



A New Unstructured Variable-Resolution Finite Element Ice Sheet Stress-Velocity Solver within the MPAS/Trilinos FELIX Dycore of PISCEES

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Sandia's Role in the PISCEES* Project

Objective: Develop Unstructured Grid Finite Element Code for Velocity-Stress Solves using MPAS/Trilinos (MPAS/Trilinos "FELIX" Dycore)

- Implement ice sheet PDE flow models of varying fidelity (Stokes, Higher-Order, L1L2).
- Uses Trilinos very heavily (**FASTMath liaison**).
 - Close connection to Perego/Gunzberger at FSU.
- Interface to MPAS framework (LANL collaboration) for mesh, advection, temperature solve, topology data.
- Interface to DAKOTA software for UQ (**QUEST liaison**) .
 - Collaboration on applications with Jackson at UT Austin.
- Work on scalability: particularly preconditioning (Tuminaro) and performance (Worley).
- Post-processing and V&V through LIVV (Kate Evans).

Sandia Staff: Salinger, Kalashnikova, Eldred, Tuminaro, Jakeman, Perego.

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Trilinos & Component-Based Software Development

Analysis Tools (black-box)
Optimization
UQ (sampling)
Parameter Studies
V&V, Calibration
OUU, Reliability
Analysis Tools (embedded)
Nonlinear Solver
Time Integration
Continuation
Sensitivity Analysis
Stability Analysis
Constrained Solves
Optimization
UQ Solver
Linear Algebra
Data Structures
Iterative Solvers
Direct Solvers
Eigen Solver
Preconditioners
Matrix Partitioning
Architecture- Dependent Kernels
Multi-Core Accelerators

Trilinos/Dakota have Greatly Expanded - Full Suite of Independent-yet-Interoperable Components

Composite Physics
MultiPhysics Coupling
System Models
System UQ

Mesh Tools
Mesh I/O
Inline Meshing
Partitioning
Load Balancing
Adaptivity
Grid Transfers
Quality Improvement
DOF map

PostProcessing
Visualization
Verification
Model Reduction

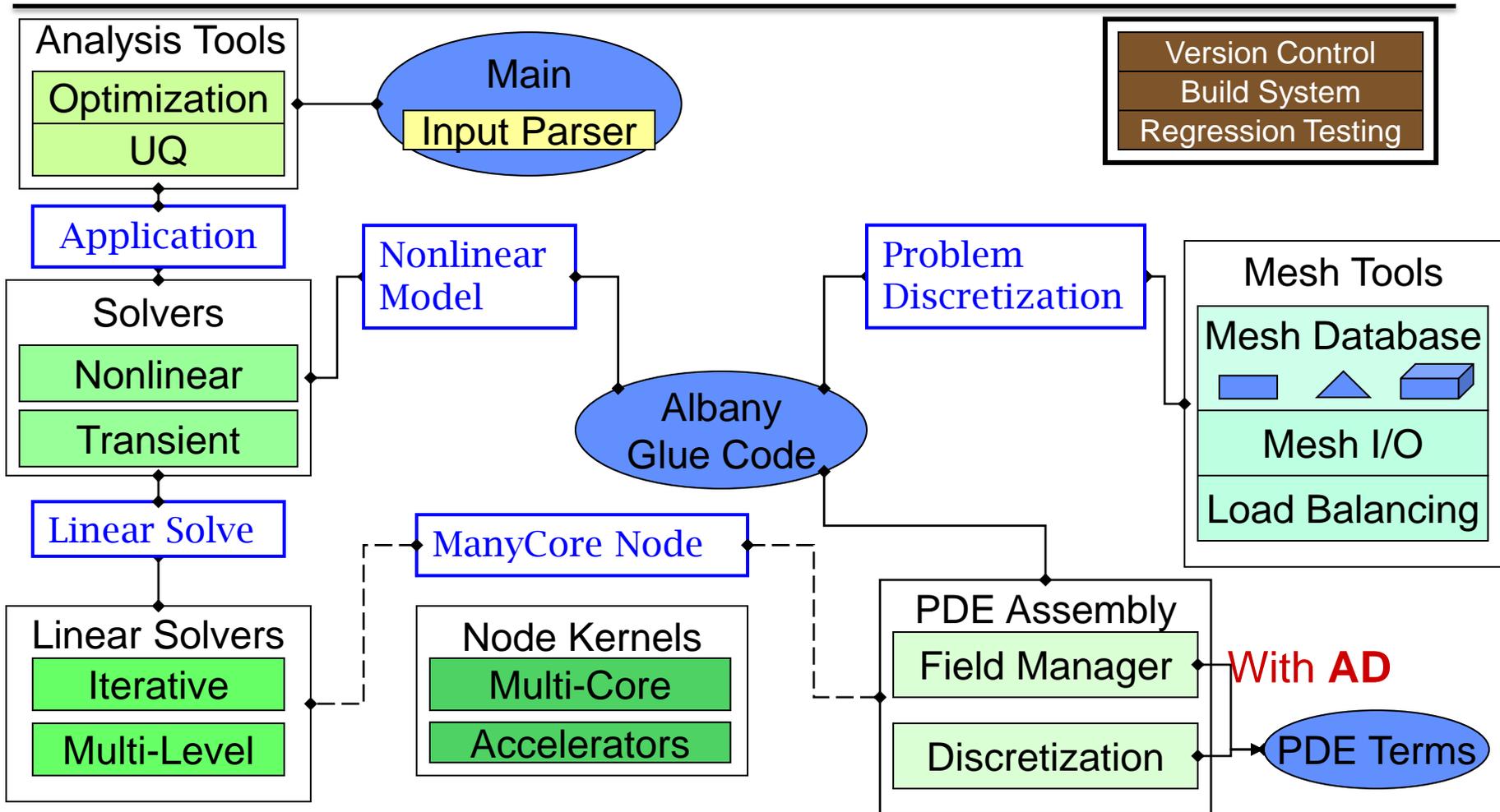
Mesh Database
Mesh Database
Geometry Database
Solution Database
Checkpoint/Restart

