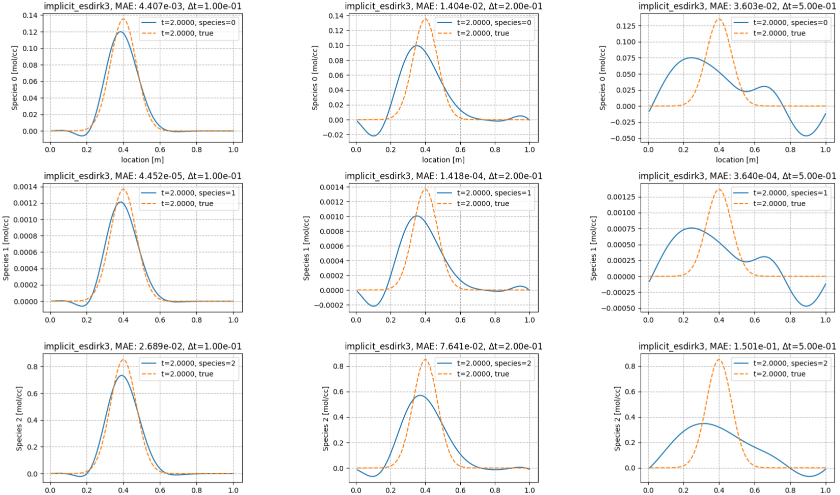

Figure 5: ESDIRK Order 3, $\Delta t = \{0.1, 0.2, 0.5\}$

Case Study: Bateman+Advection

$$\frac{\partial u}{\partial t} = Lu - v\nabla u$$

$$L = \begin{bmatrix} -1 & 0 & 0 \\ 1 & -1\times 10^2 & 0 \\ 0 & 1\times 10^2 & -1\times 10^{-2} \end{bmatrix}$$

- BCs: Periodic.
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- 2^{nd} order CG FEM. $\Delta x = 0.0156(\mathrm{m})$.
- $t_{final} = 2\mathrm{s}$. v=0.5m/s.

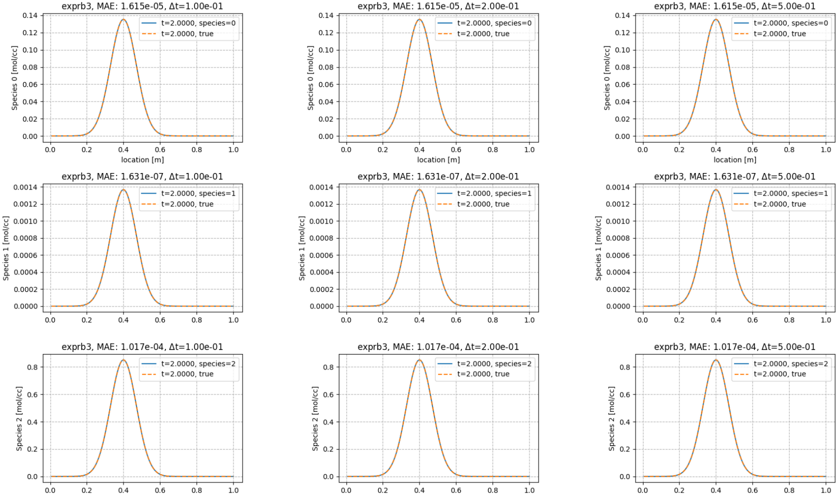

Figure 6: Exp. Rosenbrock Order 3, $\Delta t = \{0.1, 0.2, 0.5\}$

Case Study: Bateman+Advection

$$\frac{\partial u}{\partial t} = Lu - v\nabla u$$

$$L = \begin{bmatrix} -1 & 0 & 0 \\ 1 & -1\times 10^2 & 0 \\ 0 & 1\times 10^2 & -1\times 10^{-2} \end{bmatrix}$$

- BCs: Periodic.
- ICs: Smooth wave 0^{th} species.
- 2^{nd} order CG. $\Delta x = 0.0156(m)$.
- $t_{final} = 2s$. v=0.5m/s.

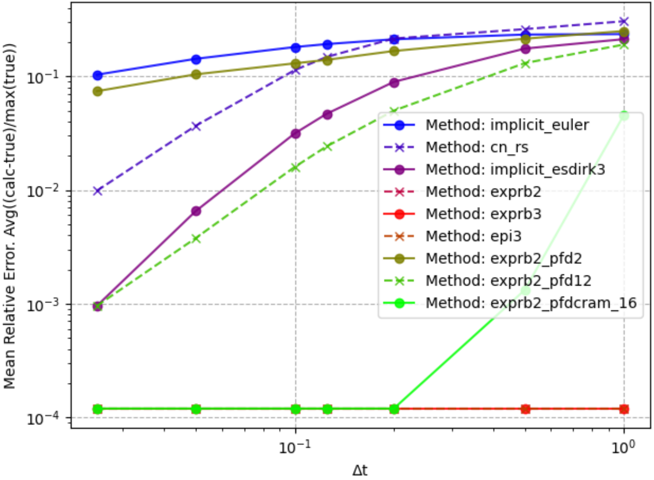

Figure 7: Error vs. Time Step Size

Questions

W. Gurecky, and K. Pieper. ORMATEX. Computer Software. `https://github.com/ORNL/ORMATEX`. USDOE. 24 Jan. 2025. Web. doi:10.11578/dc.20250124.7.

