AUTOMATIC DIFFERENTIATION FOR NONLINEAR, MULTIPHYSICS SIMULATION

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October 24 2016

MOOSE

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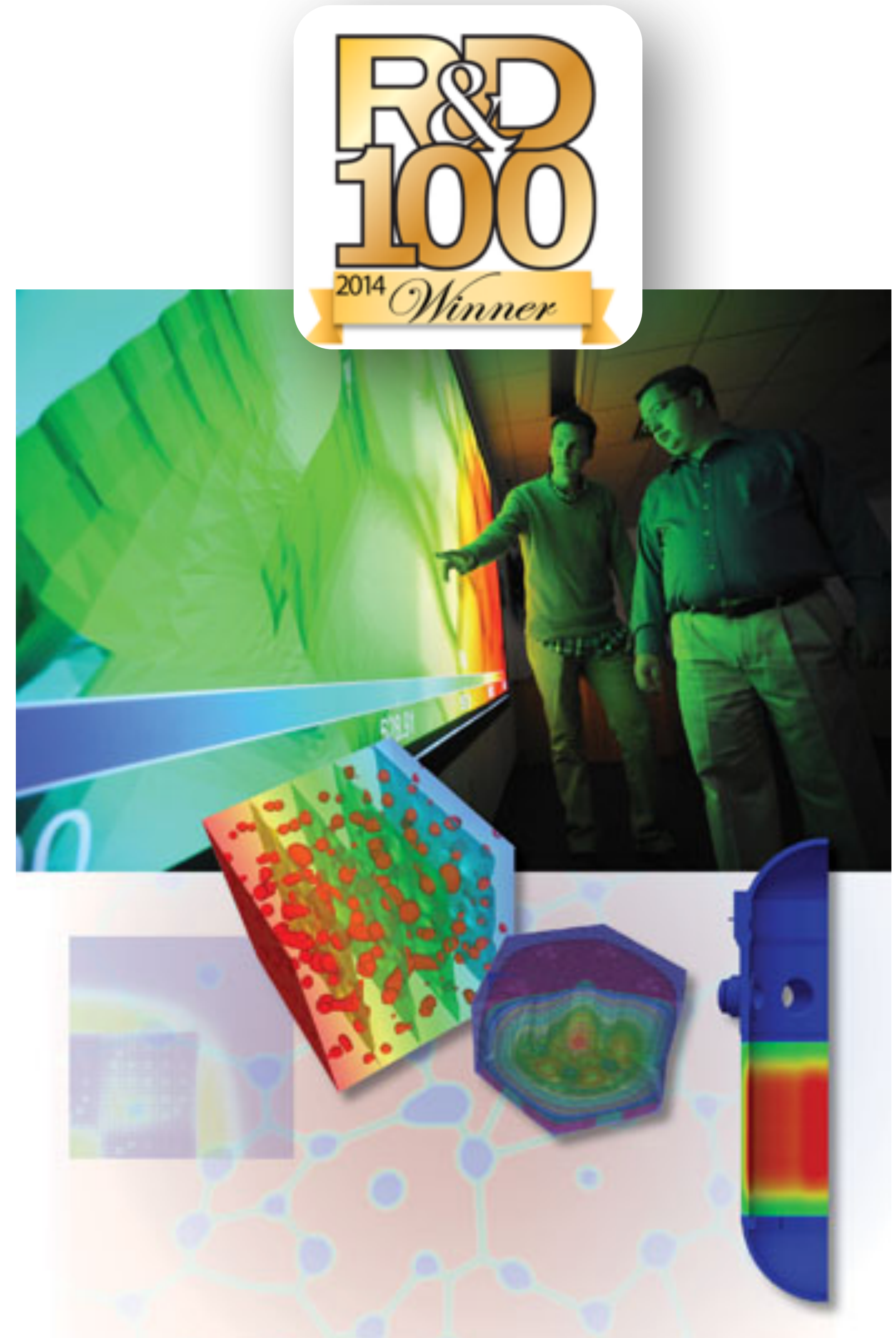
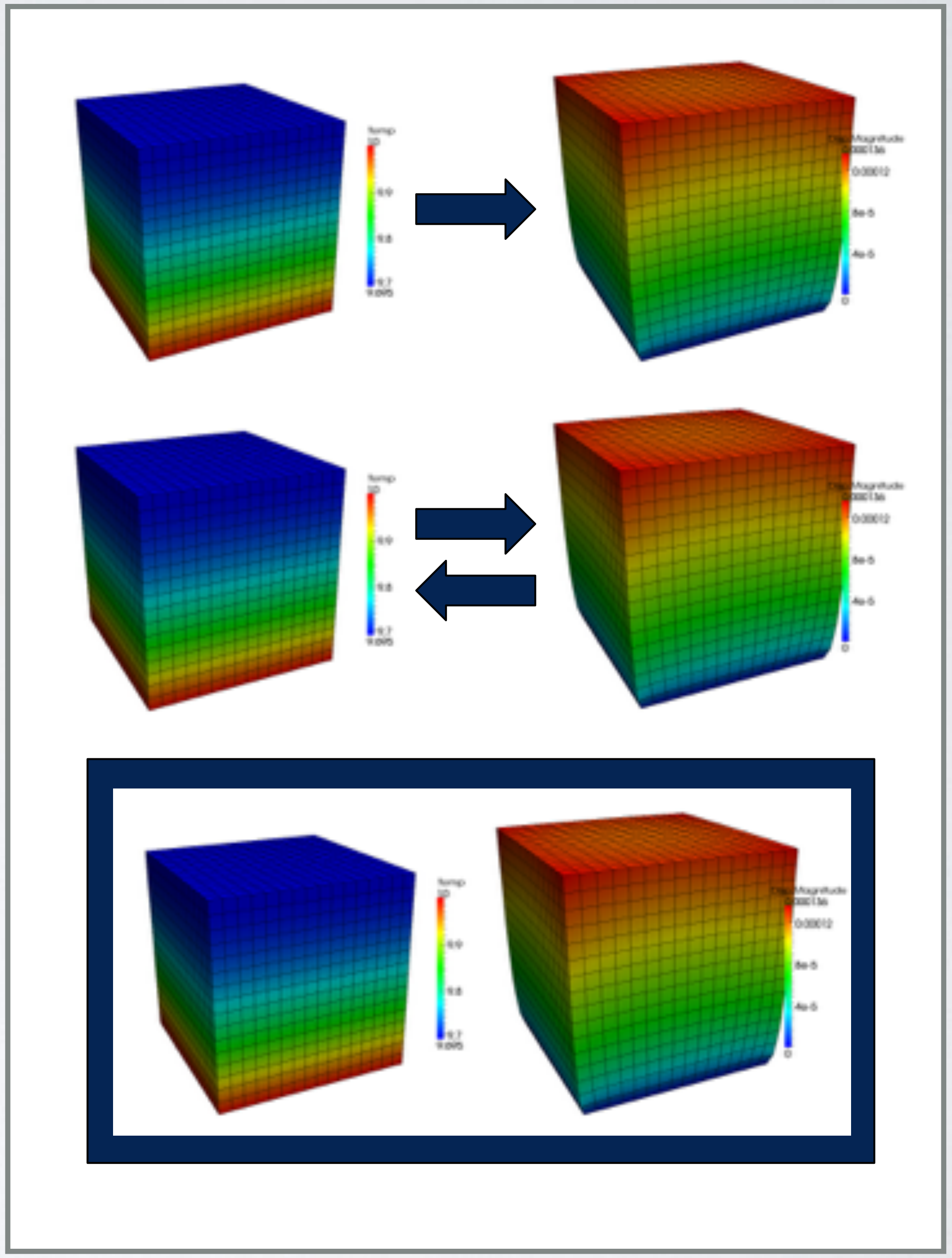
Multiphysics Object Oriented Simulation Environment

