MS17

SAND2008-1749C

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 Solving Linear Systems with Multiple Right-hand Sides using Belos

Heidi K. Thornquist, Sandia National Laboratories

Canceled

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

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 newly developed advanced numerical solver algorithms in Trilinos to build new predictive capabilities
  - **Impact:** Vertical integrated 10+ Trilinos algorithm packages from parallel linear algebra to optimization!
- **Goal:** Demonstrate new vertically integrated solver algorithms 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

Sandia National Laboratories

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

Trilinos website

http://trilinos.sandia.gov

Current Status

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

Trilinos is being developed to:

- Provide a suite of numerical solvers (and more) to support predictive simulation for Sandia's customers
- Provide a decoupled and scalable development environment to allow for algorithmic research and production capabilities
- Provide support for growing SQA requirements

At its most basic level Trilinos provides:

- A common source code repository and management system (CVS => SVN)
- Configuration and building support (autoconf/automake => CMake)
- A common infrastructure for SQA
  - Bug reporting and tracking (i.e. Bugzilla)
  - Automated regression testing and reporting (test harness, results emails and webpage)
- Developer and user communication (i.e. Mailman email lists)
- Common integrated documentation system (Trilinos website and Doxygen)
- Provides independent development environment in terms of "packages"

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 (late of 2008) and beyond

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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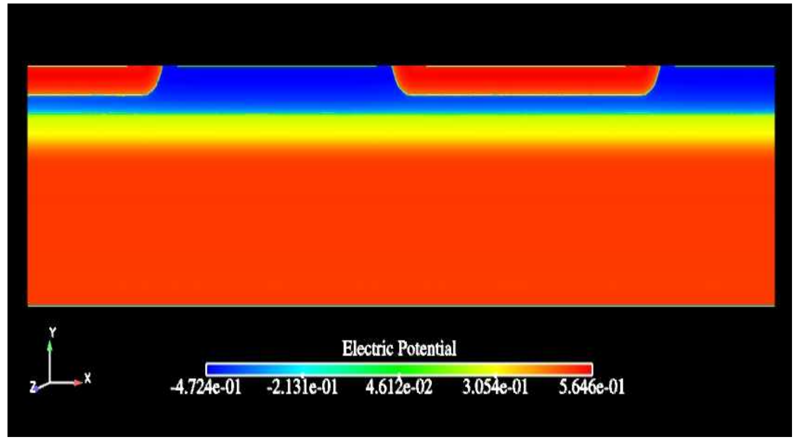
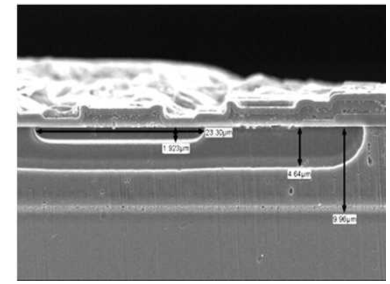
CHARON

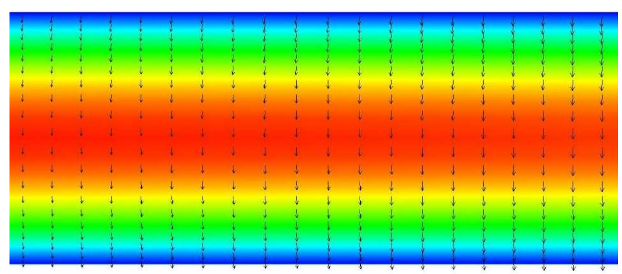
(Generalized PDE Solver)

