On the Construction of a Validated Exponential Integrator

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Outline

1. Introduction
2. Exponential integrators
3. Validated exponential integrators
4. To do
Introduction
Setting

- Discretization of PDE by method of lines yields dissipative system of ODEs.

- Stiff dissipative ODE:
  
  Traditional explicit methods require much smaller time steps than implicit methods.

- Alternative to implicit methods: Exponential integrators.
**Dissipative ODE**

- **Dissipative ODE:** \( u' = f(u) \) where \( f : D \to \mathbb{R}^m \) and \( \exists \mu \leq 0 \) s.t.

\[
< f(u) - f(v), u - v > \leq \mu < u - v, u - v > \quad \forall u, v \in D.
\]

- **Linear case:** \( u' = Au, \; A \in \mathbb{R}^{m \times m}, \; A = A^T \) is dissipative iff

\[
\lambda_{\text{max}}(A) = \sup_{\nu \neq 0} \frac{\nu^T A \nu}{\nu^T \nu} =: \mu \leq 0.
\]

- **General case:**

\[
f \text{dissipative} \Rightarrow \| u(t) - v(t) \| \leq e^{\mu (t - t_0)} \| u_0 - v_0 \| \leq \| u_0 - v_0 \|.
\]
Exponential integrators
Linearized Autonomous IVP

**IVP:**

\[ u' = f(u), \quad u(0) = u_0. \]

Linearized form:

\[ u' = -Au + g(u), \quad u(0) = u_0 \]

where \( A \in \mathbb{R}^{n \times n} \).

**Exponential Rosenbrock methods:**

\[-A = \frac{\partial}{\partial u} f(u_k), \quad g(u) = f(u) - \frac{\partial}{\partial u} f(u_k) u, \quad t \in [t_k, t_{k+1}].\]
Variation of Constants

IVP:

\[ u' = -Au + g(u), \quad u(0) = u_0. \]

VOC:

\[
    u(h) = e^{-hA}u_0 + \int_0^h e^{-(h-\tau)A}g(u(\tau)) \, d\tau \\
    = e^{-hA}u_0 + h\int_0^1 e^{-(1-\theta)hA}g(u(\theta h)) \, d\theta
\]

where \( e^A = \sum_{\nu=0}^{\infty} \frac{A^\nu}{\nu!} \).
Variation of Constants

Approximation: Replace $g(u(\theta h))$ by polynomial $p(\theta h)$:

$$u(h) \approx e^{-hA}u_0 + h \int_0^1 e^{-(1-\theta)hA} p(\theta h) \, d\theta.$$ 

Evaluation of integral: $\varphi$-functions.

Let $\varphi_0(z) = e^z$ and for $k \geq 1$

$$\varphi_k(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} \, d\theta.$$
\( \varphi \)-functions

Recurrence relation:

\[
\varphi_{k+1}(z) = \frac{\varphi_k(z) - \varphi_k(0)}{z} = \frac{\varphi_k(z) - \frac{1}{k!}}{z}.
\]

Relation with \( e^z \):

\[
\varphi_k(z) = \frac{e^z - T_{k-1}(z)}{z^k} = \sum_{\nu=k}^{\infty} \frac{z^{\nu-k}}{\nu!} = \sum_{\nu=0}^{\infty} \frac{z^{\nu}}{(\nu + k)!}
\]

where \( T_k(z) = \sum_{\nu=0}^{k} \frac{z^{\nu}}{\nu!} \).
Exponential Rosenbrock Methods

Let \( p(t) = \sum_{k=0}^{n} a_k t^k \). Then

\[
\begin{align*}
  u(h) & \approx e^{-hA}u_0 + h \int_{0}^{1} e^{-(1-\theta)hA} p(\theta h) \, d\theta \\
  & = e^{-hA}u_0 + h \int_{0}^{1} \sum_{k=0}^{n} e^{-(1-\theta)hA} a_k \theta^k h^k \, d\theta \\
  & = e^{-hA}u_0 + h \sum_{k=0}^{n} k! h^k \varphi_{k+1}(-hA) a_k.
\end{align*}
\]
Exponential Rosenbrock-Taylor Method

Let

\[ p(t) = \sum_{k=0}^{n} \frac{g^{(k)}}{k!} (u_0) t^k. \]

Then

\[ u(h) \approx e^{-hA} u_0 + h \int_0^1 e^{-(1-\theta)hA} p(\theta h) \, d\theta \]

\[ = e^{-hA} u_0 + \int_0^1 \sum_{k=0}^{n} h^{k+1} e^{-(1-\theta)hA} \frac{\theta^k}{k!} g^{(k)}(u_0) \, d\theta \]

\[ = e^{-hA} u_0 + \sum_{k=0}^{n} h^{k+1} \varphi_{k+1}(-hA) g^{(k)}(u_0). \]
Validated exponential integrators
Validated exponential RT Method

Let

\[ p(t) \in \sum_{k=0}^{n} \frac{g^{(k)}(u_0)}{k!} t^k + i. \]

Then

\[ u(h) \in e^{-hA}u_0 + \sum_{k=0}^{n} h^{k+1} \phi_{k+1}(-hA)g^{(k)}(u_0) + h^{n+2}\phi_{n+2}(-hA)i \]

where

\[ -A \supset \frac{\partial}{\partial u}f(u_0). \]
Validated exponential RT Method

Reduced dependency I:

\[ \frac{\partial}{\partial \hat{u}} f(\hat{u}_0) \in -A \in \mathbb{IR}^{n \times n} \]

for some \( \hat{u}_0 \in u_0 \).

Computation of interval matrix exponential by scaling and squaring (Goldsztejn 2009).
Reduced dependency II: Mean value form for \( g^{(k)}(u_0) \):

\[
g^{(k)}(u_0) = g^{(k)}(\hat{u}_0) + J(g^{(k)}(u_0))(u_0 - \hat{u}_0).
\]

Finally,

\[
u(h) \in e^{-hA}u_0 + \sum_{k=0}^{n} h^{k+1} \varphi_{k+1}(-hA)g^{(k)}(\hat{u}_0) \\
\quad + \left( \sum_{k=0}^{n} h^{k+1} \varphi_{k+1}(-hA)J(g^{(k)}(u_0)) \right)(u_0 - \hat{u}_0) + h^{n+2} \varphi_{n+2}(-hA)i.
\]
A priori Enclosure

Remainder bound of order $n$:

$$\sum_{k=0}^{m} g^{(k)}(\hat{u}_0) t^k + g^{(n+1)}(v) t^{m+1}$$

Computation of $v$ by FP iteration benefits from $g^{(1)}(u_0) \approx 0$.

$$u_0 + [0, h] f(v) \subseteq v$$

$$u_0 + [0, h] g(v) \subseteq v$$
Inclusion Functions for $\varphi$-Functions

1. **Scalar case:**
   
   1. Similar approach as for elementary functions: Taylor approximation.
   
   2. Scaling and squaring? Argument reduction?
   
   3. Approximation interval is very small: $[0, h]$.
   
   4. Monotonicity on $\mathbb{R}$: Only point evaluations at the endpoints of an argument interval are needed.

2. **Matrix case:**
   
   1. Is Taylor approximation accurate enough?
   
   2. Approximation interval is very small: $[0, h]$.
   
   3. Hard problem: Even if $h$ is small, $hA$ in $\varphi_k(-hA)$ may be large.
To do
To Do

- Work out details.

- Additional considerations
  (e.g. QR factorization in the propagation of $e^{-hA}u_k$).

- Library of interval matrix $\varphi$-functions.