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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

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

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

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

Local Fill

Discretizations
- Discretization Library
- Field Manager

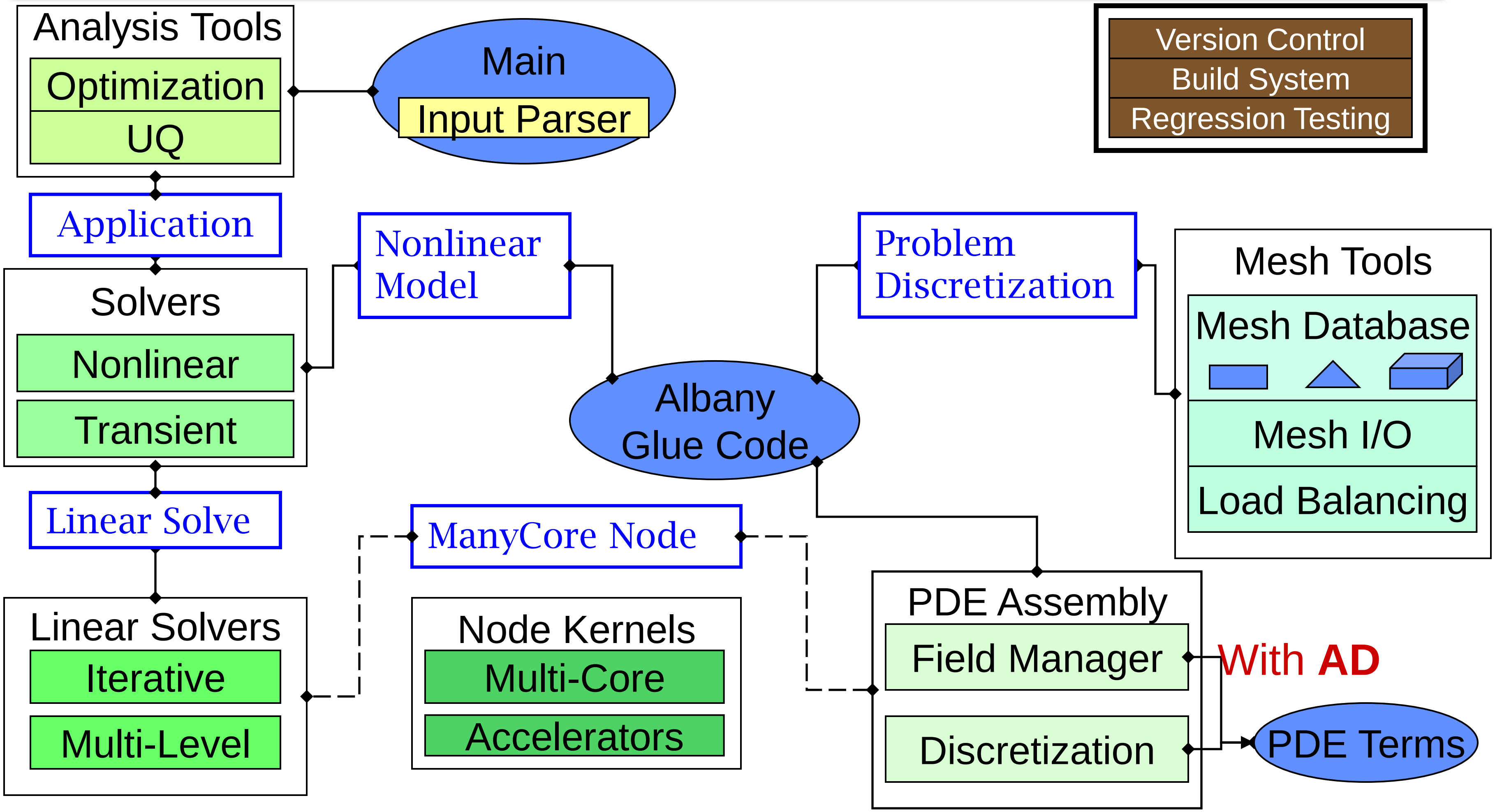
Derivative Tools
- Sensitivities
- Derivatives
- Adjoints
- UQ / PCE Propagation