- **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**

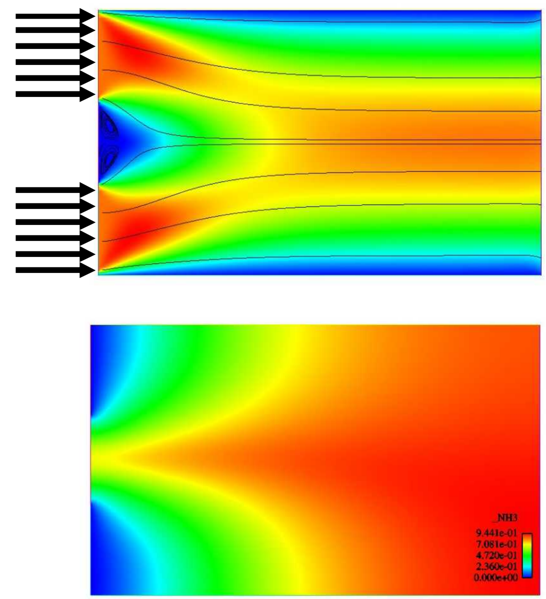




Semiconductor



MHD Pump

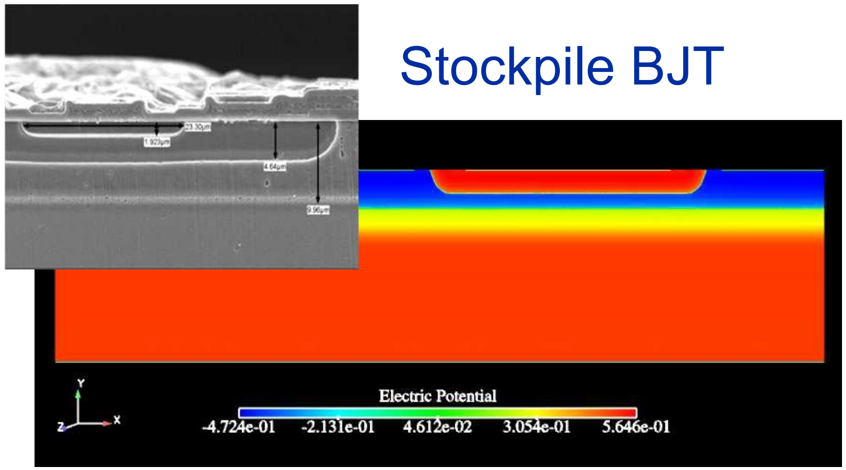


Reacting Flow

QASPR

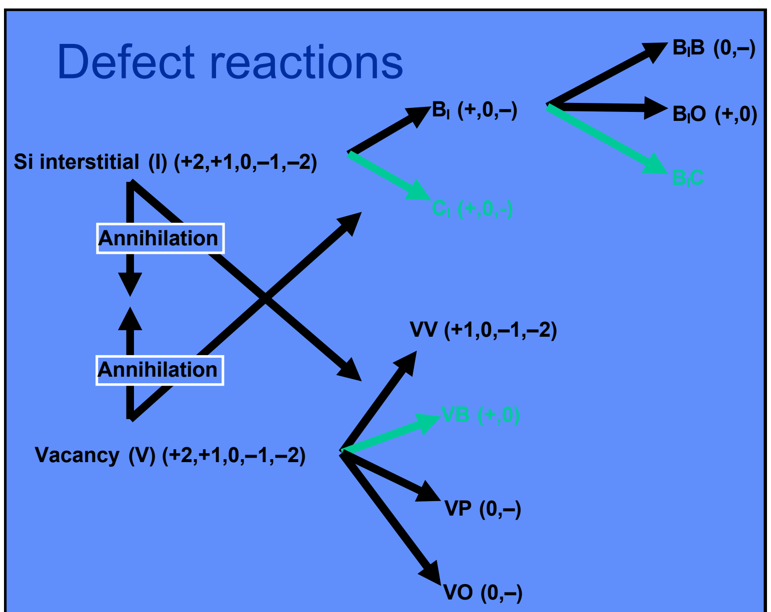
Qualification of electronic devices in hostile environments

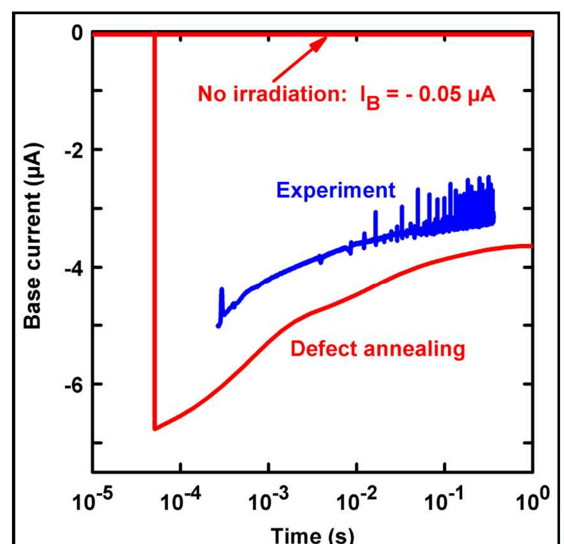
Stockpile BJT



CHARON

PDE semiconductor device simulation





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  - Serviceable: Easy to maintain and upgrade within the application environment.

