Bridging the Gap: Harnessing advanced Computational Libraries for coupled multi-physics problems

Marc Spiegelman[1,2] and **Cian R. Wilson**[1]
Plus enormous contributions from PETSc, FEniCS and AMCG groups

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BTG, Princeton, 1–2 October 2012

Introduction

Motivation

- Computation is essential for exploring non-linear multi-physics problems in Geosciences
- Major advances in hardware, software and algorithms make complex problems more accessible.
- However, still a considerable gap between Geosciences and Computational Sciences/Math.
- Some Existing Barriers:
  - Overall Complexity of both software libraries and models
  - Lack of transparency/reproducibility/reusability of current models
  - Language/Training issues between computation and Earth Sciences

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  - Language/Training issues between computation and Earth Sciences
- *We need better tools for exploring complex (and simple) models and making advanced computation accessible to more general users.*

Target Application : multi-physics models of magmatic plate boundaries

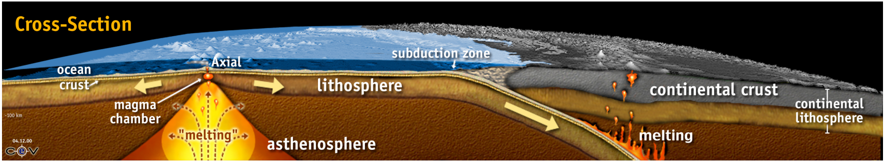

image courtesy of the Neptune project (www.neptune.washington.edu)

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  - Seismic, Volcanic and Tsunamagenic Natural Hazards
  - global tectonics and geochemical cycling

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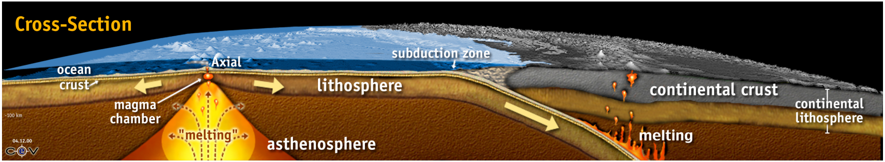

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  - Coupled fluid-solid mechanics
  - Complex solid rheologies
  - Coupled thermodynamics/geodynamics

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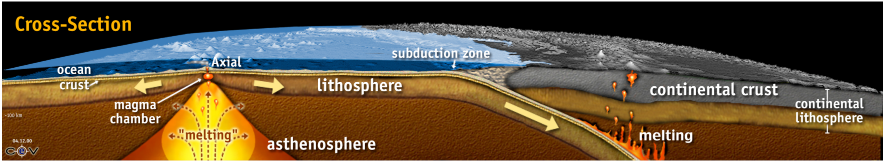

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  - Coupled fluid-solid mechanics
  - Complex solid rheologies
  - Coupled thermodynamics/geodynamics
- **Considerable uncertainty** in equations, constitutive relations and coupling

Model Requirements

User Flexibility:

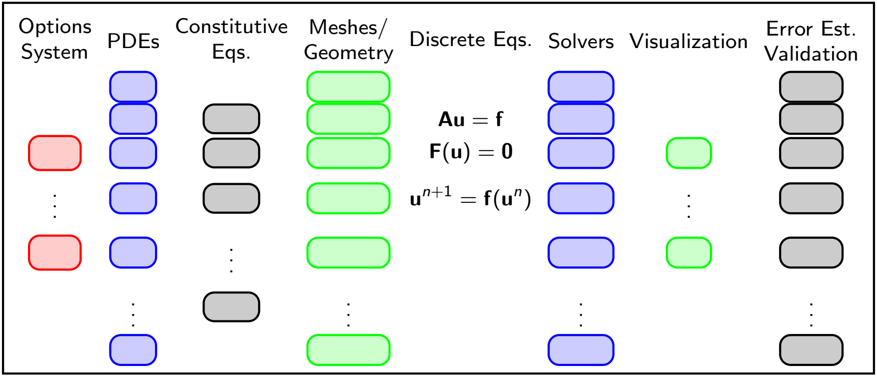
- Choice of **equations**, geometry, elements, constitutive relations, coupling
- Wide choice of solvers/preconditioners for **coupled non-linear** problems
- Ability to rapidly compose a range of models from simple process models to regional geodynamic models
- All choices available at or near run time

Model Requirements

Infrastructure:

- Residual monitoring for the *full coupled problem*
- Model reproducibility:
  - Transparent options system
  - Regression tested
- Generic model services:
  - Standardized I/O
  - Checkpointing
  - Monitoring and detectors
- Parallel, scaleable, open source, version controlled, regression tested... free

Generic Structure of PDE Based Numerical Models



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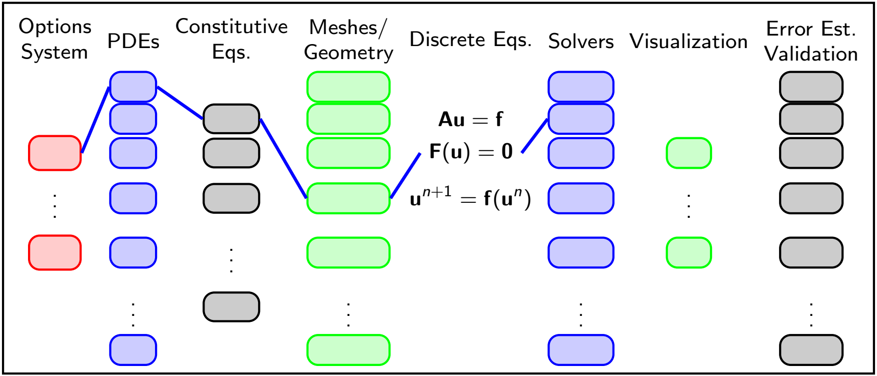

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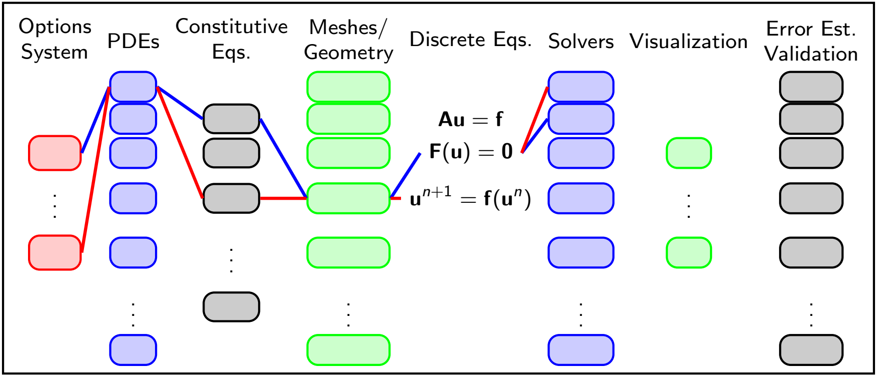

