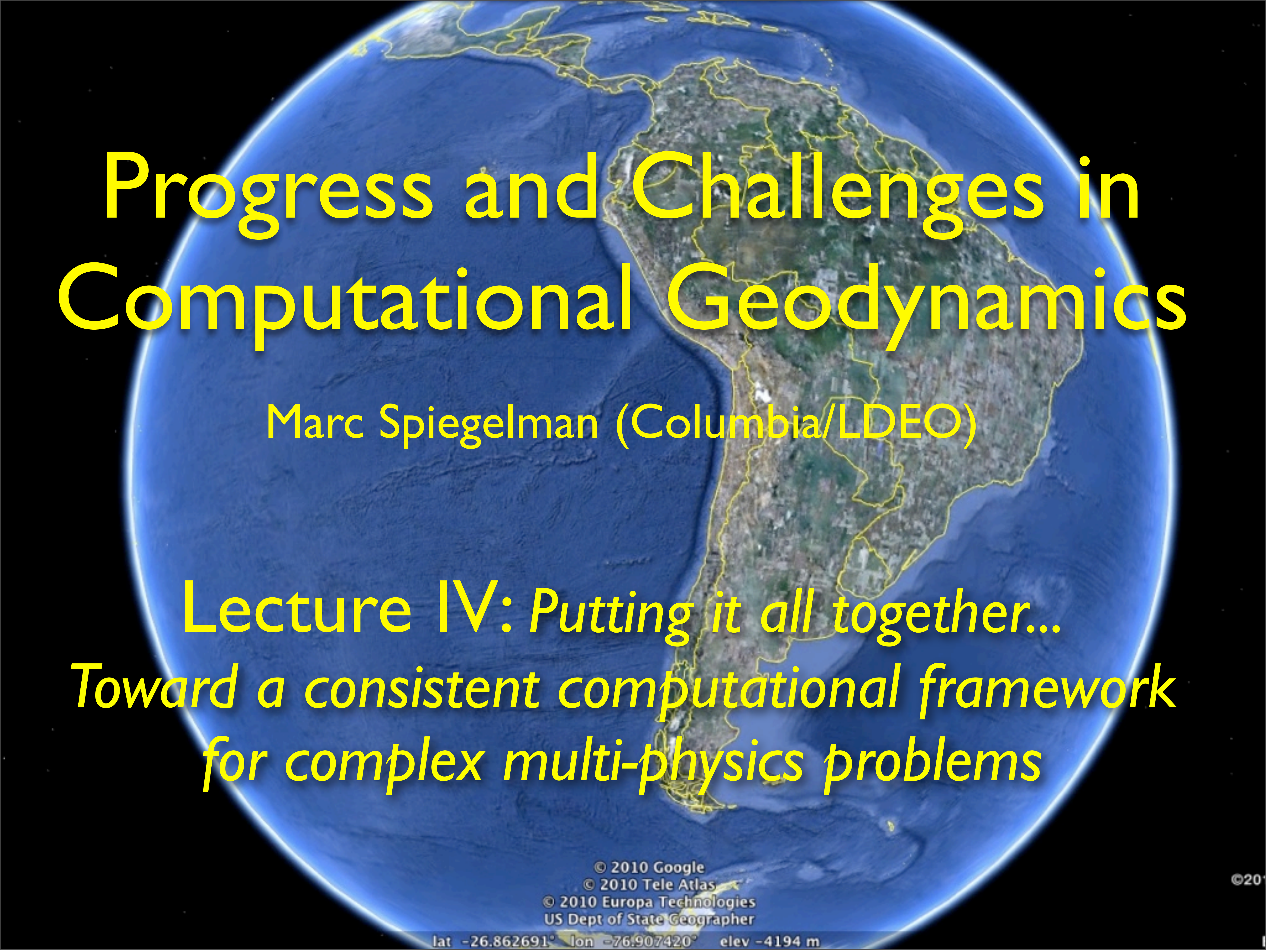
Progress and Challenges in Computational Geodynamics

Marc Spiegelman (Columbia/LDEO)

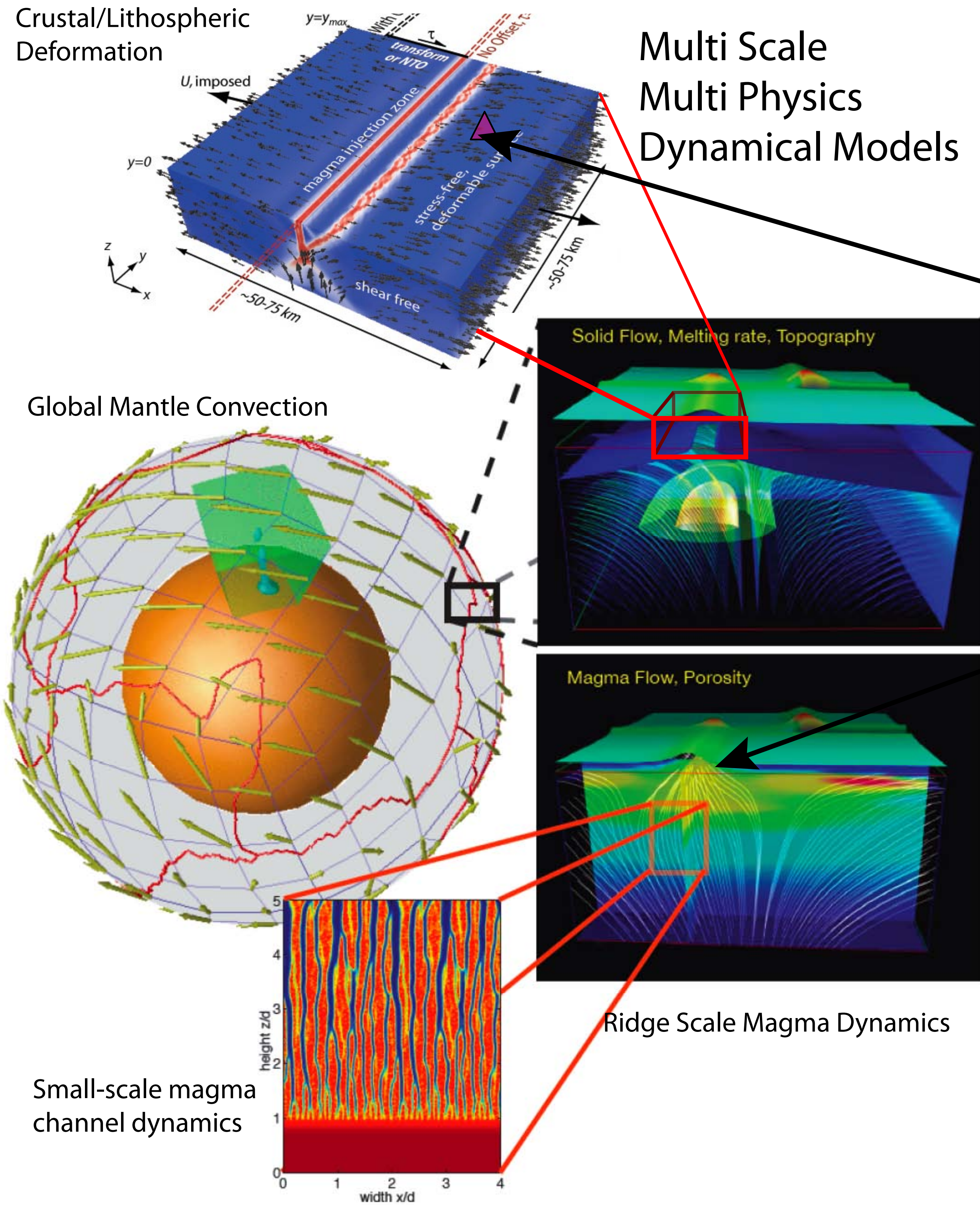
Lecture IV: *Putting it all together...*
Toward a consistent computational framework for complex multi-physics problems

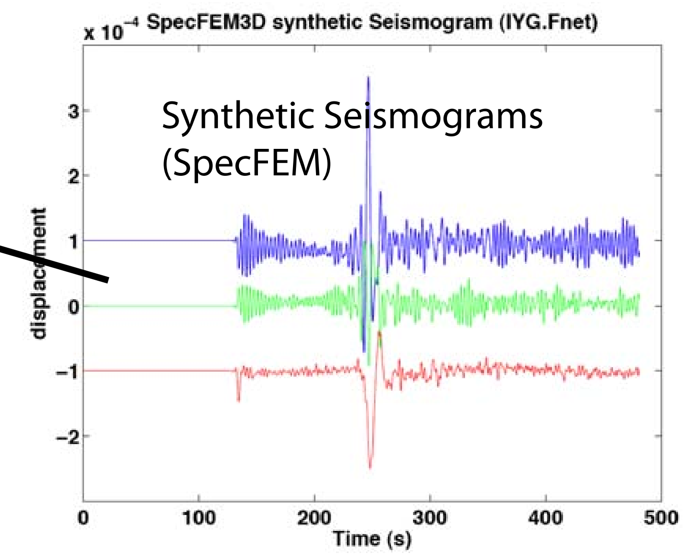


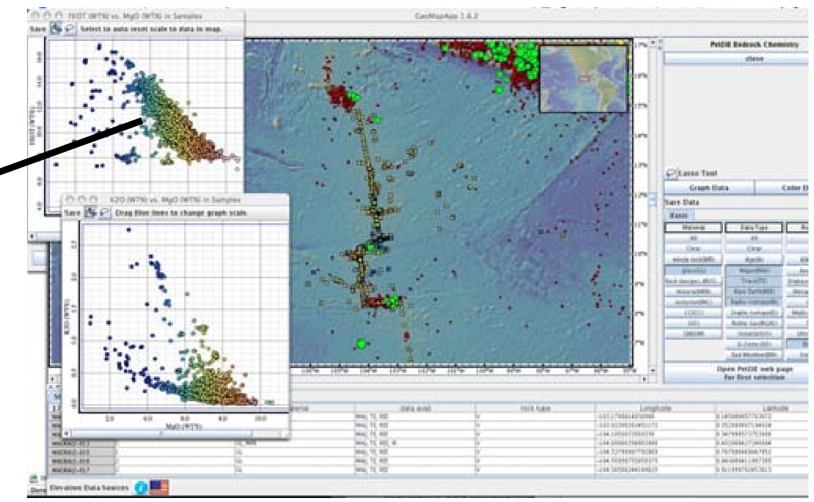
Outline

- Motivation: multi-physics issues arising from Solid Earth Geodynamics
- Some Philosophy
- Advanced software for PDE based modeling (FEniCS/PETSc)
- A model multi-physics problem: thermal convection
  - Discretization
  - Physics-based Block-Preconditioners
  - Results: Convergence/Performance
- The Future...

