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Embedded Sensitivities and Optimization

From Research to Applications

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

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

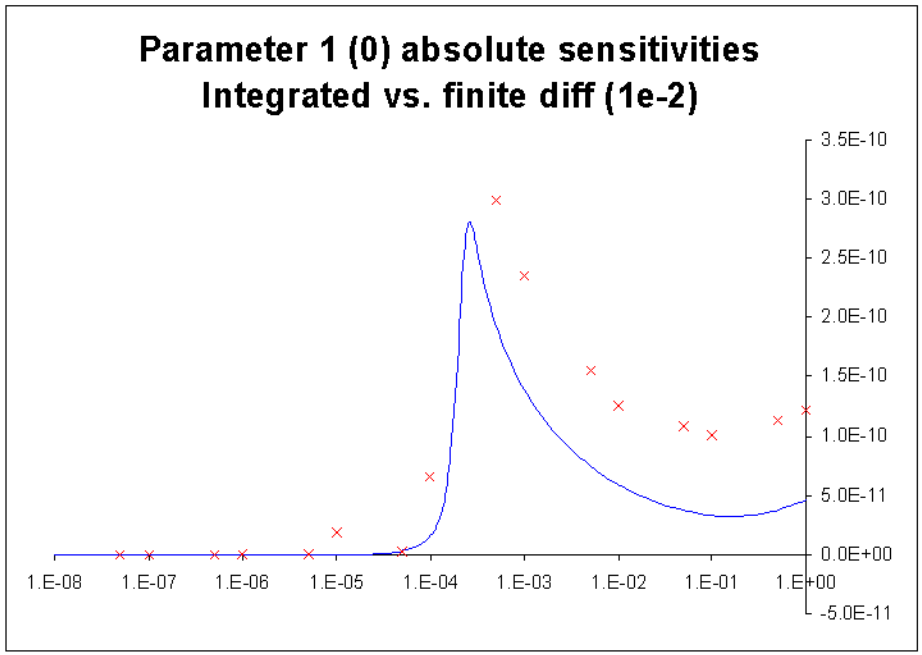
- FY07 ASC Level-2 Vertical Integration Milestone (**Lead**):
  - Charon + Trilinos Dev, vertical solver integration using Thyra
  - Optimization and transient sensitivities for QASPR problems
  - Involved members from:
    - 1411: Roscoe Bartlett, Eric Phipps, Denis Ridzal
    - 1414: Scott Collis, 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!



Bartlett, Roscoe, Scott Collis, Todd Coffey, David Day, Mike Heroux, Rob Hoekstra, Russell Hooper, Roger Pawlowski, Eric Phipps, Denis Ridzal, Andy Salinger, Heidi Thornquist, and Jim Willenbring. *ASC Vertical Integration Milestone*. SAND2007-5839, Sandia National Laboratories, 2007 [http://www.cs.sandia.gov/~rabartl/publications.html]

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!

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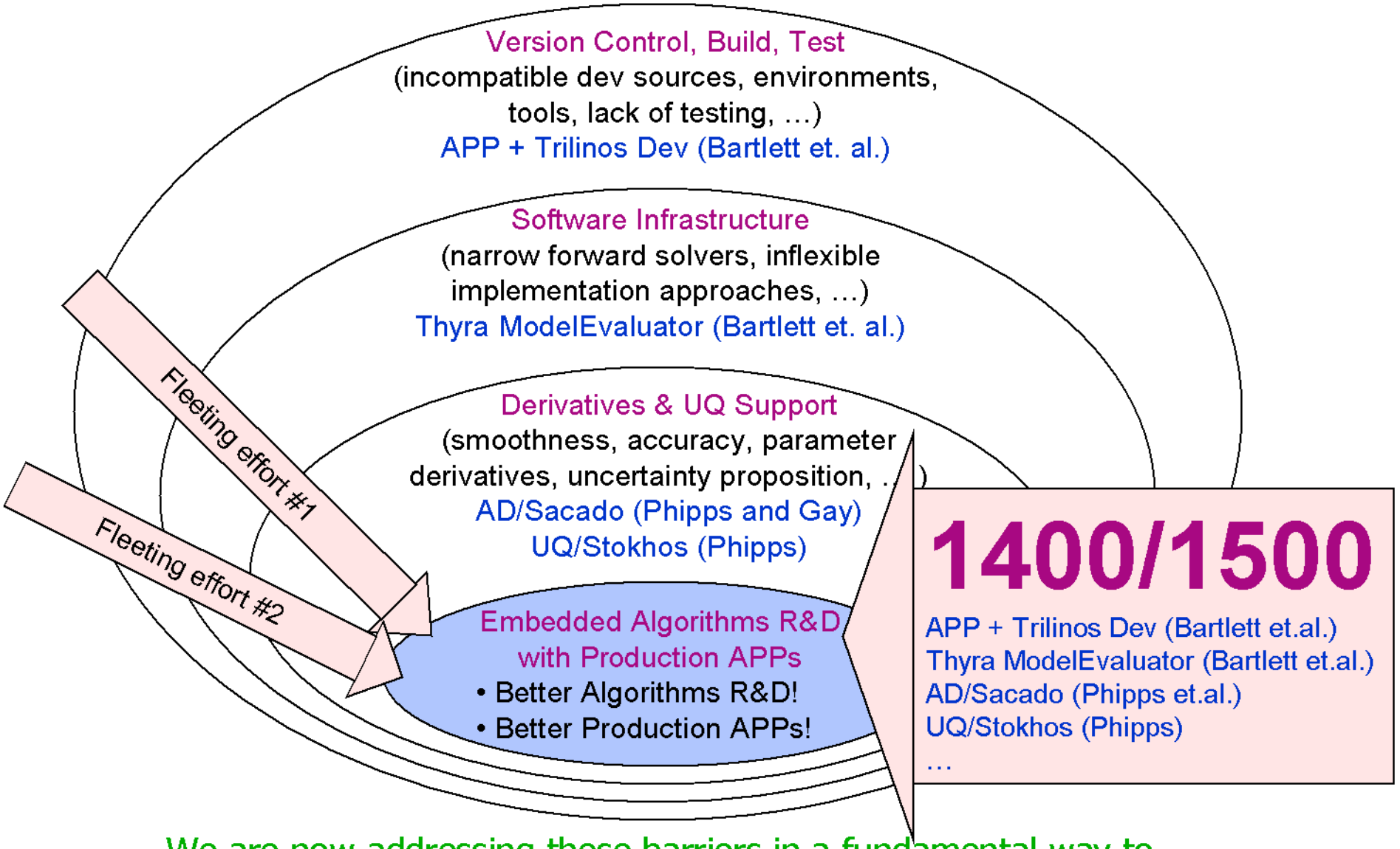
Challenges/Barriers to Embedded Analysis Algorithms



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

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APP + Trilinos Dev: Algorithms and Applications Integration

- 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!

Bartlett, Roscoe. *Daily Integration and Testing of the Development Versions of Applications and Trilinos: A stronger foundation for enhanced collaboration in application and algorithm research and development*, SAND2007-7040, Sandia National Laboratories, October 2007 [http://www.cs.sandia.gov/~rabartl/publications.html]

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The End

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