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# Enabling Predictive Simulation Through Embedded Sensitivity Analysis and Uncertainty Quantification

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**CIS External Panel Review**

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# Tight Coupling Through Automatic Differentiation Enables Predictive Simulation

- Transformation to predictive science
  - V&V, UQ, QMU
- Single-point forward simulations are insufficient
  - Forward & adjoint sensitivities
  - Error estimates
  - Probability distributions
  - Intervals

| ELEMENT \ MATURITY | Maturity Level 0<br>Low Consequence, Minimal M&S Impact, e.g., Scoping Studies | Maturity Level 1<br>Moderate Consequence, Some M&S Impact, e.g., Design Support | Maturity Level 2<br>High-Consequence, High M&S Impact, e.g., Qualification Support | Maturity Level 3<br>High-Consequence, Decision Making Based on M&S, e.g.. Qualification or Certification |
|---|---|---|---|---|
| **Representation and Geometric Fidelity**<br>What features are neglected because of simplifications or stylizations? | • Judgment only<br>• Little or no representational or geometric fidelity for the system and boundary conditions (BCs) | • Significant simplification or stylization of the system and BCs<br>• Geometry or representation of major components is defined | • Limited simplification or stylization of major components and BCs<br>• Geometry or representation is well defined for major components and some minor components<br>• Some peer review conducted | • Essentially no simplification or stylizationof components in the system and BCs<br>• Geometry or representation of all components is at the detail of "as built," e.g., gaps, material interfaces, fasteners<br>• Independent peer review conducted |
| **Physics and Material Model Fidelity**<br>How fundamental are the physics and material models and what is the level of model calibration? | • Judgment only<br>• Model forms are either unknown or fully empirical<br>• Few, if any, physics-informed models<br>• No coupling of models | • Some models are physics based and are calibrated using data from related systems<br>• Minimal or ad hoc coupling of models | • Physics-based models for all important processes<br>• Significant calibration needed using separate-effects tests (SETs) and integral-effects tests (IETs)<br>• One-way coupling of models<br>• Some peer review conducted | • All models are physics based<br>• Minimal need for calibration using SETs and IETs<br>• Sound physical basis for extrapolation and coupling of models<br>• Full, two-way coupling of models<br>• Independent peer review conducted |
| **Code Verification**<br>Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results? | • Judgment only<br>• Minimal testing of any software elements<br>• Little or no SQE procedures specified or followed | • Code is managed by SQE procedures<br>• Unit and regression testing conducted<br>• Some comparisons made with benchmarks | • Some algorithms are tested to determine the observed order of numerical convergence<br>• Some features & capabilities (F&Cs) are tested with benchmark solutions<br>• Some peer review conducted | • All important algorithms are tested to determine the observed order of numerical convergence<br>• All important F&Cs are tested with rigorous benchmark solutions<br>• Independent peer review conducted |
| **Solution Verification**<br>Are numerical solution errors and human procedural errors corrupting the simulation results? | • Judgment only<br>• Numerical errors have unknown or large effect on simulation results | • Numerical effects on relevant SRQs are qualitatively estimated<br>• Input/output (I/O) verified only by the analysts | • Numerical effects are quantitatively estimated to be small on some SRQs<br>• I/O independently verified<br>• Some peer review conducted | • Numerical effects are determined to be small on all important SRQs<br>• Important simulations are independently reproduced<br>• Independent peer review conducted |
| **Model Validation**<br>How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy? | • Judgment only<br>• Few, if any, comparisons with measurements from similar systems or applications | • Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest<br>• Large or unknown exper-imental uncertainties | • Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs<br>• Experimental uncertainties are well characterized for most SETs, but poorly known for IETs<br>• Some peer review conducted | • Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application<br>• Experimental uncertainties are well characterized for all IETs and SETs<br>• Independent peer review conducted |
| **Uncertainty Quantification and Sensitivity Analysis**<br>How thoroughly are uncertainties and sensitivities characterized and propagated? | • Judgment only<br>• Only deterministic analyses are conducted<br>• Uncertainties and sensitivities are not addressed | • Aleatory and epistemic (A&E) uncertainties propagated, but without distinction<br>• Informal sensitivity studies conducted<br>• Many strong UQ/SA assumptions made | • A&E uncertainties segregated, propagated, and identified in SRQs<br>• Quantitative sensitivity analyses conducted for most parameters<br>• Numerical propagation errors are estimated and their effect known<br>• Some strong assumptions made<br>• Some peer review conducted | • A&E uncertainties comprehensively treated and properly interpreted<br>• Comprehensive SAs conducted for parameters and models<br>• Numerical propagation errors are demonstrated to be small<br>• No significant UQ/SA assumptions made<br>• Independent peer review conducted |