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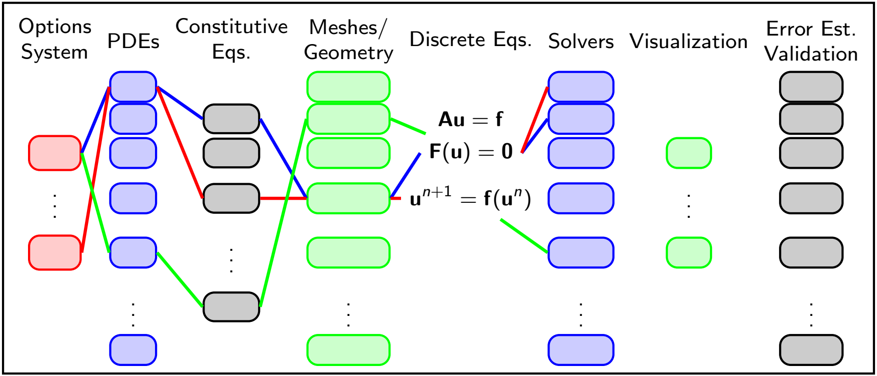

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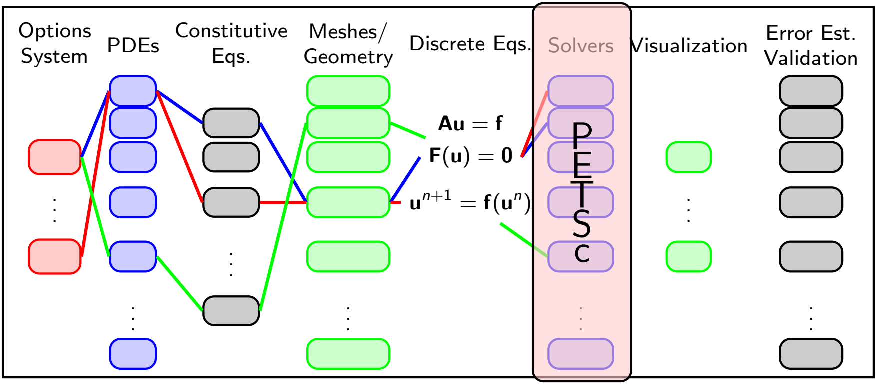

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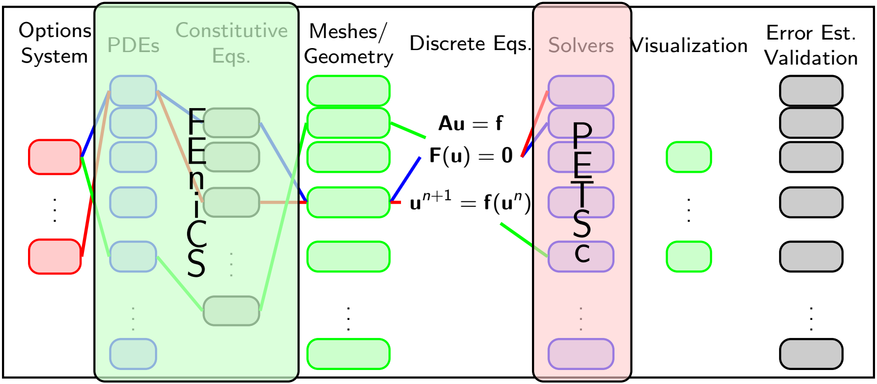

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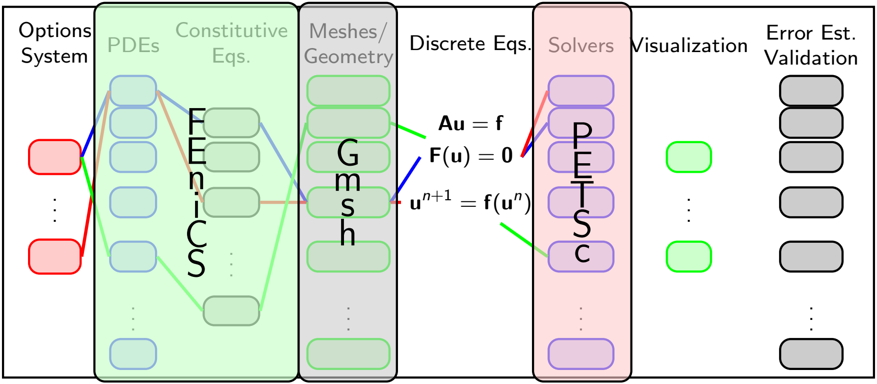

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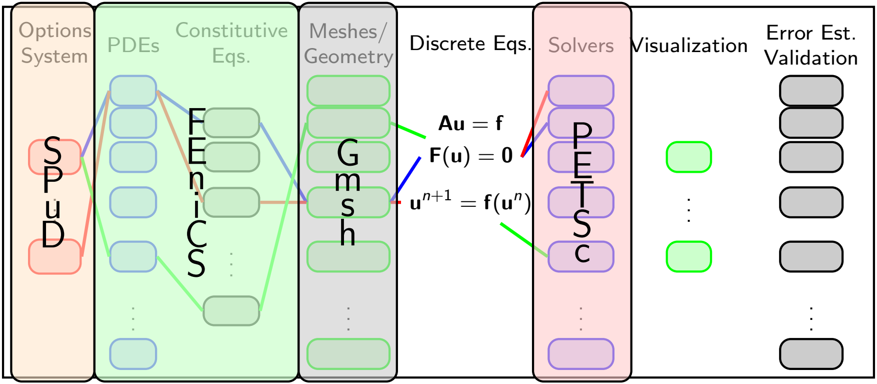
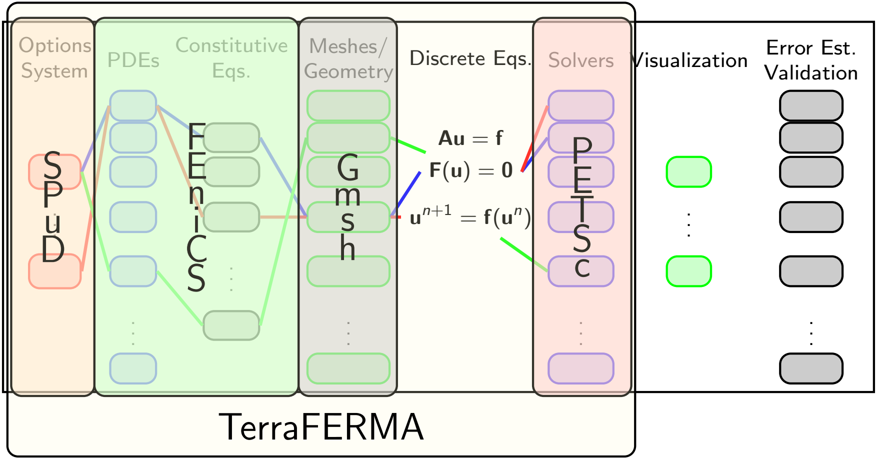
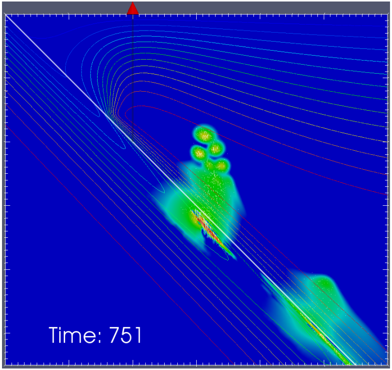




