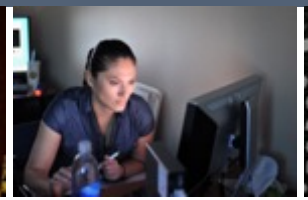
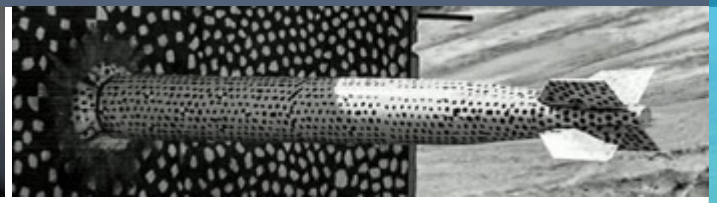
SAND2021-14942 C: UUR

Sandia National Laboratories

Nonlinear Analysis Product Area Update





PRESENTED BY

Roger Pawlowski

Current Contributors: Bartlett, Conde, Phipps, Miller, Ober, Perego, Ridzal, Tezaur, Watkins

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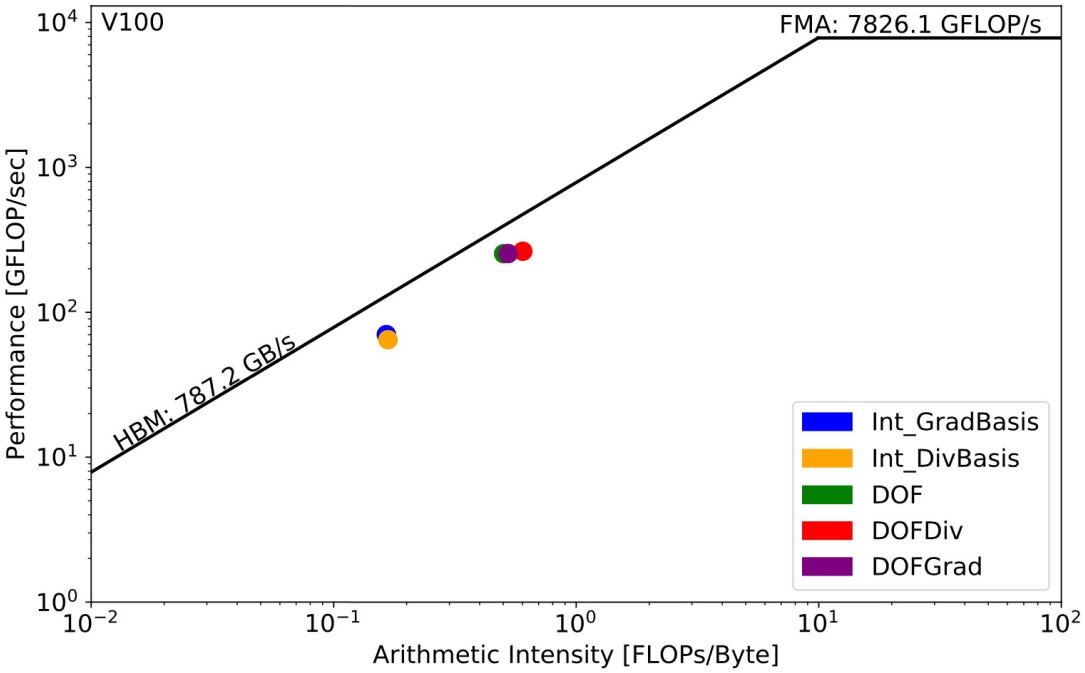
Nonlinear Product Area Updates

- Sacado (Phipps)
  - Library is UVM free
  - Tests refactored to be UVM free. Only certain DFad use-cases require UVM (and this won't change).
  - Paper on performance portability submitted to TOMS
  - Porting to HIP in FY22/Q2
  - Port to SYCL
  - Porting Sacado to the new MDSpan should happen this year, which will simplify the integration with Kokkos substantially
- NOX/LOCA (Pawlowski)
  - UVM free
  - Householder constraint solver added for Tpetra stack
  - Porting to HIP in FY22/Q2
- Rythmos (Ober)
  - Planning to deprecate at end of FY22 or early FY23
  - Replacement is Tempus

Roofline for Panzer AD Kernels on V100 with DFAD



$$\begin{bmatrix} J & A \\ B^T & C \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} F \\ G \end{bmatrix}$$

Tempus – Time-Integration Package (Ober)

- Provides time-integration methods for first and second-order ODEs
  - Explicit: $\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{p}, t)$ $\quad\quad$ $\ddot{\mathbf{x}}(t) = \mathbf{f}(\dot{\mathbf{x}}(t), \mathbf{x}(t), \mathbf{p}(t), t)$
  - Implicit: $\mathbf{f}(\dot{\mathbf{x}}(t), \mathbf{x}(t), t) = 0$ $\quad\quad$ $\mathbf{f}(\ddot{\mathbf{x}}(t), \dot{\mathbf{x}}(t), \mathbf{x}(t), t) = 0$
- Developed to support advanced analysis techniques
  - Embedded transient sensitivity analysis and UQ capabilities
    - Forward and Adjoint Sensitivities
  - Couples with ROL to provide transient optimization capabilities
- Provides "out of the box" capabilities
  - Embedded error analysis for variable time steps
  - Temporal solution interpolation
  - Solution history management
  - *47+ Steppers*
- Provides customization capabilities
  - Ability to incorporate application-specific time steppers
  - *Application-specific time-step control* for variable time steps
  - Observers – ability to insert application-specific algorithms
  - *Time-event management*, e.g.,
    - Problem-specific events – switch flipped, x-ray impingement, …
    - Solution/diagnostic/debug/in-situ visualization output