## Impacting CIS Transformation Mission

- Algorithms research for better efficiency, scalability, robustness
  - Tight algorithmic coupling to underlying physics
- Vehicle for incorporating these technologies into applications
  - Templating and (generalized) Automatic Differentiation (AD)

# Crash Course in AD 101

- How does AD work
  - Derivatives at operation level known
  - Chain rule

- What does AD compute?
  - Forward mode derivatives (Jacobians, Jacobian-vector products)
  - Reverse mode derivatives (Gradients, Jacobian-transpose products)
  - High order univariate Taylor polynomials

- How is it implemented?
  - Source transformation (Fortran)
  - Operator overloading (C++)

- Multiple derivative components propagated simultaneously
  - Big cache benefit, potential for multi-core

# AD Research Distinguished By Tools and Approach for Large-Scale Codes

- **Many AD tools and research projects**
  - × **Most geared towards Fortran (ADIFOR, OpenAD)**
  - × **Most C++ tools are slow (ADOL-C)**
  - × **Most applied in black-box fashion**

- **Sacado: Operator overloading AD tools for C++ applications**
  - ✓ **Multiple highly-optimized AD data types**
  - ✓ **Transform to template code & instantiate on Sacado AD types**
  - ✓ **Apply AD only at the "element level"**

Trilinos

- **Directly impacting QASPR through Charon**
  - ✓ **Analytic Jacobians and parameter derivatives**

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

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TIFF (Uncompressed) decompressor
are needed to see this picture.

- **This is the only successful, sustainable approach for large-scale C++ codes!**

