A Perl program for the symbolic manipulation of flows of differential equations and its application to the analysis of defect-based error estimators for splitting methods

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Problem class and splitting methods

Problem class:

$\frac{d}{dt}u(t) = H(u(t)) = A(u(t)) + B(u(t))$, in general A,B both nonlinear
$u(0) = u_0$ given

Example: cubic nonlinear Schrödinger equation:

$$A(u) = \tfrac{1}{2}\mathrm{i}\Delta u \quad \text{(linear)}$$
$$B(u) = -\mathrm{i}\,V_{\mathrm{ext}}\,u - \mathrm{i}\beta|u|^2 u$$

(or A, B exchanged)
Lie/Trotter splitting:

$$\mathcal{S}(t, u_0) = \mathcal{E}_B(t, \mathcal{E}_A(t, u_0))$$

Strang splitting:

$$\mathcal{S}(t, u_0) = \mathcal{E}_A(\tfrac{1}{2}t, \mathcal{E}_B(t, \mathcal{E}_A(\tfrac{1}{2}t, u_0)))$$

Defect and local error

Defect:

$$\mathcal{D}(t,u) \;=\; \mathcal{S}^{(1)}(t,u) \;=\; \tfrac{\partial}{\partial t}\mathcal{S}(t,u) - H(\mathcal{S}(t,u)).$$

Local error:

$$\mathcal{L}(t,u) \;=\; \mathcal{S}(t,u) - \mathcal{E}_H(t,u) \;=\; \int_0^t \mathcal{F}(\tau,t,u)\,\mathrm{d}\tau$$

with

$$\mathcal{F}(\tau,t,u) = \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(1)}(\tau,u).$$

Proof. It holds

$$\begin{aligned}
\tfrac{\partial}{\partial\tau}\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u)) &= -H(\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))) \\
&\quad +\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\tfrac{\partial}{\partial\tau}\mathcal{S}(\tau,u) \\
&= -\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot H(\mathcal{S}(\tau,u)) \\
&\quad +\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\tfrac{\partial}{\partial\tau}\mathcal{S}(\tau,u) \\
&= \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(1)}(\tau,u),
\end{aligned}$$

such that

$$\begin{aligned}
\int_0^t \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(1)}(\tau,u)\,\mathrm{d}\tau &= \mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\Big|_{\tau=0}^{t} \\
&= \mathcal{S}(t,u) - \mathcal{E}_H(t,u) = \mathcal{L}(t,u).
\end{aligned}$$

Local error for Lie/Trotter splitting

Goal: Show

$$\mathcal{S}^{(1)}(t,u) = O(t) \;\Rightarrow\; \mathcal{L}(t,u) = O(t^2).$$

$$\mathcal{S}(t,u) = \mathcal{E}_B(t, \mathcal{E}_A(t,u)).$$

$$\frac{\partial}{\partial t}\mathcal{S}(t,u) = \partial_2 \mathcal{S}(t,u)\cdot A(u) + B(\mathcal{S}(t,u)).$$

$$\begin{aligned}
\mathcal{S}^{(1)}(t,u) &= \mathcal{D}(t,u) = \frac{\partial}{\partial t}\mathcal{S}(t,u) - H(\mathcal{S}(t,u)) \\
&= \partial_2\mathcal{S}(t,u)\cdot A(u) - A(\mathcal{S}(t,u)) \\
&= \partial_2\mathcal{E}_B(t,\mathcal{E}_A(t,u))\cdot A(\mathcal{E}_A(t,u)) - A(\mathcal{E}_B(t,\mathcal{E}_A(t,u))) \\
&= \tilde{\mathcal{S}}^{(1)}(t,\mathcal{E}_A(t,u)) \qquad (1)
\end{aligned}$$

with

$$\tilde{\mathcal{S}}^{(1)}(t,v) = \partial_2\mathcal{E}_B(t,v)\cdot A(v) - A(\mathcal{E}_B(t,v)).$$