Transparent Finite Element Rapid Model Assembler

Application: Fluid Migration in Subduction Zones



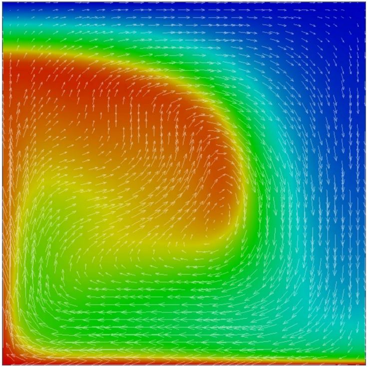
$$\nabla\cdot\left(2\eta\left(\frac{\nabla\mathbf{v_s}+\nabla\mathbf{v_s}^T}{2}\right)\right)=\nabla p^*+\varphi_0\varphi\mathbf{k}$$

$$\nabla\cdot\mathbf{v_s}=\varphi_0\frac{\mathcal{P}}{\zeta}$$

$$-\nabla\cdot\frac{K}{\mu}\nabla\mathcal{P}+\frac{\mathcal{P}}{\zeta}=-\nabla\cdot\left(\frac{K}{\mu}\mathbf{k}-\nabla p^*\right)+\Gamma\frac{\Delta\rho}{\rho_f\varphi_0}$$

$$\frac{D\varphi}{Dt}=(1-\varphi_0\varphi)\frac{\mathcal{P}}{\zeta}+\frac{\Gamma}{\varphi_0}$$

Example: Infinite Prandtl Thermal Convection



$$-\nabla\cdot\left[2\ \mu\ \left(\frac{\nabla v+\nabla v^{T}}{2}\right)\right]+\nabla p-T k=0,$$

$$\nabla\cdot v=0,$$

$$\frac{\partial T}{\partial t}+\ v\ \cdot\nabla T+\frac{1}{\mathrm{Ra}}\nabla^{2}T=0$$

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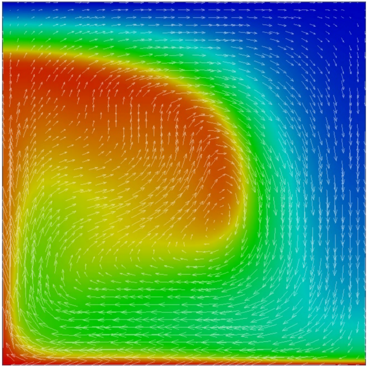

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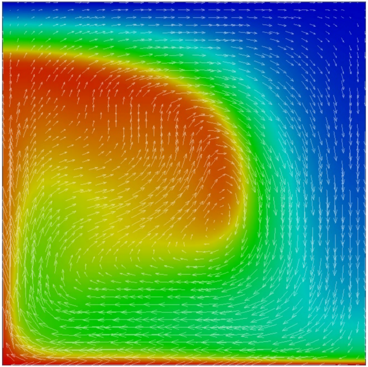

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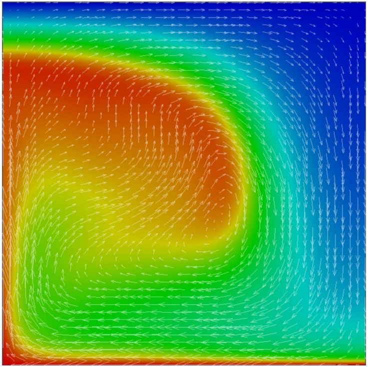

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Let $u=(v,p,T)$

$$u_{i+1}=u_i-\alpha J(u_i)^{-1}r(u_i)$$

Example: FEniCS Equation Description

Given function $u = (v, p, T)$, test function $u_t = (v_t, p_t, T_t)$ and trial function $u_a = (v_a, p_a, T_a)$:

Weak form of residual, $r(u)$:

$$r_V = \int_\Omega \left[\left(\frac{\nabla v_t + \nabla v_t^T}{2} \right) : 2\mu \left(\frac{\nabla v + \nabla v^T}{2} \right) - \nabla \cdot v_t p - (v_t)_z T \right],$$

$$r_p = \int_\Omega p_t \nabla \cdot v,$$

$$r_T = \int_\Omega \left[T_t \left((T - T_n) + \Delta t v_\theta \cdot \nabla T_\theta \right) + \frac{\Delta t}{\mathrm{Ra}} \nabla T_t \cdot \nabla T_\theta \right]$$

$$r = r_V + r_p + r_T$$

Weak form of Jacobian, $J(u)$:

$$J = r'(u)$$

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Given function $u = (v, p, T)$, test function $u_t = (v_t, p_t, T_t)$ and trial function $u_a = (v_a, p_a, T_a)$:

Weak form of residual, $r(u)$:

```
r_v = (inner(sym(grad(v_t)), 2.*mu*sym(grad(v)))
      - div(v_t)*p - T*v_t[1] )*dx
r_p = p_t*div(v)*dx
r_T = (T_t*((T - T_n) + dt*inner(v_theta, grad(T_theta)))
      + (dt/Ra)*inner(grad(T_t), grad(T_theta)) )*dx

r =   r_v + r_p + r_T
```

Weak form of Jacobian, $J(u)$:

```
J = derivative(r, u, u_a)
```

Example: PETSc Block Preconditioning & Solvers

$$J(u_i)\delta u = -r(u_i)$$

$$J = \begin{pmatrix} K_{11} & K_{12} & G_1 & C_1 \\ K_{21} & K_{22} & G_2 & C_2 \\ G_1^T & G_2^T & \mathbf{0} & \mathbf{0} \\ B_1 & B_2 & \mathbf{0} & A \end{pmatrix}$$

