MS17

A Case Study on the Vertical Integration of Trilinos Solver Algorithms with a Production Application Code

Organizer: Roscoe A. Bartlett

Sandia National Laboratories

10:00-10:25 Overview of the Vertical Integration of Trilinos Solver Algorithms in a Production Application Code

Roscoe A. Bartlett, Sandia National Laboratories

10:30-10:55 Analytic Sensitivities in Large-scale Production Applications via Automatic Differentiation with Sacado

Eric Phipps, Sandia National Laboratories

11:00-11:25 To PDE Components and Beyond

Andy Salinger, Sandia National Laboratories

Replacement

11:30-11:55 Analysis Tools for Large-scale Simulation with Application to the Stationary Magnetohydrodynamics Equations

Roger Pawlowski, Eric Phipps, Heidi K. Thornquist, and Roscoe A. Bartlett, Sandia National Laboratories

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Overview of the Vertical Integration of Trilinos Solver Algorithms in a Production Application Code

Roscoe A. Bartlett
Department of Optimization & Uncertainty Estimation

http://www.cs.sandia.gov/~rabartl

Sandia National Laboratories

March 13th, 2008

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.

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Overview of Trilinos Vertical Integration Project (Milestone)

- **Goal:** Vertically integrate Trilinos solver algorithms in Trilinos to build new predictive embedded analysis capabilities
  - **Impact:** Vertically integrated 10+ Trilinos algorithm packages
- **Goal:** Demonstrate on relevant production applications
  - **Impact:** Solved steady-state parameter estimation problems and transient sensitivities on semiconductor devices in Charon
  - **Impact:** Solved Eigen problems on MHD problem in Charon
- **Added Goal:** Explore refined models of collaboration between production application developers and algorithm researchers.
  - **Impact:** Closer collaboration between application and algorithm developers yielding better algo and app R&D

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]

Trilinos

CHARON

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Outline

- Overview of Trilinos and Charon
- Overview of vertical solver algorithm integration
- Moving beyond the forward solve
  - ⇒ Challenges/barriers to embedded analysis methods
  - ⇒ Enabling methods
- Examples of vertically integrated algorithms with Trilinos and Charon
- Steady-state parameter estimation optimization with MOOCHO/Charon

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Overview of Trilinos

- Provides a suite of numerical solvers to support predictive simulation for Sandia's customers

  => Scope has expended to include discretizations methods, …!
- Provides a decoupled and scalable development environment to allow for algorithmic research and production capabilities => "Packages"
- Provides support for growing SQA requirements
- Mostly C++ with some C, Fortran, Python …
- Advanced object-oriented and generic C++ …

Current Status

- Current release: Trilinos 8.0.x (September 2007)
- Next release Trilinos 9.0 (September 2008)

Trilinos website

http://trilinos.sandia.gov

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Trilinos (8.0 & 9.0+) Package Summary

	Objective	Package(s)
Discretizations	Meshing & Spatial Discretizations	phdMesh, Intrepid
Methods	Automatic Differentiation and UQ Prop.	Sacado, Stokos
	Mortar Methods	Moertel
Core	Linear algebra objects	Epetra, Jpetra, Tpetra
	Abstract interfaces	**Thyra**, Stratimikos, RTOp
	Load Balancing	Zoltan, Isorropia
	"Skins"	PyTrilinos, WebTrilinos, Star-P, ForTrilinos, CTrilinos
	C++ utilities, (some) I/O	Teuchos, EpetraExt, Kokkos, Triutils
Solvers	Iterative (Krylov) linear solvers	AztecOO, Belos, Komplex
	Direct sparse linear solvers	Amesos
	Direct dense linear solvers	Epetra, Teuchos, Pliris
	Iterative eigenvalue solvers	Anasazi
	ILU-type preconditioners	AztecOO, IFPACK
	Multilevel preconditioners	ML, CLAPS
	Block preconditioners	Meros
	Nonlinear system solvers	NOX, LOCA
	Time Integration & Sensitivities	Rythmos
Analysis	Optimization (SAND)	MOOCHO, Aristos

Green: Packages used in Vertical Integration Milestone

Gray: New packages that will be included in Trilinos 9.0 (September 2008) or later

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Trilinos Strategic Goals

- **Scalable Computations:** As problem size and processor counts increase, the cost of the computation will remain nearly fixed.
- **Hardened Computations:** Never fail unless problem essentially intractable, in which case we diagnose and inform the user why the problem fails and provide a reliable measure of error.
- **Full Vertical Coverage:** Provide leading edge enabling technologies through the entire technical application software stack: from problem construction, solution, analysis and optimization.

Algorithmic Goals

- ***Grand* Universal Interoperability**: All Trilinos packages will be interoperable, so that any combination of solver packages that makes sense algorithmically will be possible within Trilinos.
- **Universal Accessibility:** All Trilinos capabilities will be available to users of major computing environments: C++, Fortran, Python and the Web, and from the desktop to the latest scalable systems.
- **Universal Solver RAS**: Trilinos will be:
  - Reliable: Leading edge hardened, scalable solutions for each of these applications
  - Available: Integrated into every major application at Sandia
  - Serviceable: Easy to maintain and upgrade within the application environment.