# Efficient Sensitivity Analysis Requires Accurate Derivatives + Solver Integration

- **Spatially discretized PDE:**

$$f(\dot{x}, x, p, t) = 0$$

- **Temporal discretization (Backward Euler):**

$$f\left(\frac{x_{n+1} - x_n}{\Delta t}, x_{n+1}, p, t_{n+1}\right) = 0$$

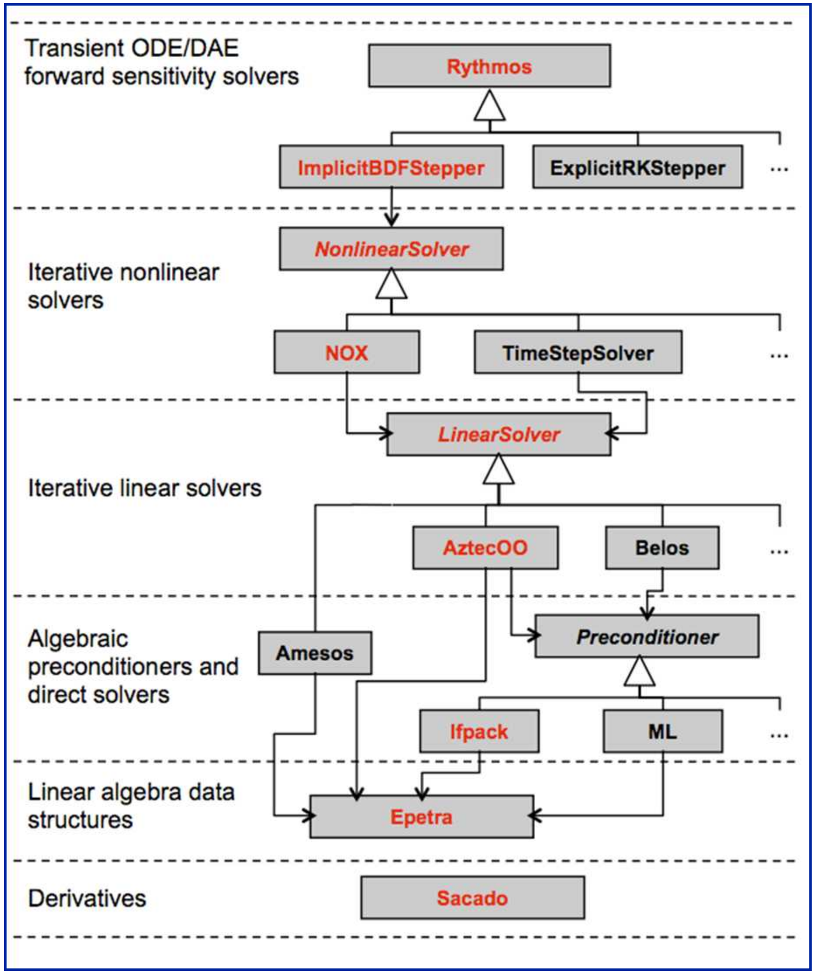
- **Forward sensitivity problem:**

$$\frac{\partial f}{\partial \dot{x}}\left(\frac{\partial \dot{x}}{\partial p}\right) + \frac{\partial f}{\partial x}\left(\frac{\partial x}{\partial p}\right) + \frac{\partial f}{\partial p} = 0$$

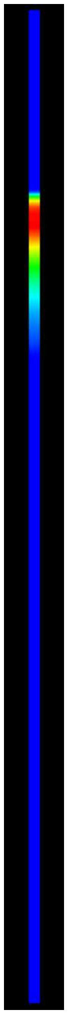
$$\frac{1}{\Delta t}\frac{\partial f}{\partial \dot{x}}\left(\frac{\partial x_{n+1}}{\partial p} - \frac{\partial x_n}{\partial p}\right) + \frac{\partial f}{\partial x}\left(\frac{\partial x_{n+1}}{\partial p}\right) + \frac{\partial f}{\partial p} = 0$$

- **Achieving transformation**
  - **Algorithm: Forward sensitivities**
  - **Tight Coupling: Analytic derivatives**
  - **Vehicle: AD + Templating**

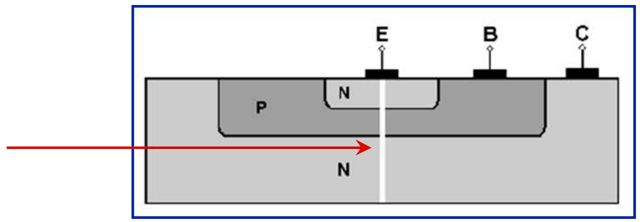
**Vertical integration of Trilinos capabilities**



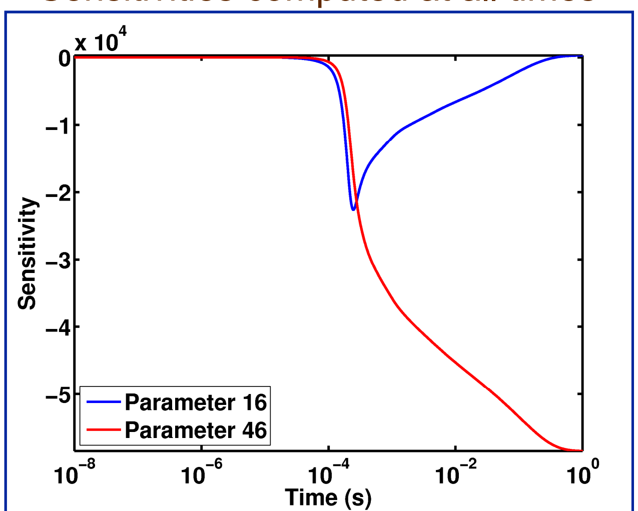
# Capability Demonstrated on the QASPR Simple Prototype*