Multi-Scale Multi-physics problems in Solid Earth Geodynamics





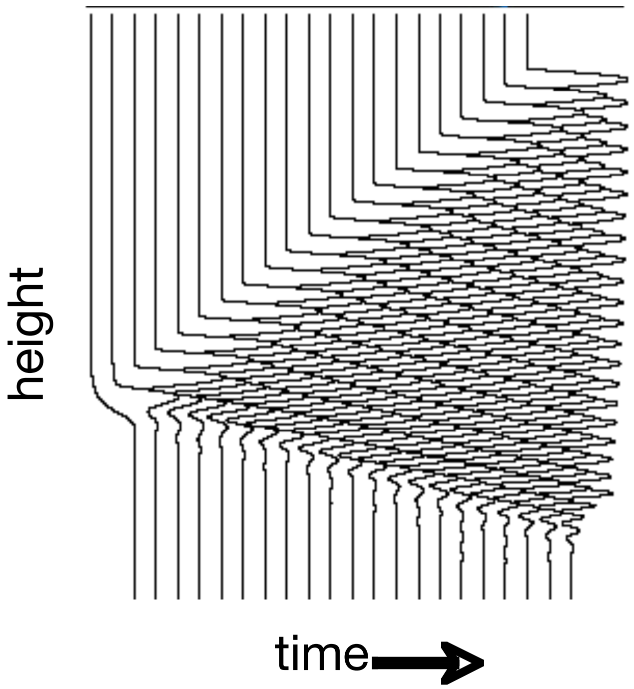


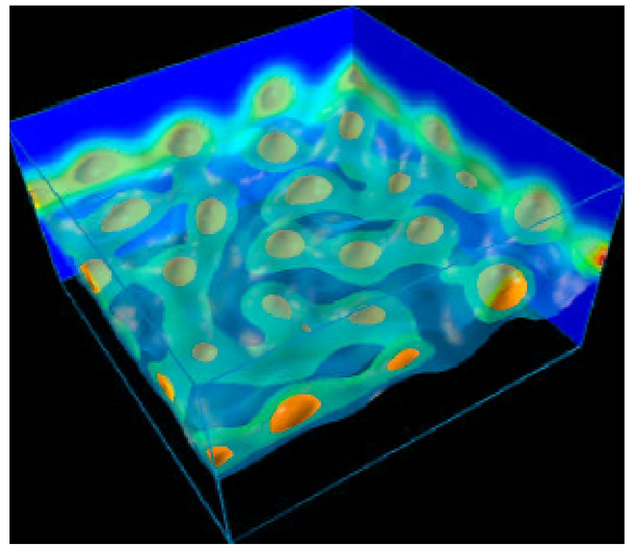
Geochemistry/Petrology (PetDB/GeoMapApp)

Observational Constraints

Basic Behavior of Magma PDEs

Nonlinear Porosity Waves

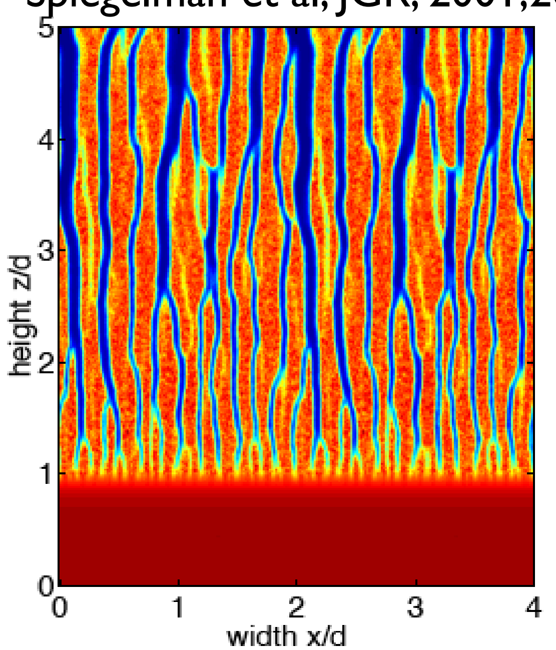


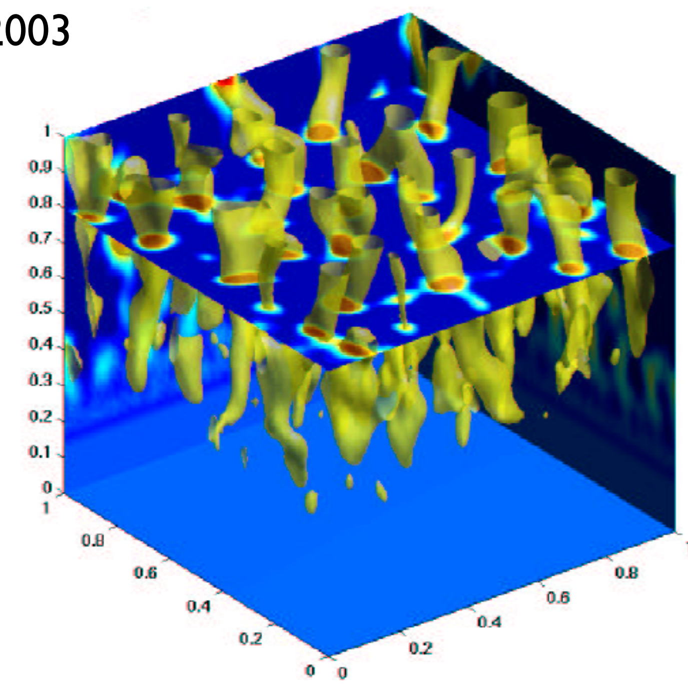


Spiegelman, JFM 93, W&S, GRL 94

Reactive Channel formation

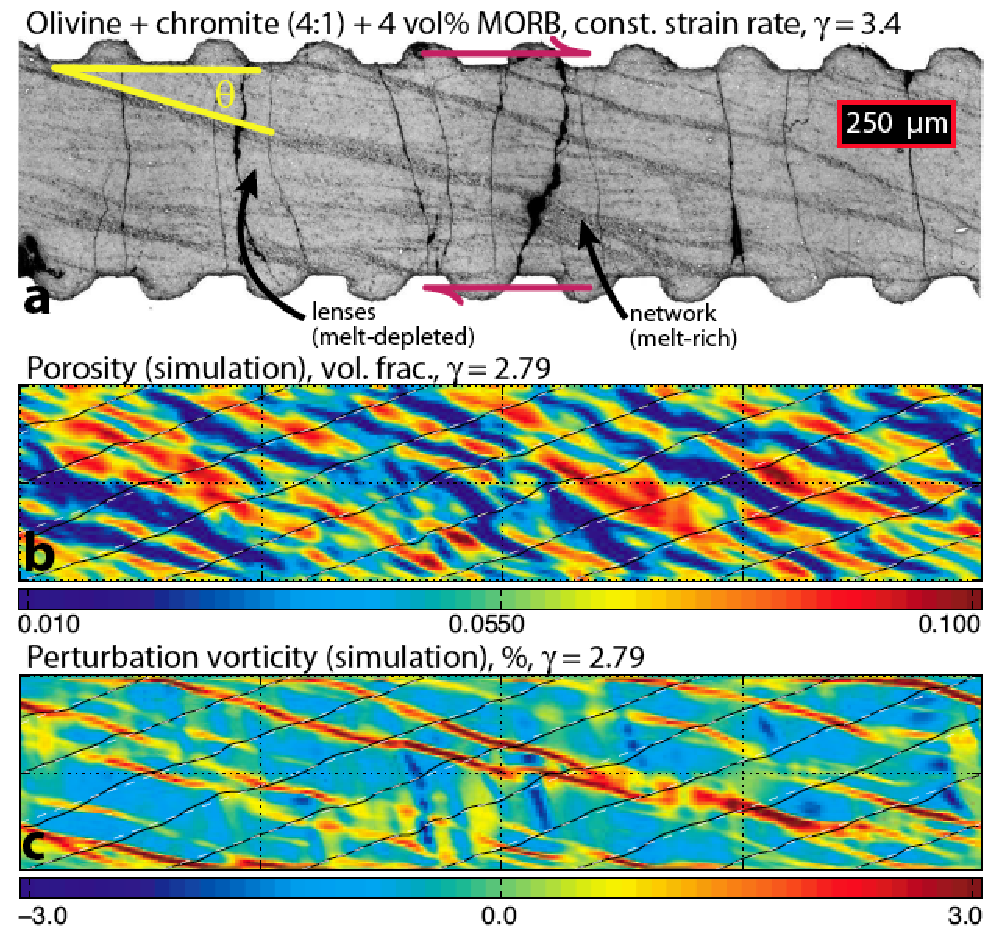
Spiegelman et al, JGR, 2001,2003





Mechanical Melt Localization

(Katz et al., 2006, Nature)