Software Goals

Courtesy of Mike Heroux, Trilinos Project Leader

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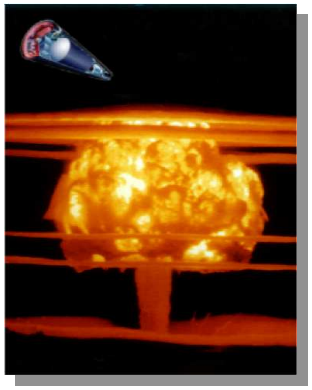
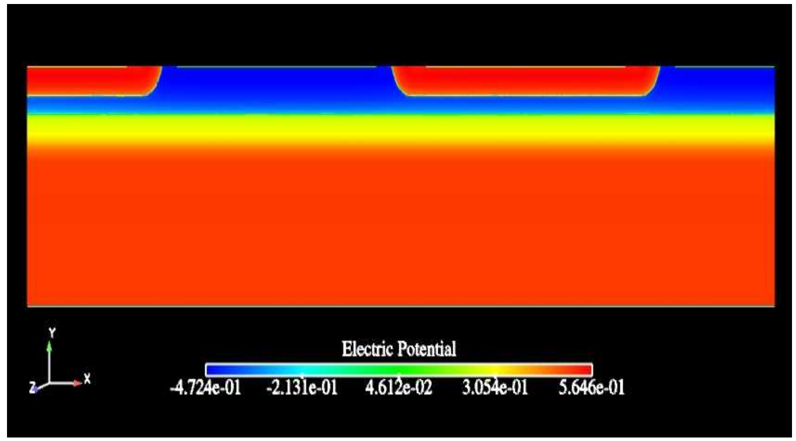
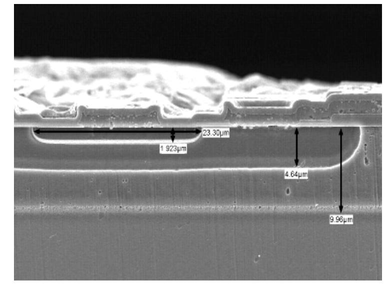
CHARON

(Generalized PDE Solver)

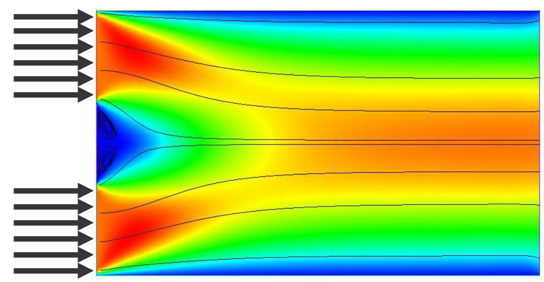


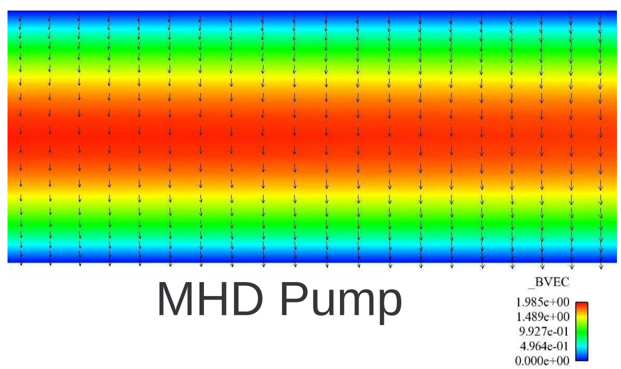
- Internal SNL Code for QASPR project
- Large-scale parallel (MPI)
- Unstructured grid finite elements
- Automatic Differentiation
- Adaptive Mesh Refinement
- Generalized operators – fast addition of new operators/equations
- Physics
  - Semiconductor Device
  - Multi-phase Aerosol
  - Reacting flows/gas-phase Combustion
  - MHD/Plasma
- Algorithms testing ground



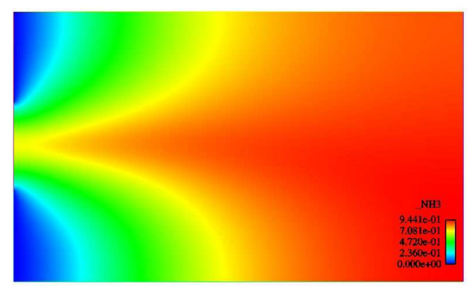


Semiconductor





MHD Pump



Reacting Flow

Outline

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  - ⇒ Challenges/barriers to embedded analysis methods
  - ⇒ Enabling methods
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Thyra is being developed to address this issue

Software Goals

Courtesy of Mike Heroux, Trilinos Project Leader

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Packages/Algorithms Most Directly to Vertical Integration Project

