Rythmos Update

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1442 Numerical Analysis and Applications

Trilinos User Group Meeting

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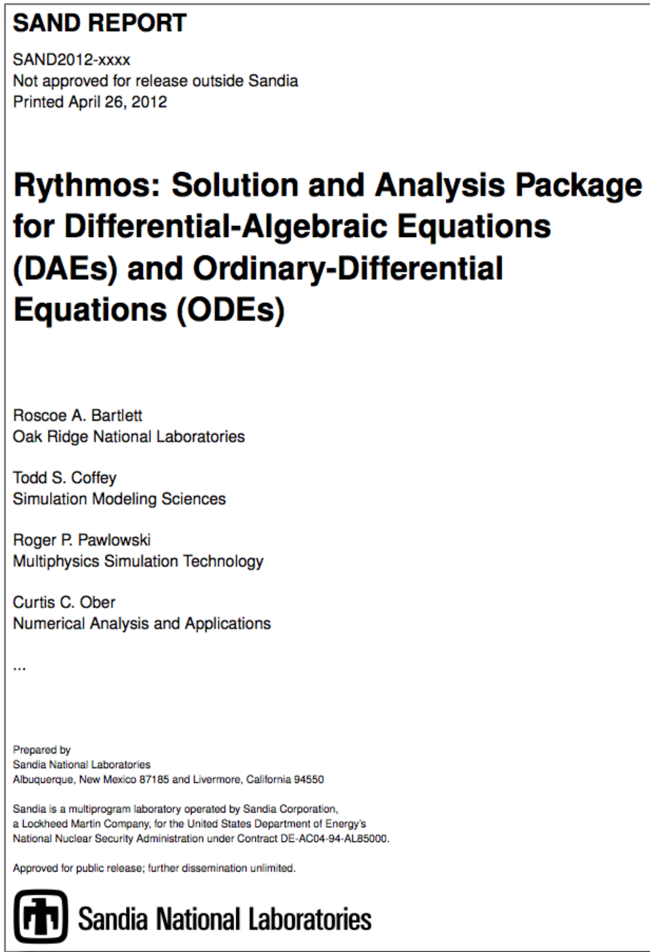
Improve Usability - New Additions to Manual

- **Under development (not R&A'ed yet)**
- **Portions are "auto-"generated (*)**
  - Scripts and verification/unit tests
- **Three parts**
  - Theory Manual
    - Description of methods
    - Convergence plots for all Steppers*
  - User's Guide
    - ParameterList Hierarchy*
    - ParameterList Descriptions*
    - Convergence Test Problems
  - Developer's Guide
    - High-level description of software infrastructure and design
    - Low-level descriptions will be hyperlinked to Rythmos Doxygen



SAND REPORT

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Rythmos: Solution and Analysis Package for Differential-Algebraic Equations (DAEs) and Ordinary-Differential Equations (ODEs)

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Sine-Cosine Problem

Canonical Sine-Cosine differential equation $\ddot{x} = -x$

Rewriting as two 1st order ODEs

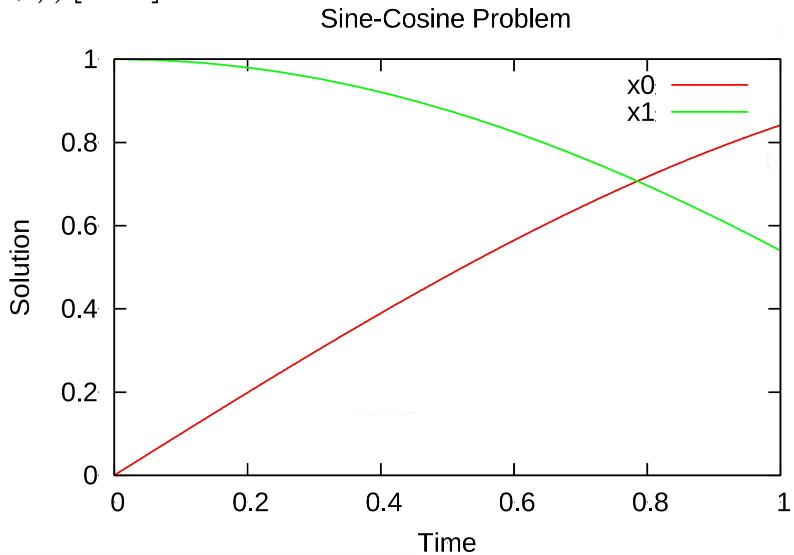
$$\frac{d}{dt}x_0(t) = x_1(t)$$
$$\frac{d}{dt}x_1(t) = \left(\frac{f}{L}\right)^2 (a - x_0(t))$$