Physics Fill
- Element Level Fill
- Material Models
- Objective Function
- Constraints
- Error Estimates
- MMS Source Terms

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

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

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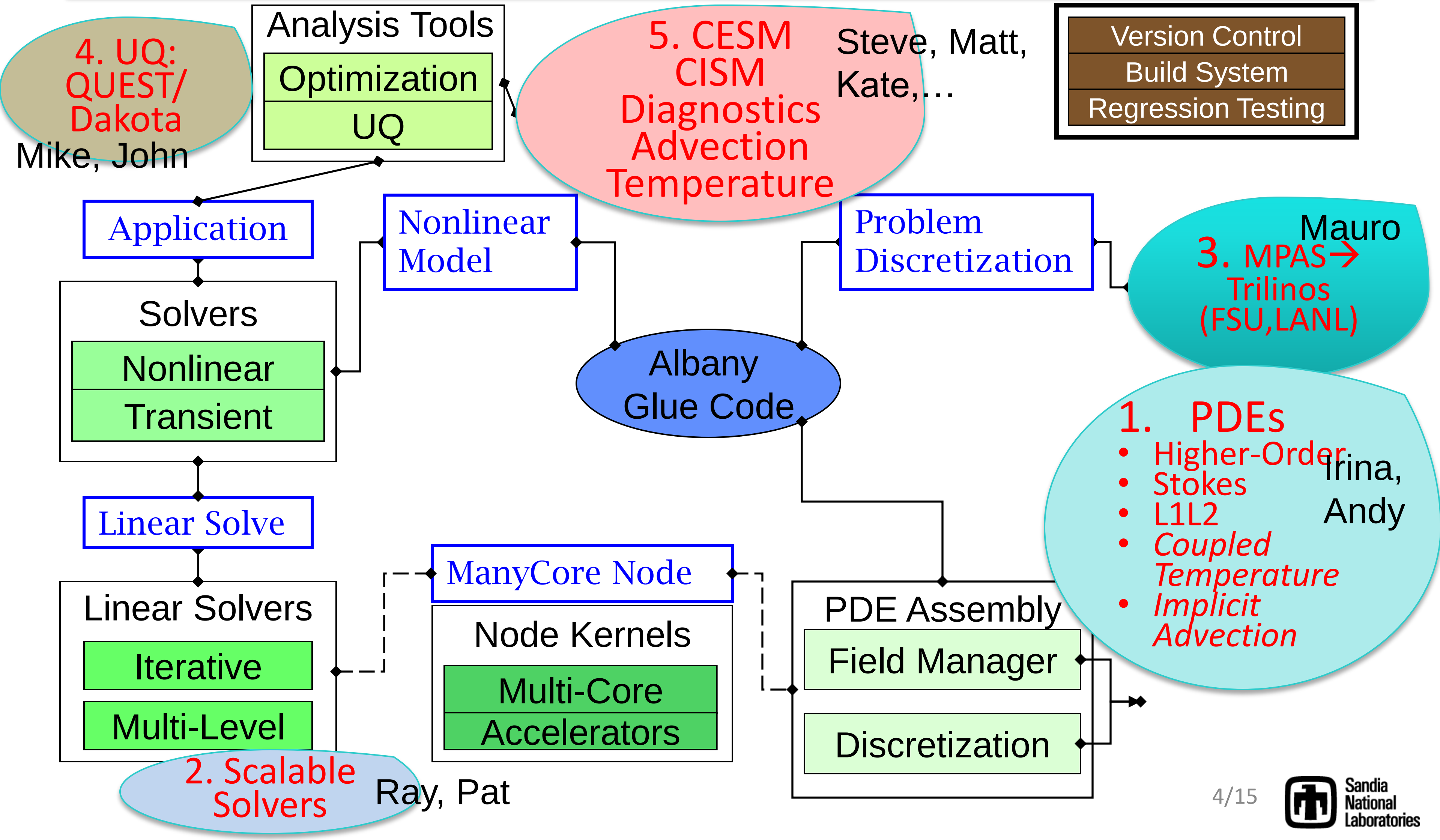
MPAS/Trilinos FELIX Dycore: Leveraging of Albany Code Base