Trilinos Packages

- Linear Problems: Given linear operator (matrix) $A \in \mathbf{R}^{n \times n}$
  - Linear equations: Solve $Ax = b$ for $x \in \mathbf{R}^n$ — Belos
  - Eigen problems: Solve $Av = \lambda v$ for (all) $v \in \mathbf{R}^n$ and $\lambda \in \mathbf{R}$ — Anasazi
- Nonlinear Problems: Given nonlinear operator $f(x,p) \in \mathbf{R}^{n+m} \to \mathbf{R}^n$
  - Nonlinear equations: Solve $f(x) = 0$ for $x \in \mathbf{R}^n$ — NOX
  - Stability analysis: For $f(x,p) = 0$ find space $p \in \mathcal{P}$ such that $\frac{\partial f}{\partial x}$ is singular — LOCA
- Transient Nonlinear Problems:
  - DAEs/ODEs: Solve $f(\dot{x}(t), x(t), t) = 0, t \in [0,T]$, $x(0) = x_0$, $\dot{x}(0) = x'_0$ for $x(t) \in \mathbf{R}^n, t \in [0,T]$ — Rythmos
  - ODE/DAE Sensitivities …
- Optimization Problems:
  - Unconstrained: Find $p \in \mathbf{R}^m$ that minimizes $g(p)$
  - Constrained: Find $x \in \mathbf{R}^n$ and $p \in \mathbf{R}^m$ that:
    minimizes $g(x,p)$
    such that $f(x,p) = 0$ — MOOCHO

Embedded Analysis Algorithms (NOX, LOCA, Rythmos, MOOCHO)

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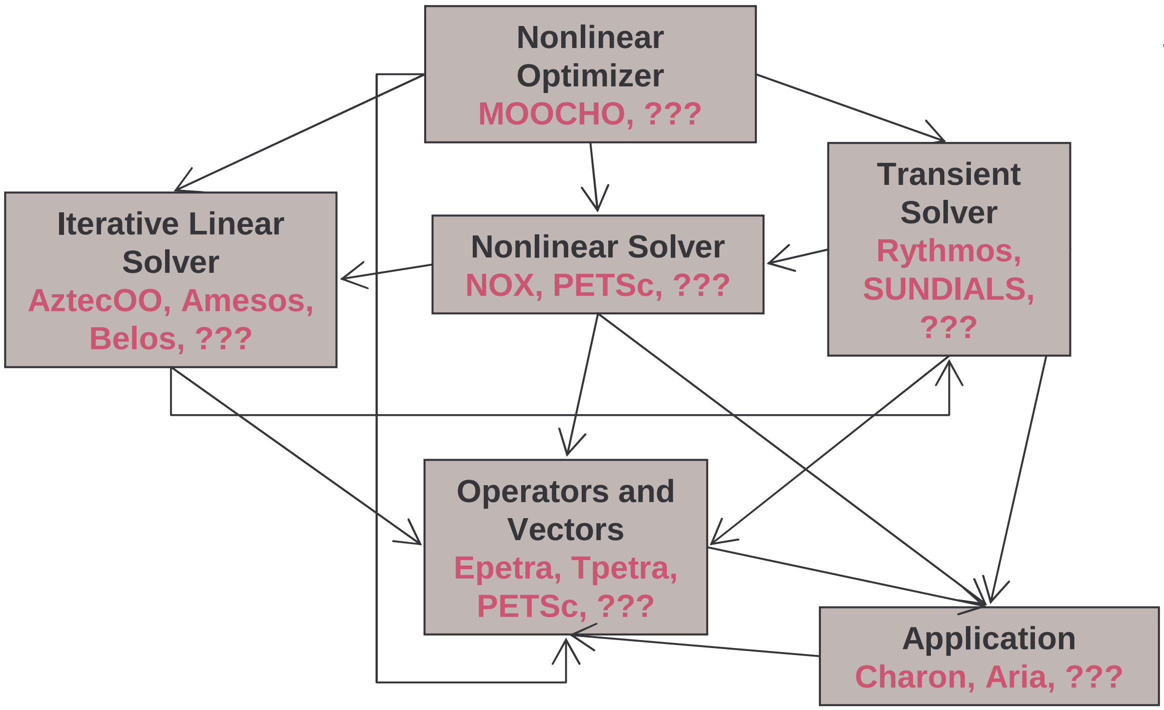
Vertical Integration and Interoperability is Important

Example: Numerous interactions exist between layers of abstract numerical algorithms (ANAs) in a transient optimization problem



What is needed to solve problem?

