Rythmos Update

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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
Sine-Cosine Problem

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

Rewriting as two 1st order ODEs
\[ \frac{d}{dt} x_0(t) = x_1(t) \]
\[ \frac{d}{dt} x_1(t) = \left( \frac{f}{L} \right)^2 \left( a - x_0(t) \right) \]

With the following coefficients and initial condition
\[
\begin{align*}
a &= 0 & \phi &= \arctan\left( ((f/L)/\gamma_1) \ast (\gamma_0 - a) \right) - (f/L) \ast t_0 & [= 0] \\
f &= 1 & b &= \gamma_1 / ((f/L) \ast \cos((f/L) \ast t_0 + \phi)) & [= 1] \\
L &= 1 & x_0(t_0 = 0) &= \gamma_0 & [= 0] \\
& & x_1(t_0 = 0) &= \gamma_1 & [= 1]
\end{align*}
\]

Exact solution
\[
\begin{align*}
x_0(t) &= a + b \ast \sin\left( (f/L) \ast t + \phi \right) \\
x_1(t) &= b \ast (f/L) \ast \cos\left( (f/L) \ast t + \phi \right)
\end{align*}
\]
Examples of Convergence Plots

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

\[
\begin{array}{c|ccc}
0 & 0 \\
1/2 & 1/2 & 0 \\
1/2 & 0 & 1/2 & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
1/6 & 1/3 & 1/3 & 1/6
\end{array}
\]

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

\[
\frac{\gamma}{1} \begin{pmatrix}
\gamma \\
1 - \gamma & \gamma
\end{pmatrix}
\]

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

\[
x_n = \frac{1}{\Delta t \beta_0} \sum_{i=0}^{s} \alpha_i x_{n-i}
\]
Example ParameterList Descriptions

• ParameterList hierarchy
  – 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
\[
\begin{align*}
gamma &= \frac{3+\sqrt{3}}{6} \rightarrow 3rd \ order \ and \ A-stable \\
gamma &= \frac{2+\sqrt{2}}{2} \rightarrow 2nd \ order \ and \ L-stable \\
c &= \begin{bmatrix} \gamma & 1-\gamma \\ \gamma & 0 \end{bmatrix} \\
A &= \begin{bmatrix} \gamma & \gamma \\ 1-2\gamma & \gamma \end{bmatrix} \\
b &= \begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix}
\end{align*}
\]

Parent(s): Runge Kutta Butcher Tableau Selection (Section 5.26)
Child(ren): None

Parameters:

3rd Order A-stable = 1 If true, set gamma to \(\gamma = \frac{3+\sqrt{3}}{6}\) to obtain a 3rd order A-stable scheme. '3rd Order A-stable' and '2nd Order L-stable' cannot both be true.

2nd Order L-stable = 0 If true, set gamma to \(\gamma = \frac{2+\sqrt{2}}{2}\) to obtain a 2nd order L-stable scheme. '3rd Order A-stable' and '2nd Order L-stable' cannot 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, \(\frac{3+\sqrt{3}}{6}\).
Improve Usability - IntegratorBuilder

• Improved access to Integrators through IntegratorBuilder
  – Create IntegratorBuilder
  – Set ParameterList
  – Set ModelEvaluator
  – Set NonlinearSolver
  – 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<Thya::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);
itegrator->getFwdPoints(time_vec,&x_vec,NULL,NULL);
New Steppers

- Explicit Trapezoidal
  - 2\textsuperscript{nd} Order method

- SDIRK 2-Stage
  - 2\textsuperscript{nd} Order L-Stable when $\gamma = (2 \pm \sqrt{2})/2$
  - 100x more accurate than previous L-Stable SDIRK

- 3-Stage 3\textsuperscript{rd} Order TVD
  - Gottlieb, Shu, Tadmor, 2001

\begin{align*}
  & \begin{array}{c|ccc}
    & 0 & 0 & \\hline
    1 & 1 & 0 \\hline
    1/2 & 1/2 & \\
  \end{array} \\
  & \begin{array}{c|ccc}
    & \gamma & \gamma & \\hline
    1 & 1-\gamma & \gamma \\hline
    1-\gamma & \gamma & \\
  \end{array} \\
  & \begin{array}{c|cccc}
    & 0 & 0 & \\hline
    1 & 1 & 0 \\hline
    1/2 & 1/4 & 1/4 & 0 \
    1/6 & 1/6 & 4/6 & \\
  \end{array}
\end{align*}
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.