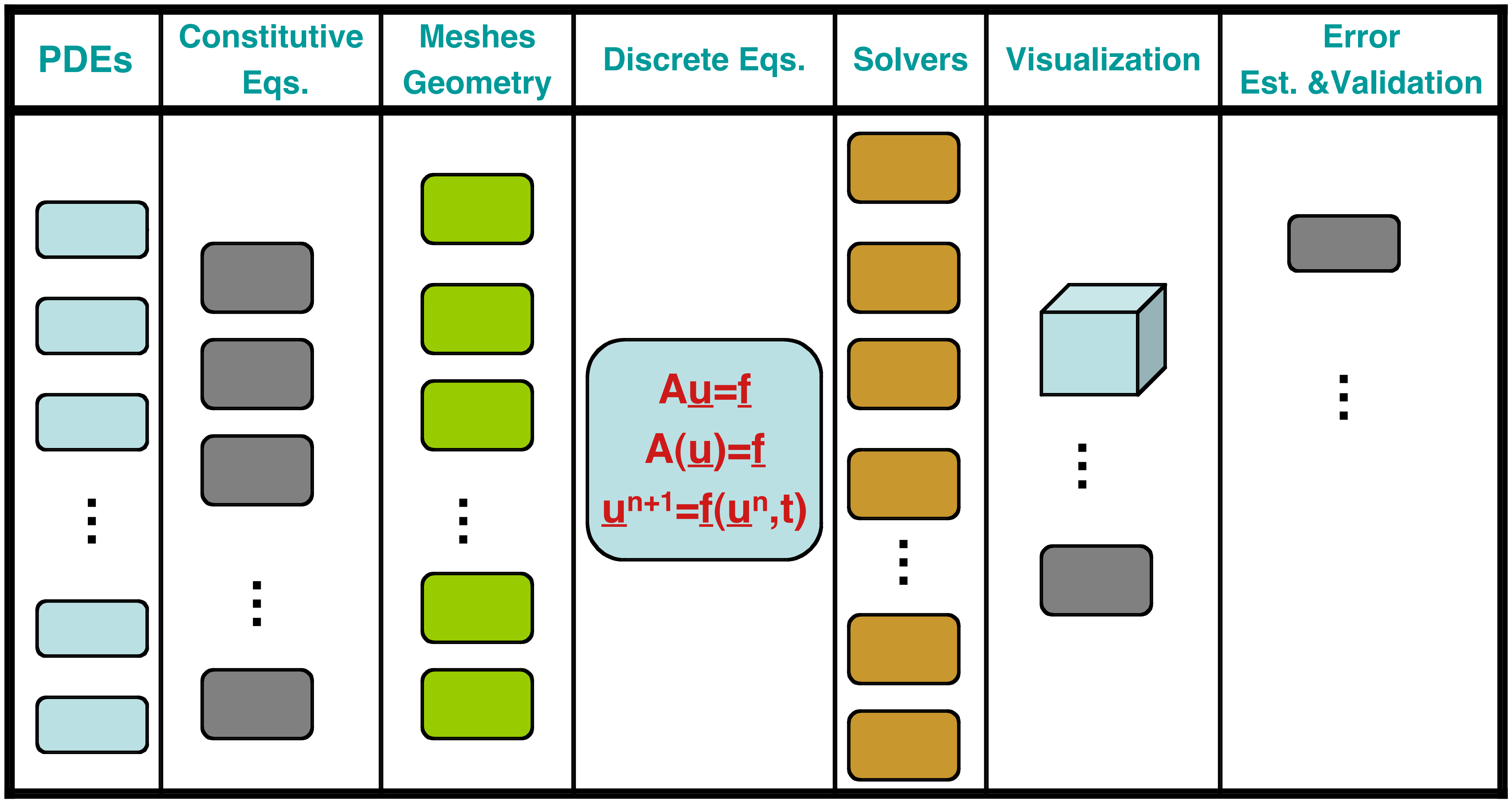


- Spontaneous formation of coherent structures at multiple scales
- Small changes in assumptions of coupling can radically change the physics
- Many questions remain about interactions and implications of multiple instabilities

Some Questions

- How do we manage the complexity of Multi-Physics, Multi-Scale problems?
- How do we sensibly explore model space and decide what is important and what can be ignored, homogenized etc?
- How do we write Multi-Physics software that
  - allows reuse, interoperability?
  - takes advantage of advanced hardware?
  - Gives flexibility to the end user to make their own decisions, and do their own science?

The Structure of Computational Problems
(numerical PDE's)



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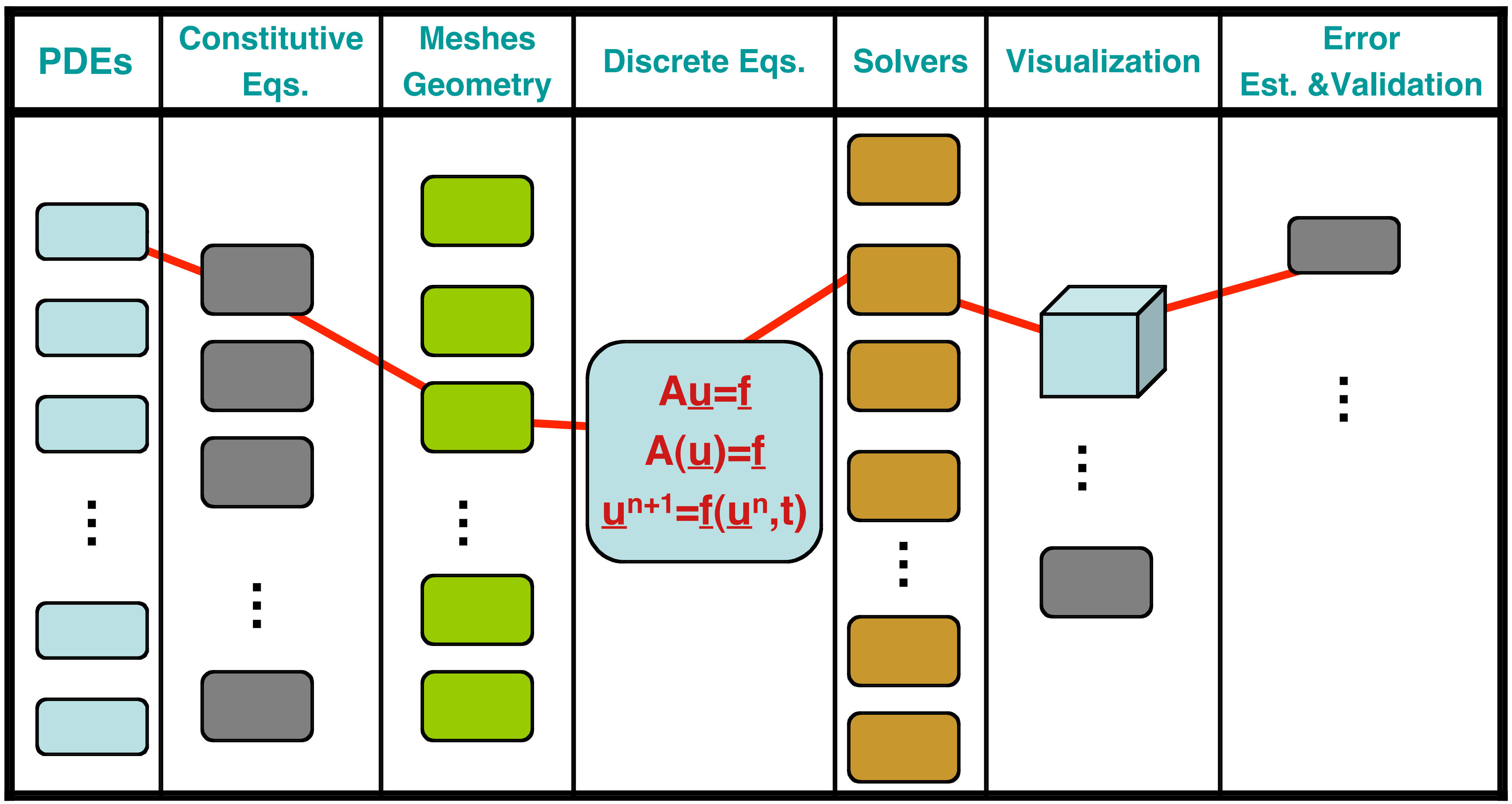