With the following coefficients and initial condition

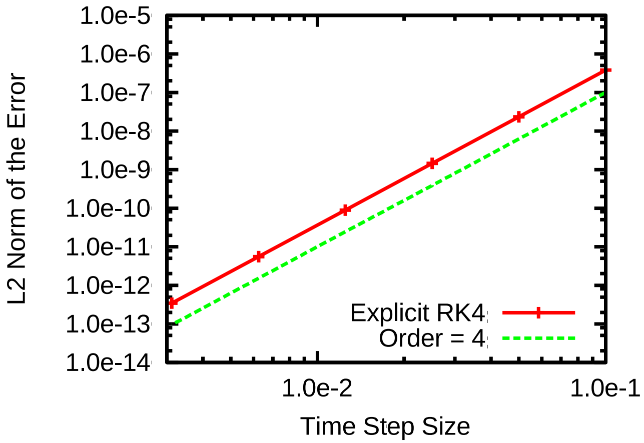
$$a = 0 \qquad \phi = \arctan(((f/L)/\gamma_1) * (\gamma_0 - a)) - (f/L) * t_0[= 0]$$
$$f = 1 \qquad b = \gamma_1/((f/L) * cos((f/L) * t_0 + \phi))[= 1]$$
$$L = 1$$
$$x_0(t_0 = 0) = \gamma_0[= 0]$$
$$x_1(t_0 = 0) = \gamma_1[= 1]$$

Exact solution

$$x_0(t) = a + b * \sin((f/L) * t + \phi)$$
$$x_1(t) = b * (f/L) * \cos((f/L) * t + \phi)$$

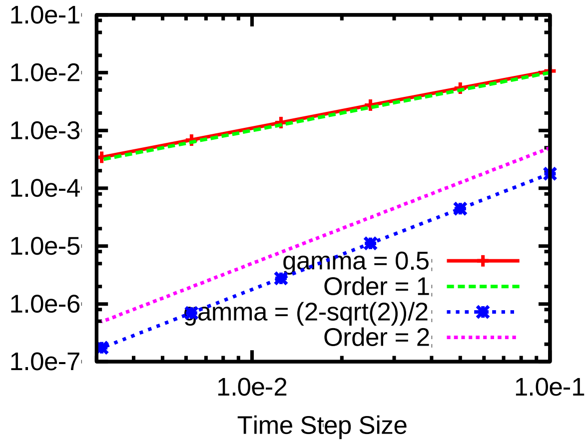


Examples of Convergence Plots



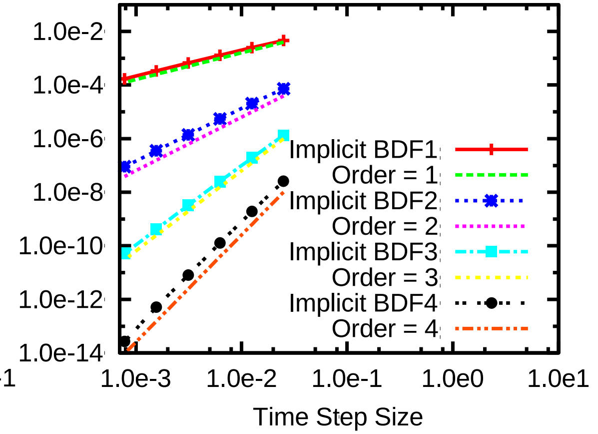
- **Explicit Runge-Kutta**
- **One-Step Method**
- **4-Stage**
- **4th Order**

$$
\begin{array}{c|cccc}
0 & 0 & & & \\
1/2 & 1/2 & 0 & & \\
1/2 & 0 & 1/2 & 0 & \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & 1/6 & 1/3 & 1/3 & 1/6
\end{array}
$$



- **Singly Diagonal Implicit Runge-Kutta (SDIRK)**
- **One-Step Method**
- **2-Stage**
- **L-Stable**

$$
\begin{array}{c|cc}
\gamma & \gamma & \\
1 & 1-\gamma & \gamma \\
\hline
 & 1-\gamma & \gamma
\end{array}
$$



- **Backward Difference Formula (BDF)**
- **Multi-Step Method**
- **Variable stepsize**
- **Fixed-Leading-Coeff. Formula**

$$
\dot{x}_n = \bar{f}(t_n, x_n) = \frac{1}{\Delta t\, \beta_0} \sum_{i=0}^{s} \alpha_i\, x_{n-i}
$$

