

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

Harald Hofstätter

Institute for Analysis and Scientific Computing
Vienna University of Technology, Austria

`mailto:hofi@harald-hofstaetter.at`

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

`substitute`

`t_derivative`

`differential`

`reduce_order`

`expand`

Elementary
differentials

Verification of
eqs. (1)-(6)

Problem class and splitting methods

Problem class:

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

Example: cubic nonlinear Schrödinger equation:

$$A(u) = \frac{1}{2}i\Delta u \quad (\text{linear})$$

$$B(u) = -iV_{\text{ext}}u - i\beta|u|^2u$$

(or A , B exchanged)

Lie/Trotter splitting:

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

Strang splitting:

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Defect and local error

Defect:

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

Local error:

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

with

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

Proof. It holds

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

such that

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

Problem class,
splitting methods

**Defect and local
error**

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Local error for Lie/Trotter splitting

Goal: Show

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

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

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

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

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

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

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Local error for Lie/Trotter splitting

Variation of constants formula

$$\frac{\partial}{\partial t} \mathcal{E}_F(t, u) = F(\mathcal{E}_F(t, u))$$

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

$\Rightarrow \partial_2 \mathcal{E}_F(t, u)$ is a "fundamental system" 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

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Local error for Lie/Trotter splitting

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

where

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

From this integral representation it follows

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

and

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

A posteriori local error estimator for Lie/Trotter splitting

Error estimator ... approximation of

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

by the trapezoidal rule:

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

Error of error estimate ... Peano representation

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

with kernel

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

Goal: show that

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

A posteriori local error estimator for Lie/Trotter splitting

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

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

where

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

with

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

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

A posteriori local error estimator for Lie/Trotter splitting

⇒ integral representation

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

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

Altogether,

$$\begin{aligned}\mathcal{P}(t, u) - \mathcal{L}(t, u) &= \int_0^t K_1(\tau, t) \frac{\partial}{\partial \tau} \mathcal{F}(\tau, t, u) d\tau \\ &= \int_0^t K_1(\tau, t) \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_B(\tau, \mathcal{E}_A(\tau, u)) \cdot [B, A](\mathcal{E}_A(\tau, u)) d\tau + O(t^3) \\ &= \int_0^t K_2(\tau, t) \frac{\partial}{\partial \tau} \left(\partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_B(\tau, \mathcal{E}_A(\tau, u)) \cdot [B, A](\mathcal{E}_A(\tau, u)) \right) d\tau + O(t^3)\end{aligned}$$

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
Differentials

Verification of
eqs. (1)-(6)

A posteriori local error estimator for Lie/Trotter splitting

i.e., we have to show

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

and this holds because

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

□

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

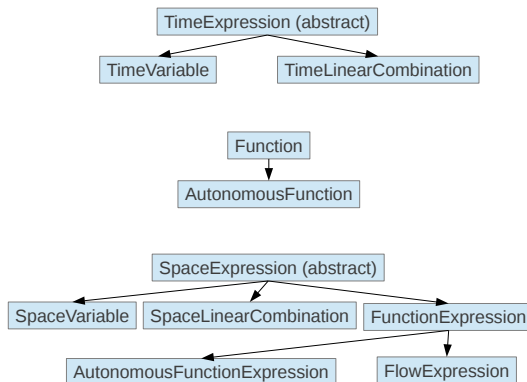
Elementary
differentials

Verification of
eqs. (1)-(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:



Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

`TimeExpression`
data types

`SpaceExpression`
data types

`substitute`

`t_derivative`

`differential`

`reduce_order`

`expand`

Elementary
differentials

Verification of
eqs. (1)-(6)

Usage of TimeExpression data types

```
1 use TimeExpression;
2 my $t = TimeVariable->new('t');
3 my $tau = TimeVariable->new('tau', '\tau');
4 my $tt1 = TimeLinearCombination->new($t, 2, $tau, 3);
5 my $tt2 = 2*$t + 3*$tau;      #overloaded operators
6 my $tt3 = TimeLinearCombination->new($tt1, 2, $t, -1);
7 my $tt4 = $tt1 - $tt2;
8 print $tt1->str() . "\n";
9 print $tt1->latex() . "\n";
10 print $tt2->str() . "\n";
11 print $tt3->str() . "\n";
12 print $tt4->str() . "\n";
```