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 $f(x,p) \in \mathbf{R}^{n+m} \rightarrow \mathbf{R}^n$
  - 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

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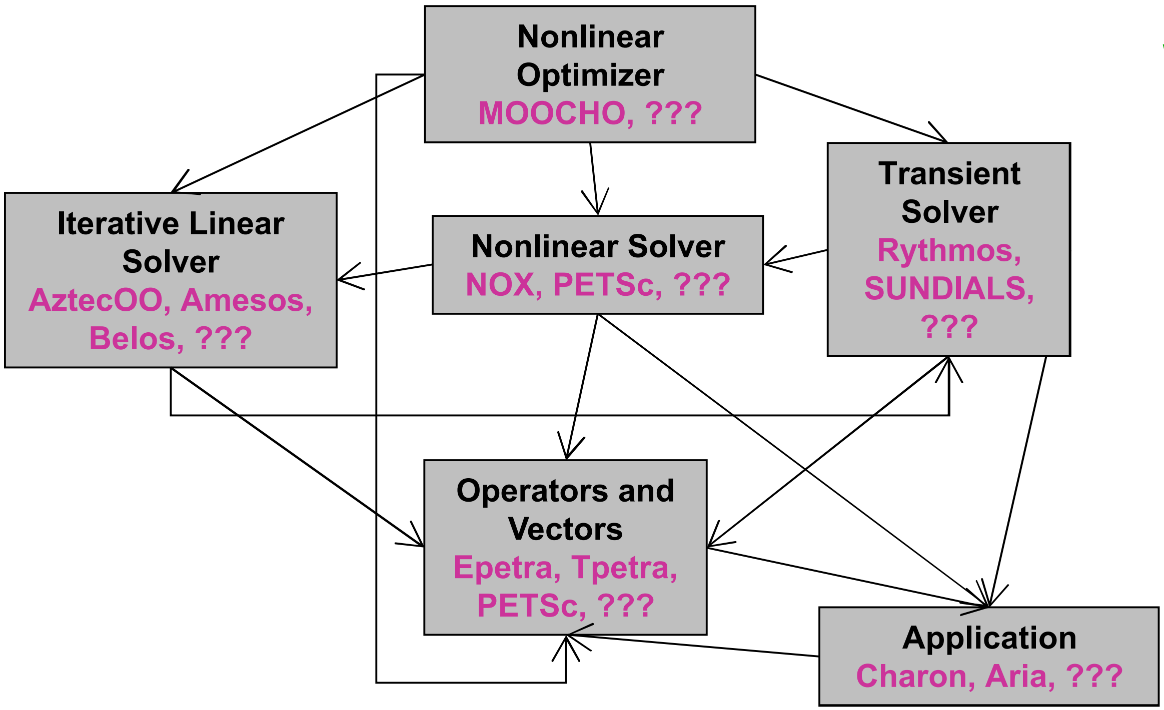
Vertical Integration and Interoperability is Important

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

Example of Vertical Interoperability : Rythmos

Solve $f(\dot{x}(t), x(t), t) = 0, t \in [t_0, t_f],\ x(t_0) = x_0,\ \dot{x}(t_0) = \dot{x}_0$

for $x(t) \in \mathbf{R}^n, t \in [t_0, t_f]$

Time Stepper

Advance $x(t_k)$ to $x(t_{k+1})$

where $t_{k+1} = t_k + \Delta t_k$

Implicit Backward Euler method

Solve $f\left(\frac{x_{k+1} - x_k}{\Delta t_k}, x_{k+1}, t_{k+1}\right) = 0$ for x_{k+1}

Nonlinear equations

Solve $r(z) = 0$ for $z \in \mathbf{R}^n$

Newton's method (e.g. NOX)

Choose initial guess z_0, tolerance η

for $k = 0, 1, \ldots$

If "converged" **Stop!**

Solve $\frac{\partial r(z_k)}{\partial z} \delta z_k = -r(z_k)$ for δz

Choose α using a line search method

$z_{k+1} = z_k + \alpha \delta z_k$

end for

Linear equations

Solve $Ax = b$ for $x \in \mathbf{R}^n$

Preconditioned GMRES

Iterate to "convergence"

$PAx = Pb$

Operator and Preconditioner applications

Apply $y = Ax$

Apply $y = Px$

Matrix-free or Matrix?