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Example ParameterList Descriptions

- ParameterList heirarchy
  - Hyperlinked to Child(ren) and Parent ParameterLists
  - Includes descriptions directly from getValidParameters()

5.38 Singly Diagonal IRK 2 Stage 3rd order

Description:

```
Singly Diagonal IRK 2 Stage 3rd order
Solving Ordinary Differential Equations I:
Nonstiff Problems, 2nd Revided Edition
E. Hairer, S. P. Norsett, and G. Wanner
Table 7.2, pg 207
gamma = (3+-sqrt(3))/6 -> 3rd order and A-stable
gamma = (2+-sqrt(2))/2 -> 2nd order and L-stable
c = [  gamma      1-gamma  ]'
A = [  gamma      0        ]
    [ 1-2*gamma  gamma     ]
b = [ 1/2        1/2       ]'
```

Parent(s): Runge Kutta Butcher Tableau Selection (Section 5.26)

Child(ren): None.

Parameters:

3rd Order A-stable = 1 If true, set gamma to gamma = (3+sqrt(3))/6 to obtain a 3rd order A-stable scheme. '3rd Order A-stable' and '2nd Order L-stable' can not both be true.

2nd Order L-stable = 0 If true, set gamma to gamma = (2+sqrt(2))/2 to obtain a 2nd order L-stable scheme. '3rd Order A-stable' and '2nd Order L-stable' can not both be true.

gamma = 0.788675 If both '3rd Order A-stable' and '2nd Order L-stable' are false, gamma will be used. The default value is the '3rd Order A-stable' gamma value, (3+sqrt(3))/6.

- Integrator Base (Section 5.1)
  - Integrator Settings (Section 5.2)
    - Integrator Selection (Section 5.3)
      - Default Integrator (Section 5.4)
        - VerboseObject (Section 5.5)
  - Integration Control Strategy Selection (Section 5.6)
    - Simple Integration Control Strategy (Section 5.7)
  - Stepper Settings (Section 5.8)
    - Stepper Selection (Section 5.9)
      - Forward Euler (Section 5.10)
      - Backward Euler (Section 5.11)
      - Implicit BDF (Section 5.12)
      - Explicit RK (Section 5.13)
      - Implicit RK (Section 5.14)
    - Step Control Settings (Section 5.15)
      - Step Control Strategy Selection (Section 5.16)
        - Implicit BDF Stepper Step Control Strategy (Section 5.17)
          - magicNumbers (Section 5.18)
        - Implicit BDF Stepper Ramping Step Control Strategy (Section 5.19)
      - Error Weight Vector Calculator Selection (Section 5.20)
        - Implicit BDF Stepper Error Weight Vector Calculator (Section 5.21)
    - Interpolator Selection (Section 5.22)
      - Linear Interpolator (Section 5.23)
      - Hermite Interpolator (Section 5.24)
      - Cubic Spline Interpolator (Section 5.25)
    - Runge Kutta Butcher Tableau Selection (Section 5.26)
      - Forward Euler (Section 5.27)
      - Explicit 2 Stage 2nd order by Runge (Section 5.28)
      - Explicit Trapezoidal (Section 5.29)
      - Explicit 3 Stage 3rd order (Section 5.30)
      - Explicit 3 Stage 3rd order by Heun (Section 5.31)
      - ...

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Improve Usability - IntegratorBuilder

- **Improved access to Integrators through IntegratorBuilder**
  - Create IntegratorBuilder
  - Set ParameterList
  - Set ModelEvaluator
  - Set NonlinearSolver
  - Create Integrator
  - Integrate forward in time
- **Testing in Piro**
  - **Interface to Albany and Panzer**
  - **Example of usage**

```
RCP<IntegratorBuilder<double> > ib = integratorBuilder<double>();
```

```
RCP<ParameterList> pl = Teuchos::parameterList();
pl->setParameters(*(ib->getValidParameters()));
pl->sublist("Stepper Settings")
    .sublist("Stepper Selection")
        .set(   "Stepper Type","Implicit RK");
pl->sublist("Stepper Settings")
    .sublist("Runge Kutta Butcher Tableau Selection")
        .set(   "Runge Kutta Butcher Tableau Type",
                "Singly Diagonal IRK 2 Stage 3rd order");
…
ib->setParameterList(pl);
```

```
RCP<SinCosModel> model = sinCosModel(true);
Thyra::ModelEvaluatorBase::InArgs<double>
  ic = model->getNominalValues();
```

```
RCP<Thyra::NonlinearSolverBase<double> > nlSolver =
  timeStepNonlinearSolver<double>();
```

