Sundance: a Trilinos package for efficient development of efficient simulators

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Kirby's Recursive Conundrum

Computers were invented to automate tedious, error-prone tasks. Computer programming is a tedious, error-prone task. (R. Kirby)

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So why not program a computer to do it?

Our goal: simplify FEM simulation development without sacrificing performance

We want everything

Provide general multiphysics and intrusive capabiities, **and** a friendly user interface, **and** high performance

Our approach

- State in mathematical form the problems that arise “writing” an efficient intrusive code
- Write (by hand, once) a code to solve those meta-problems

Differentiation provides a path to automation

The mathematics of FEM system assembly is summarized as:

$$\frac{\partial F}{\partial v_i} = \sum_{\alpha} \int_{\Omega} \frac{\partial \mathcal{F}}{\partial D_\alpha v} D_\alpha \psi_i$$

$$\frac{\partial^2 F}{\partial v_i \partial u_j} = \sum_{\alpha,\beta} \int_{\Omega} \frac{\partial^2 \mathcal{F}}{\partial D_\alpha v \partial D_\beta u} D_\alpha \psi_i \, D_\beta \phi_j$$

(From KL, Howle, Kirby, and van Bloemen Waanders 2008)

The key idea

These equations bridge high-level problem specification and low-level computation. Fréchet differentiation connects:

- The abstract problem specification $\mathcal{F}$
- The discretization specification: ψ, ϕ, and integration procedure
- The discrete matrix and vector elements $\frac{\partial^2 F}{\partial v_i \partial u_j}$ and $\frac{\partial F}{\partial v_i}$

A plan for automation

To make practical use of the "bridge theorem" we need:

- A data structure for high-level symbolic description of functionals F
  - Integrands $\mathcal{F}$ represented as DAG
- Automated selection of basis function combinations from element library, given signature of derivative
- Connection to finite element infrastructure for basis functions, mesh, quadrature, linear algebra, and solvers
- A top-level layer for problem specification
- A method to automate the organization of **efficient** in-place computations of *numerical values* of $\frac{\partial \mathcal{F}}{\partial v}$, etc, given DAG for $\mathcal{F}$

Sundance: a Trilinos package taking high-level abstractions to efficient code

Poisson-Boltzmann solver in a notebook

Poisson-Boltzmann: $\nabla^2 u = \sinh u$, $\frac{\partial u}{\partial n} = g$ on Γ_N, $u = u_D$ on Γ_D

$$\int_\Omega (\nabla v \cdot \nabla u + v \sinh u)\, d\Omega - \int_{\Gamma_N} g v \, d\Gamma = 0 \quad \forall v \in H^1$$

with $u = u_D$ on Γ_D

- use P_1 for u, v
- Do integrals exactly when possible, with 4th-order Gauss otherwise

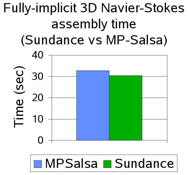
Sundance: a Trilinos package taking high-level abstractions to efficient code

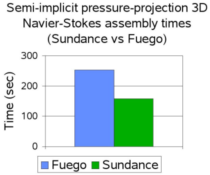
Poisson-Boltzmann solver in Sundance

```
Mesh mesh = mesher.getMesh();

/* Create a cell filter that will identify the maximal cells
 * in the interior of the domain */
CellFilter interior = new MaximalCellFilter();
CellFilter edges = new DimensionalCellFilter(1);
CellFilter left = edges.labeledSubset(1);

/* Create unknown and test functions, discretized using first-order
 * Lagrange interpolants */
int order = 1;
Expr u = new UnknownFunction(new Lagrange(order), "u");
Expr v = new TestFunction(new Lagrange(order), "v");

/* Create differential operator and coordinate functions */
Expr dx = new Derivative(0);
Expr dy = new Derivative(1);
Expr grad = List(dx, dy);

/* We need a quadrature rule for doing the integrations */
QuadratureFamily quad2 = new GaussianQuadrature(2);
QuadratureFamily quad4 = new GaussianQuadrature(4);

/* Define the weak form */
Expr eqn = Integral(interior, (grad*u)*(grad*v) + v*exp(-u), quad2);

/* Define the Dirichlet BC */
Expr bc = EssentialBC(left, v*(u-1.0), quad4);

/* Create a discrete space, and discretize the function 1.0 on it */
DiscreteSpace discSpace(mesh, new Lagrange(order), vecType);
Expr u0 = new DiscreteFunction(discSpace, 1.0, "u0");


/* Create a TSF NonlinearOperator object */
NonlinearOperator<double> F
  = new NonlinearProblem(mesh, eqn, bc, v, u, u0, vecType);
```

Math-based automated assembly is at least as efficient as matrix assembly in hand-coded, problem-tuned “gold standard” codes

- Comparison of assembly times for 3D forward problems
  - Sundance uses same solvers (Trilinos) as gold-standard codes
- MP-Salsa and Fuego don’t allow instrusion
  - Can only compare forward problem performance
  - Comparisons do *not* include additional gains enabled by Sundance’s intrusive capabilities





Parallel scalability of assembly process

Processors	Assembly time
4	54.5
16	54.7
32	54.3
128	54.4
256	54.4

- Assembly times for a model CDR problem on ASC Red Storm
- Weak scalability means: assembly time remains constant as number of processors increases in proportion to problem size
- Results demonstrate Sundance is weakly scalable

How can user-friendly, intrusion-friendly code be fast?

High performance is a result of:

- Amortization of overhead
- Careful memory management
- Effective use of BLAS
- Work reduction through data flow analysis

With our unified formulation, effort spent tuning computational kernels applies immediately to diverse problem types and arbitrary PDE

Amortization, memory managment, and BLAS

Amortize DAG traversal

- Process batches of elements and quadrature points

Minimize allocations and copies

- Maintain a stack of work vectors
- Automatically identify vectors that can operated into
  - *e.g.* identify opportunities for `x+=y` instead of `x=x+y`

BLAS

- Aggregate integral transformations, hit with level 3 BLAS

Pre-computation data flow analysis lets us avoid unnecessary work

Sparsity determination

- Don't store or compute derivatives known to be zero or unused
- Distinguish spatially-constant from spatially-variable derivatives

We must track data flow through these operations:

- Multivariable, multiargument chain rule (special cases: +,-,$\times$,/)
- Spatial differentiation

Set theoretical data flow analysis

- Tracks changes in sets of nonzero, constant, and variable derivatives through evaluation process
- Implemented using STL set/multiset classes

A key to high level simplicity without low performance: division of labor

Decouple user-level representiation from low-level evaluation

Reduces human factors / performance tradeoffs

- User-level objects optimized for human factors
- Low-level objects optimized for performance

Allows interchangeable evaluators under a common interface

- Easy to upgrade, tune, and experiment with evaluators w/o impact on user
- Future: different evaluators for different architectures

Summary

- Mathematical formulation of discrete system assembly process enables automated transition from “blackboard” mathematics to efficient PDE simulation
- Automated assembly code compares favorably in both efficiency and scalability to “gold standard” simulators
- Our method transparently enables intrusive algorithms, realizing even greater performance gains for optimization, sensitivity, and UQ
- By developing a unifying mathematical framework for PDE simulation, our results can be applied to a wide range of types of discretization methods and physical problems

The one-sentence description

We use high-level symbolic components to automate the organization of low-level high-performance numerical computations