- Standard interfaces to break $O(N^2)$ 1-to-1 couplings

Thyra is being developed to address interoperability of ANAs by defining interfaces for:

- Linear operators/vectors
- Preconditioners / Linear solvers
- Nonlinear models
- Nonlinear solvers
- Transient solvers

Key Points

- Higher level algorithms, like optimization, require a lot of interoperability
- Interoperability and vertical integration must be “easy” or these configurations will not be achieved in practice

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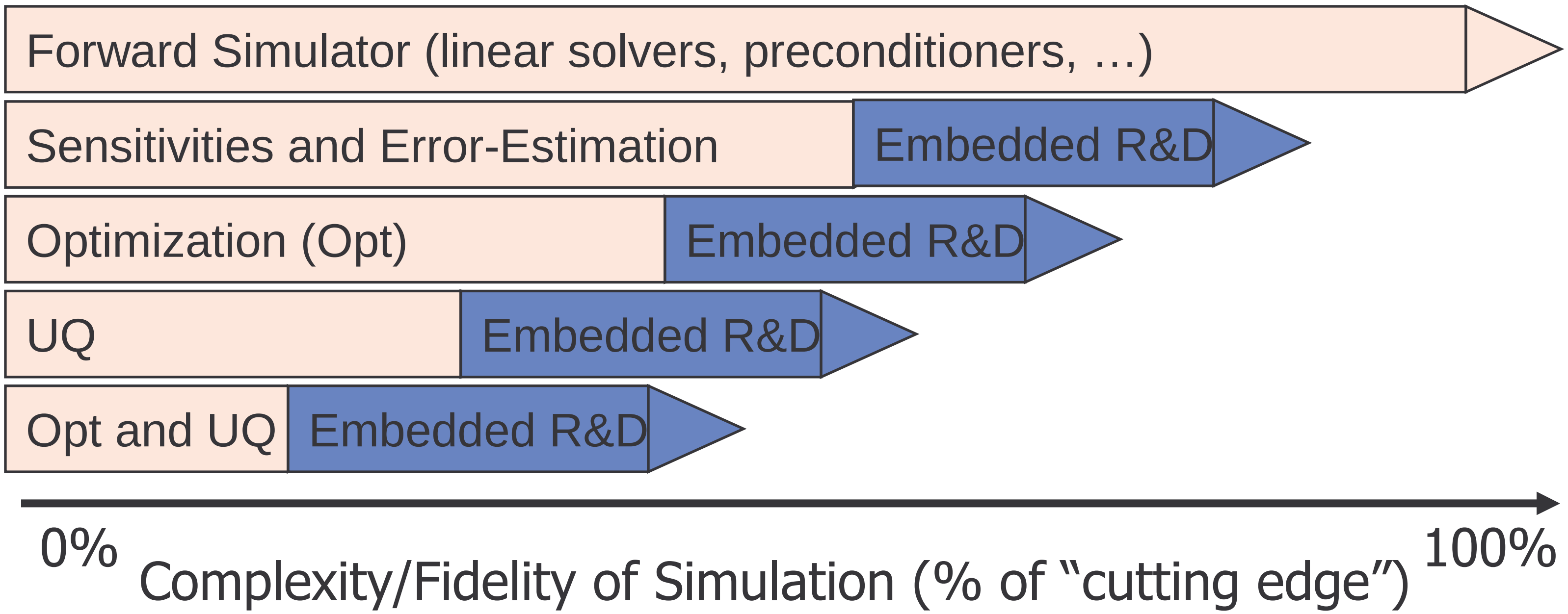
Embedded Analysis Algorithms and "The Cutting Edge"



- The "Cutting Edge" for the Forward Simulation Application
  - Drives capability computing (e.g., Gordan Bell, etc.)
  - Drives (i.e., "Pulls") R&D for linear solvers, preconditioners, …
- Advanced Analysis Methods
  - Lag behind the "cutting edge" of the forward simulation
  - R&D reduces the lag!
  - Less direct impact on the forward simulation results => Leads to "Push" instead of "Pull"
  - Requires a different approach w.r.t. working with APP developers and customers!