Tempus Steppers

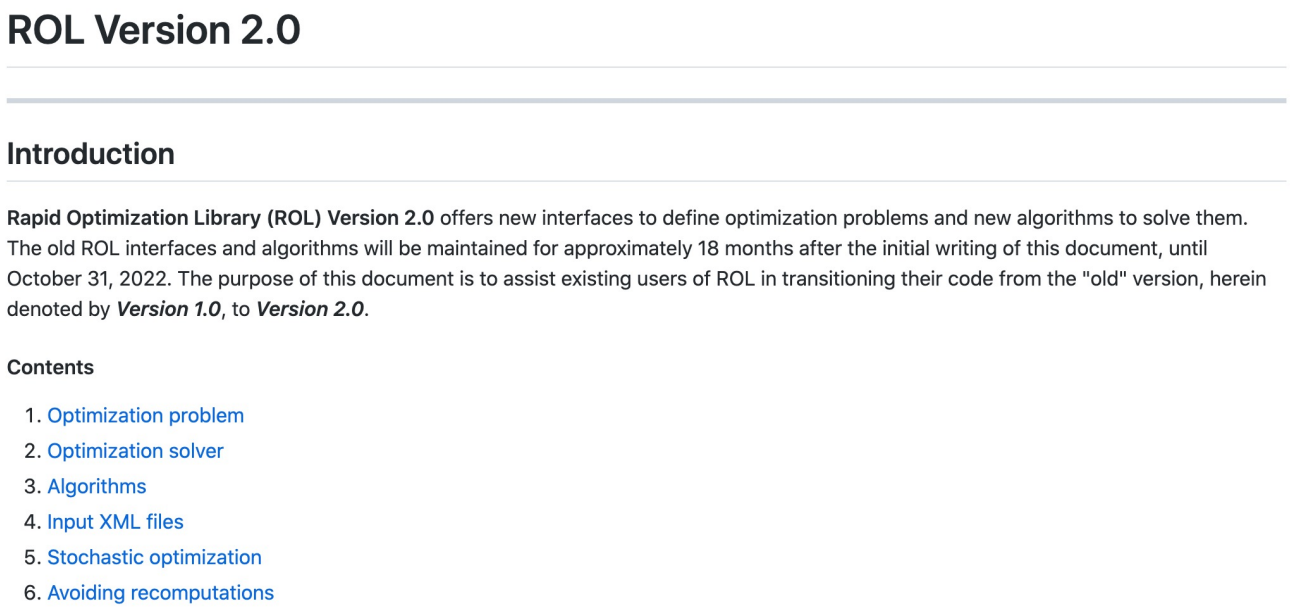
- Forward Euler
- Backward Euler
- Explicit Runge-Kutta (ERK) (*15+*)
- Diagonally Implicit Runge-Kutta (DIRK) (*20+*)
- Newmark, HHT-a, Leapfrog
- IMEX-RK (+Partitioned) (3+)
- BDF2
- Trapezoidal
- 1st Order Splitting
- *Subcycling*

- Other features
  - *Generate consistent initial conditions*
  - *FSAL when possible*
  - Extensive verification & unit testing
  - Documentation (Doxygen)

Italicized – latest development

ROL (Ridzal)

- ROL 2.0 released in April 2021
- New interfaces to define optimization problems (ROL::Problem) and solve them (ROL::Solver).
- Completely revised infrastructure for recomputing function values and derivatives.
- ROL 1.0 interfaces will be maintained until October 2022.
- Transition website: https://github.com/trilinos/Trilinos/blob/master/packages/rol/Version-2.0.md



ROL Version 2.0

Introduction

Rapid Optimization Library (ROL) Version 2.0 offers new interfaces to define optimization problems and new algorithms to solve them. The old ROL interfaces and algorithms will be maintained for approximately 18 months after the initial writing of this document, until October 31, 2022. The purpose of this document is to assist existing users of ROL in transitioning their code from the "old" version, herein denoted by ***Version 1.0***, to ***Version 2.0***.

Contents

PIRO (Perego, Tezaur)

- Continuing work on the steady-state PDE-constrained optimization capability, implementing wrappers for ROL that are based on Thyra.
  - Can solve gradient based and Newton methods (with Hessian information), in reduced-space and full-space form.
  - Can also use a Hessian-based dot-product for ROL, which proved to significantly improve the convergence for some optimization problems. The partial first (e.g. Jacobian) and second (Hessian) derivatives needs to be provided by the application.
  - Changed the way PIRO computes steady-state adjoint sensitivities. Now relies on ROL to manage the solution of the forward and adjoint system instead of directly doing that in Piro.
- Added transient adjoint sensitivities using Tempus.
  - Verified on MMS problems
  - Identified changes to Tempus for L2 Milestone
- Remove Epetra support: when Panzer users fully transition to Tpetra.

MMS Advection Problem

$$\frac{\partial u}{\partial t} + a(x)\frac{\partial u}{\partial x} = f(x, a(x))$$

$$a(x) = x(2\pi - x) + 10$$

$$u(x,t) = xsin(x - a(x)t)$$

$$g(x,t) = \frac{1}{N+1}\sum_{i=1}^{N+1} x_i t cos(x_j - a_j t)$$