- MOOSE is a finite-element, multiphysics framework that **simplifies the development** of numerical applications.
- It provides a high-level interface to **sophisticated nonlinear solvers** and **massively parallel computational capability**.
- Used to model thermomechanics, neutronics, geomechanics, reactive transport, microstructure, computational fluid dynamics…
- **Open source** and freely available at **mooseframework.org**
- High honors:
  - Early career award from President Obama
  - R&D 100 from R&D Magazine
  - Hundreds of publications, thousands of citations



MULTIPHYSICS IS TOUGH!

- Multiphysics: simultaneously solving multiple PDEs representing multiple, coupled, physical phenomena
    - Heat conduction, solid mechanics, neutronics, etc.
- Many different solution schemes
    - Loose, Picard, Fully Coupled, etc.
- Fully Coupled
    - Fast, Robust
    - Solves all equations simultaneously
    - Typically uses a Newton-like solver
- Newton solvers require **Jacobians**



Loose, Picard and Full Coupling

FINITE-ELEMENT CONSTRUCTION

Strong Form: $-\nabla \cdot D(u)\nabla u = 0$

Weak Form: $$\int_V D(u)\nabla u \cdot \nabla \psi dV - \int_S (D(u)\nabla u \cdot n)\psi dS = 0$$

Discretized Variable: $$u_h = \sum_k u_k \phi_k$$

$$\nabla u_h = \sum_k u_k \nabla \phi_k$$

Discretized Test Space: $$\psi = \{\phi_i\}$$

Break domain into "elements". Evaluate integrals using Quadrature.