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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:

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

with Glen's law viscosity:

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

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

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

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

A = flow rate factor
n = Glen's law exponent $= 3$
γ = regularization parameter
β = sliding coefficient ≥ 0

- Boundary conditions:

$$\begin{array}{lll} \dot{\boldsymbol{\epsilon}}_1 \cdot \mathbf{n} = 0, & \dot{\boldsymbol{\epsilon}}_2 \cdot \mathbf{n} = 0, & \text{on } \Gamma_s, \\ u = 0, & v = 0, & \text{on } \Gamma_0 \\ 2\mu \dot{\boldsymbol{\epsilon}}_1 \cdot \mathbf{n} + \beta u = 0, & 2\mu \dot{\boldsymbol{\epsilon}}_2 \cdot \mathbf{n} + \beta v = 0, & \text{on } \Gamma_\beta \end{array}$$

- 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.

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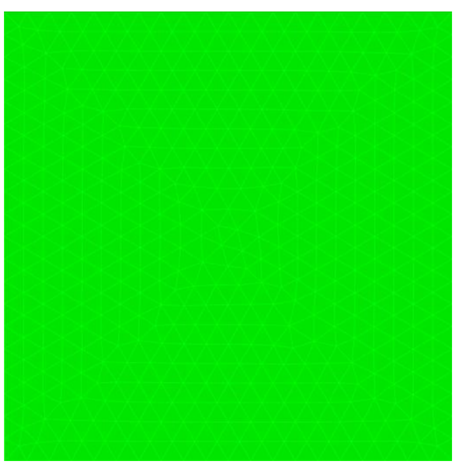
First Order (a.k.a. Higher-Order) Stokes Model: Convergence Study

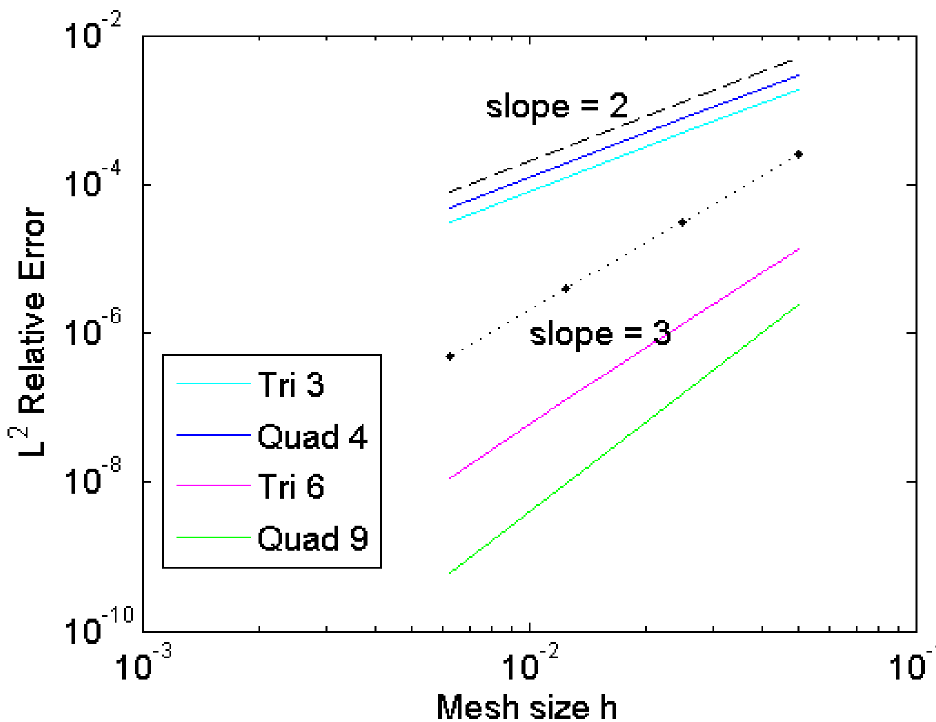
- 2D Method of Manufactured Solutions (MMS) problem: source terms f_1 and f_2 are derived such that

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

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).