Output:

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Usage of SpaceExpression data types

Define expressions

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

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

```
1 use TimeExpression;
2 use SpaceExpression;
3 my $t = TimeVariable->new('t');
4 my $u = SpaceVariable->new('u');
5 my $A = AutonomousFunction->new('A');
6 my $B = AutonomousFunction->new('B');
7 my $Stu = FlowExpression->new($B, $t,
8     FlowExpression->new($A, $t, $u));
9 my $Cu = AutonomousFunctionExpression->new($A, $u,
10     AutonomousFunctionExpression->new($B, $u))
11     -AutonomousFunctionExpression->new($B, $u,
12     AutonomousFunctionExpression->new($A, $u));
13 print $Stu->str() . "\n";
14 print $Cu->str() . "\n";
```

Output:

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Method substitute

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

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

Output:

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

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

```
20 # $Cu already defined
21 my $Du = $Cu->substitute($B, $Cu, $u);
22 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]))
```

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Method `t_derivative`

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

```
23 my $S1tu = $Stu->t_derivative($t)
24         -AutonomousFunctionExpresssion->new($A, $Stu)
25         -AutonomousFunctionExpresssion->new($B, $Stu);
26 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

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

\rightsquigarrow (1)

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

`t_derivative`

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Method differential (1)

Compute higher-order Fréchet derivatives of

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

```
27 my $F = AutonomousFunction->new('F');
28 my $Zu = AutonomousFunctionExpression->new($F,
29       FlowExpression->new($F, $t, $u))
30       -FlowExpression->new($F, $t, $u,
31       AutonomousFunctionExpression->new($F, $u));
32 my $Z1uv = $Zu->differential($u, $v);
33 my $w = SpaceVariable->new('w');
34 my $Z2uvw = $Z1uv->differential($u, $w);
35 print $Z1uv->str() . "\n";
36 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)
```

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Methods differential (2) and reduce_order

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Method `expand`

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

(multi-)linear map applied to linear combination(s)
→ linear combination of (multi-)linear maps

Examples:

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

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

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

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

↪ elementary_differentials.pl

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

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

↪ `defect_lie_trotter.pl`

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

Thank you for your attention!

**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**

Harald Hofstätter

Institute for Analysis and Scientific Computing
Vienna University of Technology, Austria

`mailto:hofi@harald-hofstaetter.at`

Problem class,
splitting methods

Defect and local
error

Local error for
Lie/Trotter

Local error
estimator for
Lie/Trotter

Perl modules

TimeExpression
data types

SpaceExpression
data types

substitute

t_derivative

differential

reduce_order

expand

Elementary
differentials

Verification of
eqs. (1)-(6)

MATHEMATIKKOLLOQUIUM

Das Institut für Mathematik lädt zu folgendem Vortrag ein:

Harald Hofstätter

TU Wien

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

For the proof of the asymptotical correctness of certain defect-based a posteriori local error estimators for splitting methods, suitable (integral) representations of local error expansions have to be derived, from which the order of the local error can directly be inferred. In the linear case this is achieved by tedious but relatively straightforward manipulations of operator exponentials. In the nonlinear case, however, to obtain these local error representations explicitly, complicated expressions involving nonlinear flows of differential equations and higher-order Frechet derivatives of such flows have to be handled. Performing these tedious and error prone calculations manually very quickly becomes unreasonable or even impossible. We describe an especially tailored tool for performing such manipulations symbolically, whose development was strongly facilitated by employing the object-orientedness and the superior string and hash manipulation features of the Perl programming language.

Zeit: Donnerstag, den 24. Januar 2013 um 17:15 Uhr

Ort: Bauing.-Gebäude, Technikerstraße 13, HSB 7

Gäste sind herzlich willkommen!

Mechthild Thalhammer