$\tilde{\mathcal{S}}^{(1)}(t,v)$ satisfies

$$\frac{\partial}{\partial t}\tilde{\mathcal{S}}^{(1)}(t,v) = B'(\mathcal{E}_B(t,v))\cdot\tilde{\mathcal{S}}^{(1)}(t,v) + [B,A](\mathcal{E}_B(t,v)) \qquad (2)$$

$$\tilde{\mathcal{S}}^{(1)}(0,v) = 0$$

$$\frac{\partial}{\partial t}\mathcal{E}_F(t,u) = F(\mathcal{E}_F(t,u))$$
$$\Rightarrow \quad \frac{\partial}{\partial t}\partial_2\mathcal{E}_F(t,u)\cdot v = F'(\mathcal{E}_F(t,u))\cdot\partial_2\mathcal{E}_F(t,u)\cdot v$$

$\Rightarrow$ $\partial_2\mathcal{E}_F(t,u)$ is a "fundamental systen" of the linear differential equation

$$\frac{\partial}{\partial t}X(t,u) = F'(\mathcal{E}_F(t,u))\cdot X(t,u).$$

$$\partial_2\mathcal{E}_F(t,u)^{-1} = \partial_2\mathcal{E}_F(-t,\mathcal{E}_F(t,u)).$$

$\Rightarrow$ Variation of constants formula:

$$\frac{\partial}{\partial t}X(t,u) = F'(\mathcal{E}_F(t,u))\cdot X(t,u) + R(t,u),$$
$$X(0,u) = X_0(u)$$

has the solution

$$X(t,u) = \partial_2\mathcal{E}_F(t,u)\cdot\left(X_0(u) + \int_0^t \partial_2\mathcal{E}_F(-\tau,\mathcal{E}_F(\tau,u))\cdot R(\tau,u)\,\mathrm{d}\tau\right).$$

Local error for Lie/Trotter splitting

$$\mathcal{S}^{(1)}(t,u) \;=\; \mathcal{D}(t,u) \;=\; \tfrac{\partial}{\partial t}\mathcal{S}(t,u) - H(\mathcal{S}(t,u)) \;=\; \tilde{\mathcal{S}}^{(1)}(t,\mathcal{E}_A(t,u))$$

where

$$\tilde{\mathcal{S}}^{(1)}(t,v) = \partial_2\mathcal{E}_B(t,v)\cdot\int_0^t \partial_2\mathcal{E}_B(-\tau,\mathcal{E}_B(\tau,v))\cdot[B,A](\mathcal{E}_B(\tau,v))\,\mathrm{d}\tau$$

From this integral representation it follows

$$\mathcal{D}(t,u) = O(t)$$

and

$$\mathcal{L}(t,u) = \int_0^t \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{D}(\tau,u)\,\mathrm{d}\tau = O(t^2)$$

A posteriori local error estimator for Lie/Trotter splitting

Error estimator . . . approximation of

$$\mathcal{L}(t,u) \;=\; \int_0^t \mathcal{F}(\tau,t,u)\,\mathrm{d}\tau \;=\; \int_0^t \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(1)}(\tau,u)\,\mathrm{d}\tau.$$

by the trapezoidal rule:

$$\mathcal{P}(t,u) = \tfrac{1}{2}t\mathcal{F}(t,t,u) = \tfrac{1}{2}t\mathcal{D}(t,u) = \tfrac{1}{2}t\mathcal{S}^{(1)}(t,u).$$

Error of error estimate . . . Peano representation

$$\mathcal{P}(t,u) - \mathcal{L}(t,u) = \int_0^t K_1(\tau,t)\tfrac{\partial}{\partial\tau}\mathcal{F}(\tau,t,u)\,\mathrm{d}\tau$$

with kernel

$$K_1(\tau,t) = \tau - \tfrac{1}{2}t = O(t).$$

Goal: show that

$$\mathcal{P}(t,u) - \mathcal{L}(t,u) = O(t^3) \quad \Rightarrow \text{ asymptotical correctnesss}$$