Utilities
Input File Parser
Parameter List
Memory Management
I/O Management
Communicators
Runtime Compiler
MultiCore
Parallelization Tools

Local Fill
Discretizations
Discretization Library
Field Manager
Derivative Tools
Sensitivities
Derivatives
Adjoints
UQ / PCE
Propagation
Physics Fill
Element Level Fill
Material Models
Objective Function
Constraints
Error Estimates
MMS Source Terms

Software Quality
Version Control
Regression Testing
Build System
Backups
Verification Tests
Mailing Lists
Unit Testing
Bug Tracking
Performance Testing
Code Coverage
Porting
Web Pages
Release Process

“Albany Code”: Component-Based Software Development in Action



Mechanics, quantum dots, fuel rod degradation, embedded UQ, MOR



Stress-Velocity Solver within the MPAS/Trilinos Dycore

- Stress-velocity finite element solver with three different fidelity ice flow models:
 - L1L2.
 - First order (a.k.a. higher-order) Stokes.
 - Nonlinear physics implemented, w/o and w/ basal sliding, and convergence verified.
 - Good agreement with published results for test cases (ISMIP-HOM, Dome).
 - Preliminary UQ studies.
 - Full Stokes.
 - Linear full Stokes physics with PSPG velocity/pressure finite elements implemented and convergence verified.
 - Nonlinear full Stokes physics with PSPG velocity/pressure finite elements implemented.
 - Accuracy limited by stabilization.

First Order (a.k.a. Higher-Order) Stokes Model

- Derived as approximation of the Stokes model under the assumption that the aspect ratio δ is small and normals to upper/lower surfaces are almost vertical.
- System of two coupled non-linear PDEs for u and v velocities of ice:

$$\begin{cases} -\nabla \cdot (2\mu\dot{\epsilon}_1) = -\rho g \frac{\partial s}{\partial x}, \\ -\nabla \cdot (2\mu\dot{\epsilon}_2) = -\rho g \frac{\partial s}{\partial y} \end{cases}$$

with Glen's law viscosity:

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\dot{\epsilon}_{xx}^2 + \dot{\epsilon}_{yy}^2 + \dot{\epsilon}_{xx}\dot{\epsilon}_{yy} + \dot{\epsilon}_{xy}^2 + \dot{\epsilon}_{xz}^2 + \dot{\epsilon}_{yz}^2 + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

$$\dot{\epsilon}_1^T = (2\dot{\epsilon}_{xx} + \dot{\epsilon}_{yy}, \dot{\epsilon}_{xy}, \dot{\epsilon}_{xz})$$

$$\dot{\epsilon}_2^T = (\dot{\epsilon}_{xy}, \dot{\epsilon}_{xx} + 2\dot{\epsilon}_{yy}, \dot{\epsilon}_{yz})$$

$$\dot{\epsilon}_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

A = flow rate factor

n = Glen's law exponent = 3

γ = regularization parameter

β = sliding coefficient ≥ 0

- Boundary conditions:

$\dot{\epsilon}_1 \cdot \mathbf{n} = 0,$	$\dot{\epsilon}_2 \cdot \mathbf{n} = 0,$	on $\Gamma_s,$
$u = 0,$	$v = 0,$	on Γ_0
$2\mu\dot{\epsilon}_1 \cdot \mathbf{n} + \beta u = 0,$	$2\mu\dot{\epsilon}_2 \cdot \mathbf{n} + \beta v = 0,$	on Γ_β
- Numerical Method:
 - Discretization: classical Galerkin FEM with structured or unstructured mesh.
 - Nonlinear solver: Newton's method
 - Automatic differentiation (AD) Jacobians using Sacado package of Trilinos.
 - Continuation in $\gamma \rightarrow 10^{-10}$ using LOCA package of Trilinos.
 - Linear solver: preconditioned GMRES with ILU or algebraic multigrid preconditioner.

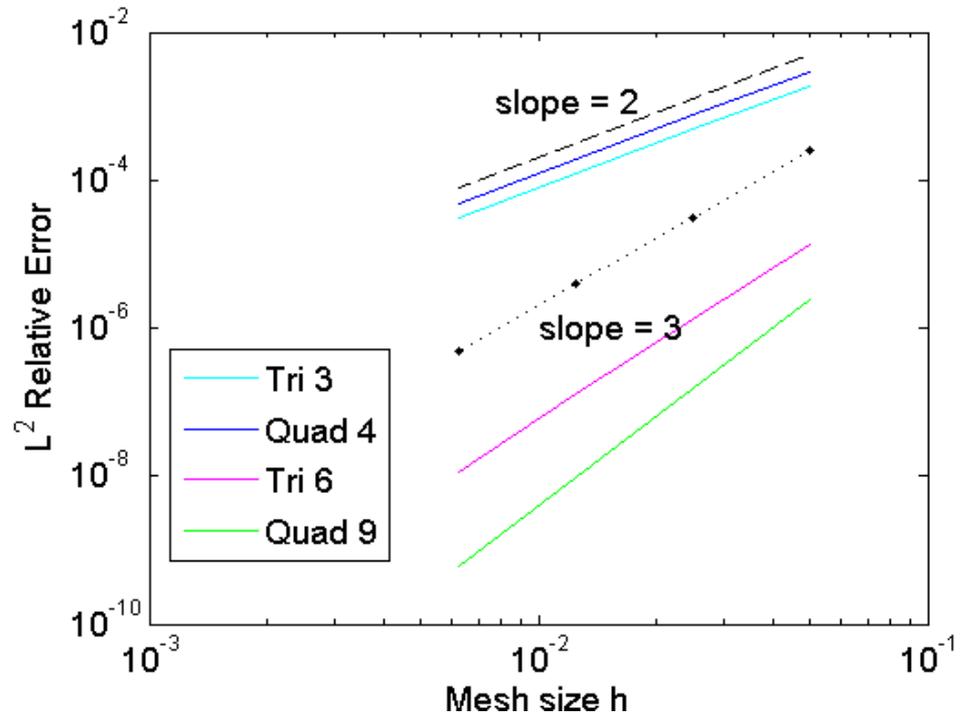
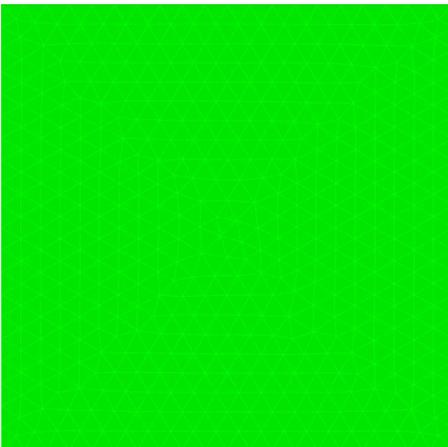
First Order (a.k.a. Higher-Order) Stokes Model: Convergence Study