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Stokes Advection-Diffusion

Example: PETSc Block Preconditioning & Solvers

$$\tilde{J}_{\mathrm{PC}}(u_i)^{-1} J(u_i)\delta u = -\tilde{J}_{\mathrm{PC}}(u_i)^{-1} r(u_i)$$

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System
(fgmres, fieldsplit)

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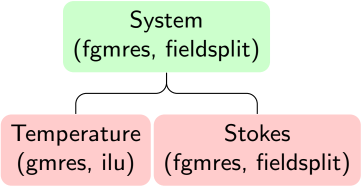

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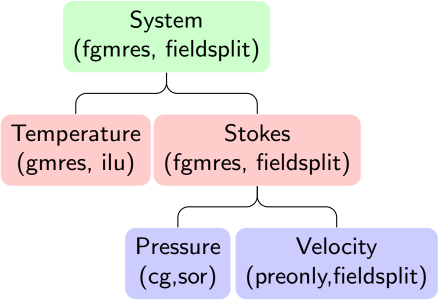

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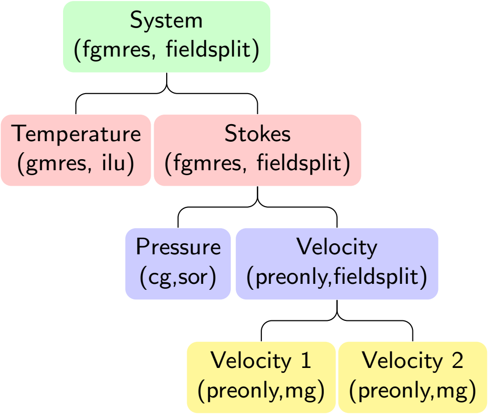

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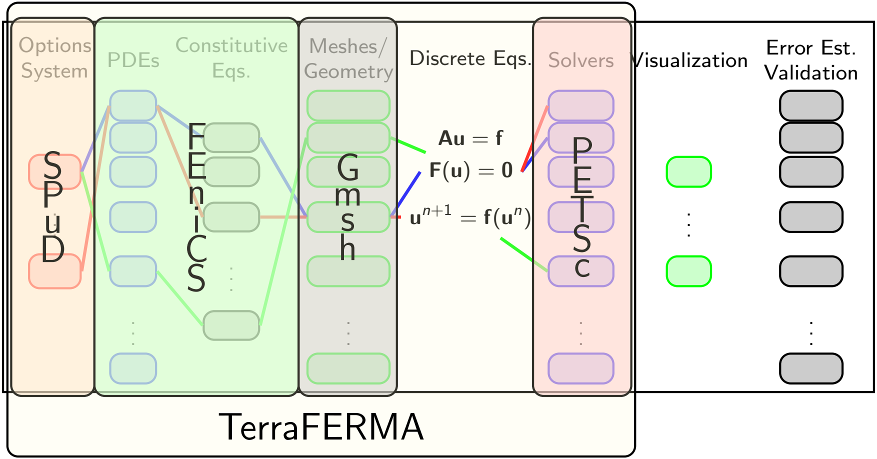
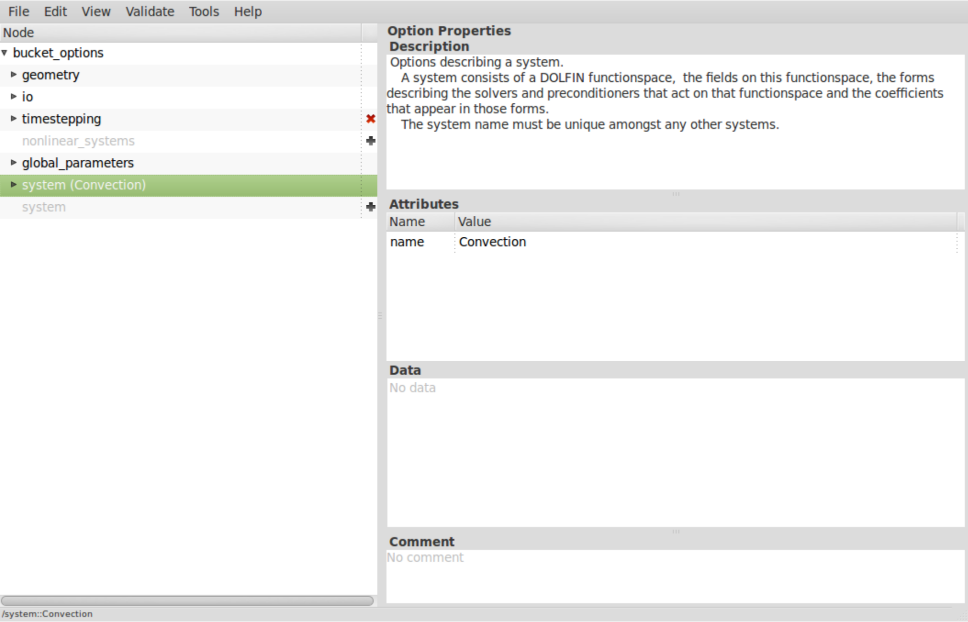