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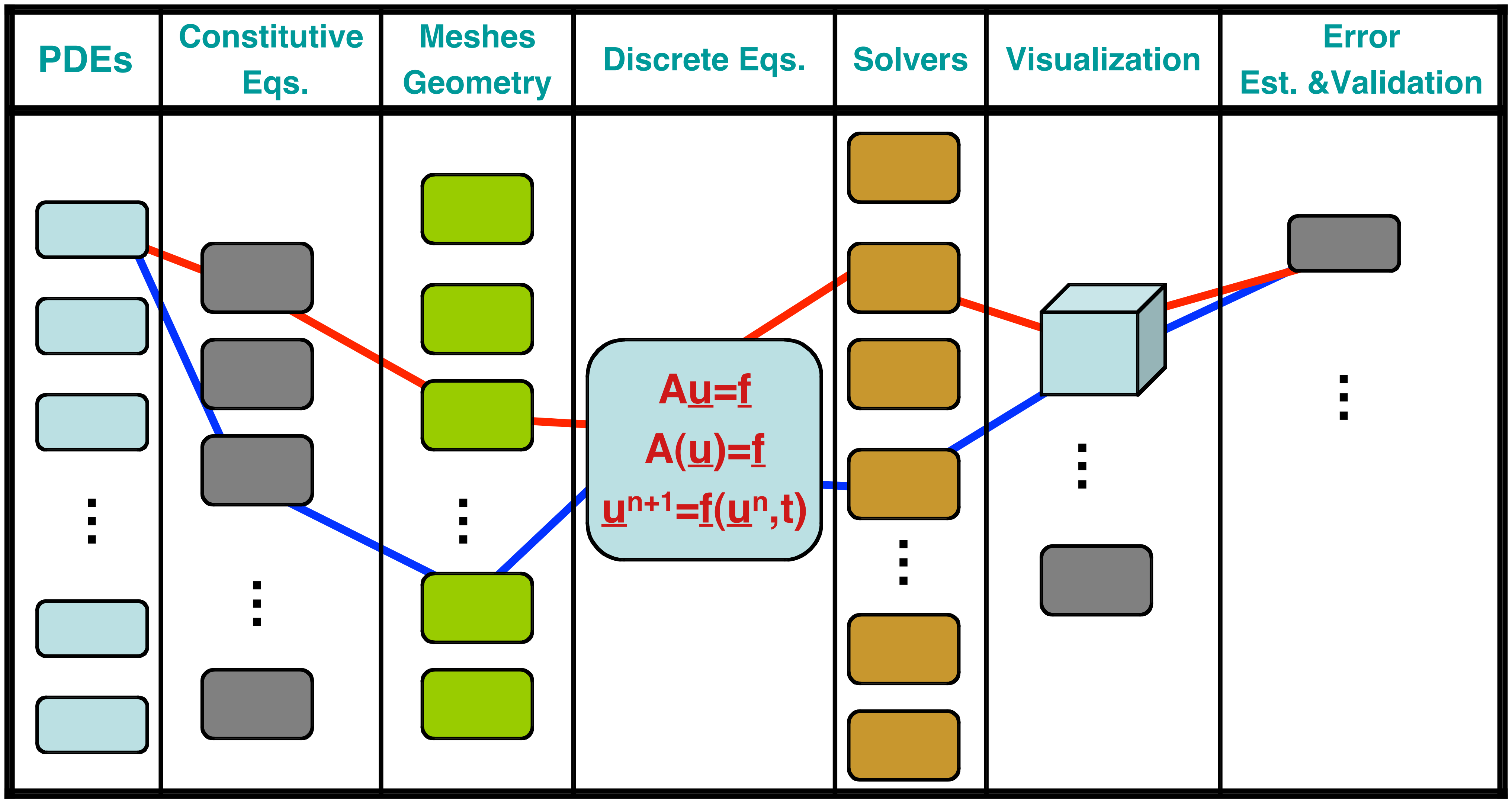

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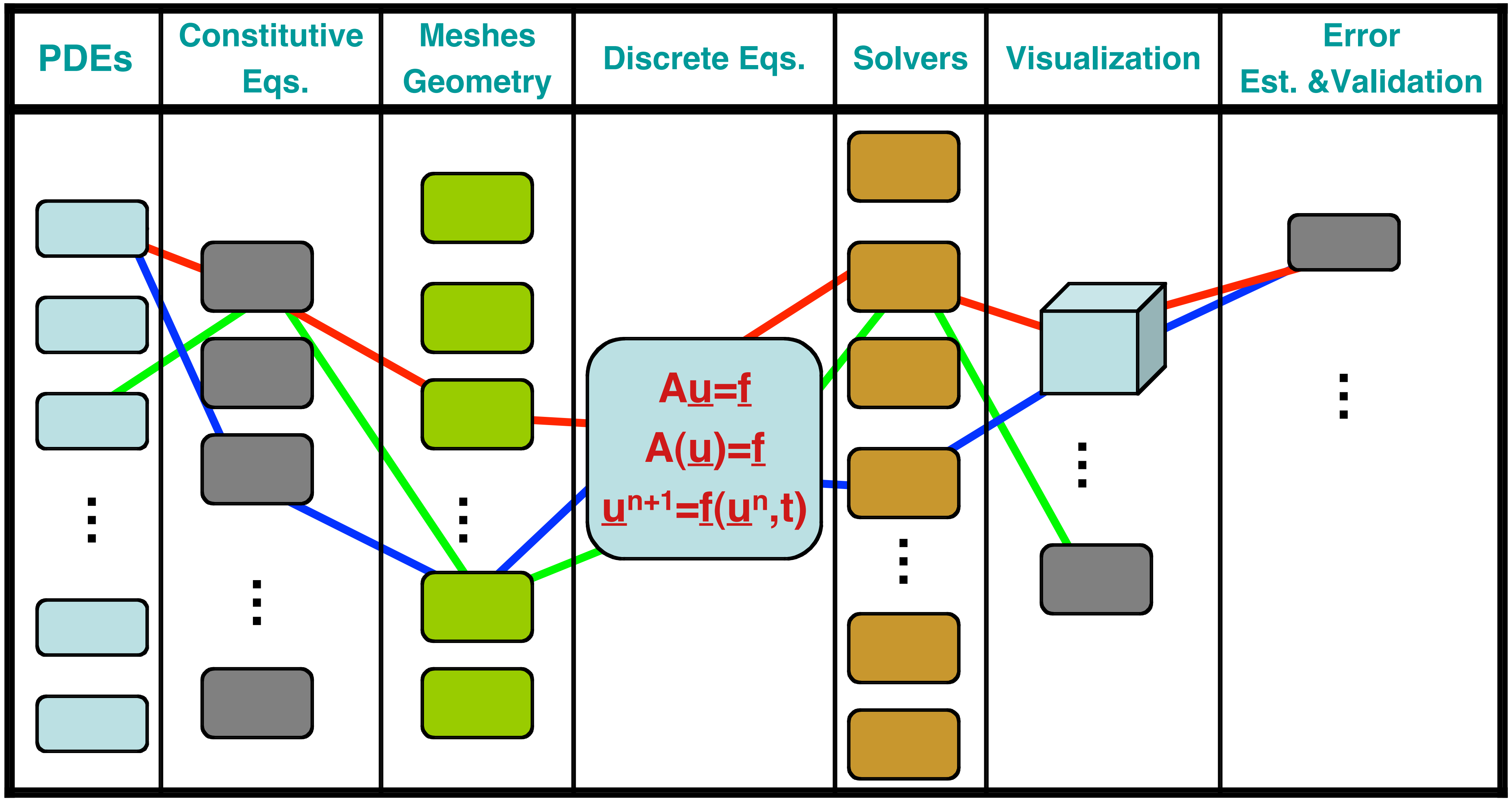