- 2D Method of Manufactured Solutions (MMS) problem: source terms f_1 and f_2 are derived such that

$$\begin{aligned}u &= \sin(2\pi x) \cos(2\pi y) + 3\pi x, \\v &= -\cos(2\pi x) \sin(2\pi y) - 3\pi y\end{aligned}$$

is the exact solution to

$$\begin{cases} -\nabla \cdot (2\mu \dot{\epsilon}_1) = f_1, \\ -\nabla \cdot (2\mu \dot{\epsilon}_2) = f_2 \end{cases}$$



- Low order elements attain expected convergence rates; super-convergence in higher-order elements observed (above).

First Order (a.k.a. Higher-Order) Stokes Model: ISMIP-HOM Test C

- Standard test case of Stokes models with basal sliding.

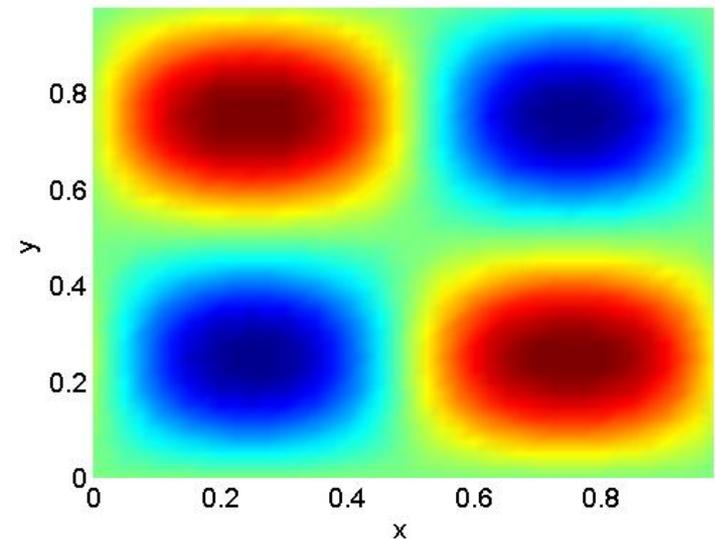
- Bedrock and top surfaces are given by:

$$\begin{aligned} s(x, y) &= -x \tan \alpha, \\ b(x, y) &= s(x, y) - 1 \end{aligned}$$

- Sliding boundary conditions prescribed on basal boundary with:

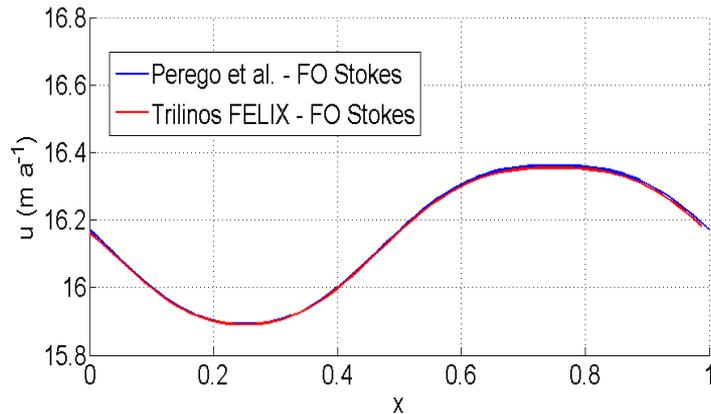
$$\beta(x, y) = 1 + \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right)$$

- Periodic boundary conditions in lateral directions x and y .
- Excellent agreement between results computed in Trilinos FELIX dycore and published results.