Transparent Finite Element Rapid Model Assembler

Example: TerraFERMA Options



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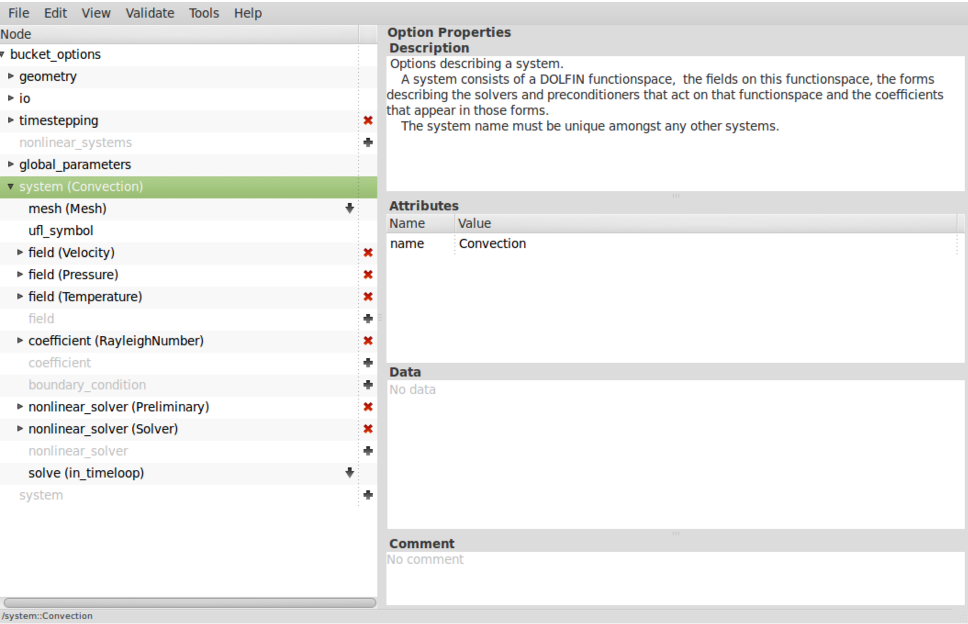
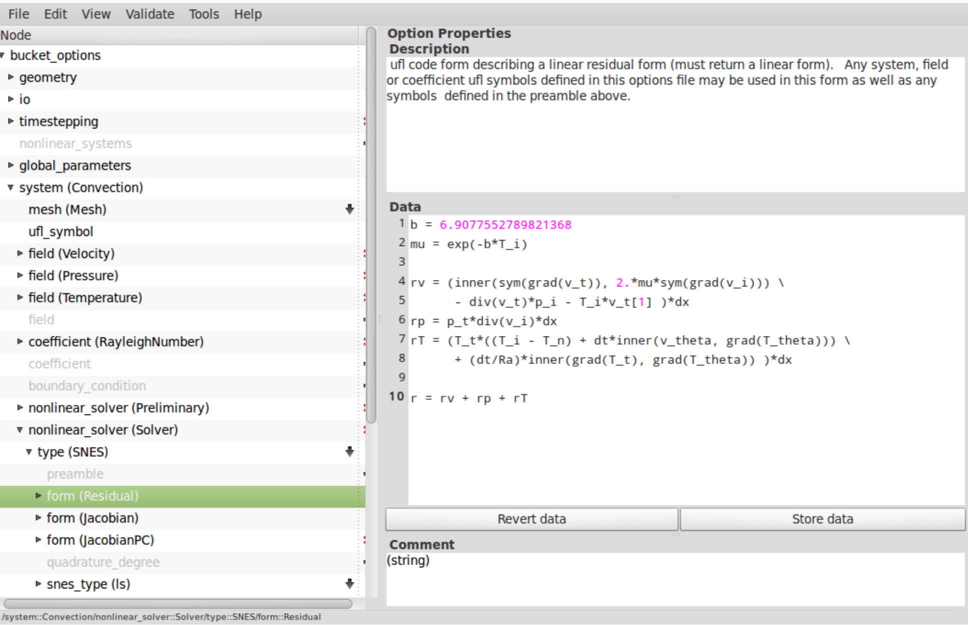


Example: Setting Equations in TerraFERMA



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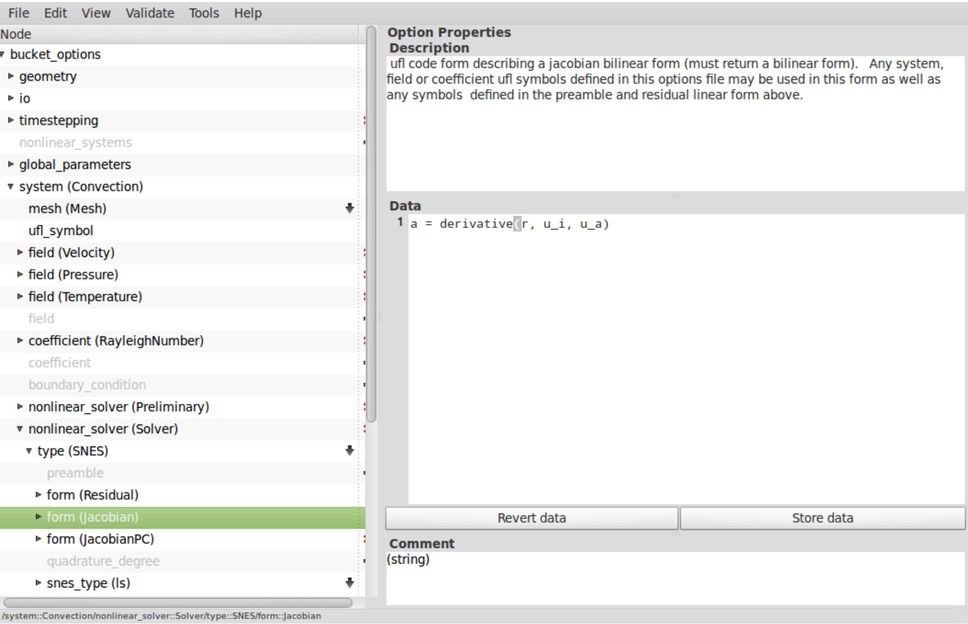
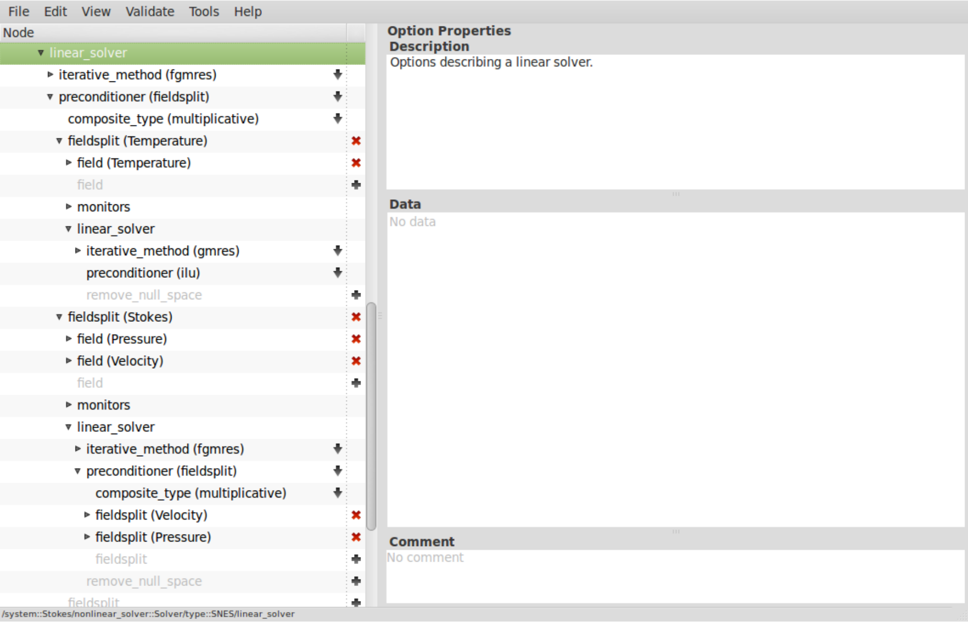