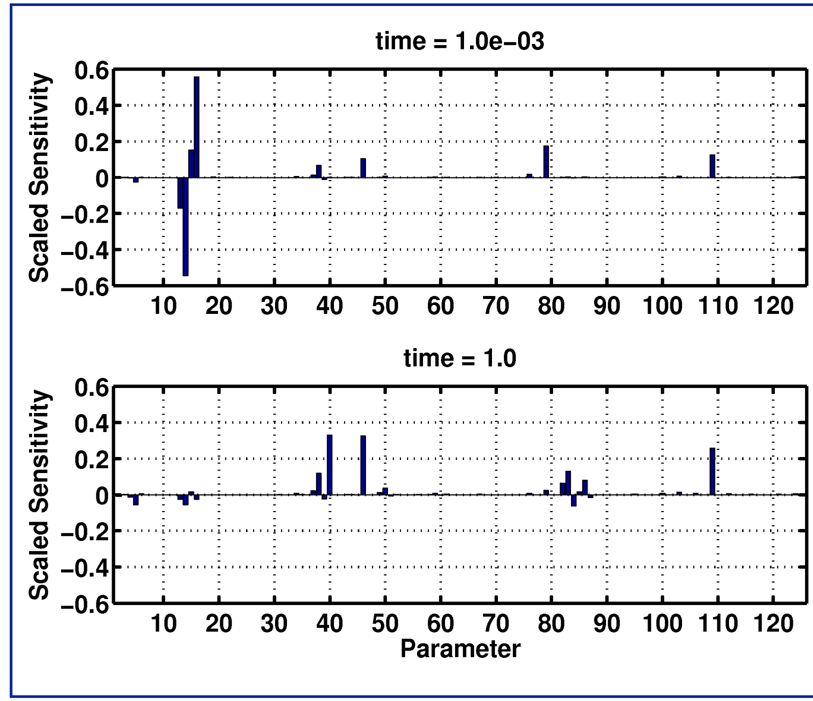
- **Pseudo 1D Bipolar Junction Transistor (9x0.1 micron)**
- **Full defect physics**
- **126 parameters**




Sensitivities computed at all times




Sensitivities at early/late time show dominant physics




**Comparison to standard FD approach:**

- ✓ **Sensitivities at all time points**
- ✓ **14x faster**
- ✓ **More accurate**
- ✓ **More robust**

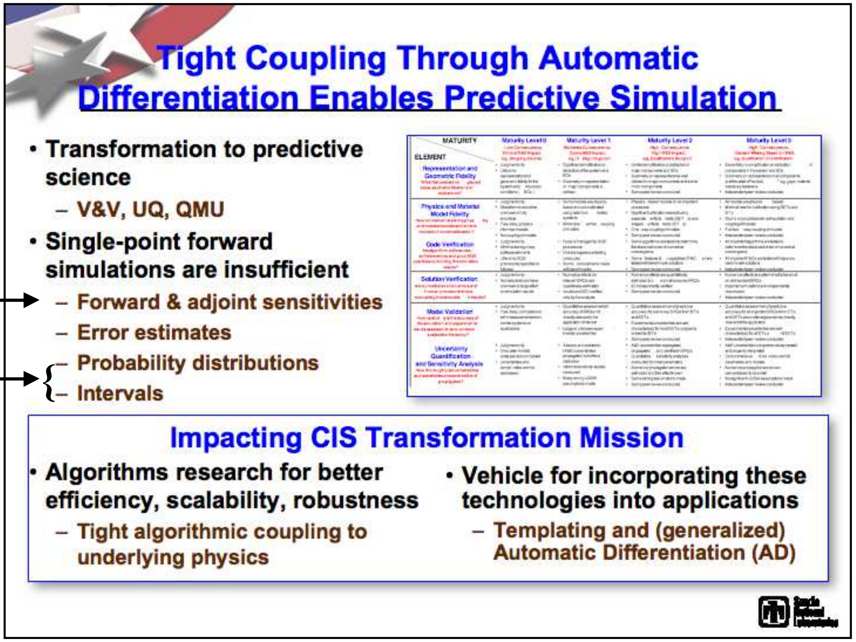
***ASC Level II Milestone (Bartlett *et al*)**

# Impacting CIS Transformation to Predictive Science Through Templating and AD

- AD impact:
  - Forward sensitivity analysis (completed)
  - Adjoint sensitivity analysis (on going 1400-1500 collaboration)

- Templating provides deep interface to applications

- Impacting UQ:
  - Stochastic Galerkin methods (on going)
  - Taylor methods (near term)
  - Intervals (mid term)
  - Probability boxes (long term)

