Argonne NATIONAL LABORATORY

... for a brighter future

Scalable Ice-sheet Solvers and Infrastructure for Petascale, High-resolution, Unstructured Simulations (SISIPHUS)

A Brief Summary

Ice Sheet Kickoff Meeting
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A One-sentence Description

"For this project, we propose to develop techniques for solving the fully 3D Stokes problem, for continent-scale ice sheets, integrated over hundreds or thousands of years, on petascale computers ..."

[by developing]

"... more accurate, high-performing ice sheet modeling methods, and a framework for constructing the models, connecting them to solvers,and coupling them to regional and global climate models."

Technical Outline

- Modeling methods
  - 3D Stokes solver
  - High-order shallow ice model
  - Energy balance model
  - Regional ocean model
- Enabling technologies
  - Mesh generation & geometry
  - Solvers & physics-based preconditioning
  - Solution coupling
  - Adjoint & inverse methods
- Model integration

Non-Newtonian Stokes system

$$-\nabla \cdot (\eta D\boldsymbol{u}) + \nabla p - \boldsymbol{f} = 0$$
$$\nabla \cdot \boldsymbol{u} = 0$$

$$D\boldsymbol{u} = \tfrac{1}{2}\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right)$$
$$\gamma(D\boldsymbol{u}) = \tfrac{1}{2} D\boldsymbol{u} : D\boldsymbol{u}$$
$$\eta(\gamma) = B(\Theta, \dots)(\epsilon + \gamma)^{\frac{\mathfrak{p}-2}{2}}$$
$$\mathfrak{p} = 1 + \tfrac{1}{\mathfrak{n}} \approx \tfrac{4}{3}$$
$$T = \mathbf{1} - \boldsymbol{n} \otimes \boldsymbol{n}$$

with boundary conditions

$$(D\boldsymbol{u} - p\mathbf{1}) \cdot \boldsymbol{n} = \begin{cases} \mathbf{0} & \text{free surface} \\ -\rho_w z \boldsymbol{n} & \text{ice-ocean interface} \end{cases}$$

$$\boldsymbol{u} = \mathbf{0} \qquad \text{frozen bed, } \Theta < \Theta_0$$

$$\left.\begin{aligned} \boldsymbol{u} \cdot \boldsymbol{n} &= \boldsymbol{g}_{\text{melt}}(T\boldsymbol{u}, \dots) \\ T(D\boldsymbol{u} - p\mathbf{1}) \cdot \boldsymbol{n} &= \boldsymbol{g}_{\text{slip}}(T\boldsymbol{u}, \dots) \end{aligned}\right\} \text{nonlinear slip, } \Theta \geq \Theta_0$$

$$\boldsymbol{g}_{\text{slip}}(T\boldsymbol{u}) = \beta_{\mathfrak{m}}(\dots)|T\boldsymbol{u}|^{\mathfrak{m}-1} T\boldsymbol{u}$$

Navier $\mathfrak{m} = 1$, Weertman $\mathfrak{m} \approx \frac{1}{3}$, Coulomb $\mathfrak{m} = 0$.

Other critical equations

- Mesh motion

$$-\nabla \cdot \boldsymbol{\sigma} = 0 \qquad \boldsymbol{\sigma} = \mu\left[2D\boldsymbol{w} + (\nabla \boldsymbol{w})^T \nabla \boldsymbol{w}\right] + \lambda \operatorname{tr}(\nabla \boldsymbol{w})\mathbf{1}$$

surface: $(\dot{\boldsymbol{x}} - \boldsymbol{u}) \cdot \boldsymbol{n} = q_{BL}, \; T\boldsymbol{\sigma} \cdot \boldsymbol{n} = 0 \qquad \boldsymbol{w} = \boldsymbol{x} - \boldsymbol{x}_0$

- Enthalpy transport

$$\rho\left[\frac{\partial}{\partial t}\Theta + (\boldsymbol{u} - \dot{\boldsymbol{x}}) \cdot \nabla\Theta\right] - \nabla \cdot \left[\kappa(\Theta)\nabla\Theta + \boldsymbol{q}_D(\Theta)\right] - \eta D\boldsymbol{u} : D\boldsymbol{u} = 0$$

  - ALE advection
  - Fourier/Fick diffusion
  - Darcy flow
  - Strain heating

Note: $\kappa(\Theta)$ and $\boldsymbol{q}_D(\Theta)$ are very sensitive near $\Theta = \Theta_0$

Summary of primal variables in DAE

u	velocity	algebraic
p	pressure	algebraic
x	mesh location	algebraic in domain, differential at surface
Θ	enthalpy	differential

Going Deeper...