References:

- Tokman, Mayya. ”A new class of exponential propagation iterative methods of Runge–Kutta type (EPIRK).” Journal of Computational Physics 230.24 (2011): 8762-8778.
- Hochbruck, Marlis, Alexander Ostermann, and Julia Schweitzer. ”Exponential Rosenbrock-type methods.” SIAM Journal on Numerical Analysis 47.1 (2009): 786-803.

Acknowledgements

This research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle LLC for the US Department of Energy under contract no. DE-AC05-00OR22725.

Appendix

Case Study: Nonlinear Lotka-Volterra

- Verify time integration method order of convergence.

$$\frac{d}{dt}\begin{bmatrix} u_0 \\ u_1 \end{bmatrix} = \begin{bmatrix} \alpha u_0 - \beta u_0 u_1 \\ -\gamma u_1 + \delta u_0 u_1 \end{bmatrix} ; \; \alpha = \beta = \gamma = \delta = 1$$

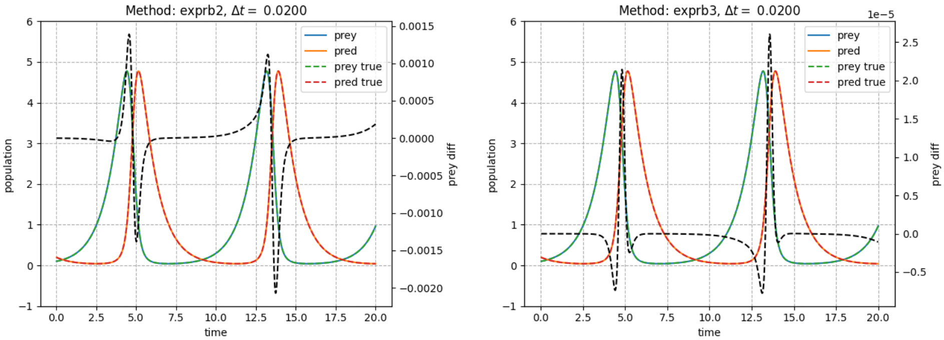

Figure 8: Exp. Rosen. 2 (Left) vs Exp. Rosen. 3 (Right), $\Delta t = 0.02(s)$

Case Study: Nonlinear Lotka-Volterra

- Verify time integration method order of convergence.

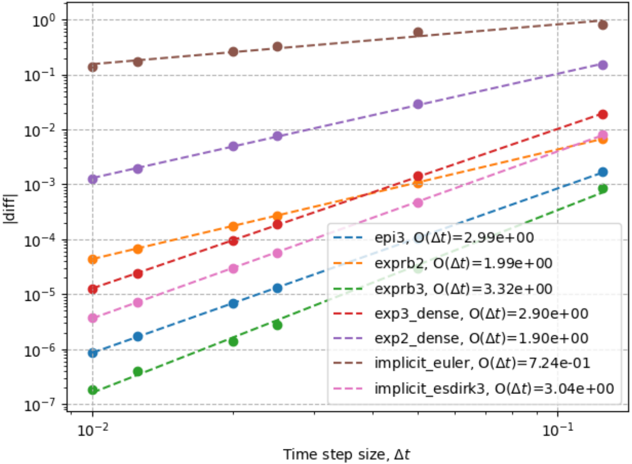

Figure 9: Method time step size convergence order

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Case Study: Bateman+Advection

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{Lu} - v\nabla \mathbf{u}$$

$$L = \begin{bmatrix} -1 & 0 & 0 \\ 1 & -1 \times 10^2 & 0 \\ 0 & 1 \times 10^2 & -1 \times 10^{-2} \end{bmatrix}$$

- BCs: Periodic.
- ICs: Smooth wave 0^{th} species.
- 2^{nd} order CG.
- $t_{final} = 2$s. v=0.5m/s.

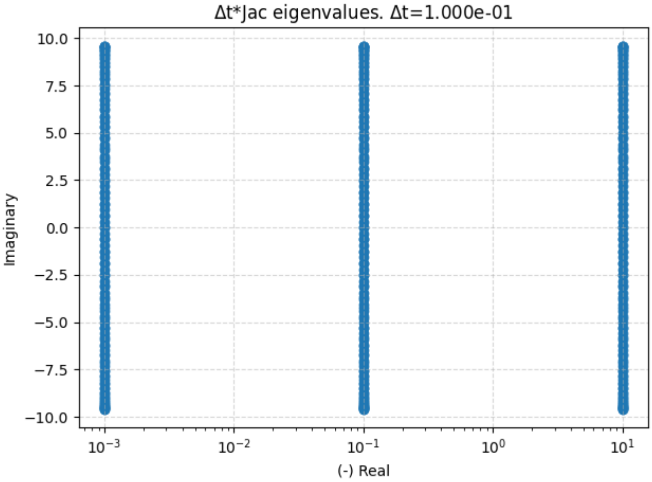

Figure 10: Eigenvalues of Jacobian