Preconditioners can be defined in many different ways

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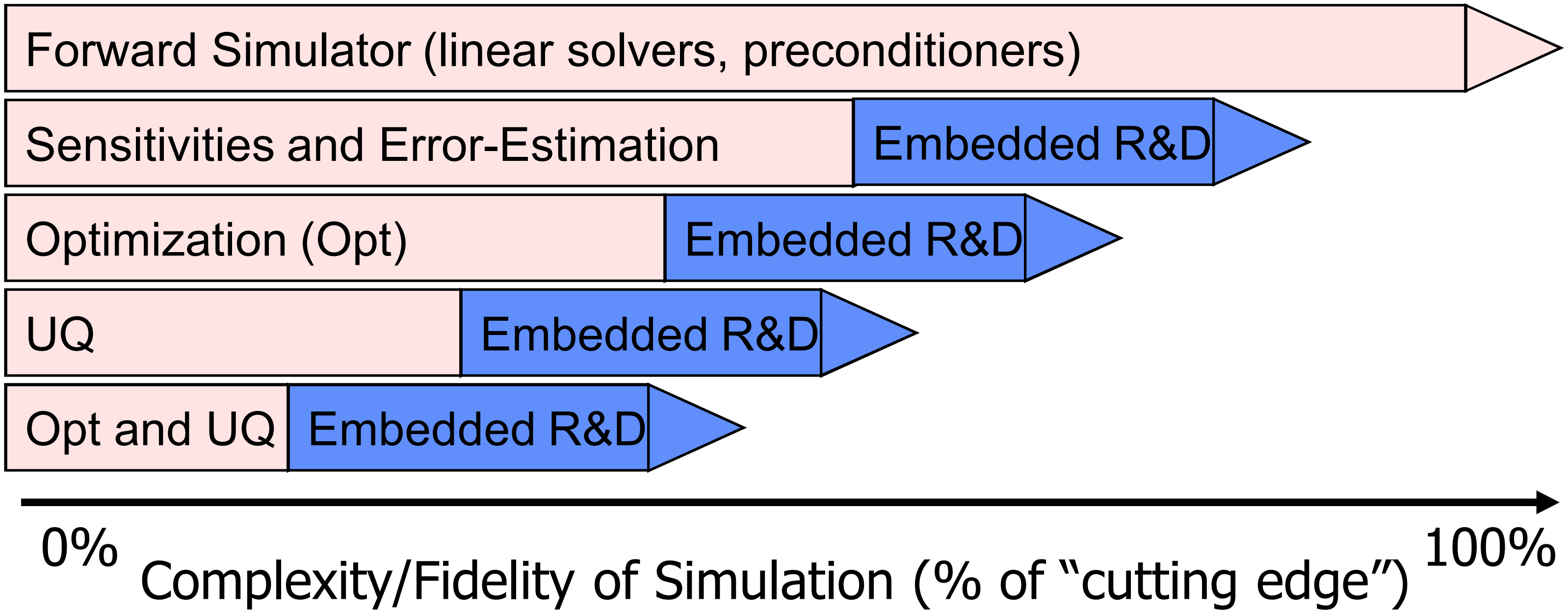
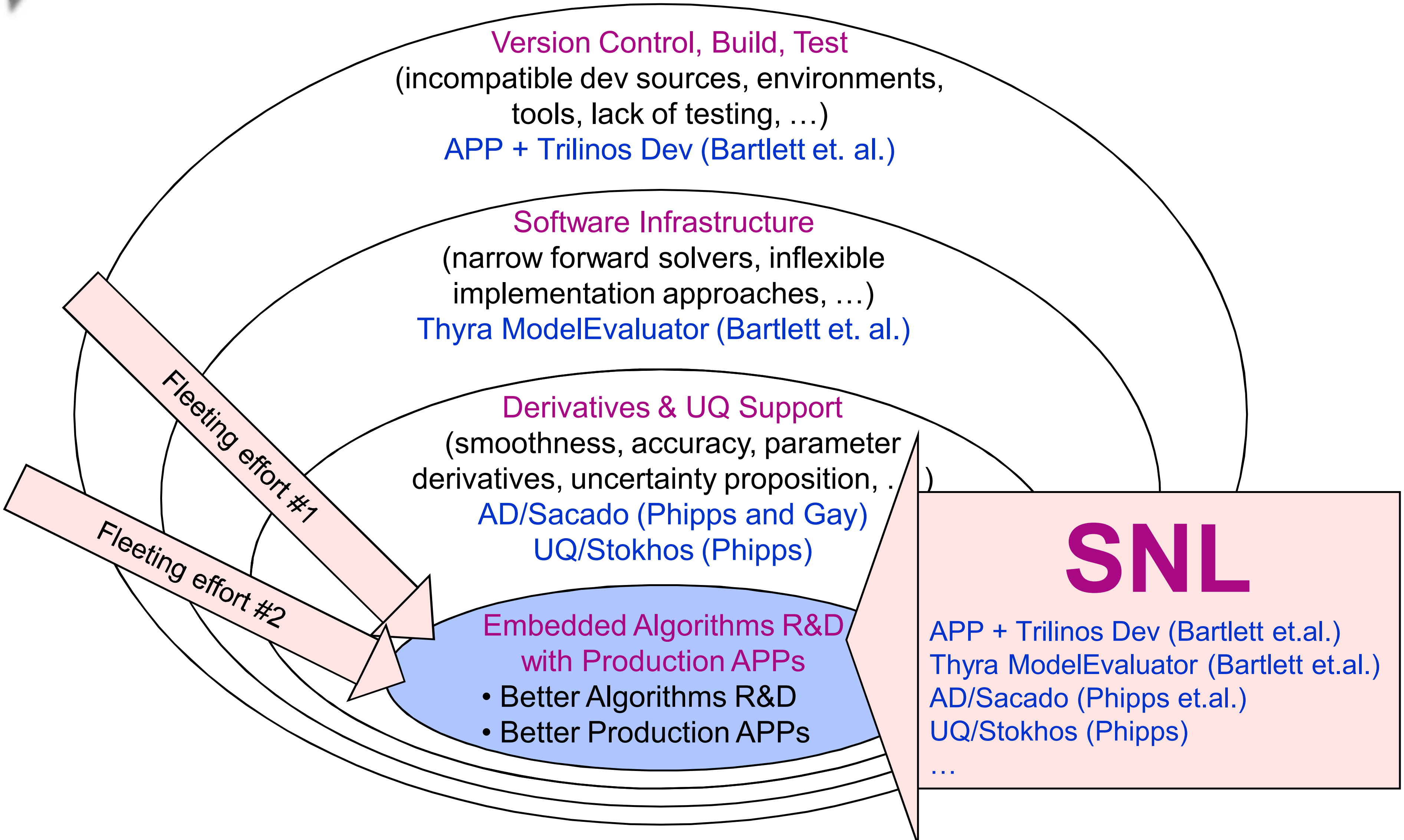
Embedded Analysis Algorithms and "The Cutting Edge"