Example: Solver Options in TerraFERMA



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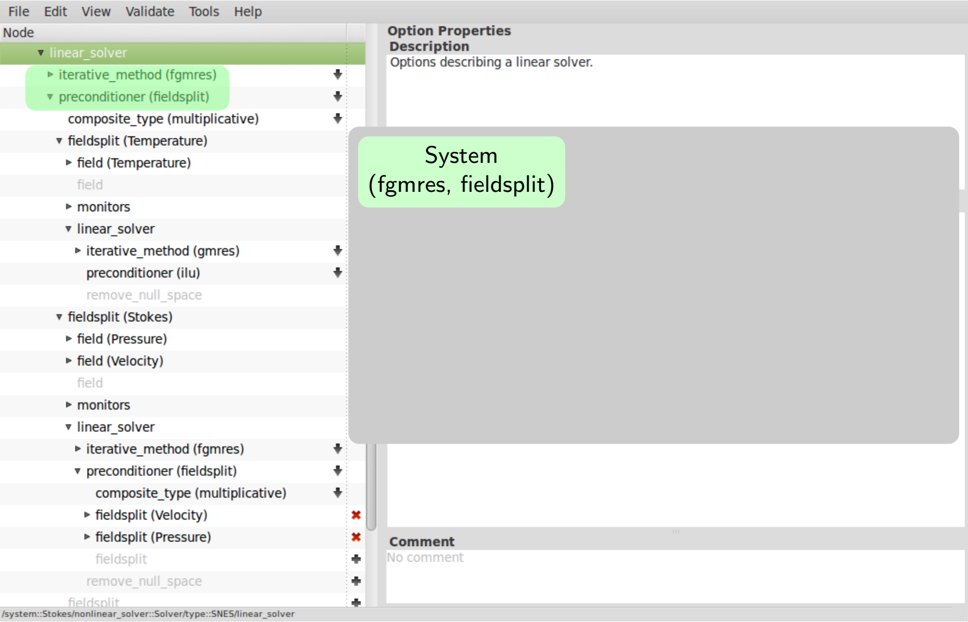

System
(fgmres, fieldsplit)

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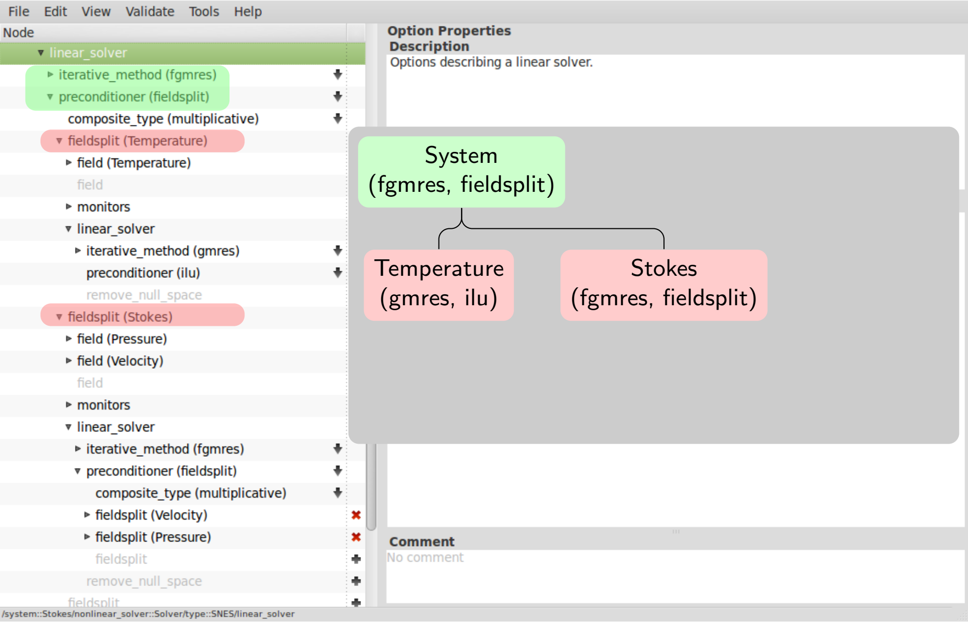

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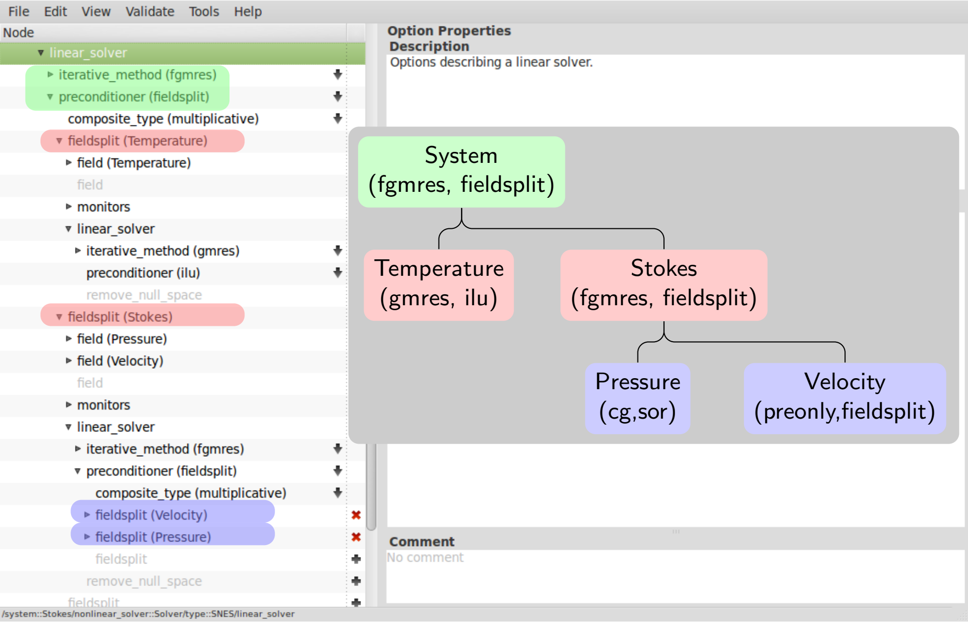
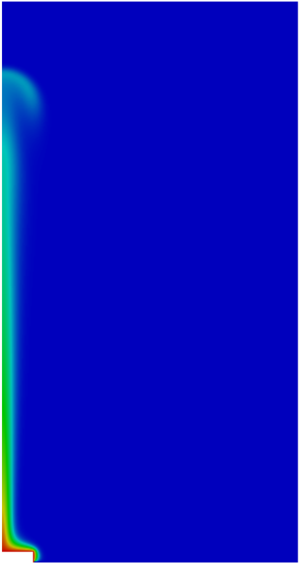