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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:

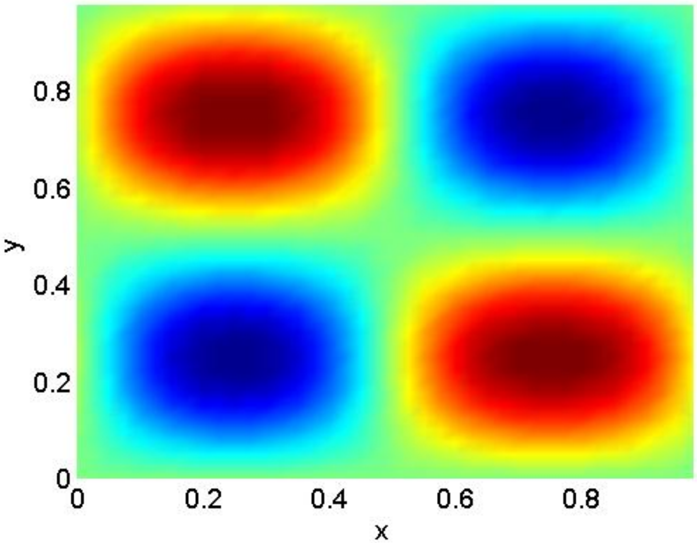
$$\begin{aligned} s(x,y) &= -x\tan\alpha, \\ b(x,y) &= s(x,y) - 1 \end{aligned}$$

- Sliding boundary conditions prescribed on basal boundary with:

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

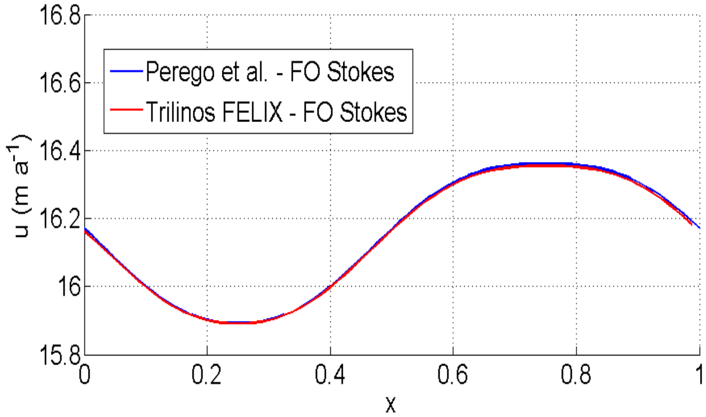
- Periodic boundary conditions in lateral directions x and y.

- Excellent agreement between results computed in Trilinos FELIX dycore and published results.

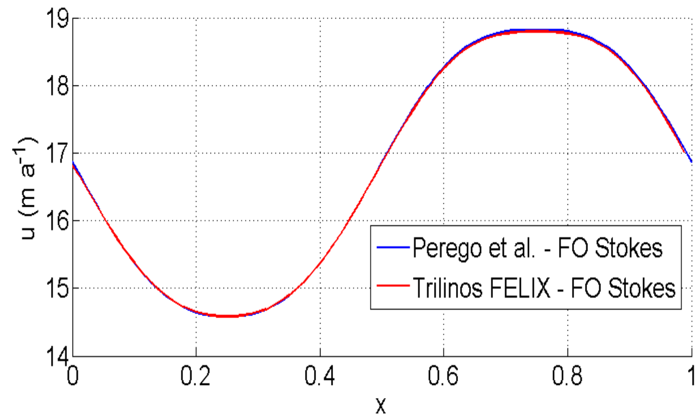


Velocity u at top surface ($L = 20$)