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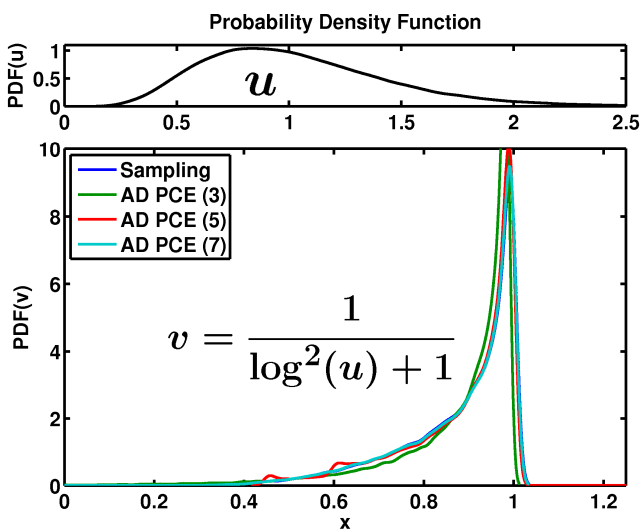
# Templating Enables Automatic Embedded Uncertainty Propagation Research

**Stochastic Galerkin method**

$$f(x,\xi)=0 \rightarrow \hat{x}(\xi)=\sum_{i=0}^{P} x_i\phi_i(\xi) \rightarrow f_i(x_0,\ldots,x_P)\equiv\int f(\hat{x}(\xi),\xi)\phi_i(\xi)d\mu=0$$

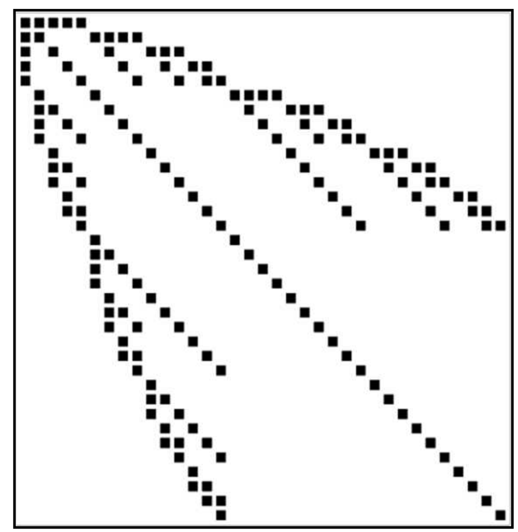
**Embedded SG techniques using AD-like procedure (completed)**

- Compute projection op-by-op




**Trilinos interfaces for solving block SG linear systems (on going)**

- Linear algebra research



**Encapsulated in new Trilinos package *Stokhos***

- Collaboration with Roger Ghanem (USC)

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# Impacting Sandia's Mission & External Community

- **Sandia mission impact**
  - Rapid physics development
    - Charon semiconductor device modeling for QASPR (ASC)
    - Charon chemical laser (Air Force WFO)
    - Charon extended MHD (ASCR)
    - SIERRA/Aria and Xyce (ASC)
  - Charon transient sensitivity analysis for QASPR
  - Potential for automatic embedded UQ in all of these codes
- **Internal recognition (including Algorithms Integration)**
  - 2 IPA awards, 2 ERA nominations, 1 ERA award
- **External visibility**
  - Collaboration with USC
  - 3 publications
  - 4 conference presentations
  - Program committee member for AD 2008

# Auxiliary Slides

# What is Automatic Differentiation (AD)?

- **Technique to compute analytic derivatives without hand-coding the derivative computation**
- **How does it work -- freshman calculus**
  - **Computations are composition of simple operations (+, *, sin(), etc…) with known derivatives**
  - **Derivatives computed line-by-line, combined via chain rule**
- **Derivatives accurate as original computation**
  - **No finite-difference truncation errors**
- **Provides analytic derivatives without the time and effort of hand-coding them**

$$y = \sin(e^x + x \log x), \quad x = 2$$

| Operation | Derivative | $x$ | $\frac{d}{dx}$ |
|---|---|---|---|
| $x \leftarrow 2$ | $\frac{dx}{dx} \leftarrow 1$ | 2.000 | 1.000 |
| $t \leftarrow e^x$ | $\frac{dt}{dx} \leftarrow t\frac{dx}{dx}$ | 7.389 | 7.389 |
| $u \leftarrow \log x$ | $\frac{du}{dx} \leftarrow \frac{1}{x}\frac{dx}{dx}$ | 0.301 | 0.500 |
| $v \leftarrow xu$ | $\frac{dv}{dx} \leftarrow u\frac{dx}{dx} + x\frac{du}{dx}$ | 0.602 | 1.301 |
| $w \leftarrow t + v$ | $\frac{dw}{dx} \leftarrow \frac{dt}{dx} + \frac{dv}{dx}$ | 7.991 | 8.690 |
| $y \leftarrow \sin w$ | $\frac{dy}{dx} \leftarrow \cos(w)\frac{dw}{dx}$ | 0.991 | -1.188 |