- 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!

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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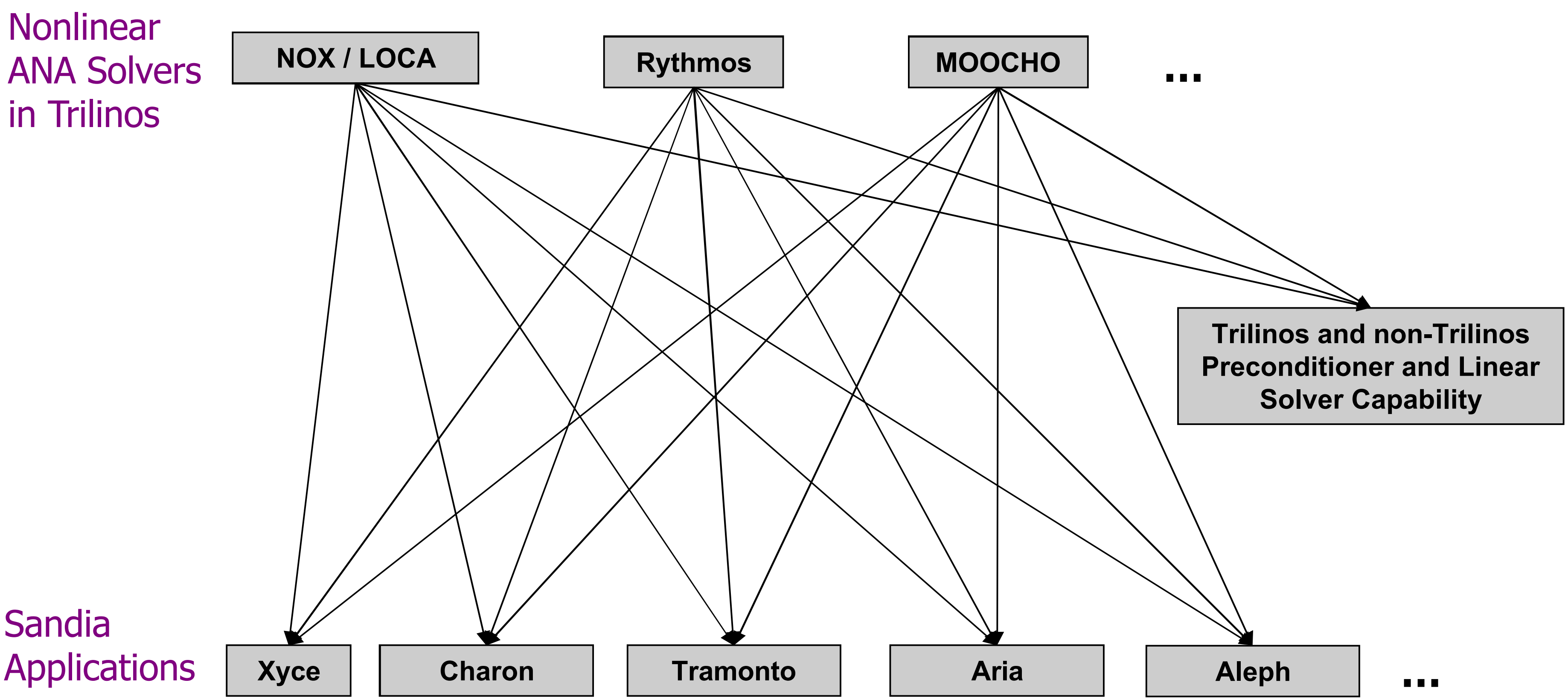
Some Nonlinear Problems Supported by the ModelEvaluator