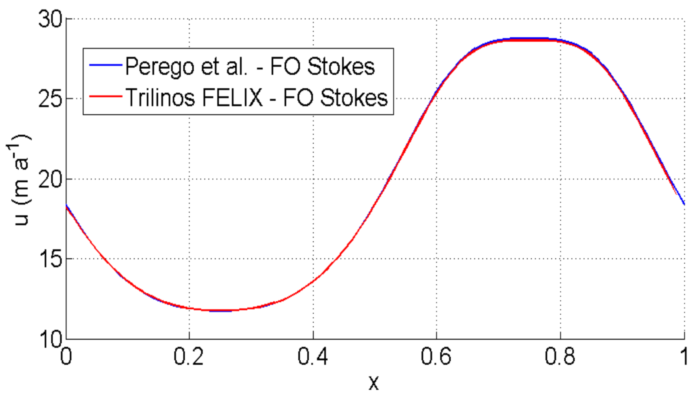
First Order (a.k.a. Higher-Order) Stokes Model: ISMIP-HOM Test C (continued)



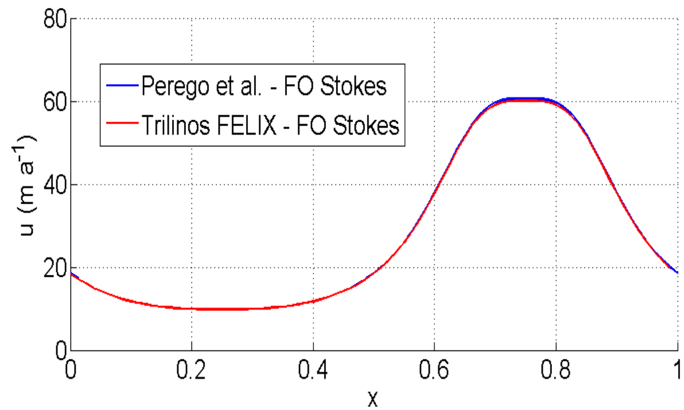
$L = 10$



$L = 20$



$L = 40$

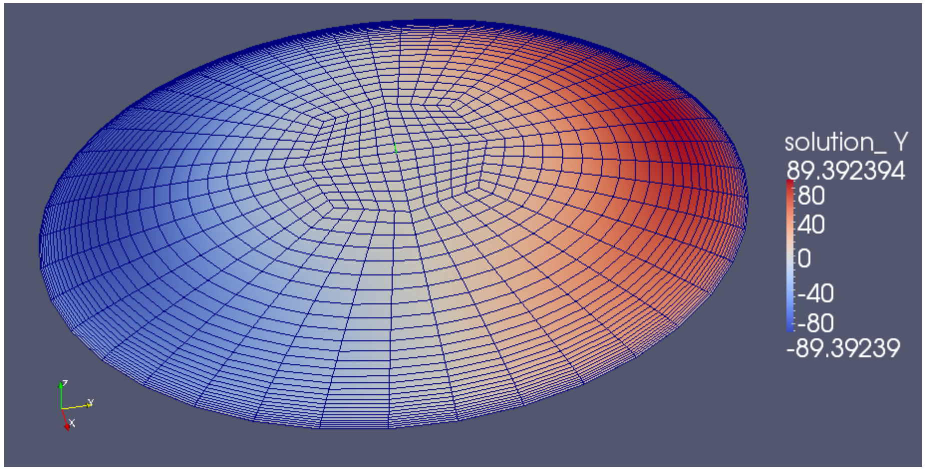


$L = 80$

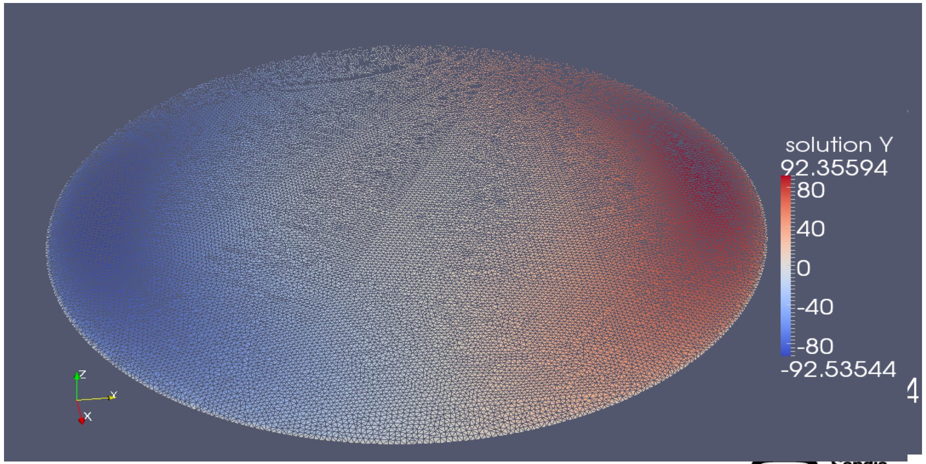
Surface velocity u as a function of x at $y = L/4$, $80x80x20$ mesh