# AD Takes Three Basic Forms

$$x \in \mathrm{R}^n,\ f : \mathrm{R}^n \rightarrow \mathrm{R}^m$$

- **Forward Mode:**

$$(x,\ V) \longrightarrow \left(f,\ \frac{\partial f}{\partial x} V\right)$$

  - **Propagate derivatives of intermediate variables w.r.t. independent variables forward**
  - **Directional derivatives, tangent vectors, square Jacobians,** $\partial f / \partial x$ **when** $m \geq n$

- **Reverse Mode:**

$$(x,\ W) \longrightarrow \left(f,\ W^T \frac{\partial f}{\partial x}\right)$$

  - **Propagate derivatives of dependent variables w.r.t. intermediate variables backwards**
  - **Gradient of a scalar value function with complexity** $\approx 4\ \text{ops}(f)$
  - **Gradients, Jacobian-transpose products (adjoints),** $\partial f / \partial x$ **when** $n > m$

- **Taylor polynomial mode:**

$$x(t) = \sum_{k=0}^{d} x_k t^k \longrightarrow \sum_{k=0}^{d} f_k t^k = f(x(t)) + O(t^{d+1}),\quad f_k = \frac{1}{k!} \frac{d^k}{dt^k} f(x(t))$$

- **Basic modes combined for higher derivatives:**

$$\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x} V_1\right) V_2,\quad W^T \frac{\partial^2 f}{\partial x^2} V,\quad \frac{\partial f_k}{\partial x_0}$$

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# Efficiency of AD in Charon

Set of N hypothetical chemical species:

$$2X_j \rightleftharpoons X_{j-1} + X_{j+1}, \quad j = 2, \ldots, N-1$$

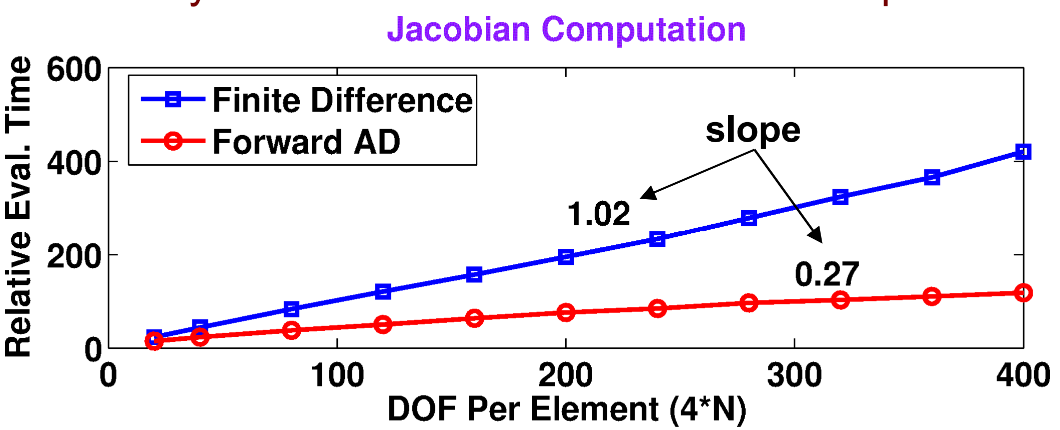
Steady-state mass transfer equations:

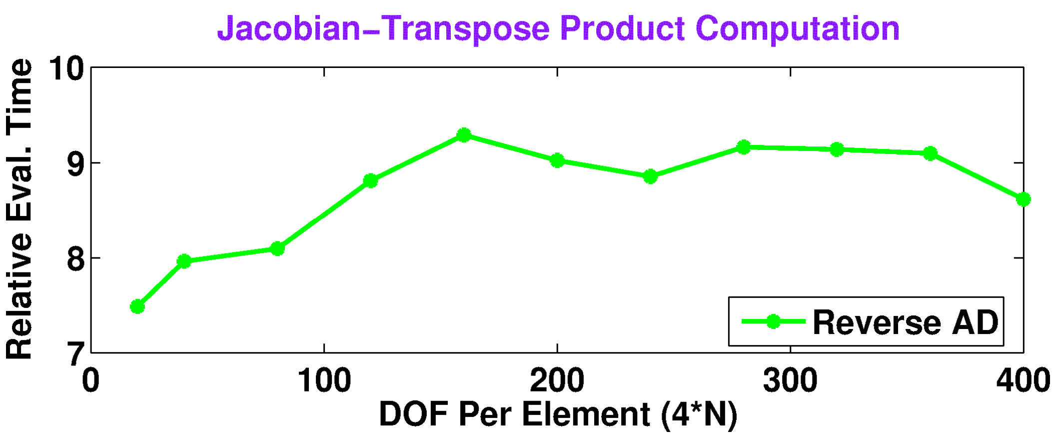
$$\nabla^2 Y_j + \mathbf{u} \cdot \nabla Y_j = \dot{\omega}_j, \quad j = 1, \ldots, N-1$$