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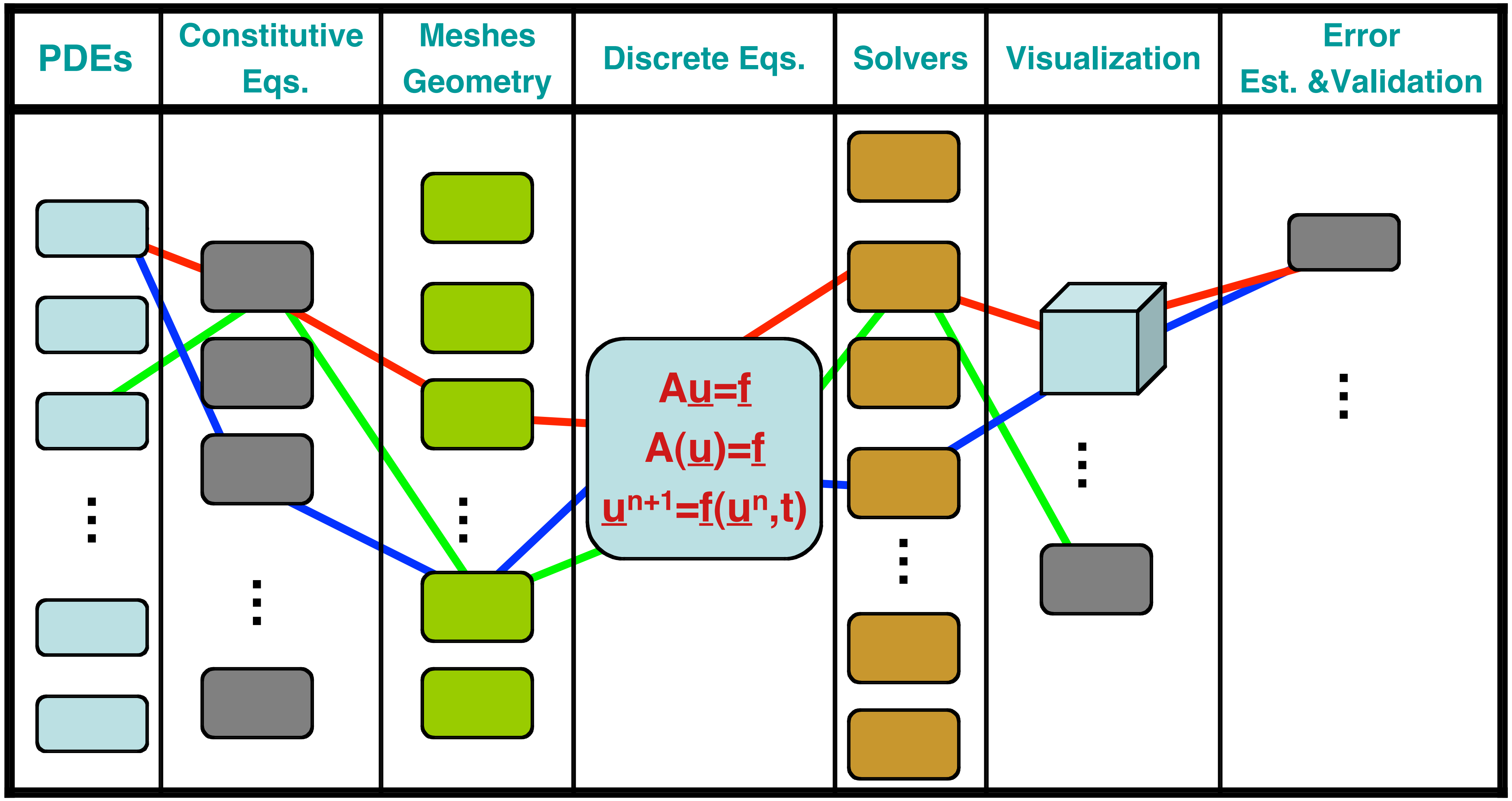
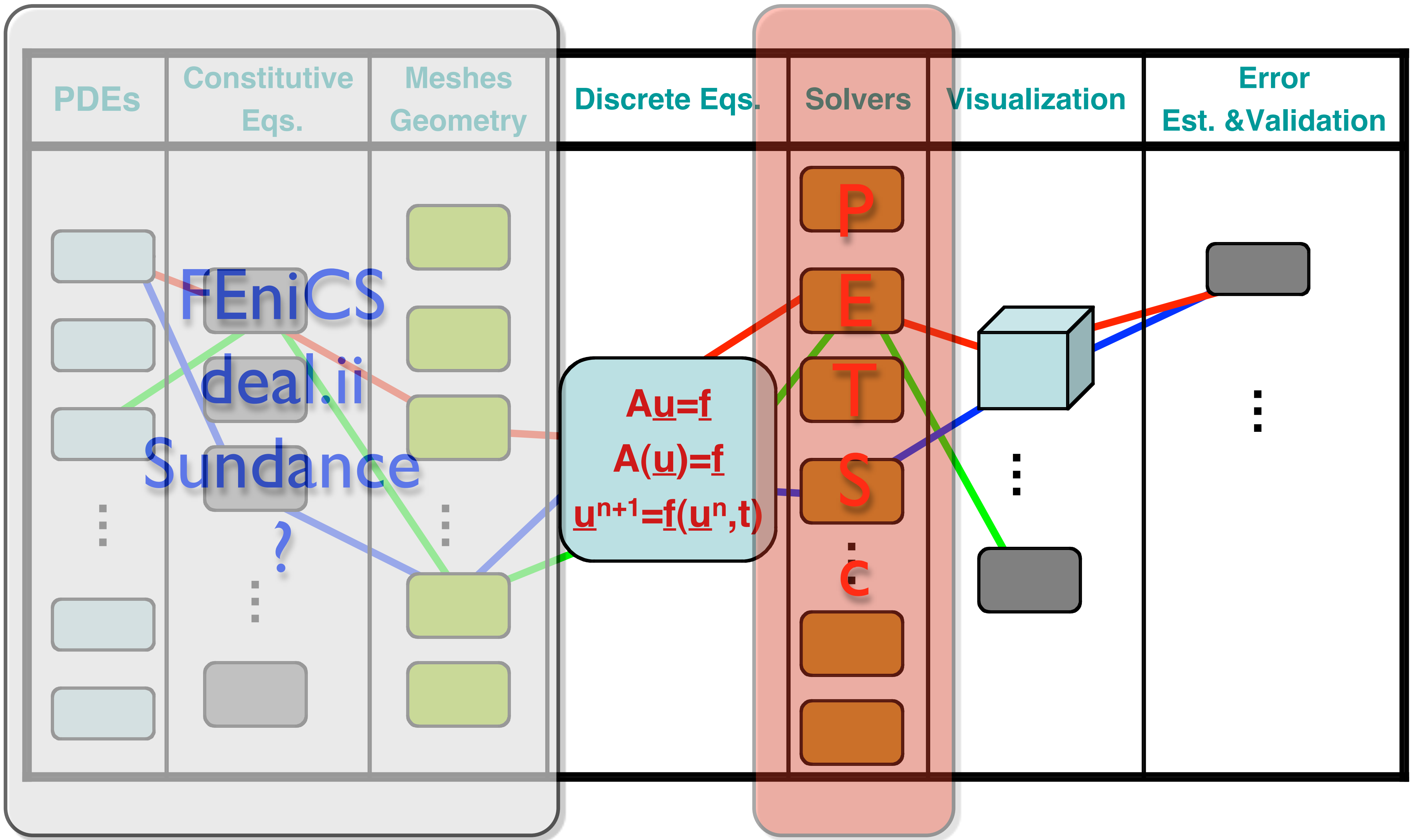


- Computation is really a set of (educated) choices
- Traditionally those choices are made early and hardwired into codes
- Some of this approach is still central to GPU programming.
- Is there a better way?

Software for Multi-physics computation

- PETSc (www.mcs.anl.gov/petsc)
  - Parallel Linear/non-linear solvers
  - Wide range of solver options
    - sparse Direct (umfpack/MUMPS etc.)
    - Algebraic Multi-Grid (HYPRE, ml)
    - Preconditioned Newton-Krylov
    - *Composite & FieldSplit Block Preconditioners*
  - *All chooseable at run time (command line options)*
- The user is responsible for providing A,b or F(u),J(u), PETSc provides interfaces to everything else.

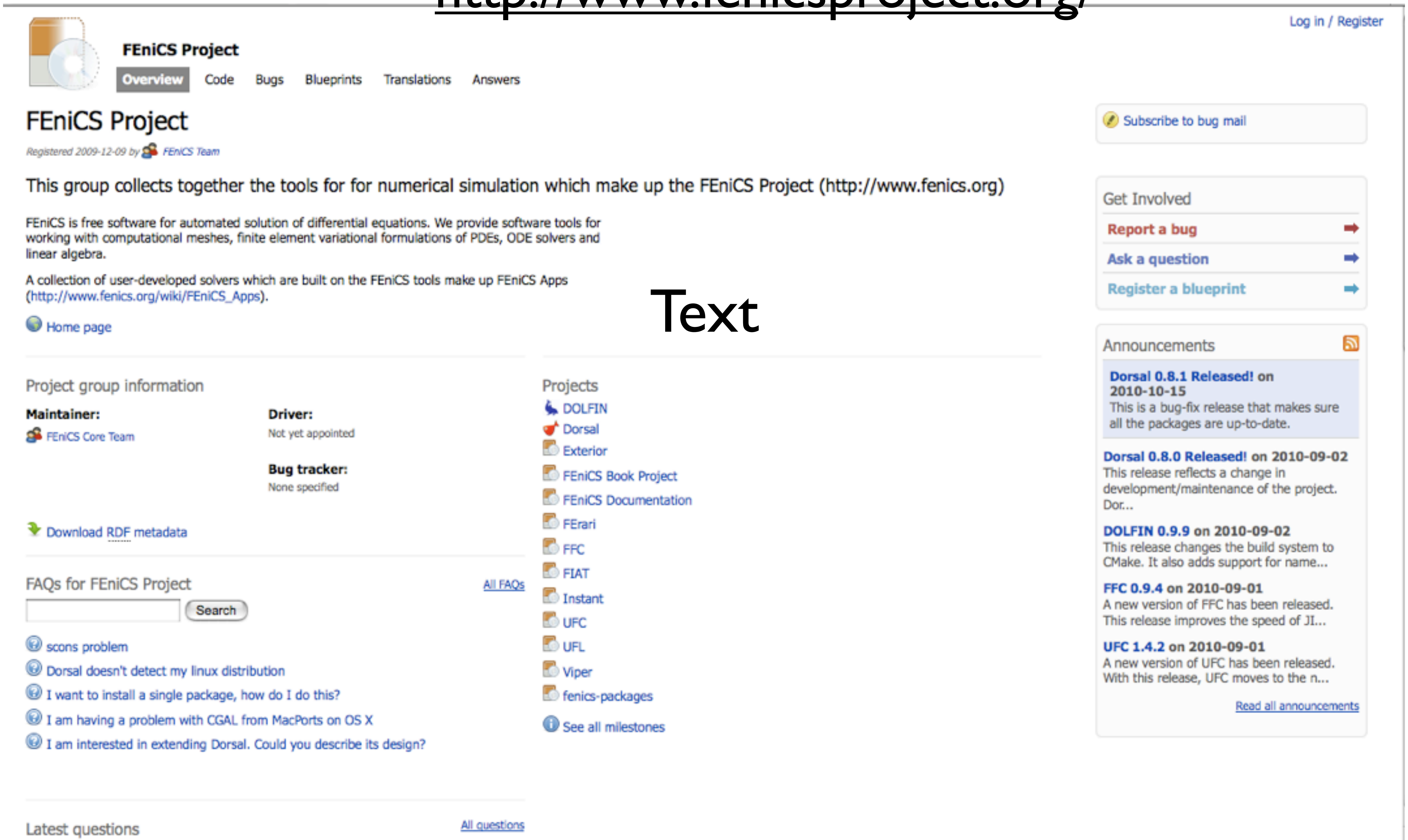
The Structure of Computational Problems (numerical PDE's)