A posteriori local error estimator for Lie/Trotter splitting

$$
\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{F}(\tau,t,u) &= \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(2)}(\tau,u) \\
&\quad +\partial_2^2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))(\mathcal{S}^{(1)}(\tau,u),\mathcal{S}^{(1)}(\tau,u)) \qquad (3) \\
&= \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(2)}(\tau,u)+O(t)
\end{aligned}
$$

where

$$
\begin{aligned}
\mathcal{S}^{(2)}(t,u) &= \frac{\partial}{\partial t}\mathcal{S}^{(1)}(t,u)-H'(\mathcal{S}(t,u))\cdot\mathcal{S}^{(1)}(t,u) \\
&= \tilde{\mathcal{S}}^{(2)}(t,\mathcal{E}_A(t,u)) \qquad (4)
\end{aligned}
$$

with

$$\tilde{\mathcal{S}}^{(2)}(t,v)=\partial_2\tilde{\mathcal{S}}^{(1)}(t,v)\cdot A(v)-A'(\mathcal{E}_B(t,v))\cdot\tilde{\mathcal{S}}^{(1)}(t,v)+[B,A](\mathcal{E}_B(t,v)).$$

$\tilde{\mathcal{S}}^{(2)}(t,v)$ satisfies

$$
\begin{aligned}
\frac{\partial}{\partial t}\tilde{\mathcal{S}}^{(2)}(t,v) &= B'(\mathcal{E}_B(t,v))\cdot\tilde{\mathcal{S}}^{(2)}(t,v) \\
&\quad +B''(\mathcal{E}_B(t,v))(\tilde{\mathcal{S}}^{(1)}(t,v),\tilde{\mathcal{S}}^{(1)}(t,v)) \\
&\quad -[B,[B,A]](\mathcal{E}_B(t,v))-[A,[B,A]](\mathcal{E}_B(t,v)) \\
&\quad +2[B,A]'(\mathcal{E}_B(t,v))\cdot\tilde{\mathcal{S}}^{(1)}(t,v), \qquad (5) \\
\tilde{\mathcal{S}}^{(2)}(0,v) &= [B,A](v).
\end{aligned}
$$

A posteriori local error estimator for Lie/Trotter splitting

$\Rightarrow$ integral representation

$$\begin{aligned}\tilde{\mathcal{S}}^{(2)}(t,v) \quad = \quad & \partial_2\mathcal{E}_B(t,v)\cdot[B,A](v) + \partial_2\mathcal{E}_B(t,v)\cdot\int_0^t \partial_2\mathcal{E}_B(-\tau,\mathcal{E}_B(\tau,v))\cdot \\ & \Big(B''(\mathcal{E}_B(\tau,v))(\tilde{\mathcal{S}}^{(1)}(\tau,v),\tilde{\mathcal{S}}^{(1)}(\tau,v)) \\ & -[B,[B,A]](\mathcal{E}_B(\tau,v)) - [A,[B,A]](\mathcal{E}_B(\tau,v)) \\ & +2[B,A]'(\mathcal{E}_B(\tau,v))\cdot\tilde{\mathcal{S}}^{(1)}(\tau,v)\Big)\,\mathrm{d}\tau\end{aligned}$$

$$\Rightarrow \mathcal{S}^{(2)}(\tau,u) = \partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))\cdot[B,A](\mathcal{E}_A(\tau,u)) + O(t)$$

Altogether,

$$\mathcal{P}(t,u)-\mathcal{L}(t,u) = \int_0^t K_1(\tau,t)\tfrac{\partial}{\partial\tau}\mathcal{F}(\tau,t,u)\,\mathrm{d}\tau$$

$$= \int_0^t K_1(\tau,t)\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))\cdot[B,A](\mathcal{E}_A(\tau,u))\,\mathrm{d}\tau + O(t^3)$$

$$= \int_0^t K_2(\tau,t)\tfrac{\partial}{\partial\tau}\Big(\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))\cdot[B,A](\mathcal{E}_A(\tau,u))\Big)\,\mathrm{d}\tau + O(t^3)$$

where $K_2(\tau,t)=\frac{1}{2}\tau(t-\tau)=O(t^2)$ by partial integration.