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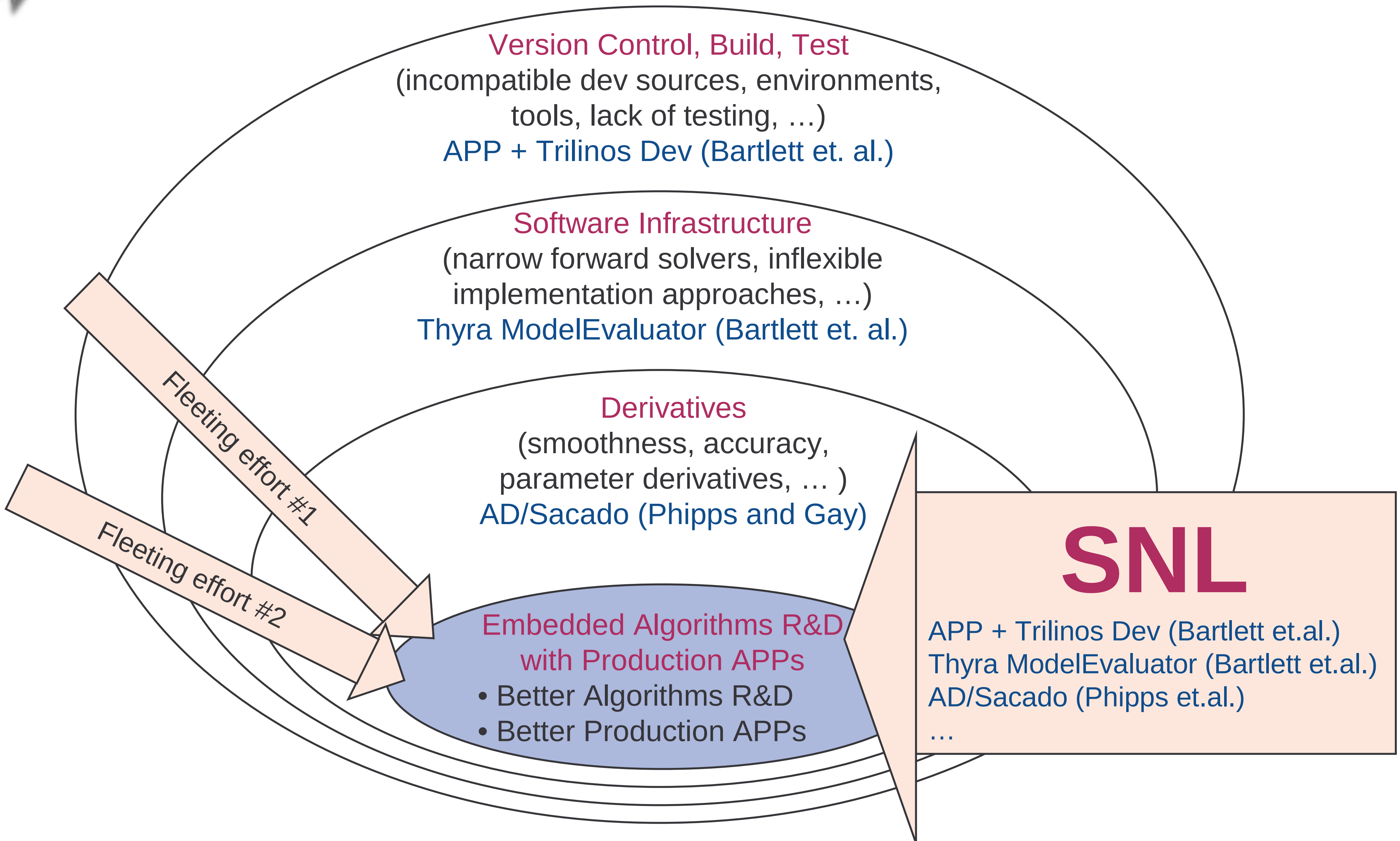
Challenges/Barriers to Embedded Analysis Algorithms



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

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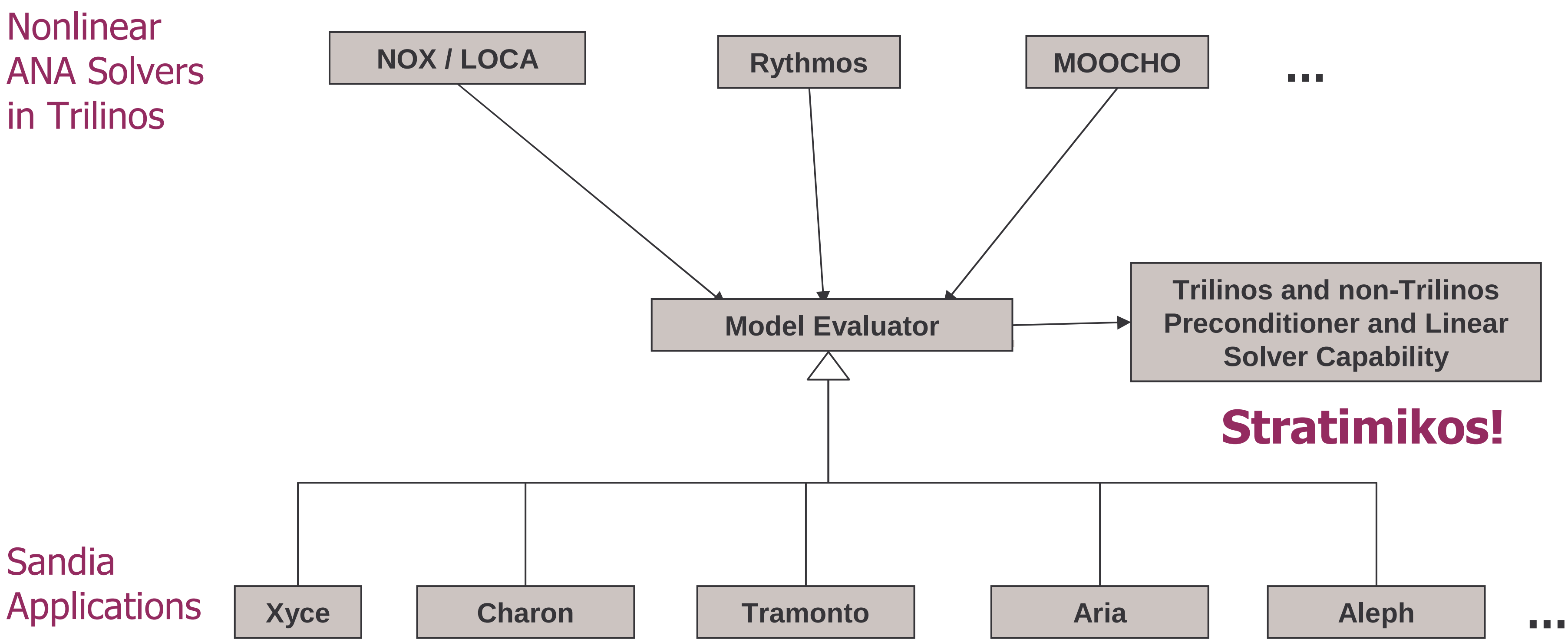
Nonlinear Algorithms and Applications : Thyra & Model Evaluator!