Software for Multi-physics computation

https://launchpad.net/fenics-project

http://www.fenicsproject.org/



Text

Advanced Software for Multi-physics computation

- FEniCS (www.fenicsproject.org)
  - UFL: (Unified Form Language), a python extension for describing variational forms
  - FFC: Form Compiler for automatic FEM code generation from .ufl
  - Dolfin: high-level C++ libraries (and Python bindings) for mesh handling, automatic discretization/assembly and Function abstraction (u.eval(x))

Example: Poisson's Equation

- Strong form: Find $u \in \mathcal{C}^2(\Omega)$ with $u = 0$ on $\partial\Omega$ such that

$$-\nabla^2 u = f \text{ in } \Omega$$

- Weak Form: Find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega \mathbf{\nabla} v(x) \cdot \mathbf{\nabla} u(x) dx = \int_\Omega v(x) f(x) dx \text{ for all } v \in H_0^1(\Omega)$$

- Standard notation: Find $u \in V$ such that

$$a(v, u) = L(v) \text{ for all } v \in \hat{V}$$

with $a : \hat{V} \times V \to \mathbb{R}$ a *bilinear form* and $L : \hat{V} \to \mathbb{R}$ a *linear form*

Poisson.ufl

```
element = FiniteElement("Lagrange", triangle, 1)

v = TestFunction(element)
u = TrialFunction(element)
f = Coefficient(element)
g = Coefficient(element)

a = inner(grad(v), grad(u))*dx
L = v*f*dx + v*g*ds
```

compile with

```
ffc -l dolfin -O Poisson.ufl
```

(generates 2110 lines of compilable C++ code as Poisson.h)

Full solution of Poisson with Python interface

```
from dolfin import *

# Create mesh and define function space
mesh = UnitSquare(32, 32)
V = FunctionSpace(mesh, "Lagrange", 1)

# Define Dirichlet boundary (x = 0 or x = 1)
def boundary(x):
    return x[0] < DOLFIN_EPS or x[0] > 1.0 - DOLFIN_EPS

# Define boundary condition
u0 = Constant(0.0)
bc = DirichletBC(V, u0, boundary)

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("10*exp(-(pow(x[0] - 0.5, 2) + pow(x[1] - 0.5, 2)) / 0.02)")
g = Expression("sin(5*x[0])")
a = inner(grad(u), grad(v))*dx
L = f*v*dx + g*v*ds

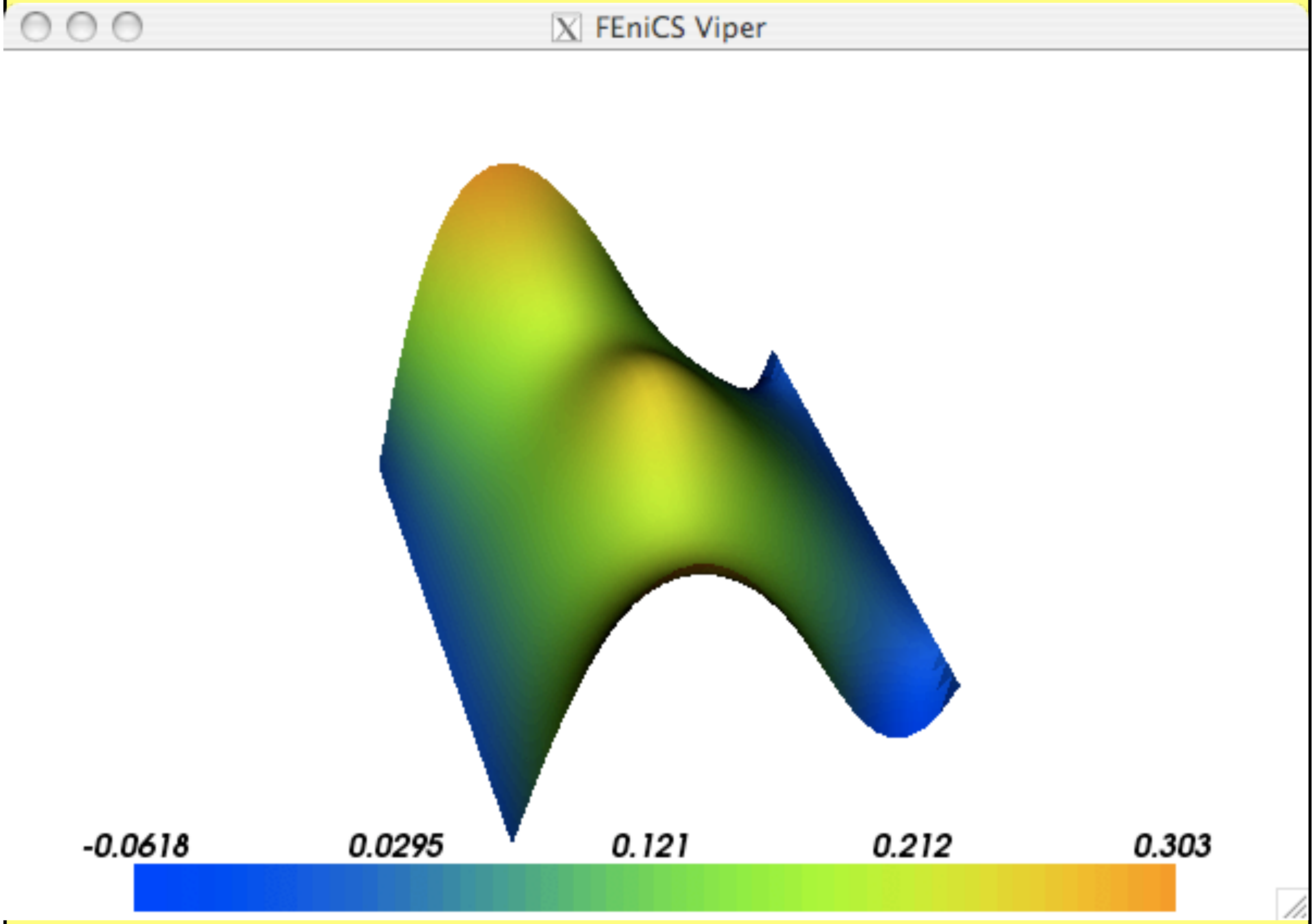
# Compute solution
problem = VariationalProblem(a, L, bc)
u = problem.solve()

# Save solution in VTK format
file = File("poisson.pvd")
file << u

# Plot solution
plot(u, interactive=True)
```

Full solution of Poisson with Python interface

```
from dolfin import *
```



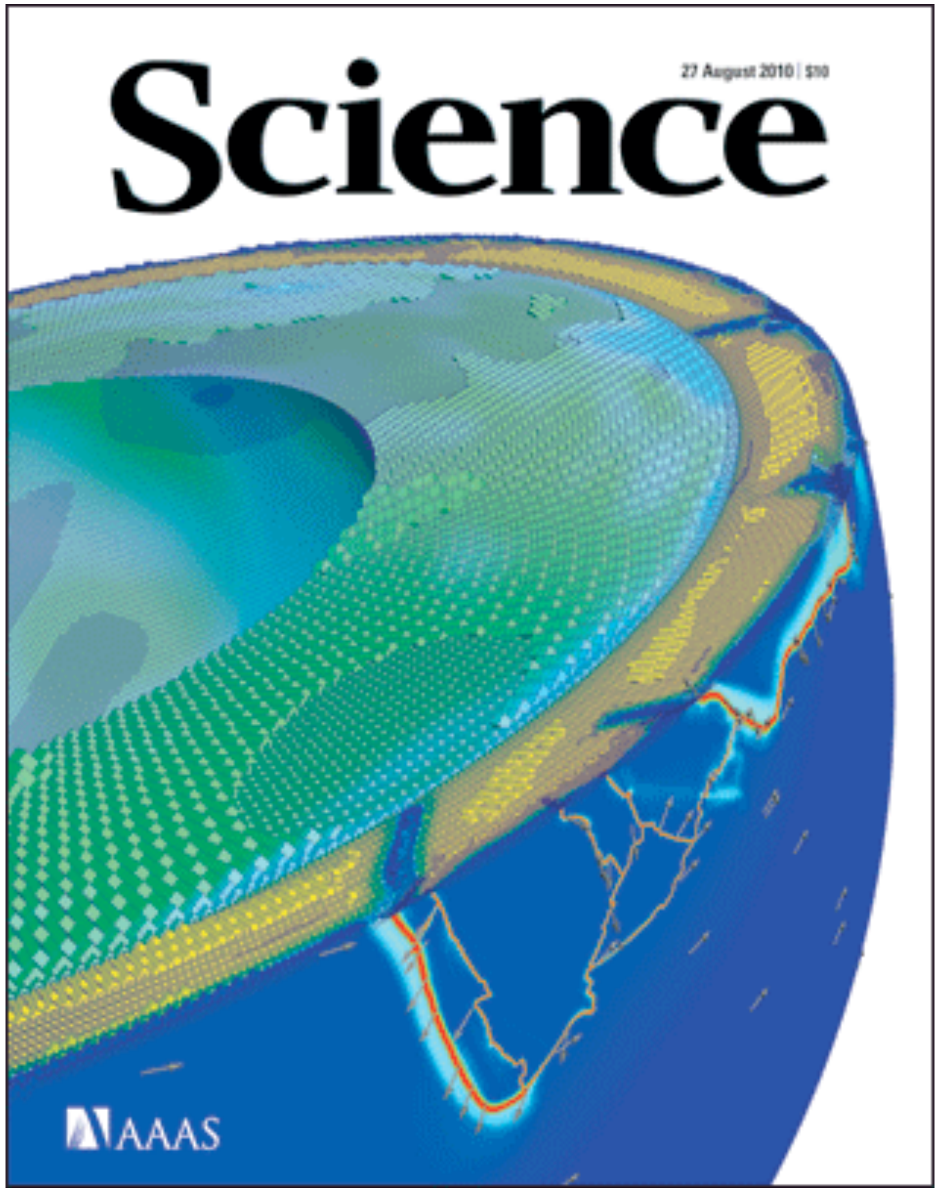

```
# Plot solution
plot(u, interactive=True)
```