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 $x(0) = x_0$

Nonlinear Algorithms and Applications : Everyone for Themselves?

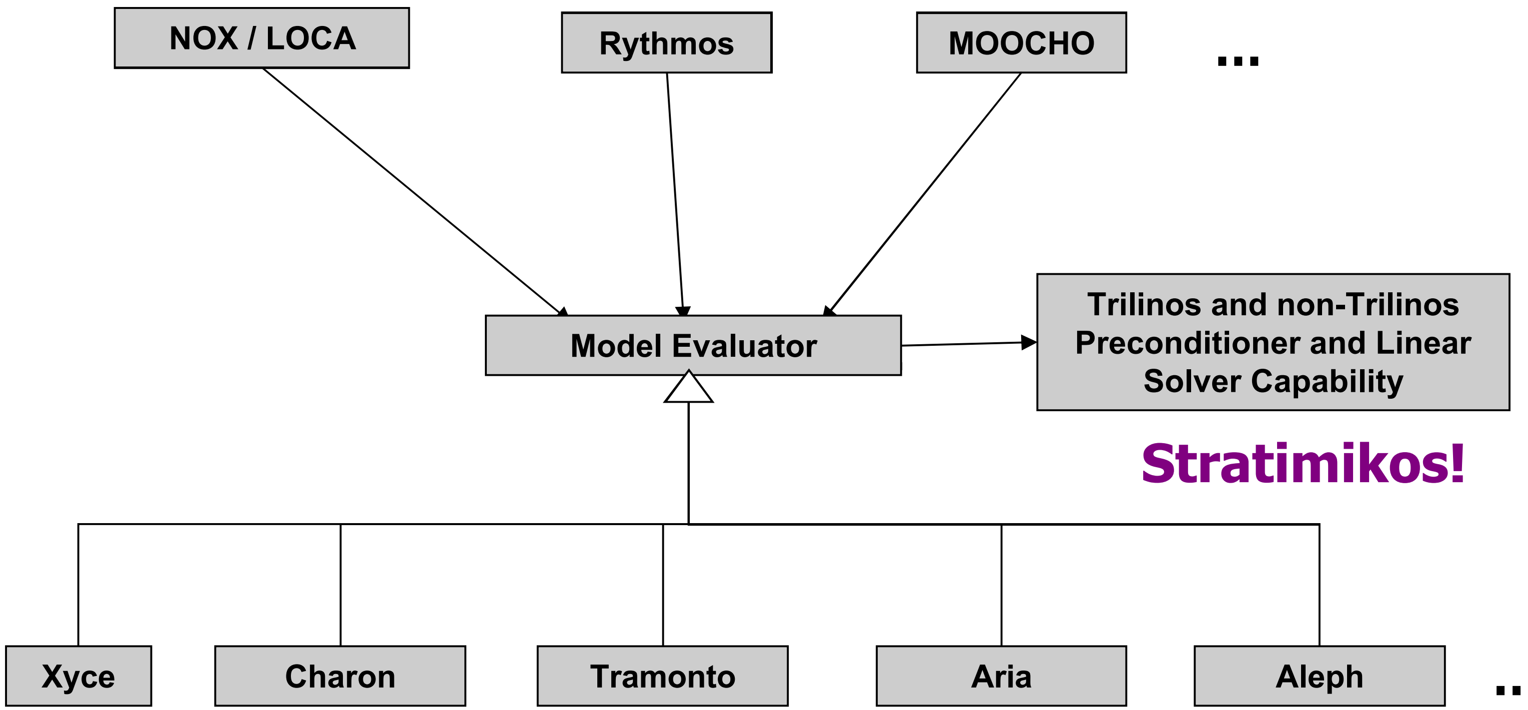


Key Point

- BAD

Nonlinear Algorithms and Applications : Thyra & Model Evaluator!