A posteriori local error estimator for Lie/Trotter splitting

I.e., we have to show

$$\frac{\partial}{\partial\tau}\Big(\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))\cdot[B,A](\mathcal{E}_A(\tau,u))\Big)=O(1),$$

and this holds because

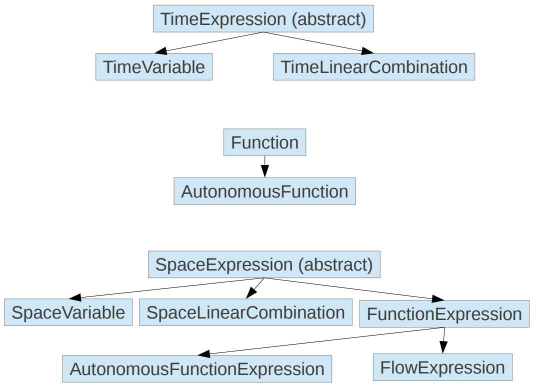
$$\begin{aligned}
&\frac{\partial}{\partial\tau}\Big(\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))\cdot[B,A](\mathcal{E}_A(\tau,u))\Big)\\
&\qquad= \Big[\partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v))\cdot\partial_2\mathcal{E}_B(\tau,v)\cdot[[B,A],A](v)\\
&\qquad\quad+\partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v))\cdot\partial_2\tilde{\mathcal{S}}^{(1)}(\tau,v)\cdot[B,A](v)\\
&\qquad\quad+\partial_2^2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v))\big(\tilde{\mathcal{S}}^{(1)}(\tau,v),\partial_2\mathcal{E}_B(\tau,v)\cdot[B,A](v)\big)\Big]_{v=\mathcal{E}_{\boldsymbol{A}}(\boldsymbol{t},\boldsymbol{u})}
\end{aligned}\tag{6}$$

□

Perl modules for the symbolic manipulation of flows of differential equations

Functionality provided by 2 Perl modules `TimeExpression.pm` and `SpaceExpression.pm`

Data types / class hierarchy:



Usage of TimeExpression data types

```perl
use TimeExpression;
my $t = TimeVariable->new('t');
my $tau = TimeVariable->new('tau', '\tau');
my $tt1 = TimeLinearCombination->new($t, 2, $tau, 3);
my $tt2 = 2*$t + 3*$tau;      #overloaded operators
my $tt3 = TimeLinearCombination->new($tt1, 2, $t, -1);
my $tt4 = $tt1 - $tt2;
print $tt1->str() . "\n";
print $tt1->latex() . "\n";
print $tt2->str() . "\n";
print $tt3->str() . "\n";
print $tt4->str() . "\n";
```

Output:

```
2t+3tau
2t+3\tau
2t+3tau
3t+6tau
0
```

Usage of SpaceExpression data types

Define expressions

$$\mathcal{S}(t,u) = \mathcal{E}_B(t, \mathcal{E}_A(t,u))$$

$$C(u) = [A,B](u) = A'(u)\cdot B(u) - B'(u)\cdot A(u)$$

```
use TimeExpression;
use SpaceExpression;
my $t = TimeVariable->new('t');
my $u = SpaceVariable->new('u');
my $A = AutonomousFunction->new('A');
my $B = AutonomousFunction->new('B');
my $Stu = FlowExpression->new($B, $t,
            FlowExpression->new($A, $t, $u));
my $Cu = AutonomousFunctionExpression->new($A, $u,
            AutonomousFunctionExpression->new($B, $u))
        -AutonomousFunctionExpression->new($B, $u,
            AutonomousFunctionExpression->new($A, $u));
print $Stu->str() . "\n";
print $Cu->str() . "\n";
```