Key Points

- Provide single interface from nonlinear ANAs to applications
- Provides for shared, uniform access to linear solver capabilities
- Once an application implements support for one ANA, support for other ANAs can be added incrementally

Some Nonlinear Problems Supported by the ModelEvaluator

Nonlinear equations:	Solve $f(x) = 0$ for $x \in \mathbf{R}^n$
Stability analysis:	For $f(x,p) = 0$ find space $p \in \mathcal{P}$ such that $\frac{\partial f}{\partial x}$ is singular
Explicit ODEs:	Solve $\dot{x} = f(x,t) = 0, t \in [0,T]$, $x(0) = x_0$, for $x(t) \in \mathbf{R}^n, t \in [0,T]$
DAEs/Implicit ODEs:	Solve $f(\dot{x}(t), x(t), t) = 0, t \in [0,T]$, $x(0) = x_0$, $\dot{x}(0) = x'_0$ for $x(t) \in \mathbf{R}^n, t \in [0,T]$
Explicit ODE Forward Sensitivities:	Find $\frac{\partial x}{\partial p}(t)$ such that: $\dot{x} = f(x,p,t) = 0, t \in [0,T]$, $x(0) = x_0$, for $x(t) \in \mathbf{R}^n, t \in [0,T]$
DAE/Implicit ODE Forward Sensitivities:	Find $\frac{\partial x}{\partial p}(t)$ such that: $f(\dot{x}(t), x(t), p, t) = 0, t \in [0,T]$, $x(0) = x_0$, $\dot{x}(0) = x'_0$, for $x(t) \in \mathbf{R}^n, t \in [0,T]$
Unconstrained Optimization:	Find $p \in \mathbf{R}^m$ that minimizes $g(p)$
Constrained Optimization:	Find $x \in \mathbf{R}^n$ and $p \in \mathbf{R}^m$ that: minimizes $g(x,p)$ such that $f(x,p) = 0$
ODE Constrained Optimization:	Find $x(t) \in \mathbf{R}^n$ in $t \in [0,T]$ and $p \in \mathbf{R}^m$ that: minimizes $\int_0^T g(x(t),p)$ such that $\dot{x} = f(x(t),p,t) = 0$, on $t \in [0,T]$ where $x(0) = x_0$

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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
  - 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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Vertical Integrations of Trilinos Capabilities: Example 1

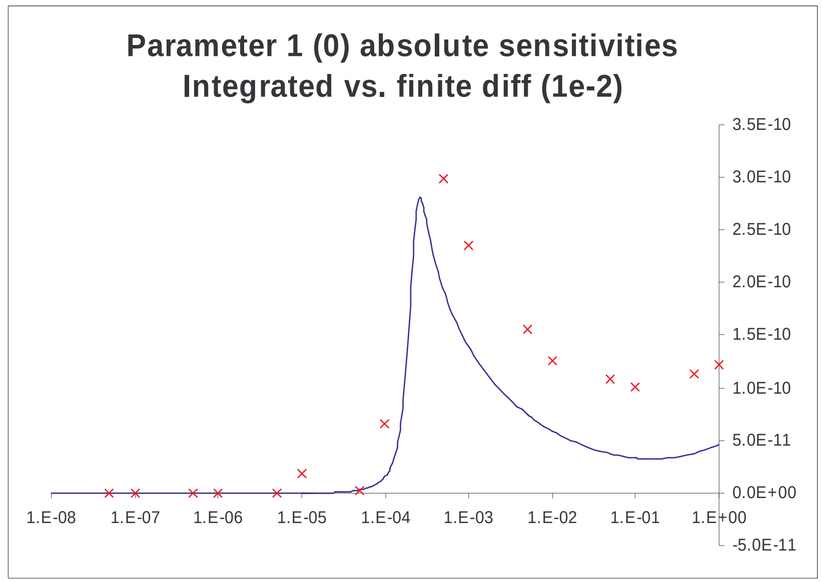
See Andy Salinger's Talk at 11:00 AM

Trilinos Capabilities

Analysis Tools *(embedded)*
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Constrained Solves
- Optimization