Example: Benchmark (Blankenbach, 1989)

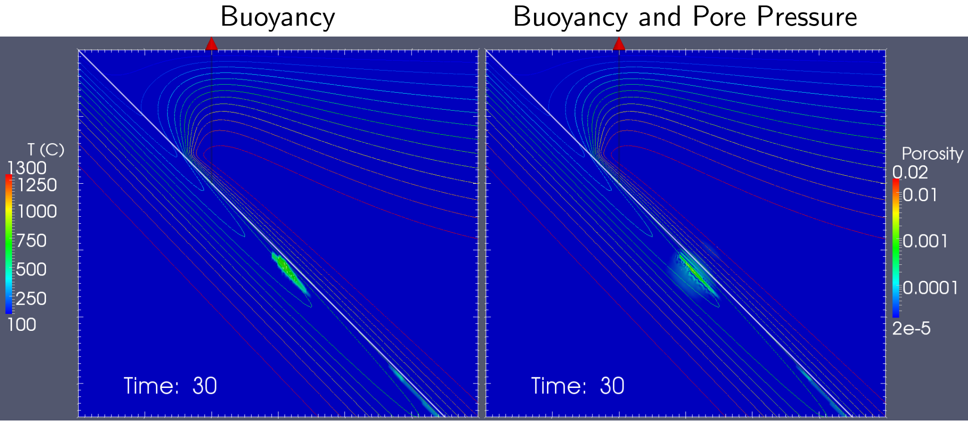
		Nu	v_{rms}	q_1	q_2	T_e	z_e
$\mathrm{Ra} = 10^4$ isoviscous	32×32	4.887	42.865	8.060	0.589	0.422	0.226
	64×64	4.885	42.865	8.059	0.589	0.422	0.226
	128×128	4.885	42.865	8.059	0.589	0.422	0.225
	Benchmark	4.884	42.865	8.059	0.589	0.422	0.225
$\mathrm{Ra} = 10^5$ isoviscous	32×32	10.539	193.222	19.081	0.722	0.428	0.114
	64×64	10.535	193.215	19.080	0.723	0.428	0.111
	128×128	10.534	193.215	19.080	0.723	0.428	0.112
	Benchmark	10.534	193.214	19.079	0.723	0.428	0.112
$\mathrm{Ra} = 10^6$ isoviscous	32×32	21.982	834.024	46.008	0.877	0.432	0.059
	64×64	21.971	833.990	45.972	0.877	0.432	0.058
	128×128	21.972	833.989	45.967	0.877	0.432	0.058
	Benchmark	21.972	833.990	45.964	0.877	0.432	0.058
$\mathrm{Ra} = 10^4$ T-dep viscosity	32×32	10.069	479.951	17.533	1.007	0.739	0.062
	64×64	10.066	480.385	17.531	1.008	0.740	0.063
	128×128	10.064	480.257	17.528	1.008	0.740	0.063
	Benchmark	10.066	480.433	17.531	1.009	0.741	0.062

Current Benchmarks

- Incompressible 2D Convection (Blankenbach et al, 1989)
- Incompressible 3D Convection (Busse et al., 1994)
- Cylindrical Laminar Plumes (Vatteville et al., 2009)
- Compressible 2D Convection (King et al., 2009)
- Kinematic Subduction Zones (van Keken et al., 2008)
- Linearized Free Surface Evolution (Kramer et al., 2012)
- Non-linear magma waves (Simpson and Spiegelman, 2011)
- Cylindrical Convection (Rhodri Davies: rhodri.davies@imperial.ac.uk)



Fluid Migration



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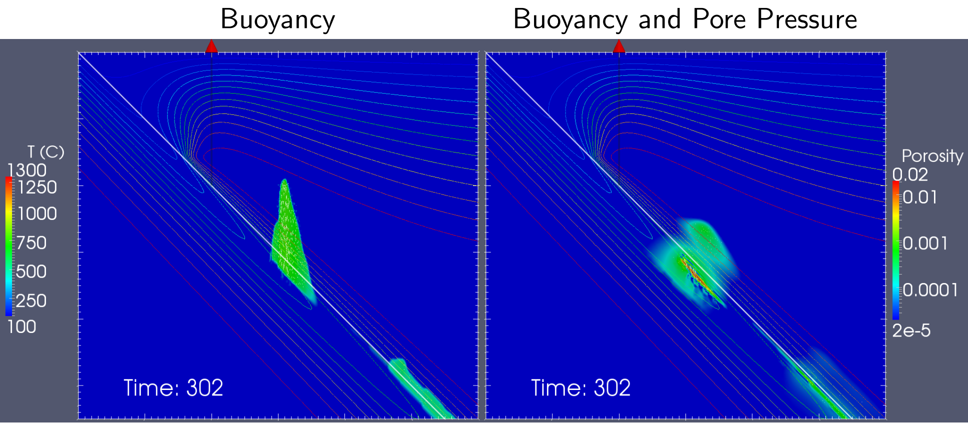
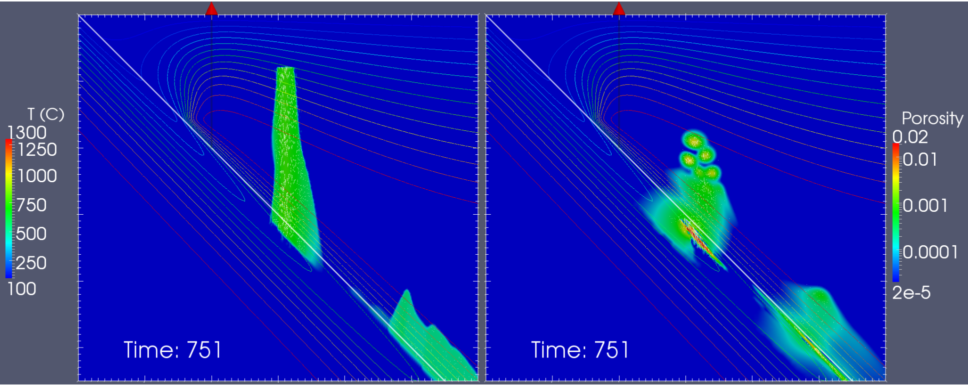


