Sacado: Automatic Differentiation Tools for C++ Codes

Eric Phipps and David Gay

Sandia National Laboratories

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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

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

	x	$\frac{d}{dx}$
$x \leftarrow 2$	2.000	1.000
$t \leftarrow e^x$	7.389	7.389
$u \leftarrow \log x$	0.301	0.500
$v \leftarrow xu$	0.602	1.301
$w \leftarrow t + v$	7.991	8.690
$y \leftarrow \sin w$	0.991	-1.188

Sacado: AD Tools for C++ Codes

- Sacado provides several modes of Automatic Differentiation (AD)
  - Forward (Jacobians, Jacobian-vector products, …)
  - Reverse (Gradients, Jacobian-transpose-vector products, …)
  - Taylor (High-order univariate Taylor series)

- Sacado implements AD via operator overloading and C++ templating
  - Expression templates for OO efficiency
  - Application code templating for easy incorporation

- Designed for use in large-scale C++ codes
  - Apply AD at “element-level”
  - Very successful in Charon application code
  - `Sacado::FEApp` example demonstrates approach

- Sacado provides other useful utilities
  - Scalar flop counting (Ross Bartlett)
  - Scalar parameter library
  - Template utilities

The Usual Suspects

- Configure options
  - `--enable-sacado` — Enables Sacado at Trilinos top-level
  - `--enable-sacado-tests, --enable-tests` — Enables unit, regression, and performance tests
    - `--with-cppunit-prefix=[path]` — Path to CppUnit for unit tests
    - `--with-adolc=[path]` — Enables Taylor polynomial unit tests with ADOL-C
  - `--enable-sacado-examples, --enable-examples` — Enables examples
    - `nox/examples/epetra/LOCA_Sacado_FEApp` — Continuation example using `Sacado::FEApp` 1D finite element application
- Mailing lists
  - Sacado-announce@software.sandia.gov, Sacado-checkins@software.sandia.gov, Sacado-developers@software.sandia.gov, Sacado-regression@software.sandia.gov, Sacado-users@software.sandia.gov
- Bugzilla: http://software.sandia.gov/bugzilla
- Bonsai: http://software.sandia.gov/bonsai/cvsqueryform.cgi
- Web: http://software.sandai.gov/Trilinos/packages/sacado (not much there yet)
- Doxygen documentation (not all that useful)
- Examples are best way to learn how to use Sacado

sacado/example/dfad_example.cpp

```cpp
#include "Sacado.hpp"

// The function to differentiate
template <typename ScalarT>
ScalarT func(const ScalarT& a, const ScalarT& b, const ScalarT& c) {
  ScalarT r = c*std::log(b+1.)/std::sin(a);

  return r;
}

int main(int argc, char **argv) {
  double a = std::atan(1.0);                              // pi/4
  double b = 2.0;
  double c = 3.0;
  int num_deriv = 2;                                      // Number of independent variables

  // Fad objects
  Sacado::Fad::DFad<double> afad(num_deriv, 0, a); // First (0) indep. var
  Sacado::Fad::DFad<double> bfad(num_deriv, 1, b); // Second (1) indep. var
  Sacado::Fad::DFad<double> cfad(c);               // Passive variable
  Sacado::Fad::DFad<double> rfad;                  // Result

  // Compute function
  double r = func(a, b, c);

  // Compute function and derivative with AD
  rfad = func(afad, bfad, cfad);

  // Extract value and derivatives
  double r_ad = rfad.val();     // r
  double drda_ad = rfad.dx(0);  // dr/da
  double drdb_ad = rfad.dx(1);  // dr/db
```

Differentiating Element-Based Codes

- Global residual computation (ignoring boundary computations):

$$f(x) = \sum_{i=1}^{N} Q_i^T e_{k_i}(P_i x)$$

- Jacobian computation:

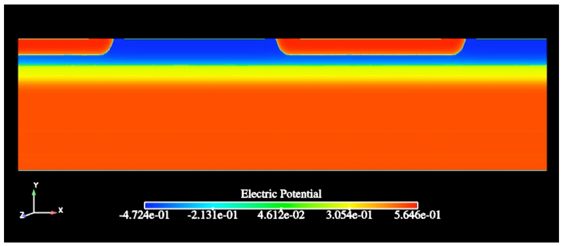
$$\frac{\partial f}{\partial x} = \sum_{i=1}^{N} Q_i^T J_{k_i} P_i, \quad J_{k_i} = \frac{\partial e_{k_i}}{\partial x_i}, \quad x_i = P_i x$$

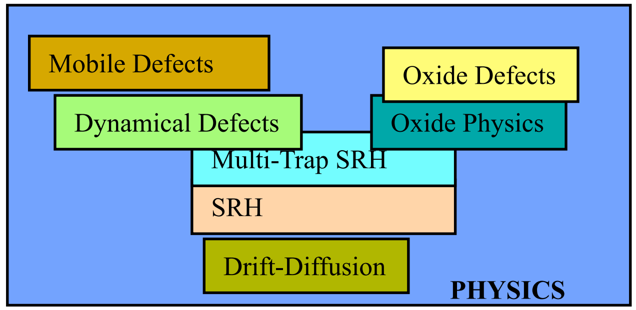
- Jacobian-transpose product computation:

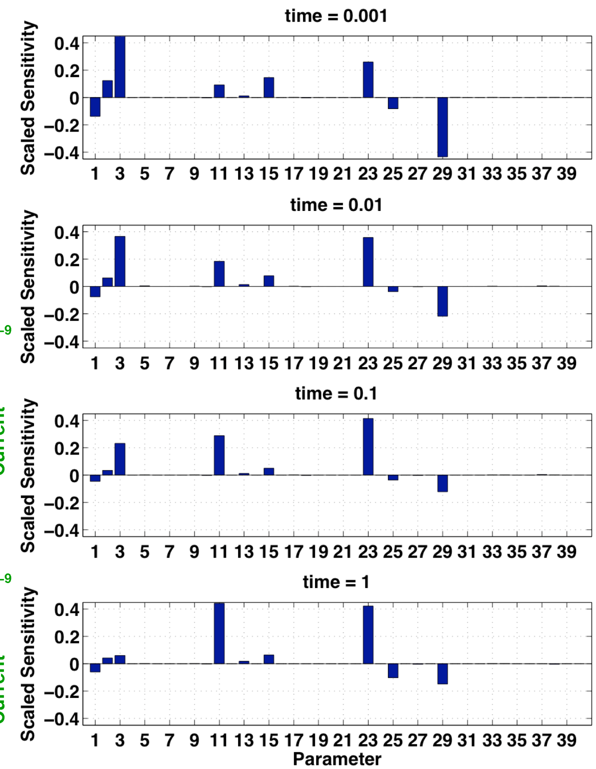
$$w^T \frac{\partial f}{\partial x} = \sum_{i=1}^{N} (Q_i w)^T J_{k_i} P_i$$

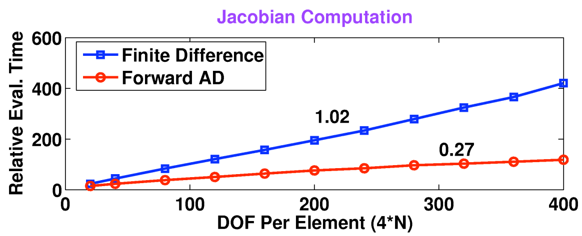
- Hybrid symbolic/AD procedure
  - Element-level derivatives computed via AD
  - Exactly the same as how you would do this "manually"
  - Avoids parallelization issues

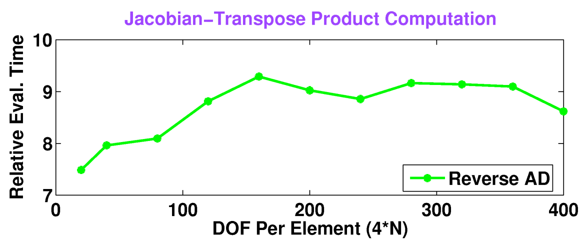
Impacts of AD in Charon

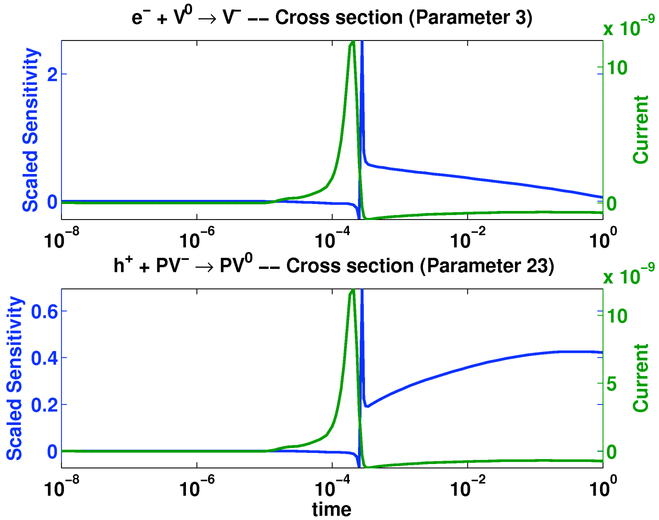


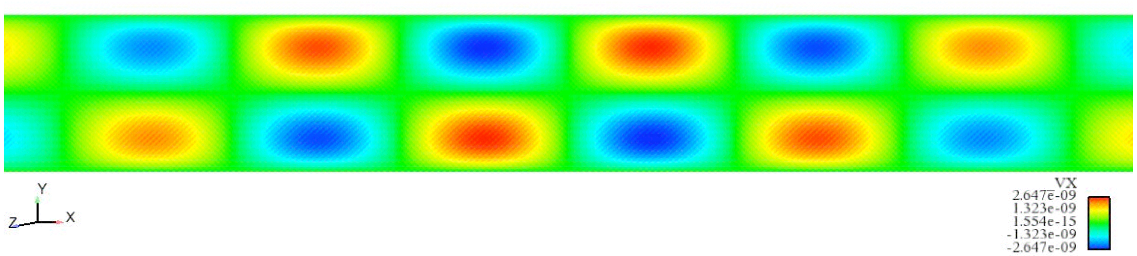


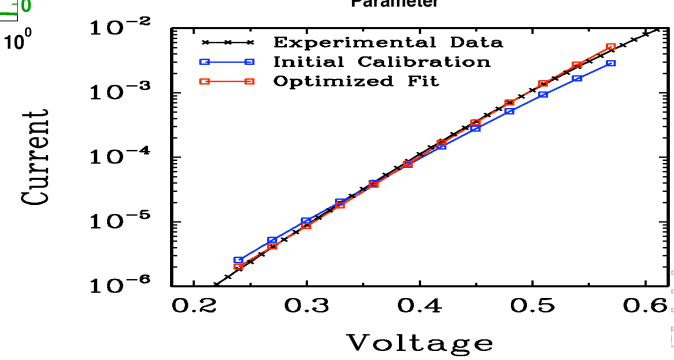












Where Sacado is going in the future

- Documentation
  - Website, tutorials, papers, etc…
- Performance improvements
  - Expression level reverse-mode (`Sacado::ELRFad`)
- Leveraging AD technology for intrusive uncertainty quantification
  - Polynomial chaos expansions via operator overloading
- Impacting more applications
  - Using Sacado is more about software engineering than AD
- SESS presentation 11/13/07
  - More in-depth tutorial on using Sacado in applications