Embedded Sensitivities and Optimization

From Research to Applications

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Department Review, January 30, 2008
Roscoe Bartlett in a Nut Shell

• Came to Sandia in 2001 directly into 1411
• Ph.D. background (CMU Chemical Engineering) is in large-scale embedded derivative-based optimization: rSQP++ => MOOCHO
• Primary algorithms research area continues to be embedded derivative-based optimization (MOOCHO/Trilinos)
• Talent and interests lie at the intersection of advanced numerical algorithms and modern software engineering methods (e.g. Thyra)
• Object-Oriented Software Engineering and C++ Expert
• Leading efforts to bridge transformational embedded analysis methods (sensitivities, optimization, ...) and applications:
  – Thyra/Trilinos: Interoperability of numerical algorithms
  – Thyra ModelEvaluator: Infrastructure for support of embedded algorithms
  – Rythmos/Trilinos (Coffey (1414)): Transient sensitivities for optimization, ...
  – Stratimikos/Trilinos: Unification of linear solvers and preconditioners
  – APP + Trilinos Dev: Keep APPs and algorithms working together, driving R&D
    – Charon + Trilinos Dev (ASC FY07 Level-2 Vertical Integration Milestone)
    – Aria/SIERRA + Trilinos Dev (1400/1500 Collaboration)

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Notable Projects for Roscoe Bartlett

• FY07 ASC Level-2 Vertical Integration Milestone (Lead):
  – Charon + Trilinos Dev, vertical solver integration using Thyra
  – Optimization and transient sensitivities for QASPR problems
  – Involved members from:
    • 1411: Roscoe Bartlett, Eric Phipps, Denis Ridzal
    • 1414: Scott Collis, Todd Coffey, David Day, Russell Hooper, Roger Pawlowski, Andy Salinger
    • 1416: Mike Heroux, Jim Willenbring
    • 1437: Rob Hoeskstra, Heidi Thornquist

• ASC Algorithms:
  – Trilinos Framework: Addressing scalability and interoperability from build tools through
    advanced numerical algorithms (Teuchos, Thyra, Rythmos, MOOCHO, ...)
  – Optimization:
    • R&D of embedded optimization methods (MOOCHO)
    • Bridging embedded (Trilinos) and non-invasive (Dakota)
  – Aria/SIERRA + Trilinos Dev Integration (Lead):
    • Add embedded algorithms to Aria/SIERRA for sensitivities, error-estimation, optimization, ...
    • Bridge between SIERRA application developers and Trilinos algorithm researchers
    • Joint 1400/1500 Collaboration:
      – 1411: Roscoe Bartlett, Eric Phipps
      – 1414: Todd Coffey, Russell Hooper, Bart vBW
      – 1541: Brian Carnes, Kevin Copps, Derek Gaston, Pat Notz

• SCIDAC TOPS-2: Trilinos Fortran/C++ interoperability for Office of Science customers
• CSRF Componentizing Effort (Salinger (1414)): Leading three working groups
Potential of Embedded Analysis Algorithms

For appropriate problems, embedded derivative-based analysis methods (e.g., sensitivities, optimization, UQ, error estimation ...) potentially provide large improvements in speed, accuracy, and/or capability over other approaches.

Example: QASPR transient current sensitivities w.r.t. reaction parameters for an irradiated semiconductor device modeled with Charon

- Embedded sensitivities with AD/Sacado (Phipps) & Rythmos
- Finite differences (steplen=1e-2) (optimal steplen=1e-1)
- Embedded sensitivities vs. finite diff.
  - Much more accurate and robust!
  - 10x faster for 40 parameters!


Since coming to Sandia in August 2001 I have been involved a number of projects related to embedded sensitivities and optimization and have had mixed experiences => I have learned a lot about how to apply embedded methods!
Challenges/Barriers to Embedded Analysis Algorithms

Version Control, Build, Test
(incompatible dev sources, environments, tools, lack of testing, ...)
APP + Trilinos Dev (Bartlett et. al.)

Software Infrastructure
(narrow forward solvers, inflexible implementation approaches, ...)
Thyra ModelEvaluator (Bartlett et. al.)

Derivatives & UQ Support
(smoothness, accuracy, parameter derivatives, uncertainty proposition, ...)
AD/Sacado (Phipps and Gay)
UQ/Stokhos (Phipps)

Embedded Algorithms R&D with Production APPs
• Better Algorithms R&D!
• Better Production APPs!

We are now addressing these barriers in a fundamental way to provide the foundation for sustained embedded algorithms R&D

1400/1500
APP + Trilinos Dev (Bartlett et. al.)
Thyra ModelEvaluator (Bartlett et. al.)
AD/Sacado (Phipps et. al.)
UQ/Stokhos (Phipps)
• The Idea:
  – Keep the development versions of APP and Trilinos code updated and tested daily
  – Also keep APP and Trilinos Release updated
  – Automated daily integrations tests
  – Results in better production capabilities and better research

• Charon + Trilinos Dev
  – Development versions of Charon and Trilinos are kept up-to-date every day!
  – New embedded optimization and sensitivity capabilities are run and tested every day!

• Aria/SIERRA + Trilinos Dev
  – We have automated configuration and daily integration testing of Aria/SIERRA VOTD against Trilinos Dev working!
  – Now, we are addressing Aria/SIERRA software infrastructure issues and will start adding new embedded Trilinos analysis algorithms!

The End