Nonlinear
ANA Solvers
in Trilinos



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Applications

Key Points

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

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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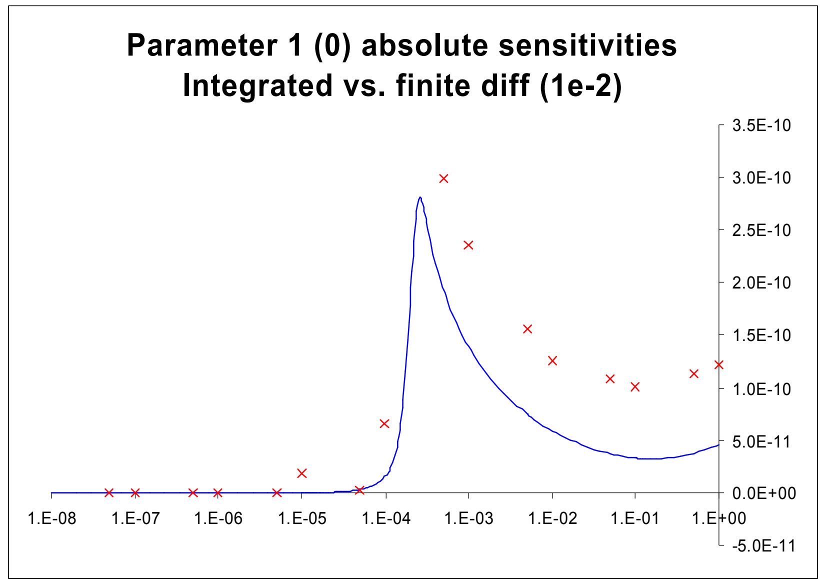
Vertical Integrations of Trilinos Capabilities: Example 1

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

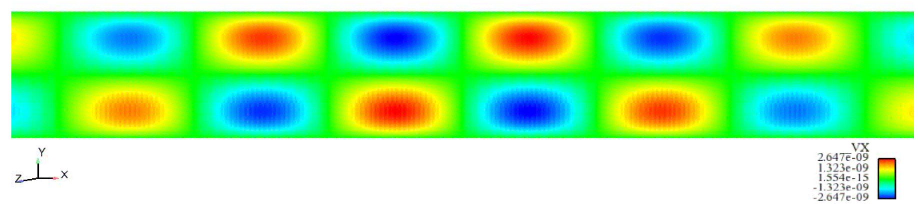
Vertical Integrations of Trilinos Capabilities: Example 2

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
- Matrix Partitioning

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

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

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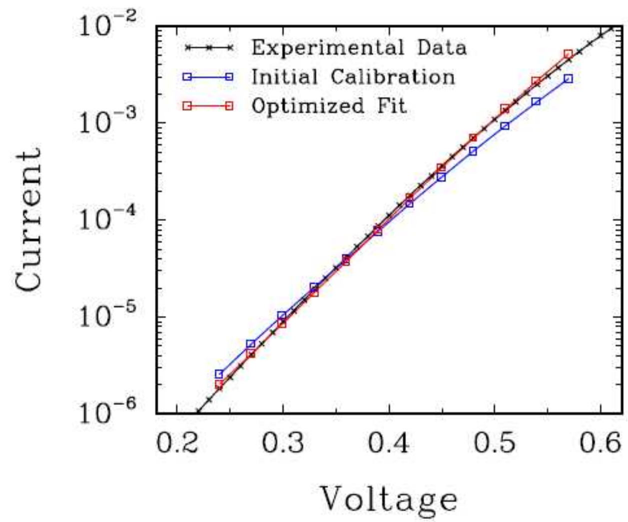
Derivative Tools
- Derivatives
- Sensitivities

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



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

I am talking about this next

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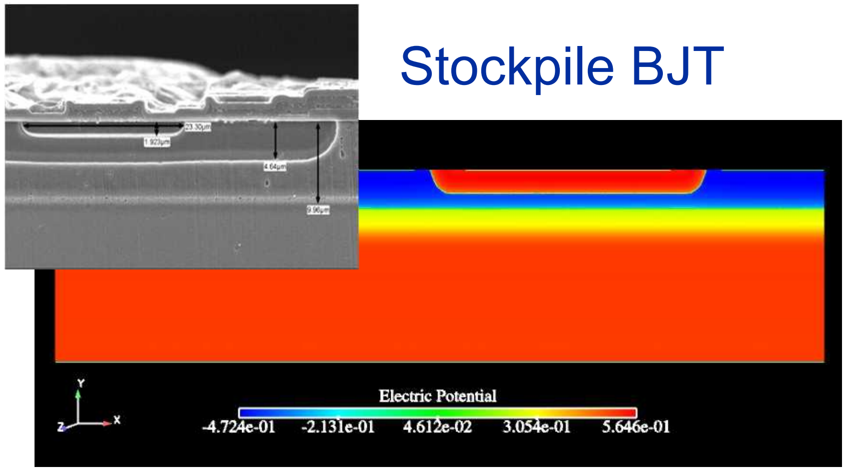
QASPR