Output:

```
E_B[t,E_A[t,u]]
-B{1}[u](B[u])+A{1}[u](B[u])
```

Method `substitute`

Define $\mathcal{S}(t,u)$ by substituting $v \to \mathcal{E}_A(t,u)$ in $\mathcal{E}_B(t,v)$:

```
my $v = SpaceVariable->new('v');
my $E_Atu = FlowExpression->new($A, $t, $u);
my $E_Btv = FlowExpression->new($B, $t, $v);
my $Stu = $E_Btv->substitute($v, $E_Atu);
print $Stu->str() . "\n";
```

Output:

```
E_B[t,E_A[t,u]]
```

Define $D(u) = [A,[A,B]](u)$ by substituting $B \to [A,B]$ in $C(u) = [A,B](u)$:

```
# $Cu already defined
my $Du = $Cu->substitute($B, $Cu, $u);
print $Du->str() . "\n";
```

Output:

```
-A{2}[u](B[u],A{1}[u](B[u])-B{1}[u](B[u]))-A{1}[u](B{1}
[u](A{1}[u](B[u])-B{1}[u](B[u])))+B{2}[u](B[u],A{1}[u](
B[u])-B{1}[u](B[u]))+B{1}[u](B{1}[u](A{1}[u](B[u])-B{1}
[u](B[u]))+A{1}[u](A{1}[u](B[u])-B{1}[u](B[u]))
```

Method t_derivative

Define $\mathcal{S}^{(1)}(t,u) = \frac{\partial}{\partial t}\mathcal{S}(t,u) - A(\mathcal{S}(t,u)) - B(\mathcal{S}(t,u))$:

```
my $S1tu = $Stu->t_derivative($t)
          -AutonomousFunctionExpresssion->new($A, $Stu)
          -AutonomousFunctionExpresssion->new($B, $Stu);
print $S1tu->str() . "\n";
```

Output:

```
E_B{0,1}[t,E_A[t,u]](A[E_A[t,u]])-A[E_B[t,E_A[t,u]]]
```

Note that the output corresponds to

$$\mathcal{S}^{(1)}(t,u) = \partial_2\mathcal{E}_B(t,\mathcal{E}_A(t,u)) \cdot A(\mathcal{E}_A(t,u)) - A(\mathcal{E}_B(t,\mathcal{E}_A(t,u)))$$

$\rightsquigarrow$ (1)

Method `differential` (1)

Compute higher-order Fréchet derivatives of

$$Z(u) = F(\mathcal{E}_F(t,u)) - \partial_2\mathcal{E}_F(t,u)\cdot F(u) = 0$$

```
my $F = AutonomousFunction->new('F');
my $Zu = AutonomousFunctionExpression->new($F,
            FlowExpression->new($F, $t, $u))
        -FlowExpression->new($F, $t, $u,
            AutonomousFunctionExpression->new($F, $u));
my $Z1uv = $Zu->differential($u, $v);
my $w = SpaceVariable->new('w');
my $Z2uvw = $Z1uv->differential($u, $w);
print $Z1uv->str() . "\n";
print $Z2uvw->str() . "\n";
```

Output:

```
-E_F{0,1}[t,u](F{1}[u](v))+F{1}[E_F[t,u]](E_F{0,1}[t,u]
(v))-E_F{0,2}[t,u](F[u],v)
-E_F{0,1}[t,u](F{2}[u](v,w))+F{2}[E_F[t,u]](E_F{0,1}[t,
u](v),E_F{0,1}[t,u](w))-E_F{0,2}[t,u](F{1}[u](w),v)+F{1
}[E_F[t,u]](E_F{0,2}[t,u](v,w))-E_F{0,2}[t,u](F{1}[u](v
),w)-E_F{0,3}[t,u](F[u],v,w)
```