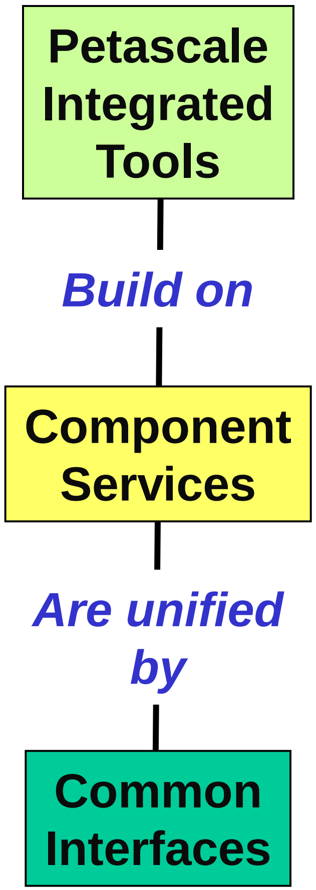
- Geometry/mesh
  - Ustructured, hexahedral grid (sweepable in 3 parts)
  - Discrete/mesh-based geometry for bed, w/ smooth normals
  - Can adapt to coastline & near bed, while remaining sweep-meshed
- Modeling
  - Method of lines approach (discretize over space – DAE, then over time)
  - hp-adaptive FE method w/ assembly-free solution
- Preconditioning
  - "Dual-order" scheme over space – high-order FE, preconditioned with low-order (linear) elements from high-order nodes
  - Apply block-ILU to Jacobian, replacing specific parts with "strategically-chosen" (physics-based) preconditioners
- Adjoints in component-based code
  - Differentiate through component APIs
  - Designing solver approach so it's also applicable to adjoint

Implementation Details

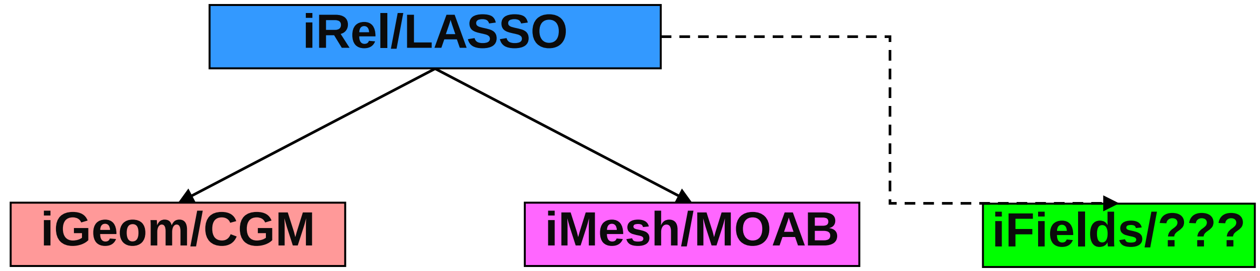
- Broader goal: use component-based solvers & tools (e.g. Petsc, ITAPS) to solve a challenging physics problem at scale
  - Higher-level interface to Petsc for expressing physics and physics-based preconditioners in component form
    - *Separates overall solution strategy from specifics of physics models, allowing variations on either side of that interface*
    - *Facilitates coupling to other parts of GCM*
  - Petsc Data Manager (DM) implementation based on ITAPS mesh interface
    - *Re-usable for other types of physics*
    - *Use DMComposite to express coupling between meshes*

ITAPS In One Slide

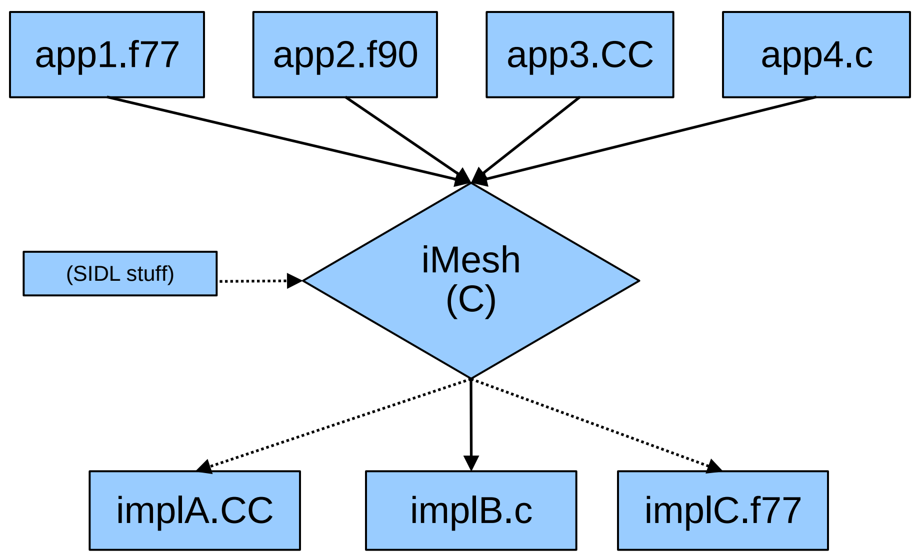
37k foot view:



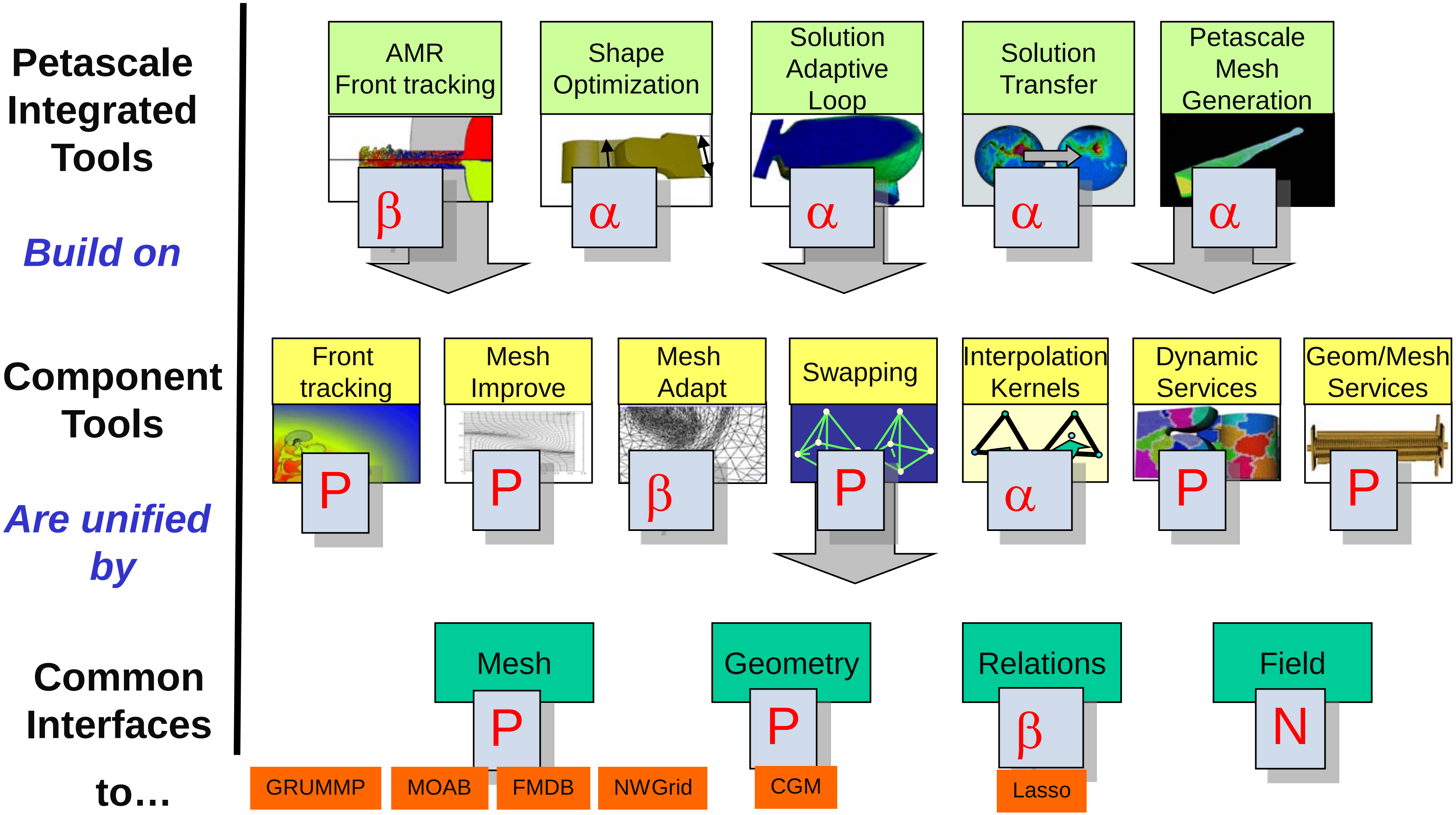
Interface relationships:



Application view:



ITAPS Tools & Services



P = production   β = Beta   α = alpha   N = new