SOLVING NONLINEAR FE

Nonlinear Vector Equation: $R_i(u_h) = 0$

Vector Newton's Method:

$$\mathbf{J}(u_h^n)\delta u_h^{n+1} = -R_i(u_h^n)$$

$$u_k^{n+1} = u_k^n + \delta u_k^{n+1}$$

$$\mathbf{J}_{i,j}(u_h^n) = \frac{\partial R_i(u_h^n)}{\partial u_j}$$

$$\frac{\partial u_h}{\partial u_j} = \sum_k \frac{\partial}{\partial u_j}(u_k \phi_k) = \phi_j \qquad \frac{\partial (\nabla u_h)}{\partial u_j} = \sum_k \frac{\partial}{\partial u_j}(u_k \nabla \phi_k) = \nabla \phi_j$$

JACOBIAN

- The Jacobian gets out of control quickly:
  - NxN matrix to store
  - NxN matrix to compute
  - Differentiation of non-smooth properties
  - Tons of analytic derivatives
  - Grows as number of equations **squared**
- Could use "Jacobian-Free" methods: JFNK
- Could use Automatic Differentiation (AD)…

$$\mathbf{J}(u_h, v_h) = \begin{bmatrix} \frac{\partial R_u(u_h, v_h)}{\partial u_k} & \frac{\partial R_u(u_h, v_h)}{\partial v_k} \\ \frac{\partial R_v(u_h, v_h)}{\partial u_k} & \frac{\partial R_v(u_h, v_h)}{\partial v_k} \end{bmatrix}$$

Block Structured Jacobian

AUTOMATIC DIFFERENTIATION

- Automatically compute derivative of code
- Many options:
  - Code transformation
  - Reverse Mode
  - Template Metaprogramming
  - Forward Mode via operator overloading
  - …

```
function residual(args)
    return D*grad_u*grad_psi
end

function jacobian(args)
    return (dD_du*grad_u + D*grad_phi)
           * grad_psi
end
```

Manual Derivatives

FORWARDDIFF.JL

- Developed by Jarrett Revels (MIT)
    - https://github.com/JuliaDiff/ForwardDiff.jl
- Implements AD via "Dual" number Type and function overloading (perfect for Julia!)
- "Dual" holds both the value and partial derivatives
- As a Dual is operated on the partials are automatically accumulated
- By seeding the partials with orthogonal components, the derivative with respect to multiple variables can be computed simultaneously
- One evaluation of "f" can also evaluate the entire gradient

Dual Number

$$f(x + \sum_{i=1}^{k} y_i \epsilon_i) = f(x) + f'(x) \sum_{i=1}^{k} y_i \epsilon_i$$

Vector Form

$$f(\vec{x}_\epsilon) = f(\vec{x}) + \sum_{i=1}^{k} \frac{\partial f(\vec{x})}{\partial x_i} \epsilon_i$$

2016, Revels, J. and Lubin, M. and Papamarkou, T. (view online)
Forward-Mode Automatic Differentiation in Julia

FE AD

Solution Coefficients: (u_1, u_2, u_3, u_4)

Dual Numbers:

$$\mathtt{u}_1 = [u_1, 1, 0, 0, 0]$$
$$\mathtt{u}_2 = [u_2, 0, 1, 0, 0]$$
$$\mathtt{u}_3 = [u_3, 0, 0, 1, 0]$$
$$\mathtt{u}_4 = [u_4, 0, 0, 0, 1]$$

Field Value: $u_h = \sum_k u_k \phi_k$

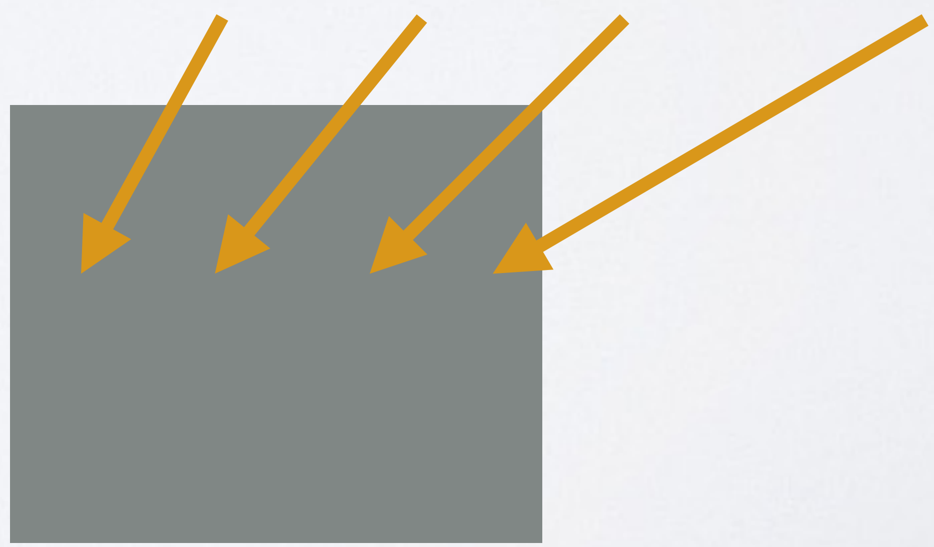
Dual Field Value:

$$\mathtt{u}_h = [u_h, \phi_1, \phi_2, \phi_3, \phi_4]$$

Residual Entry: $R_i = R(u_h, \psi_i)$

Dual Residual: $\mathtt{R}_i = R(\mathtt{u}_h, \psi_i) = [R_i, \frac{\partial R_i}{\partial u_1}, \frac{\partial R_i}{\partial u_2}, \frac{\partial R_i}{\partial u_3}, \frac{\partial R_i}{\partial u_4}]$

$\mathbf{J}_{i,j} =$

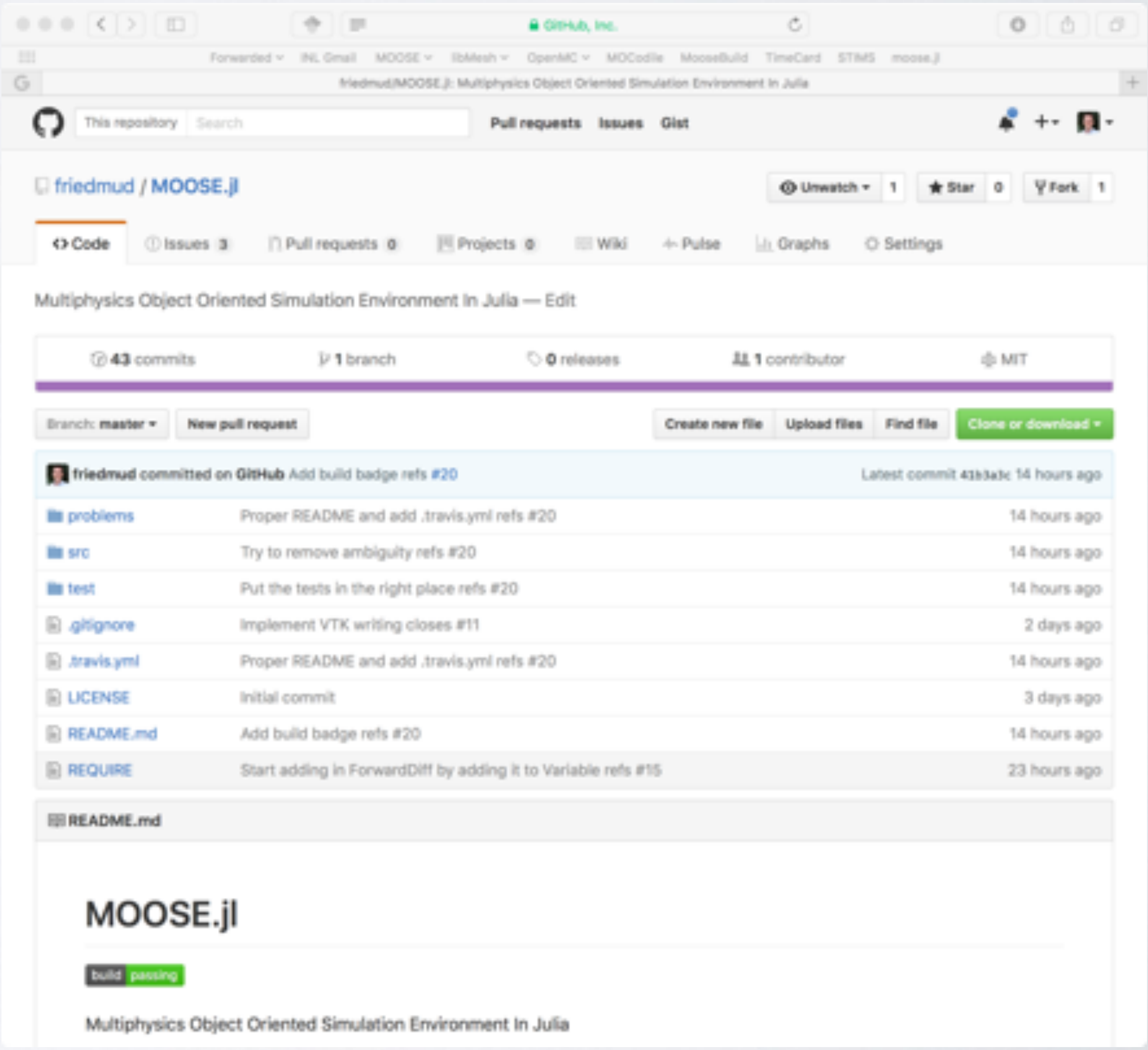


MAX_CHUNK_SIZE

- ForwardDiff.jl defines: MAX_CHUNK_SIZE = 10
- Prohibitive!
  - Can only solve for 2 variables on a Quad4 grid!
- I modified ForwardDiff.jl to set MAX_CHUNK_SIZE = 256
- WARNING: This parameter controls procedurally generated type definitions!
  - Setting this too high (I tried 1000) will cause Julia to take forever to compile ForwardDiff.jl!

MOOSE.JL

- Reimplementation of MOOSE in Julia
    - https://github.com/friedmud/moose.jl
    - Pkg.clone("https://github.com/friedmud/MOOSE.jl.git")
    - Full test suite with CI: https://travis-ci.org/friedmud/MOOSE.jl
- "plug-and-play" equation system construction
- Automatic differentiation for Jacobian calculation
- Built on:
    - ForwardDiff.jl (Jarrett Revels)
    - JuAFEM.jl (Kristoffer Carlsson)
    - ContMechTensors.jl (Kristoffer Carlsson)
    - FastGaussQuadrature.jl (Alex Townsend)
- Much more left to do! (Final Project)



EXAMPLE INPUT/SOLUTION

```julia
using MOOSE

include("CoupledConvection.jl")

mesh = buildSquare(0, 1, 0, 1, 20, 20)

diffusion_system = System{Float64}(mesh)

u = addVariable!(diffusion_system, "u")
v = addVariable!(diffusion_system, "v")

addKernel!(diffusion_system, Diffusion(u))

addKernel!(diffusion_system, CoupledConvection(u, v))
addKernel!(diffusion_system, Diffusion(v))

addBC!(diffusion_system, DirichletBC(u, [4], 0.0))
addBC!(diffusion_system, DirichletBC(u, [2], 1.0))

addBC!(diffusion_system, DirichletBC(v, [4], 0.0))
addBC!(diffusion_system, DirichletBC(v, [2], 1.0))

initialize!(diffusion_system)

solver = JuliaDenseNonlinearImplicitSolver(diffusion_system)
solve!(solver, nl_max_its=5)

out = VTKOutput()
output(out, solver, "coupled_convection_out")
```

Solves:

$$-\nabla \cdot \nabla u + \nabla v \cdot \nabla u = 0$$

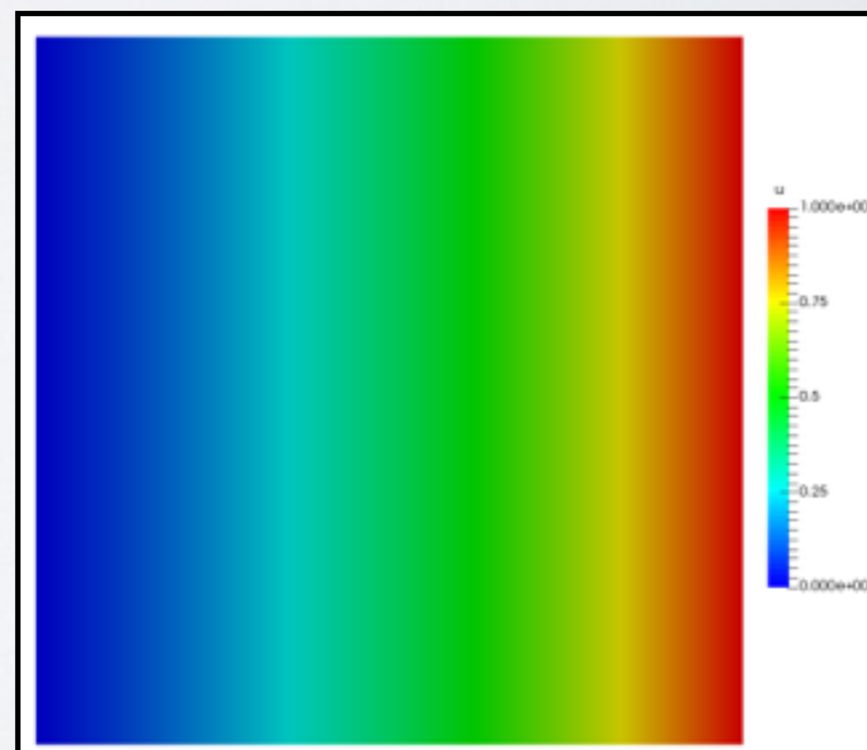
$$u = 0, u \in S_{left}$$

$$u = 1, u \in S_{right}$$

$$-\nabla \cdot \nabla v = 0$$