$$\sum_{j=1}^{N} Y_j = 1$$

- **Forward mode AD**
  - **Faster than FD**
  - **Better scalability in number of PDEs**
  - **Analytic derivative**
  - **Provides Jacobian for all Charon physics**
- **Reverse mode AD**
  - **Scalable adjoint/gradient** $J^T w = \nabla(w^T f(x))$

Efficiency of the element-level derivative computation




Results published, presented at ICCS 2006, Reading, UK

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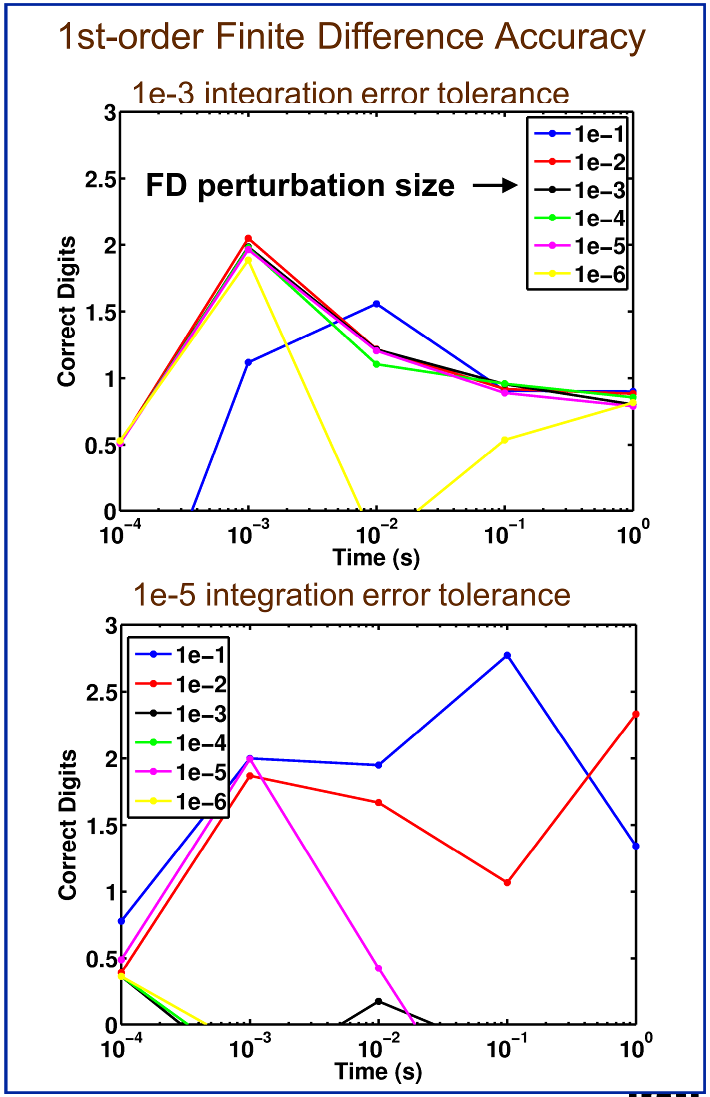
# Tight Coupling Provides More Accurate, Efficient, and Robust Sensitivity Algorithm

- **Run-times (1e-3 integration error):**
  - **Forward simulation: 105 min.**
  - **Rythmos sensitivities: 931 min.**
  - **First-order FD: ~13,000 min.**