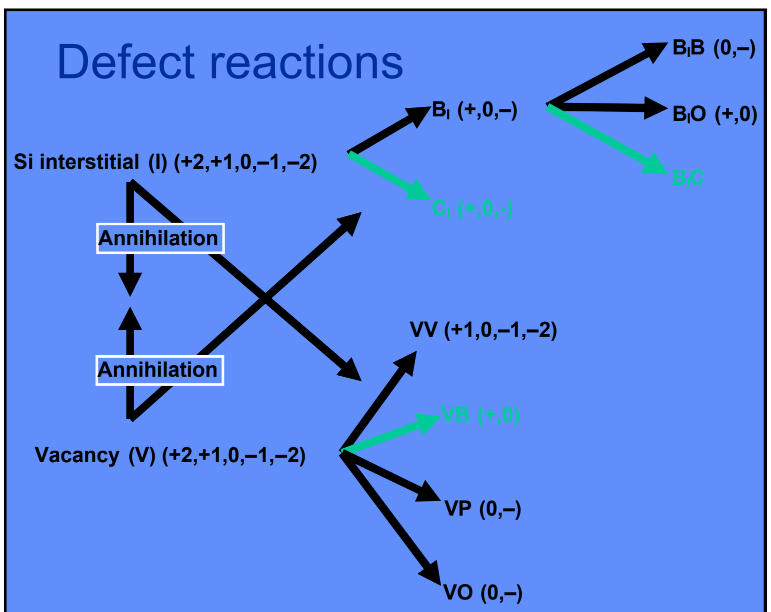
Qualification of electronic devices in hostile environments

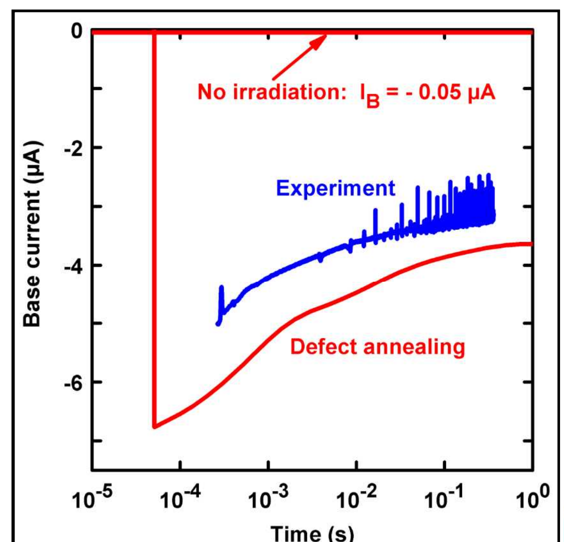
Stockpile BJT



CHARON

PDE semiconductor device simulation



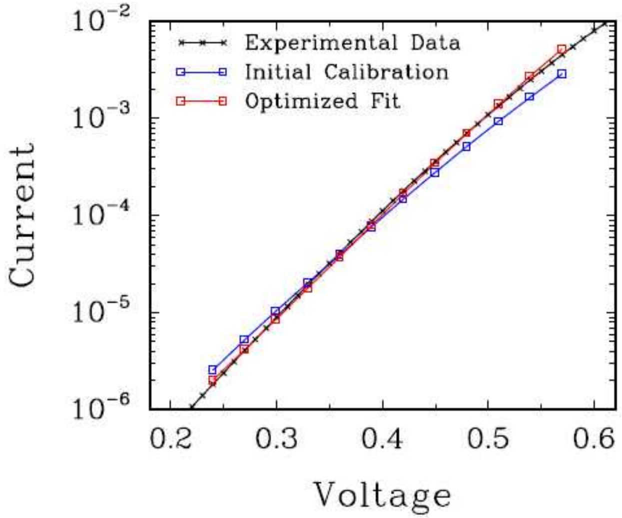


Steady-State Parameter Estimation with Charon/MOOCHO

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

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

- 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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