$$v = 0, v \in S_{left}$$

$$v = 1, v \in S_{right}$$



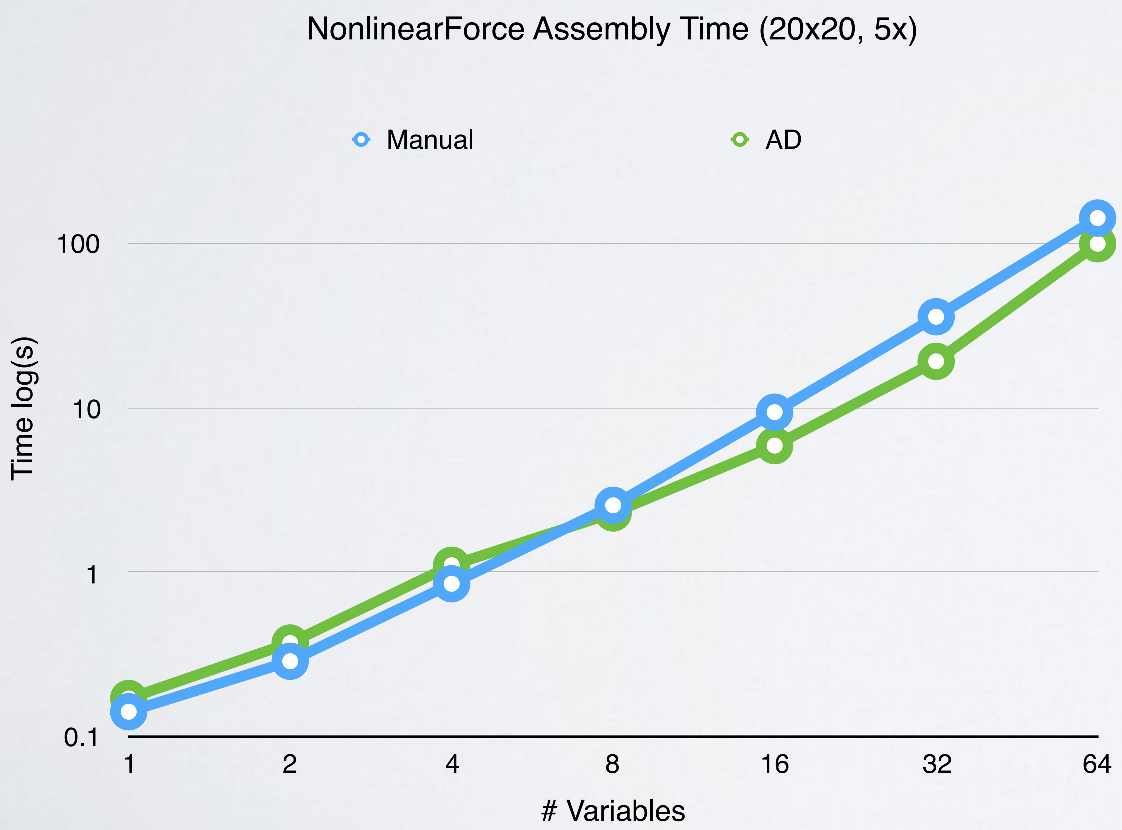
"NO COUPLING" PERFORMANCE

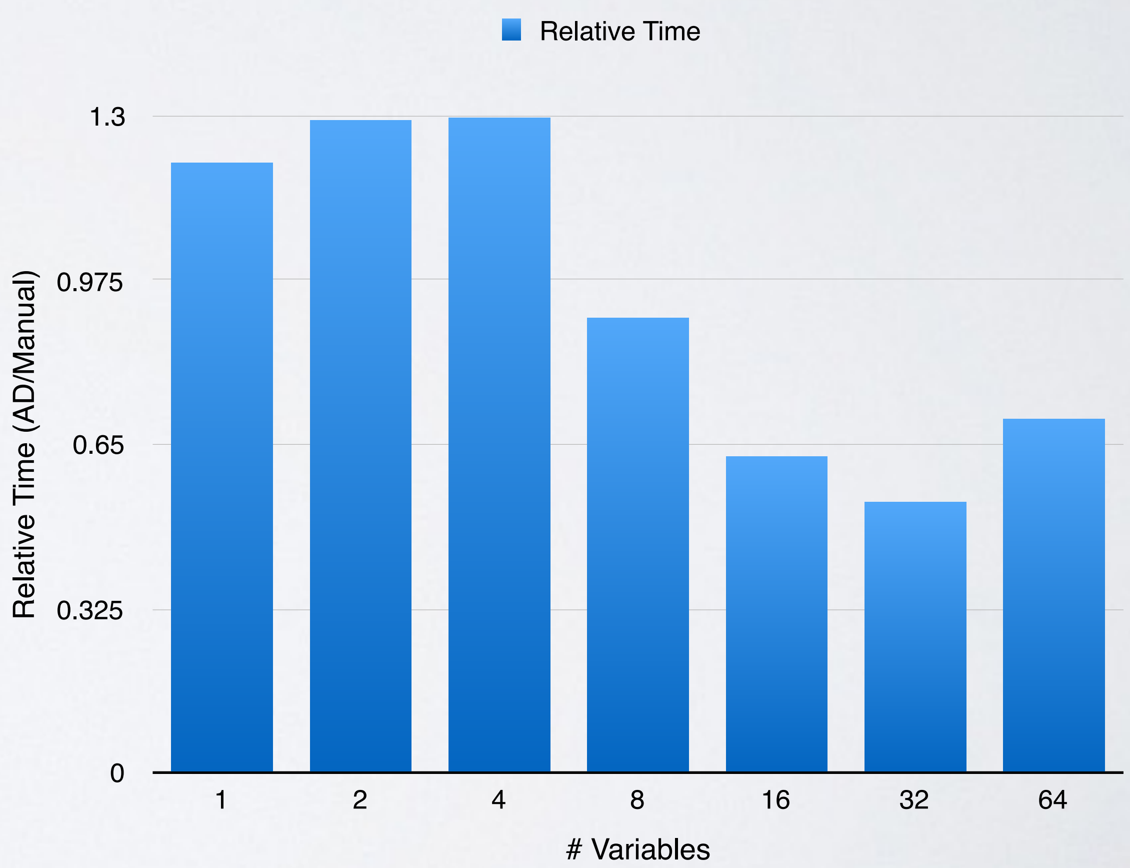
Equations:

$$-\nabla \cdot \nabla u_i + u_i^2 = 0$$

$$u_i = 0, u_i \in S_{left}$$

$$u_i = 1, u_i \in S_{right}$$





20x20 Mesh, 5 Assembly Calculations

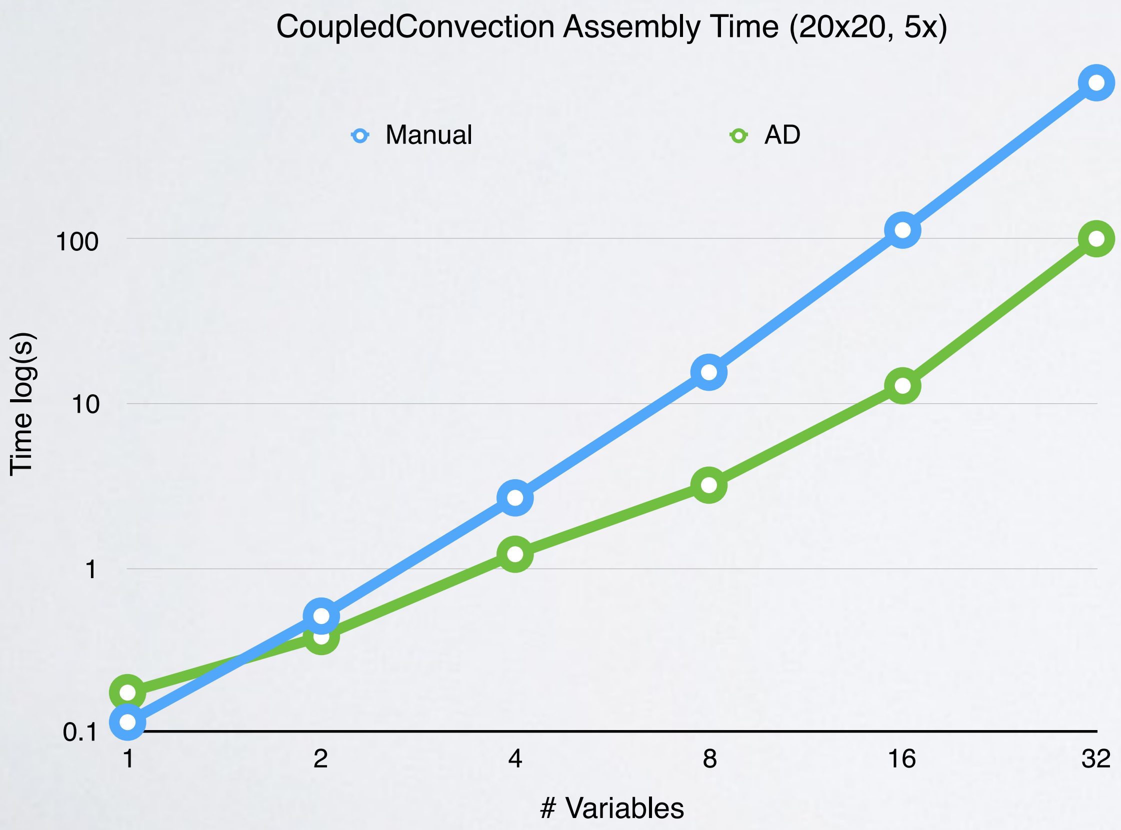
"FULLY COUPLED" PERFORMANCE

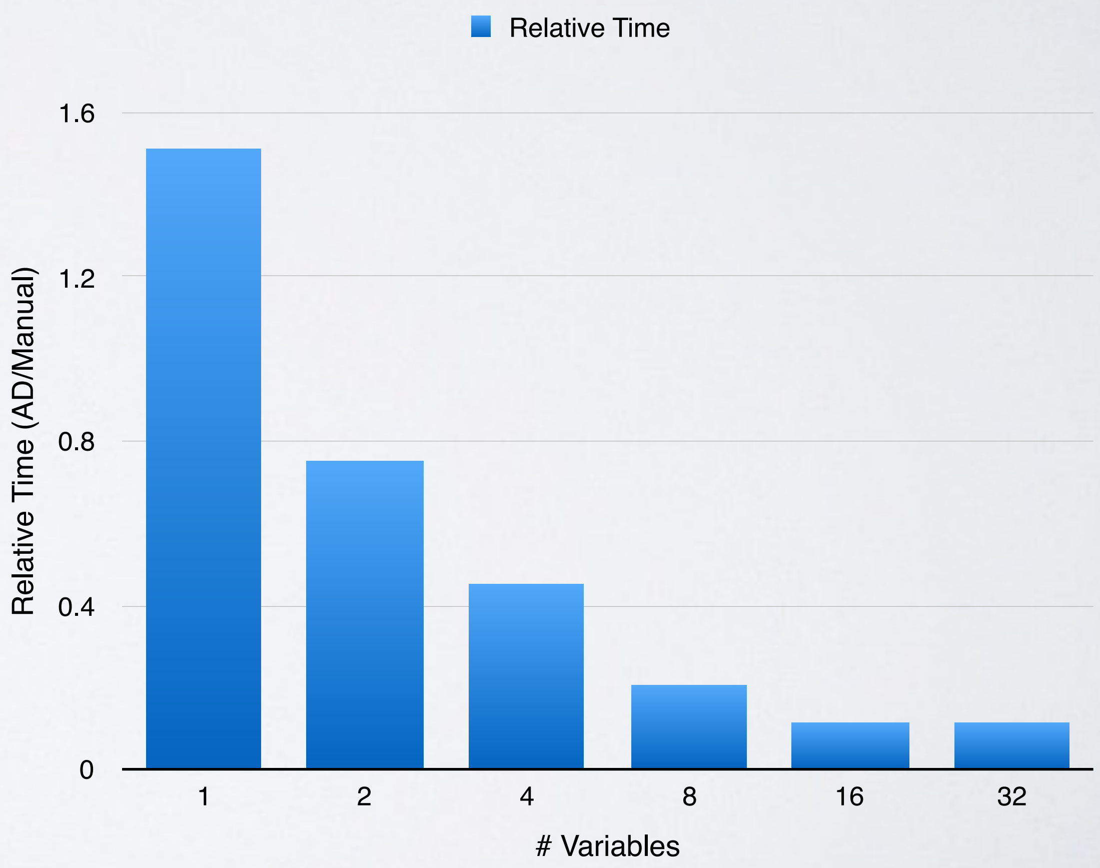
Equations:

$$-\nabla \cdot \nabla u_i + \sum_{k,k\neq i} \nabla u_k \nabla u_i = 0$$

$$u_i = 0, u_i \in S_{left}$$

$$u_i = 1, u_i \in S_{right}$$





20x20 Mesh, 5 Assembly Calculations

CONCLUSIONS

- Julia is working well for Multiphysics!
- Open source packages accelerate development
- ForwardDiff.jl provides effective AD for FE
- MOOSE.jl is now available (and will continue to improve)