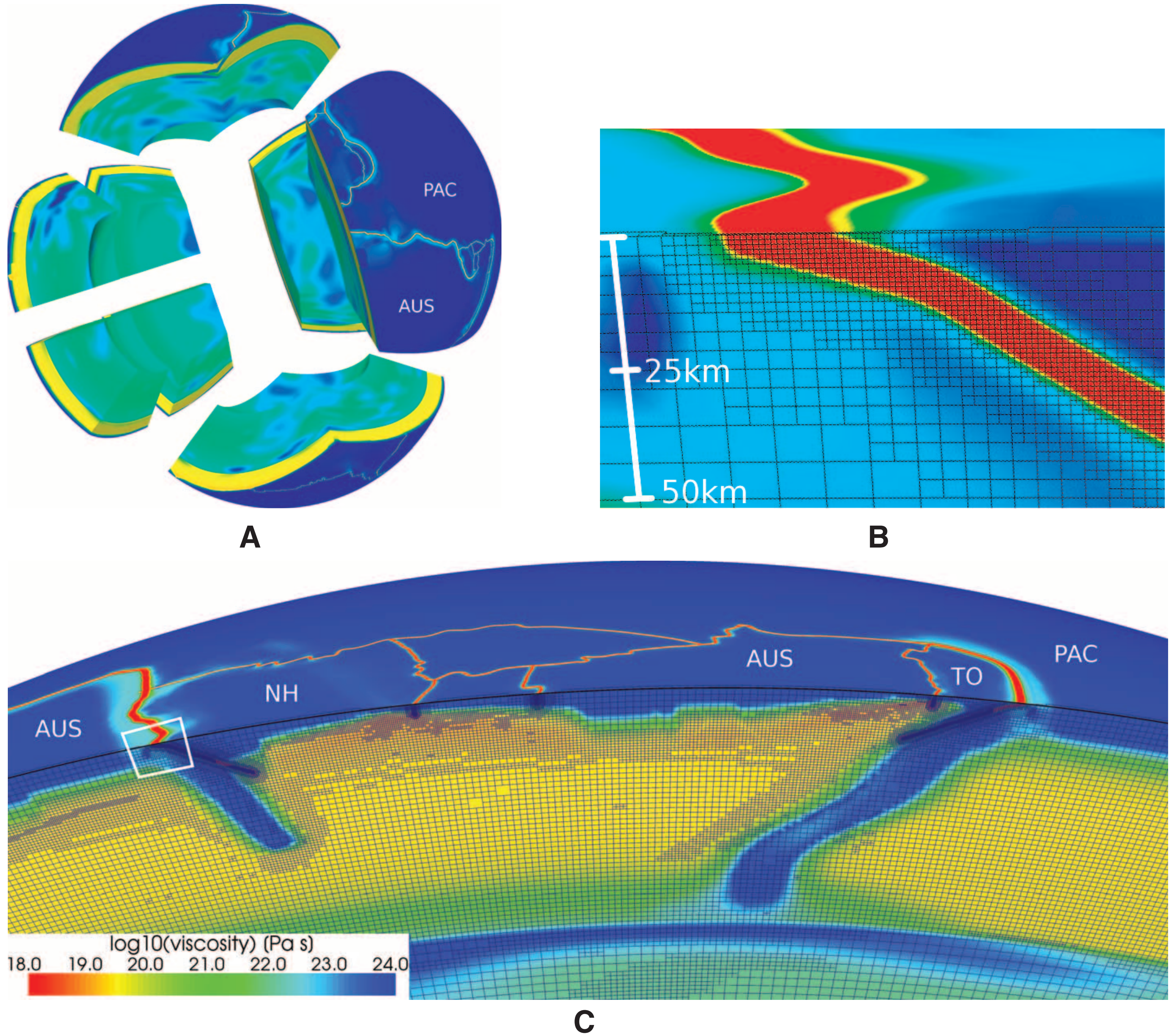
Issues for Multi-physics problems:

- How to rapidly explore/compose different multi-physics models/couplings
- How to maintain control on convergence of global non-linear problem
- How to rapidly change solvers/pre-conditioners as problems change/evolve (defer solver bets)
- How to leverage *existing* algorithms and intuition in designing effective physics-based preconditioners

A model problem:

Infinite Prandtl Number Thermal Convection





The Dynamics of Plate Tectonics and Mantle Flow: From Local to Global Scales

Georg Stadler,[1] Michael Gurnis,[2]* Carsten Burstedde,[1] Lucas C. Wilcox,[1]†
Laura Alisic,[2] Omar Ghattas[1,3,4]

A model problem:

Infinite Pr thermal convection

$$\frac{DT}{Dt} = \frac{1}{\mathrm{Ra}} \nabla^2 T$$

$$-\boldsymbol{\nabla} \cdot \eta(\boldsymbol{\nabla}\mathbf{V} + \boldsymbol{\nabla}\mathbf{V}^T) + \boldsymbol{\nabla} P = T\mathbf{k}$$

$$\boldsymbol{\nabla} \cdot \mathbf{V} = 0$$

with $\eta = \eta(T, \mathbf{V}, \ldots)$

A model problem:

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with $\eta = \eta(T, \mathbf{V}, \ldots)$

- Coupled Parabolic/Elliptic problem (Adv diff + Stokes)
- usually solved with splitting/Picard iteration assuming quasi-linearity of each equation

Discretization

- FEM in space with mixed element [P2, (P2,P2), P1] for [T,V,P]
- 2nd order Semi-Lagrangian Crank-Nicolson scheme for Energy Equation

Semi-Lagrangian Crank-Nicolson scheme for Energy Equation

$$\frac{T - T^*}{\Delta t} = \frac{1}{2\mathrm{Ra}} \left(\nabla^2 T + (\nabla^2 T)^* \right)$$

where $T^* = T_n(x^*)$ i.e. Temperature at the previous time step and take-off point. Alternatively