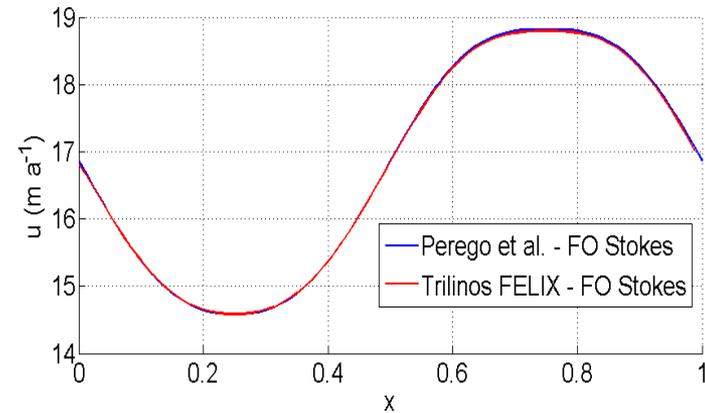


Velocity u at top surface
($L = 20$)

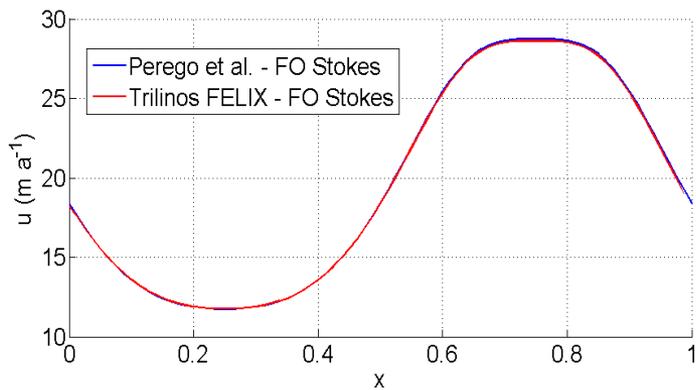
First Order (a.k.a. Higher-Order) Stokes Model: ISMIP-HOM Test C (continued)