- **Rythmos approach more efficient**
  - **14x speed-up**

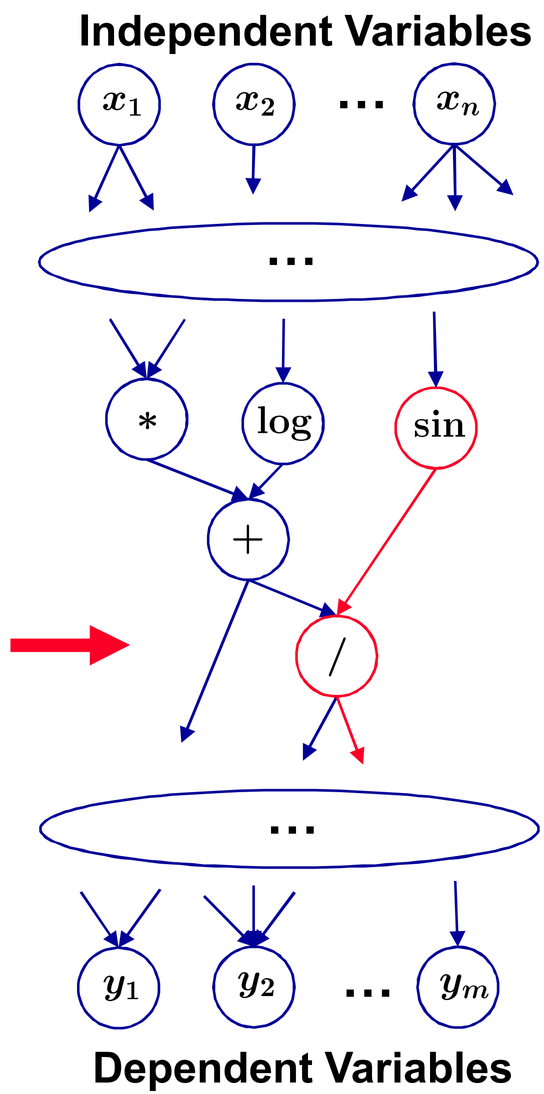
- **Rythmos approach more accurate**
  - **FD only provides square root of time integration accuracy**

- **Rythmos approach more robust**
  - **Accuracy solely dictated by time-integration accuracy**
  - **Picking FD perturbation size difficult**



# Verification of Automatic Differentiation

- **Verification of the AD tools**
  - **Unit-test with respect to known derivatives**
  - **Composite tests**
    - **Compare to other tools**
    - **Compare to hand-derived**
    - **Compare to finite differences**
- **Verification of AD in application code**
  - **Compiler drastically simplifies this**
  - **All of the standard hand-coded verification techniques**
    - **Compare to finite differences**
    - **Nonlinear convergence**




**Compiler type mechanism will not allow breaking the chain from independent to dependent variables**

# Charon Drift-Diffusion Formulation with Defects

**Current Conservation for e- and h+**

$$\frac{\partial n}{\partial t} - \nabla \cdot J_n = -R_n(\psi, n, p, Y_1, \ldots, Y_N), \quad J_n = -n\mu_n \nabla\psi + D_n \nabla n$$

$$\frac{\partial p}{\partial t} + \nabla \cdot J_p = -R_p(\psi, n, p, Y_1, \ldots, Y_N), \quad J_p = -p\mu_p \nabla\psi - D_p \nabla p$$

**Defect Continuity**

$$\frac{\partial Y_i}{\partial t} + \nabla \cdot J_{Y_i} = -R_{Y_i}(\psi, n, p, Y_1, \ldots, Y_N), \quad J_{Y_i} = -\mu_i Y_i \nabla\psi - D_i \nabla Y_i$$

**Electric potential**

$$-\nabla(\varepsilon \nabla \psi(x)) = -q\left(p(x) - n(x) + N_D^+(x) - N_A^-(x)\right) - \sum_{i=1}^{N} q_i Y_i(x)$$

**Recombination/ generation source terms**

$R_X$ **Include electron capture and hole capture by defect species and reactions between various defect species**

**Electron emission/capture**

$Z^i \leftrightarrow Z^{i+1} + e^-$

$$R_{[Z^i \to Z^{i+1}+e^-]} \propto \sigma_{[Z^i \to Z^{i+1}+e^-]} Z^i \exp\left(\frac{\Delta E_{[Z^i \to Z^{i+1}+e^-]}}{kT}\right)$$

**Activation Energy**

**Cross section**

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