

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

SAND2012-xxxx

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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

$$a = 0 \quad \phi = \arctan(((f/L)/\gamma_1) * (\gamma_0 - a)) - (f/L) * t_0 [= 0]$$

$$f = 1 \quad b = \gamma_1 / ((f/L) * \cos((f/L) * t_0 + \phi)) [= 1]$$

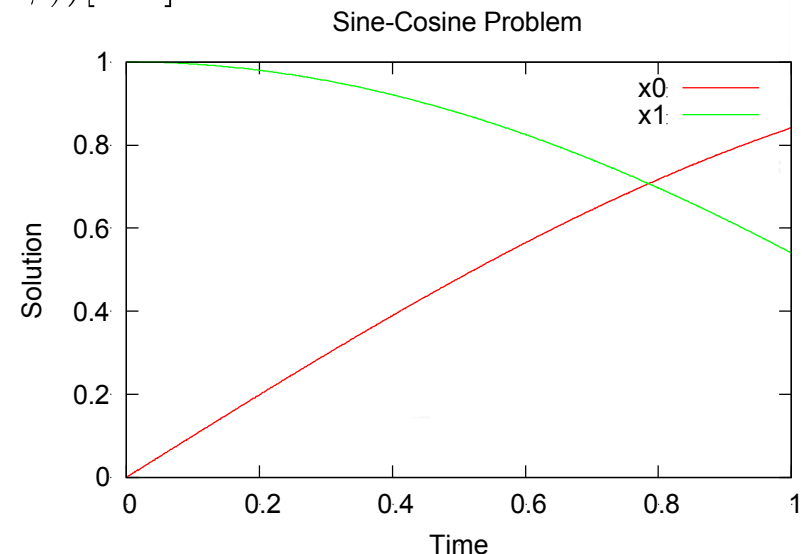
$$x_0(t_0 = 0) = \gamma_0 [= 0]$$

$$L = 1 \quad x_1(t_0 = 0) = \gamma_1 [= 1]$$

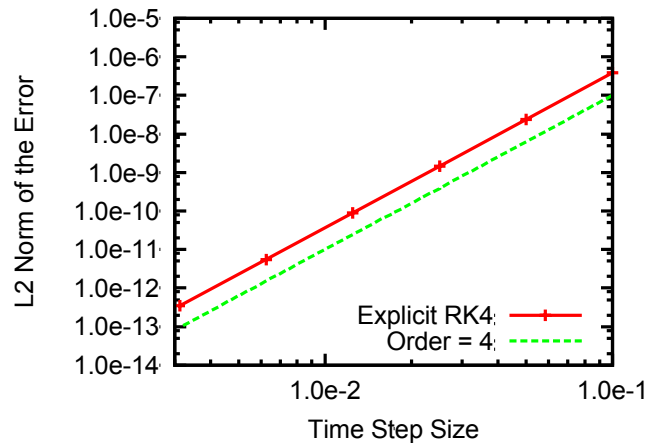
Exact solution

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

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

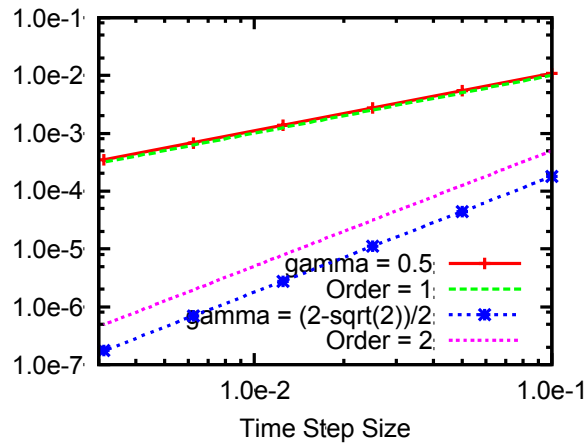


Examples of Convergence Plots



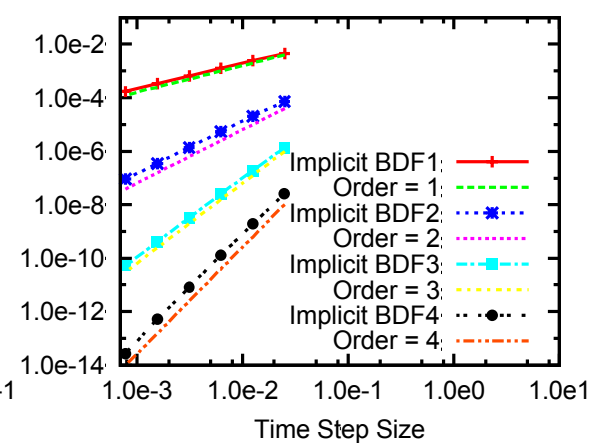
- **Explicit Runge-Kutta**
- **One-Step Method**
- **4-Stage**
- **4th Order**