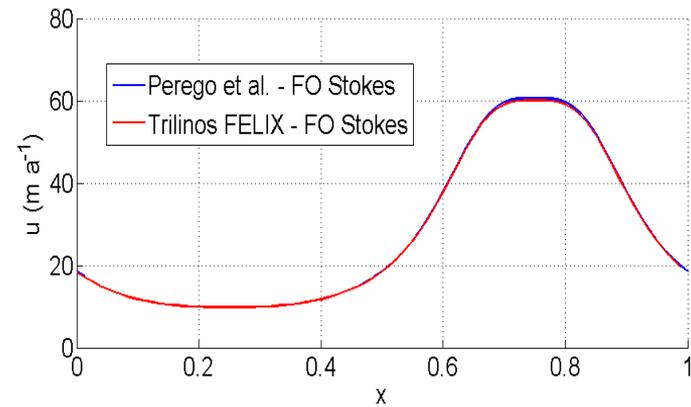
$L = 10$



$L = 20$



$L = 40$

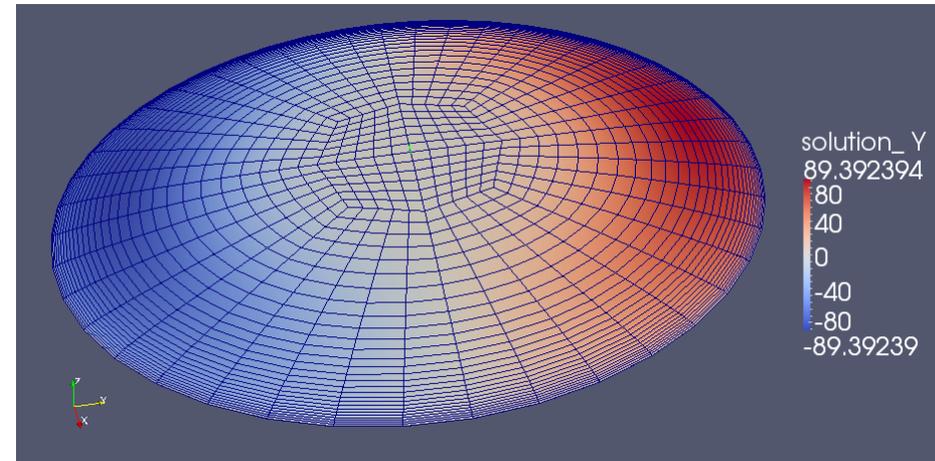


$L = 80$

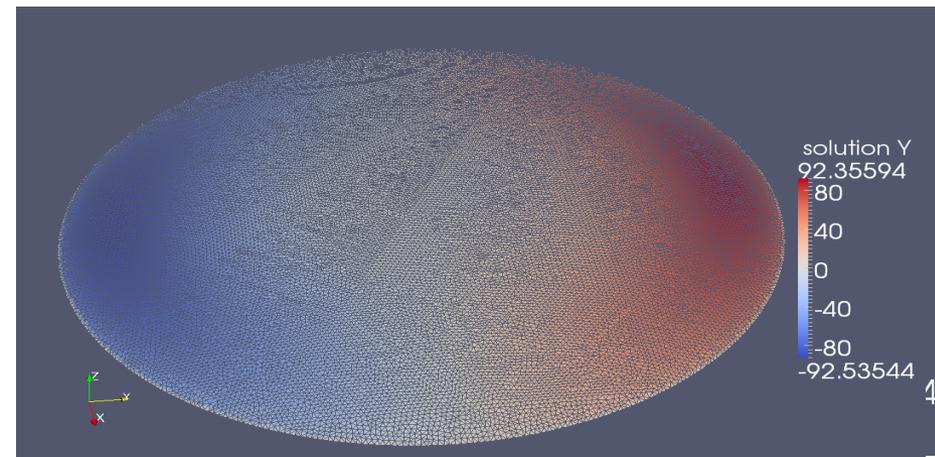
Surface velocity u as a function of x at $y = L/4$, $80 \times 80 \times 20$ mesh

First Order (a.k.a. Higher-Order) Stokes Model: Dome Test Case

- Test case that simulates 3D flow field within an isothermal, parabolic shaped dome of ice with circular base.
- No-sliding (no-slip) boundary conditions at basal boundary.
- Stress-free boundary conditions at top surface.
- No-slip boundary conditions in lateral directions x and y .
- Robust unstructured mesh generation using Sandia in-house Cubit meshing package.
- Good agreement between results computed in Trilinos FELIX dycore and in Glimmer CISM and LifeV.