Linear Algebra
- Data Structures
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
- Matrix Partitioning

Derivative Tools
- Derivatives
- Sensitivities



Transient sensitivity analysis of a 2n2222 BJT in Charon *w/AD+Rythmos: 14x faster than FD*

See Eric Phipp's Talk at 10:30 AM

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Vertical Integrations of Trilinos Capabilities: Example 2

Trilinos Capabilities

Analysis Tools (*embedded*)
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Constrained Solves
- Optimization

Linear Algebra
- Data Structures
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
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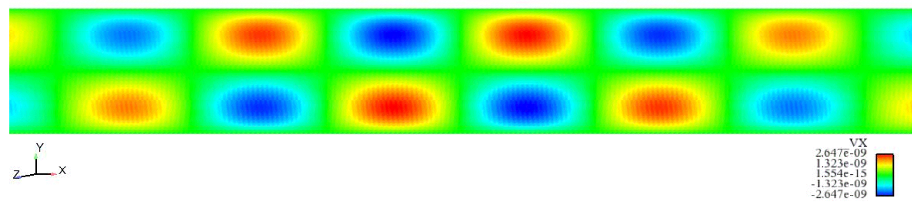
Derivative Tools
- Derivatives
- Sensitivities



Destabilizing eigen-vector for heated fluid in magnetic field

See Roger Pawlowski's Talk at 11:30 AM

Vertical Integrations of Trilinos Capabilities: Example 3

Trilinos Capabilities

Analysis Tools *(embedded)*
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Constrained Solves
- Optimization

Linear Algebra
- Data Structures
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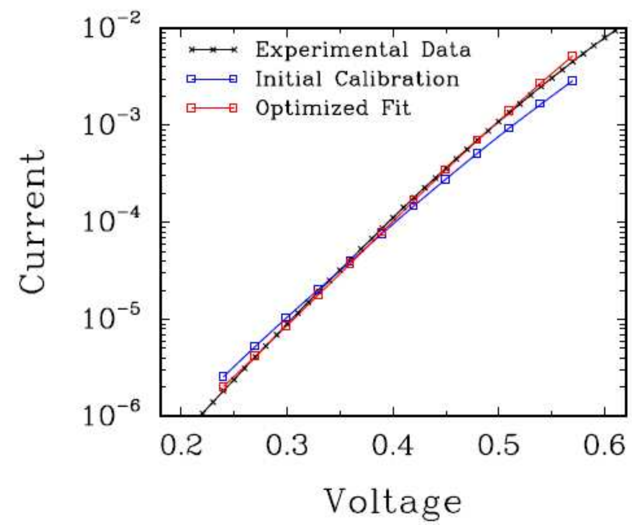
Derivative Tools
- Derivatives
- Sensitivities

$$\begin{aligned} &\text{minimize} && \tfrac{1}{2}\|g(x,p) - g^*\|_2^2 + \tfrac{1}{2}\beta\|p\|_2^2 \\ &\text{subject to} && f(x,p) = 0 \end{aligned}$$



Steady-Sate Parameter Estimation Problem using 2n2222 BJT in Charon *MOOCHO + AD*

I am talking about this next

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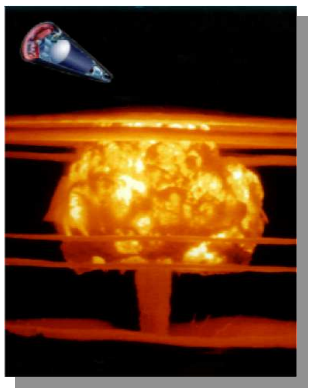
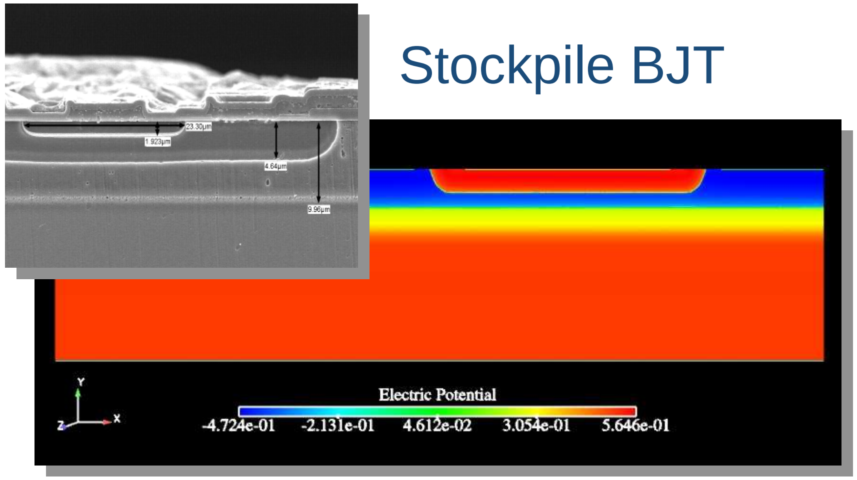
QASPR