0	0			
1/2	1/2	0		
1/2	0	1/2	0	
1	0	0	1	0
	1/6	1/3	1/3	1/6



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

γ	γ
1	$1 - \gamma$ γ
	$1 - \gamma$ γ



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

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



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 Revised Edition
E. Hairer, S. P. Norsett, and G. Wanner
Table 7.2, pg 207
 $\gamma = (3 + \sqrt{3})/6 \rightarrow$ 3rd order and A-stable
 $\gamma = (2 + \sqrt{2})/2 \rightarrow$ 2nd order and L-stable
 $c = \begin{bmatrix} \gamma & 1-\gamma \end{bmatrix}$,
 $A = \begin{bmatrix} \gamma & 0 \\ 1-2\gamma & \gamma \end{bmatrix}$
 $b = \begin{bmatrix} 1/2 & 1/2 \end{bmatrix}$

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

Child(ren): None.

Parameters: **3rd Order A-stable = 1** If true, set γ 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 γ 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, γ will be used. The default value is the '3rd Order A-stable' γ 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)

...



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**

0	0	
1	1	0
	1/2	1/2

- **SDIRK 2-Stage**

- **2nd Order L-Stable when $\gamma = (2 \pm \sqrt{2})/2$**

- 100x more accurate than previous L-Stable SDIRK

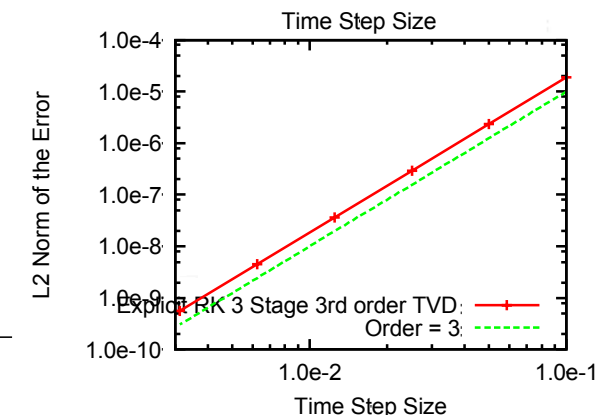
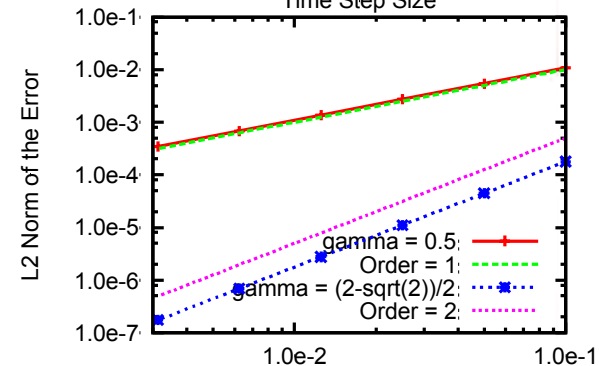
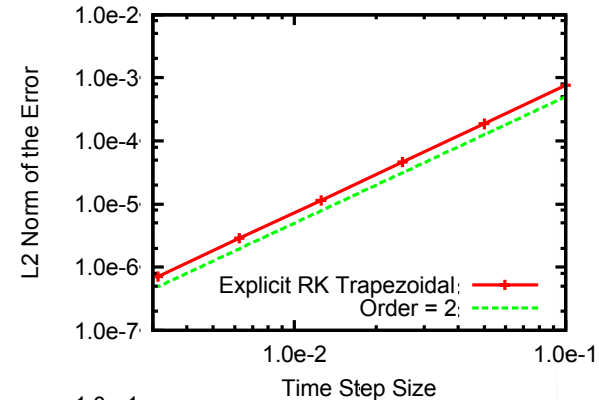
- **Solving Ordinary Differential Equations I: Nonstiff Problems, E. Hairer, et al.**

γ	γ	
1	$1 - \gamma$	γ
	$1 - \gamma$	γ

- **3-Stage 3rd Order TVD**

- **Gottlieb, Shu, Tadmor, 2001**

0	0		
1	1	0	
1/2	1/4	1/4	0
	1/6	1/6	4/6



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.**