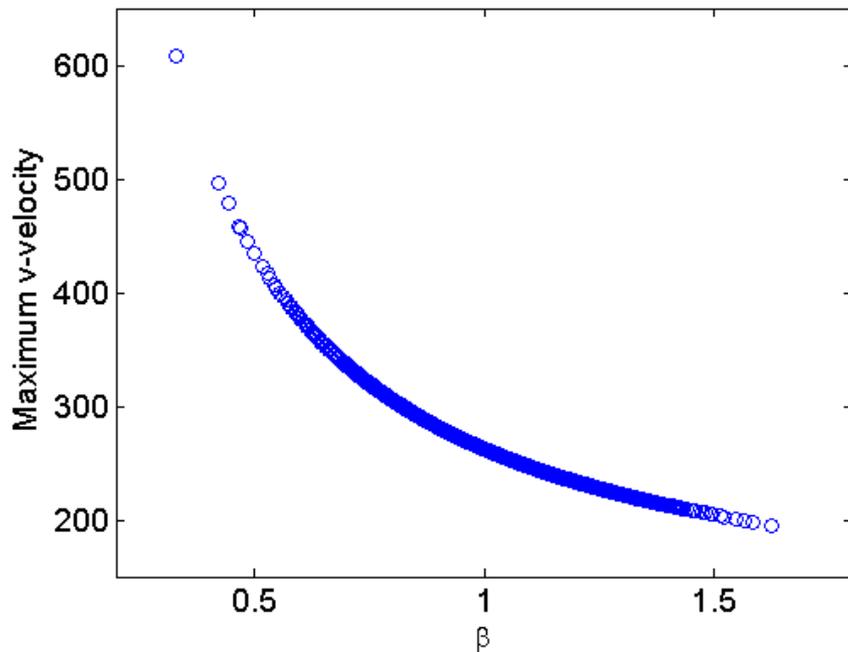
Trilinos FELIX



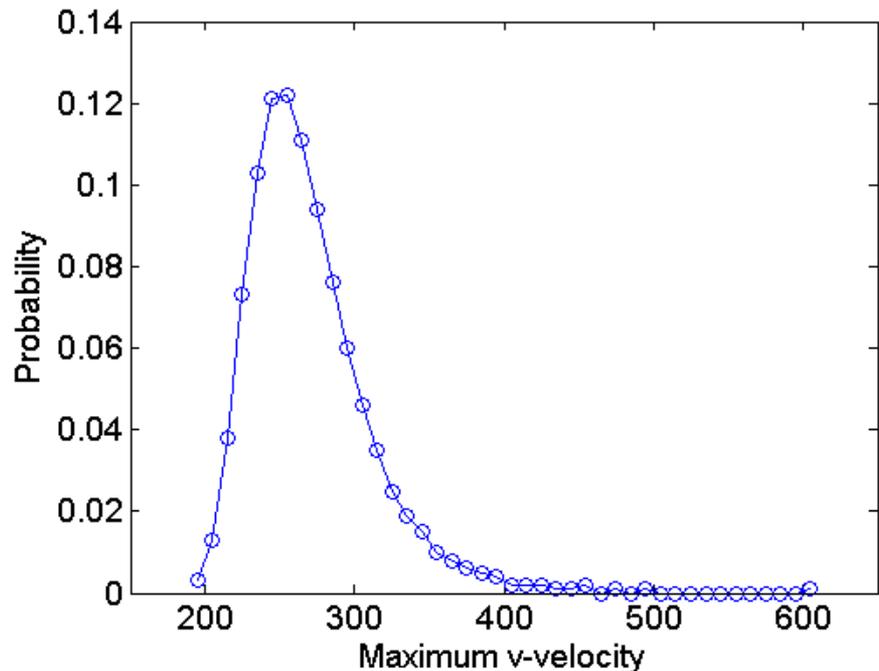
LifeV (Perego *et al.*) 10/15

First Order (a.k.a. Higher-Order) Stokes Model: UQ Study for Dome

- Modified dome test case to have basal sliding boundary condition at bedrock with:
 $\beta \sim \text{Normal}(\text{mean} = 1 \text{ kPa a/m}, \text{std. dev.} = 0.2 \text{ kPa a/m})$
- UQ study with 1000 samples of β .



β vs. max v -velocity



PDF of max v -velocity 12/15

Full Stokes Model

- Ice flow modeled as non-Newtonian incompressible fluid obeying Stokes' equations:

$$\begin{cases} -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}} - p\mathbf{I}) = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

with Glen's law viscosity:

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}^2 + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

$$\dot{\epsilon}_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

A = flow rate factor

n = Glen's law exponent = 3

γ = regularization parameter

β = sliding coefficient ≥ 0

- Boundary conditions:

$$\begin{aligned} (2\mu \dot{\boldsymbol{\epsilon}} - p\mathbf{I}) \cdot \mathbf{n} &= \mathbf{0}, && \text{on } \Gamma_s \\ \mathbf{u} &= \mathbf{0}, && \text{on } \Gamma_0 \\ \mathbf{u} \cdot \mathbf{n} &= \mathbf{0} \text{ and } [(2\mu \dot{\boldsymbol{\epsilon}} - p\mathbf{I}) \cdot \mathbf{n} + \beta \mathbf{u}]_{||} = \mathbf{0}, && \text{on } \Gamma_\beta \end{aligned}$$