Fluid Migration

Buoyancy | Buoyancy and Pore Pressure



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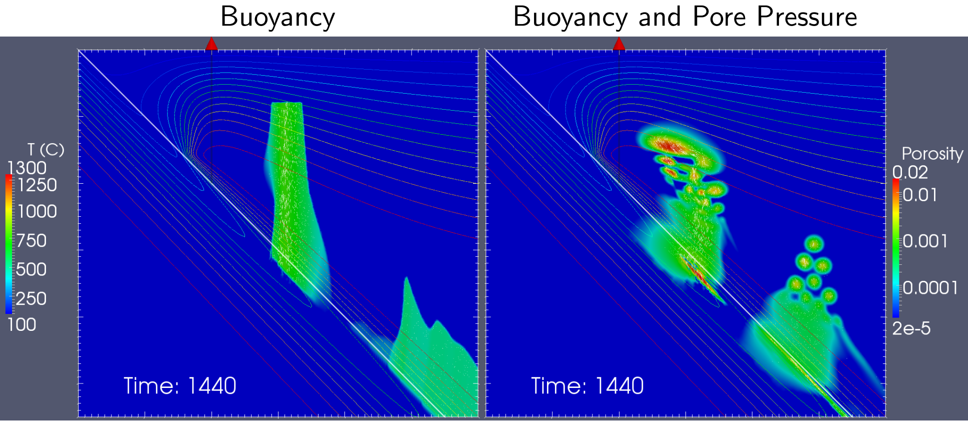
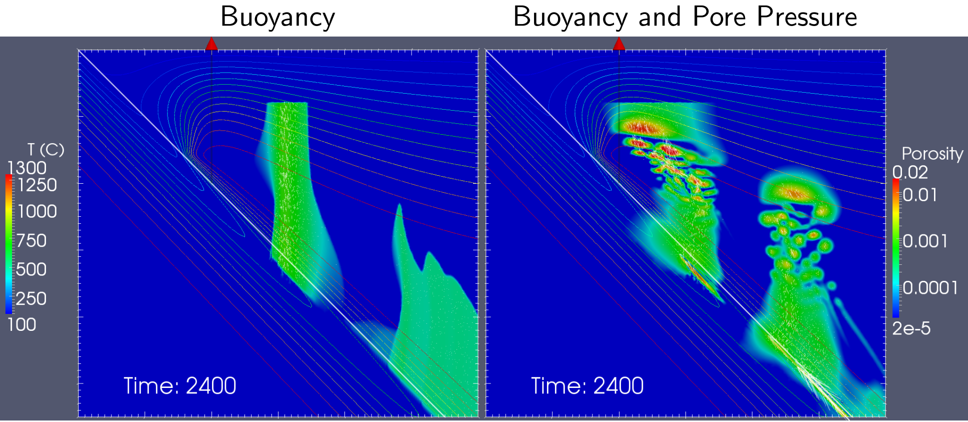


Fluid Migration



Conclusions

- Many important problems in Earth Sciences can be described by non-linear coupled systems of partial differential equations.
- Much of the complexity modelling these systems stems from the nature of multi-physics where small changes in the coupling between fields or constitutive relations can lead to radical changes in behavior and the resulting demands on discretizations and solvers.
- Many established "single-physics" models have locked in solution strategies that are unsuited or difficult to extend to the more challenging non-linear behaviour of a multi-physics system.
- We require a significant increase in flexibility for users for both composing problems (from simple model problems to more 'realistic' coupled simulations) and changing solver strategies.
- Several advanced, open-source computational libraries mean that it is now possible to provide much greater flexibility to the user.
- TerraFERMA is a model building framework that gives access to these libraries while also providing a transparent description of the model.

Equations (Katz et al., 2007)

Solid flow for solid velocity, $\mathbf{v_s}$, and dynamic pressure, p^*:

$$\nabla \cdot \left(2\,\eta\,\left(\frac{\nabla \mathbf{v_s} + \nabla \mathbf{v_s}^T}{2}\right)\right) = \nabla p^* + \varphi_0\,\varphi\,\mathbf{k}$$

$$\nabla \cdot \mathbf{v_s} = \varphi_0 \frac{\mathcal{P}}{\zeta}$$

Fluid flow for pore pressure, $\mathcal{P}$, and porosity, φ:

$$-\nabla \cdot \frac{K}{\mu} \nabla \mathcal{P} + \frac{\mathcal{P}}{\zeta} = -\nabla \cdot \left(\frac{K}{\mu} \mathbf{k} - \nabla p^* \right) + \Gamma \frac{\Delta\rho}{\rho_f \varphi_0}$$

$$\frac{D\varphi}{Dt} = \left(1 - \varphi_0 \varphi\right) \frac{\mathcal{P}}{\zeta} + \frac{\Gamma}{\varphi_0}$$

Constitutive relations:

$$\eta = \eta\left(T, \dot{\epsilon}, \varphi\right), \quad \zeta = \eta \varphi^{-m}, \quad K = \varphi^n$$

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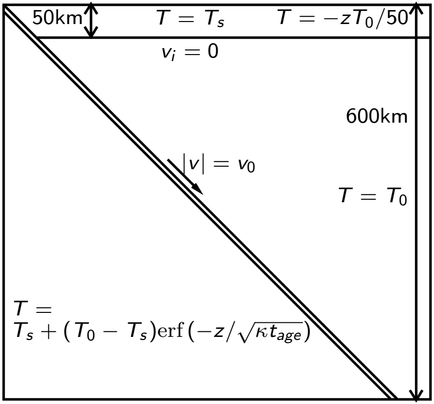
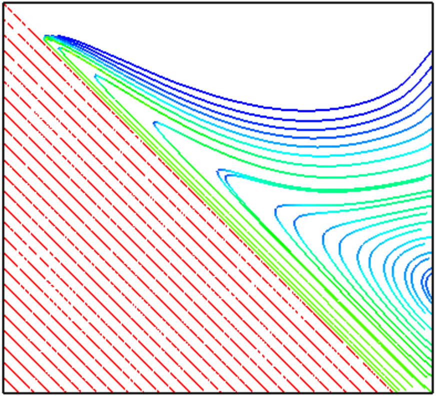
Solid Flow



Velocity streamlines



Equations

Buoyancy and Pore Pressure:

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Equations

Buoyancy (zero compaction length approximation):

$$\frac{D\varphi}{Dt} = -\nabla \cdot \frac{K}{\mu}\mathbf{k} + \frac{\Gamma}{\varphi_0}\left(\frac{\Delta\rho}{\rho_f} + 1\right)$$

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