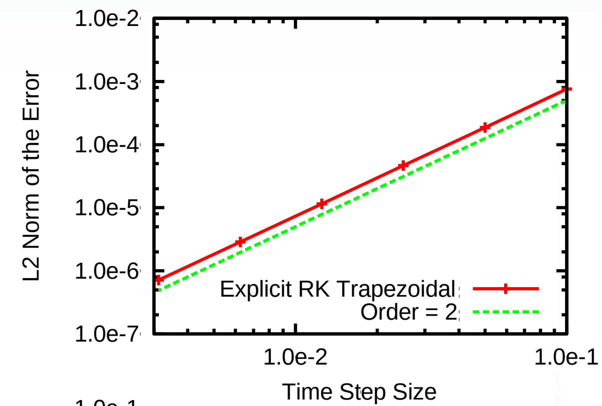
```
RCP<IntegratorBase<double> >
  integrator = ib->create(model,ic,nlSolver);
```

```
Teuchos::Array<double> time_vec;
Teuchos::Array<RCP<const VectorBase<double> > > x_vec;
time_vec.push_back(finalTime);
integrator->getFwdPoints(time_vec,&x_vec,NULL,NULL);
```

New Steppers

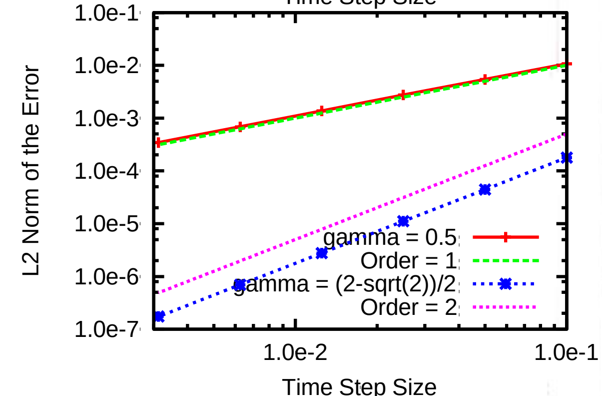
- **Explicit Trapezoidal**
  - **2nd Order method**

$$\begin{array}{c|cc} 0 & 0 & \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$



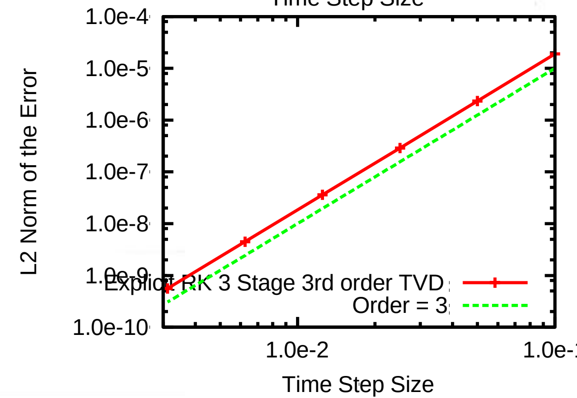
- **SDIRK 2-Stage**
  - **2nd Order L-Stable when** $\gamma = (2 \pm \sqrt{2})/2$
    - **100x more accurate than previous L-Stable SDIRK**
  - **Solving Ordinary Differential Equations I: Nonstiff Problems, E. Hairer, et al.**

$$\begin{array}{c|cc} \gamma & \gamma & \\ 1 & 1-\gamma & \gamma \\ \hline & 1-\gamma & \gamma \end{array}$$



- **3-Stage 3rd Order TVD**
  - **Gottlieb, Shu, Tadmor, 2001**

$$\begin{array}{c|ccc} 0 & 0 & & \\ 1 & 1 & 0 & \\ 1/2 & 1/4 & 1/4 & 0 \\ \hline & 1/6 & 1/6 & 4/6 \end{array}$$



Summary

- Programmatic development
  - Improve usability
    - Documentation
    - Integrators through IntegratorBuilder
  - Expand usage
    - Looking for "friendly" ASC codes
- Technical development
  - Expand available Steppers
    - Explicit Trapezoid, L-Stable SDIRK, and 3rd order TVD
    - Others?
  - Develop response sensitivities (Thyra versions)
    - Terminal response sensitivities
    - Distributed-in-time response sensitivities
  - Many others, but based on priorities.

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