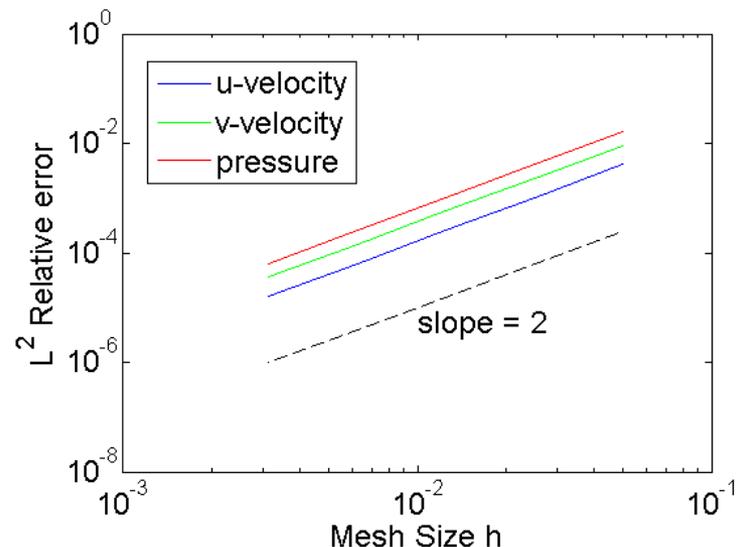
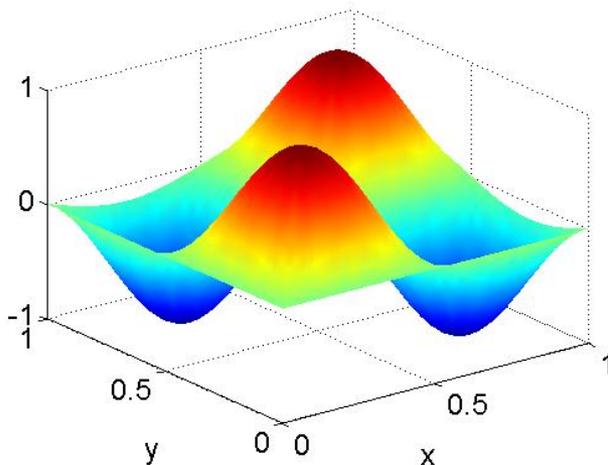
- Numerical Method:

- Discretization: classical Galerkin FEM with structured or unstructured mesh.
 - Currently, code only supports *equal*-order velocity/pressure finite elements with PSPG stabilization.
- Nonlinear solver: Newton's method
 - Automatic differentiation (AD) Jacobians using Sacado package of Trilinos.
 - Continuation in $\gamma \rightarrow 10^{-10}$ using LOCA package of Trilinos.
- Linear solver: preconditioned GMRES with ILU or algebraic multigrid preconditioner.

Full Stokes Model: Convergence Study for Linear and Non-linear Stokes

☺ Constant-coefficient Stokes flow physics with PSPG velocity/pressure finite elements verified on MMS problems, e.g., problem with the following exact solution:

$$\mathbf{u}^T = \left(\sin(2\pi x) \sin(2\pi y), \cos(2\pi x) \cos(2\pi y) \right)$$
$$p = 2\mu \sin(2\pi x) \sin(2\pi y)$$



☹ For non-linear Stokes flow physics with Glen's law viscosity, accuracy of solution with PSPG velocity/pressure finite elements is limited by stabilization.

- Future work: add capability to employ mixed velocity/pressure finite elements.



Summary and Future Work

- Development of stress-velocity solver within the MPAS/Trilinos FELIX Dycore of PISCEES is well underway.
 - Rapid code development due to leveraging of dozens of Trilinos capabilities.
 - First order (a.k.a. higher-order) Stokes physics implemented and verified.
 - Full Stokes nonlinear physics to be completed after addition of mixed pressure/velocity finite element capability into code (coming soon).
 - L1L2 physics coming soon.
- Also coming soon:
 - Interface to MPAS for mesh advection/temperature solve (Perego).
 - Interface to DAKOTA for UQ (Eldred, Jakeman).
 - Optimization algorithms for inversion/calibration (collaboration with C. Jackson).
 - Performance/scalability studies on larger problems/more realistic geometries (Worley/Tuminaro).
 - Post-processing and V&V using LIVV (Evans).

Thank you for your attention!
Questions?



References

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