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.*)

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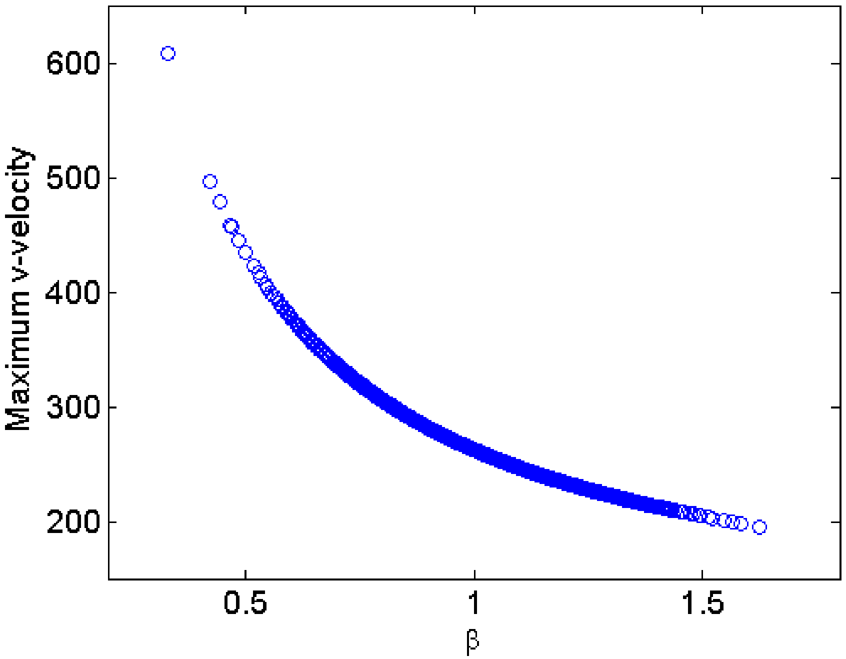
First Order (a.k.a. Higher-Order) Stokes Model: UQ Study for Dome

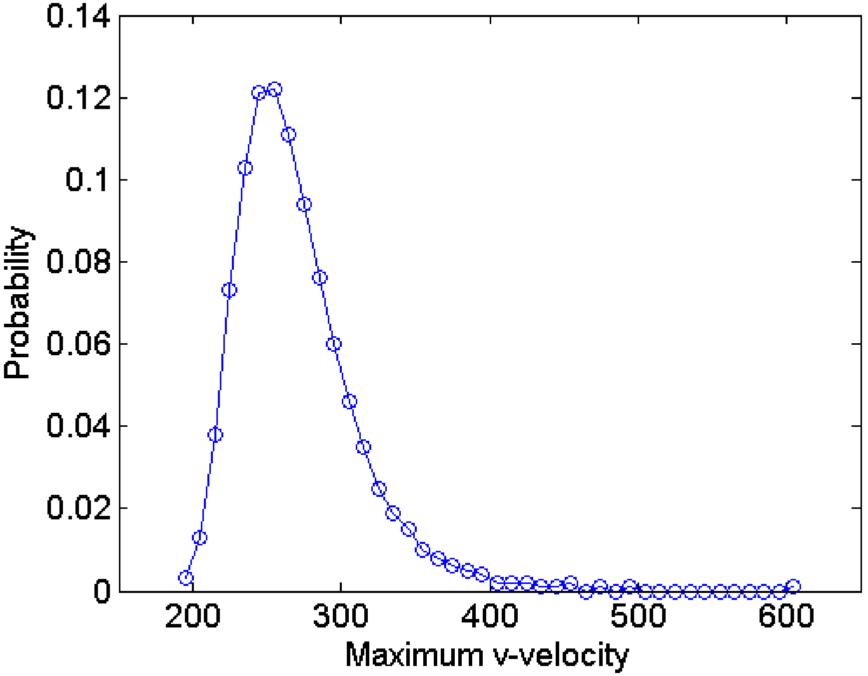
- Modified dome test case to have basal sliding boundary condition at bedrock with:

$$\beta \sim \text{Normal(mean = 1 kPa a/m, std. dev. = 0.2 kPa a/m)}$$

- UQ study with 1000 samples of β.



β vs. max v-velocity



PDF of max v-velocity

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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:

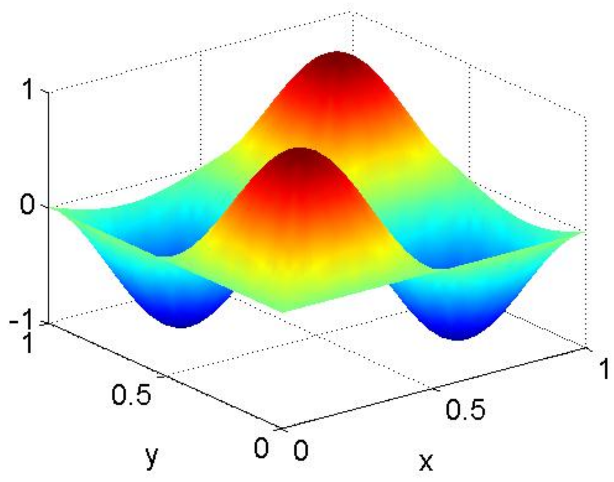
$$\begin{aligned} &(2\mu\dot{\boldsymbol{\epsilon}} - p\mathbf{I}) \cdot \mathbf{n} = \mathbf{0}, && \text{on } \Gamma_s \\ &\mathbf{u} = \mathbf{0}, && \text{on } \Gamma_0 \\ &\mathbf{u} \cdot \mathbf{n} = \mathbf{0} \text{ and } [(2\mu\dot{\boldsymbol{\epsilon}} - p\mathbf{I}) \cdot \mathbf{n} + \beta\mathbf{u}]_{||}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

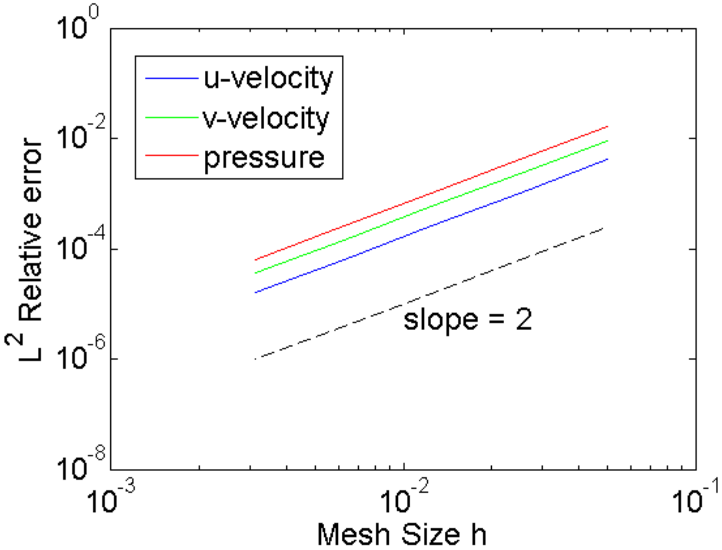
- Numerical Method:
  - Discretization: classical Galerkin FEM with structured or unstructured mesh.
    - Currently, code only supports *equal*-order velocity/pressure finite elements with PSPG stabilization.
  - Nonlinear solver: Newton's method
    - Automatic differentiation (AD) Jacobians using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

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





☹ 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.

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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?

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