Qualification of electronic devices in hostile environments

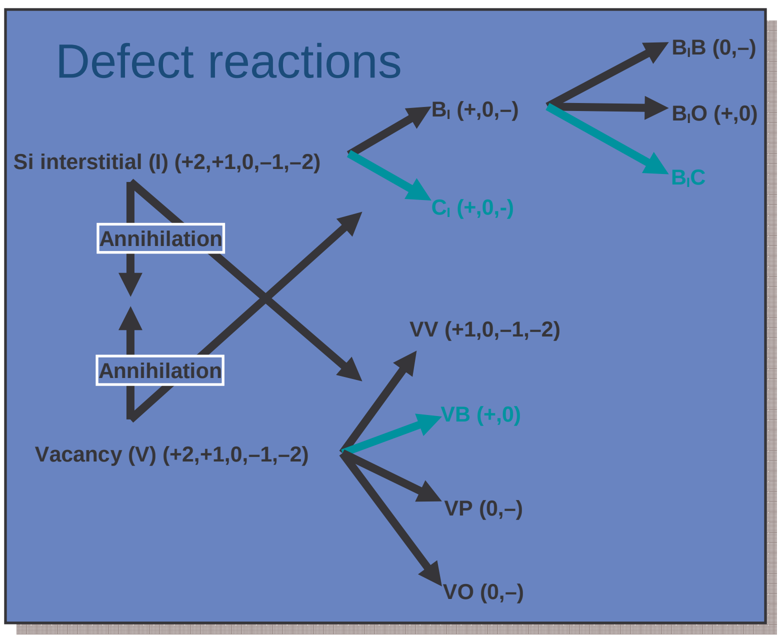


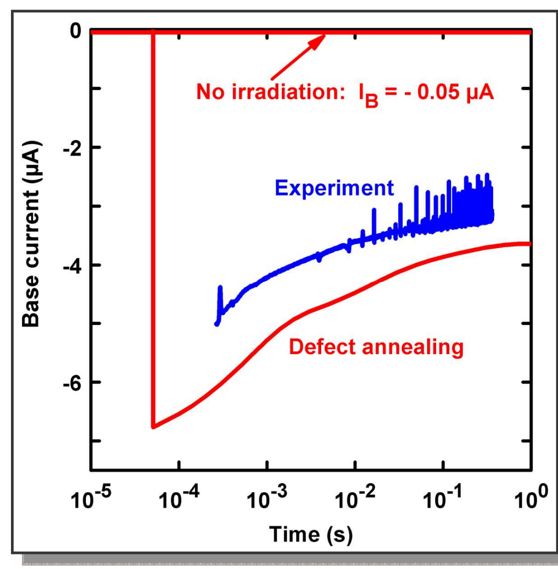
Stockpile BJT



CHARON

PDE semiconductor device simulation





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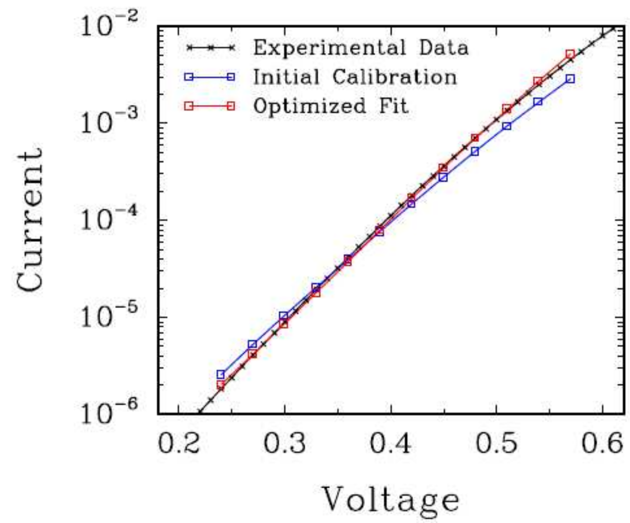
Steady-State Parameter Estimation with Charon/MOOCHO

Minimize	Current model vs. target mismatch
Subject to:	Steady-state semiconductor defect physic FE model

$$\begin{array}{ll} \text{minimize} & \tfrac{1}{2}\|g(x,p) - g^*\|_2^2 + \tfrac{1}{2}\beta\|p\|_2^2 \\ \text{subject to} & f(x,p) = 0 \end{array}$$

- Solved current matching optimization problems to calibrate model parameters against target currents
- MOOCHO (Bartlett) optimization solver converges simulation model and optimality at same time
  - Faster and more robust than black-box optimization methods
  - More accurate solutions
- Successes
  - Very accurate inversion of currents and model parameters for contrived "inverse" problems
- Challenges
  - Extremely difficult nonlinear solver convergences on model convergence
    => Opportunities for algorithm research
  - Inability to match experimental data
    => May indicate incomplete FE model



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