We obtain the identities

$$F(\mathcal{E}_F(t,u)) - \partial_2\mathcal{E}_F(t,u)\cdot F(u) = 0$$

$$F'(\mathcal{E}_F(t,u))\cdot\partial_2\mathcal{E}_F(t,u)\cdot v - \partial_2^2\mathcal{E}_F(t,u)(F(u),v) - \partial_2\mathcal{E}_F(t,u)\cdot F'(u)\cdot v = 0$$

$$\begin{aligned} F''(\mathcal{E}_F(t,u))(\partial_2\mathcal{E}_F(t,u)\cdot v, \partial_2\mathcal{E}_F(t,u)\cdot w) + F'(\mathcal{E}_F(t,u))\cdot\partial_2^2\mathcal{E}_F(t,u)(v,w) \\ -\partial_2^3\mathcal{E}_F(t,u)(F(u),v,w) - \partial_2^2\mathcal{E}_F(t,u)(F'(u)\cdot v, w) \\ -\partial_2^2\mathcal{E}_F(t,u)(F'(u)\cdot w, v) - \partial_2\mathcal{E}_F(t,u)\cdot F''(u)(v,w) = 0 \end{aligned}$$

The method `reduce_order` transforms expressions of the form of the highest order derivative in these identities by means of these identities:

$$\partial_2\mathcal{E}_F(t,u)\cdot F(u) \;\rightarrow\; F(\mathcal{E}_F(t,u))$$

$$\partial_2^2\mathcal{E}_F(t,u)(F(u),v) \;\rightarrow\; F'(\mathcal{E}_F(t,u))\cdot\partial_2\mathcal{E}_F(t,u)\cdot v - \partial_2\mathcal{E}_F(t,u)\cdot F'(u)\cdot v$$

$$\begin{aligned} \partial_2^3\mathcal{E}_F(t,u)(F(u),v,w) \;\rightarrow\; & F''(\mathcal{E}_F(t,u))(\partial_2\mathcal{E}_F(t,u)\cdot v, \partial_2\mathcal{E}_F(t,u)\cdot w) \\ & +F'(\mathcal{E}_F(t,u))\cdot\partial_2^2\mathcal{E}_F(t,u)(v,w) - \partial_2^2\mathcal{E}_F(t,u)(F'(u)\cdot v, w) \\ & -\partial_2^2\mathcal{E}_F(t,u)(F'(u)\cdot w, v) - \partial_2\mathcal{E}_F(t,u)\cdot F''(u)(v,w) \end{aligned}$$

Similarly for higher derivatives of analogous form

Method `expand`

(Higher-order) Fréchet derivative ... (multi-)linear map

(multi-)linear map applied to linear combination(s)
$\longrightarrow$ linear combination of (multi-)linear maps

Examples:

$$\partial_2 \mathcal{E}_A(t,u)\cdot(2v+3w) \;\longrightarrow\; 2\partial_2 \mathcal{E}_A(t,u)\cdot v + 3\partial_2 \mathcal{E}_A(t,u)\cdot w$$

$$A''(u)(v+w,v+w) \;\longrightarrow\; A''(u)(v,v)+2A''(u)(v,w)+A''(u)(w,w)$$

Demonstration: elementary differentials

$$
\begin{aligned}
y'(t) &= F(y(t)) \\
y''(t) &= F'(y(t)) \cdot F(y(t)) \\
y'''(t) &= F''(y(t))(F(y(t), F(y(t)) + F'(y(t)) \cdot F'(y(t)) \cdot F(y(t)) \\
&\vdots
\end{aligned}
$$

terms = # elementary differentials (Butcher trees) of given order

available from the literature:

order	1	2	3	4	5	6	7	8	9	10	11
# terms	1	1	2	4	9	20	48	115	286	719	1842

$\rightsquigarrow$ `elementary_differentials.pl`

Demonstration: verification of equations (1)-(6)

⇝ `defect_lie_trotter.pl`

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