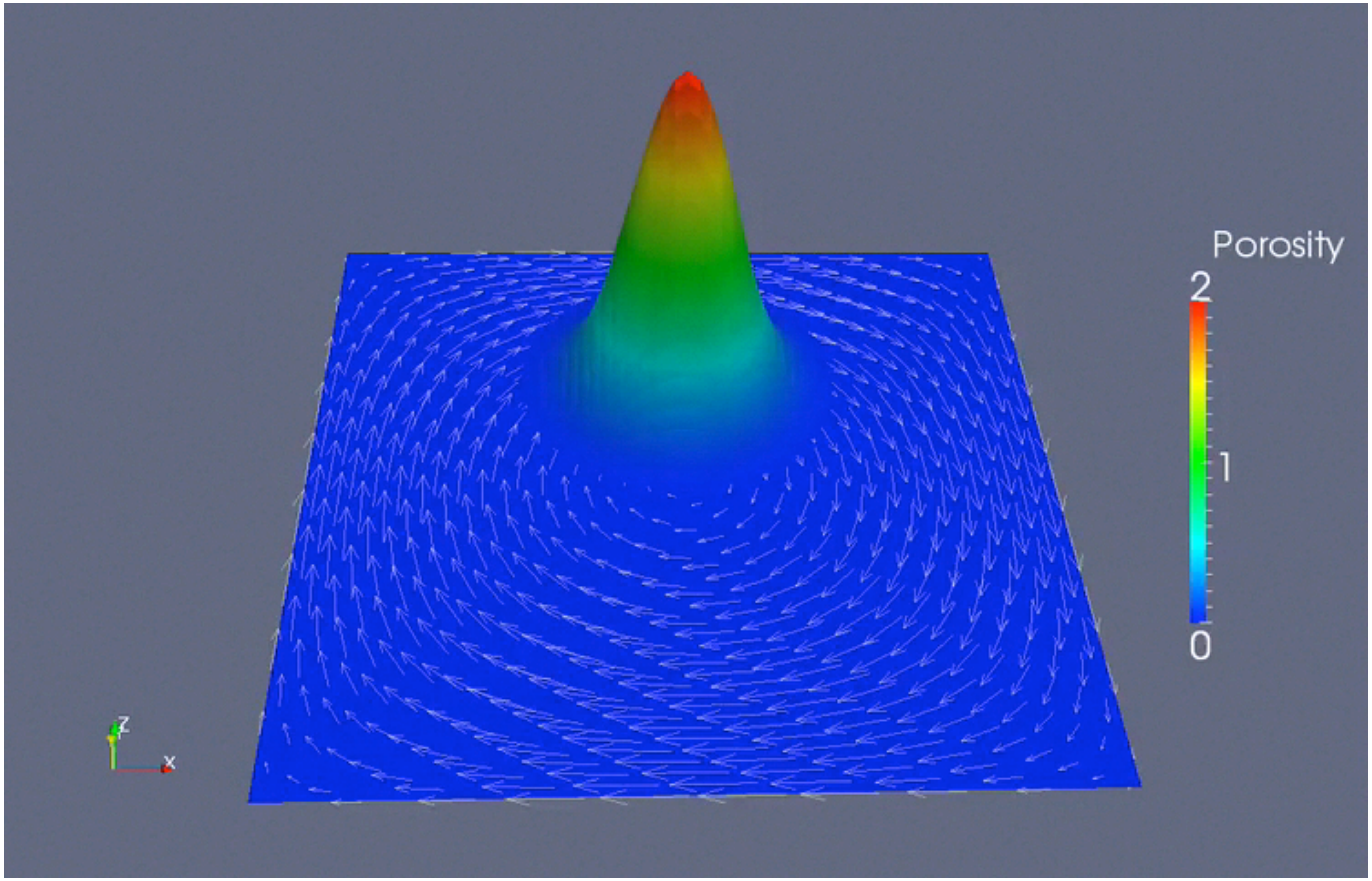
SLCN

$$T - \frac{\Delta t}{2\mathrm{Ra}} \nabla^2 T = g(x^*)$$

where

$$g(x) = T_n + \frac{\Delta t}{2\mathrm{Ra}} \nabla^2 T_n$$

Semi-Lagrangian Advection schemes in FEM



Weak Forms

Weak form of Residual $L = F[u] = F_T + F_V + F_P$

$$
\begin{aligned}
F_T &= \int_\Omega \left[s(T - g^*) + \frac{\Delta t}{2\mathrm{Ra}} \boldsymbol{\nabla} s \cdot \boldsymbol{\nabla} T \right] dx \\
F_V &= \int_\Omega \left[2\eta \boldsymbol{\nabla}^s \mathbf{u} : \boldsymbol{\nabla}^s \mathbf{V} - p \boldsymbol{\nabla} \cdot \mathbf{u} - T \mathbf{u} \cdot \mathbf{k} \right] dx \\
F_P &= \int_\Omega q \boldsymbol{\nabla} \cdot \mathbf{V} dx
\end{aligned}
$$

Weak form of Jacobian $J[u]$

$$a(v, \delta u) = \delta L = \delta F = J[u] \delta u$$

RayleighBenard.ufl

```
#  Choose a mixed vector space
#          for u = [ T,V, P]
P2 = FiniteElement("Lagrange", triangle,2)
P2v = VectorElement("Lagrange", triangle, 2)
P1 = FiniteElement("Lagrange", triangle, 1)
ME  =  MixedElement([P2,P2v, P1])

# quadrature element for Semi-Lagrangian
QE = FiniteElement("Quadrature", triangle,4)

#set test functions and trial functions
(s,u, q) = TestFunctions(ME)
du = TrialFunction(ME)

# solution from last iteration
u0 = Coefficient(ME)

# split mixed functions
(dT,dv, dp,) = split(du)
(T,v, p) = split(u0)

# SemiLagrangianFunctions
gstar = Coefficient(QE)
g = Coefficient(P2)

#parameters and functions
Ra = Constant(triangle)
dt = Constant(triangle) # time step
hdt = 0.5*dt # half time step

#Viscosity function
b = Constant(triangle)
c = Constant(triangle)
x = P2.cell().x
eta = exp(-b*T + c*(1-x[1]))

# weak form of residuals
L1= (s*(T-gstar)+hdt/Ra*inner(grad(s),grad(T)))*dx
L2 = (inner(sym(grad(u)), 2*eta*sym(grad(v))) - div(u)*p - T*u[1])*dx
L3 = q*div(v)*dx

L = L1 + L2 + L3

# Bilinear form for Jacobian with
#         added approximate Semi-Lagrangian block

a = derivative(L,u0,du) +  s*hdt*inner(grad(g),dv)*dx
```

RayleighBenard.ufl

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```

Assembled Weak Form for Newton

Assembled Block Newton form (iso-viscous Stokes)

$$J\delta\mathbf{u} = \begin{bmatrix} A & B & 0 \\ -M & K & G \\ 0 & G^T & 0 \end{bmatrix} \begin{bmatrix} \delta_T \\ \delta_{\mathbf{V}} \\ \delta_P \end{bmatrix} = -\mathbf{F}$$

where

$$\begin{aligned} A &= M + \frac{\Delta t}{2\mathrm{Ra}}\mathcal{L} \\ B &= -\frac{\Delta t}{2}\int_\Omega s\boldsymbol{\nabla} g \cdot \delta\mathbf{V} dx \end{aligned}$$

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Stokes

where

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Assembled Weak Form for Newton

Variable Viscosity adds additional blocks

$$J\delta\mathbf{u} = \begin{bmatrix} A & B & 0 \\ -M + \eta_T & K + \eta_V & G \\ 0 & G^T & 0 \end{bmatrix} \begin{bmatrix} \delta_T \\ \delta_{\mathbf{V}} \\ \delta_P \end{bmatrix} = -\mathbf{F}$$

where

$$\begin{aligned} A &= M + \frac{\Delta t}{2\mathrm{Ra}}\mathcal{L} \\ B &= -\frac{\Delta t}{2}\int_\Omega s\boldsymbol{\nabla} g \cdot \delta\mathbf{V} dx \end{aligned}$$

Some Physics Based Preconditioners
(iso-viscous Stokes)

GSP-Picard Splitting as approximate Jacobian

$$P = \begin{bmatrix} A & \\ \begin{bmatrix} -M \\ 0 \end{bmatrix} & \begin{bmatrix} K & G \\ G^T & 0 \end{bmatrix} \end{bmatrix}$$

Nested GSP - iterative Stokes Solver

$$P = \begin{bmatrix} A & \\ \begin{bmatrix} -M \\ 0 \end{bmatrix} & \begin{bmatrix} \hat{K} & G \\ 0 & \hat{S} \end{bmatrix} \end{bmatrix}$$

Software Requirements

- Rapid and Flexible Composition and Assembly of residuals and block Jacobians.
- Flexible Composition of block preconditioners
- Both Functionalities currently exist in available software
    - FEniCS (www.fenics.org): UFL/FFC/Dolfin
    - PETSc (www.anl.gov/...): PCFieldsplit

PETSc FieldSplit Preconditioners

- Define splits (memory layout done in main code):
  - fieldsplit_0 T
  - fieldsplit_1: Stokes [V, P]
  - Define Nested Splits (for fieldsplit stokes PC's)
    - fieldsplit_1_fieldsplit_0: P
    - fieldsplit_1_fieldsplit_1: V

- Then individual (PC/KSP) pairs can be defined for any split at runtime with command line options
- For Block Triangular Preconditioners use

```
-pc_fieldsplit_type multiplicative
```

PETSc FieldSplit Preconditioners: Examples

-options_file petsc_direct.options

```
# Options file describing (LU,preonly)
# Direct solve of full Jacobian
#
# Set tolerance for Newton iteration
-snes_rtol 1.e-6
-snes_atol 1.e-9
-snes_monitor

# Set (KSP/PC) for Linear solve
-ksp_type preonly
-pc_type lu
-pc_factor_mat_solver_package umfpack
```

PETSc FieldSplit Preconditioners: Examples

petsc_fieldsplit_direct.options

```
# Set Tolerance for Newton Iteration
-snes_rtol 1.e-6
-snes_atol 1.e-9

# KSP for full Jacobian
-ksp_type fgmres      change to preonly for classic picard it
-ksp_rtol 1.e-4

# Fieldsplit Block Preconditioner for Jacobian
-pc_fieldsplit_type multiplicative

# solve Temperature Block (split 0) directly
-fieldsplit_0_ksp_type preonly
-fieldsplit_0_pc_type lu
-fieldsplit_0_pc_factor_mat_solver_package umfpack
# solve Stokes Block (split 1) directly
-fieldsplit_1_ksp_type preonly
-fieldsplit_1_pc_type lu
-fieldsplit_1_pc_factor_mat_solver_package umfpack
```

PETSc FieldSplit Preconditioners: Examples

petsc_nested_fieldsplit.options

```
# Set Tolerance for Newton Iteration
-snes_rtol 1.e-6
-snes_atol 1.e-9

# KSP for full Jacobian
-ksp_type fgmres
-ksp_rtol 1.e-3 -ksp_atol 1.e-10

# Fieldsplit Block Preconditioner for Jacobian
-pc_fieldsplit_type multiplicative

# precondition Temperature Block (split 0) iteratively
-fieldsplit_0_ksp_type cg
-fieldsplit_0_pc_type sor
-fieldsplit_0_ksp_rtol 1.e-4

# precondition Stokes Block (split 1) with Fieldsplit UT
```

PETSc FieldSplit Preconditioners: Examples

petsc_nested_fieldsplit.options (cont'd)

```
# precondition Stokes Block (split 1)
# Stokes: use upper triangular preconditioner

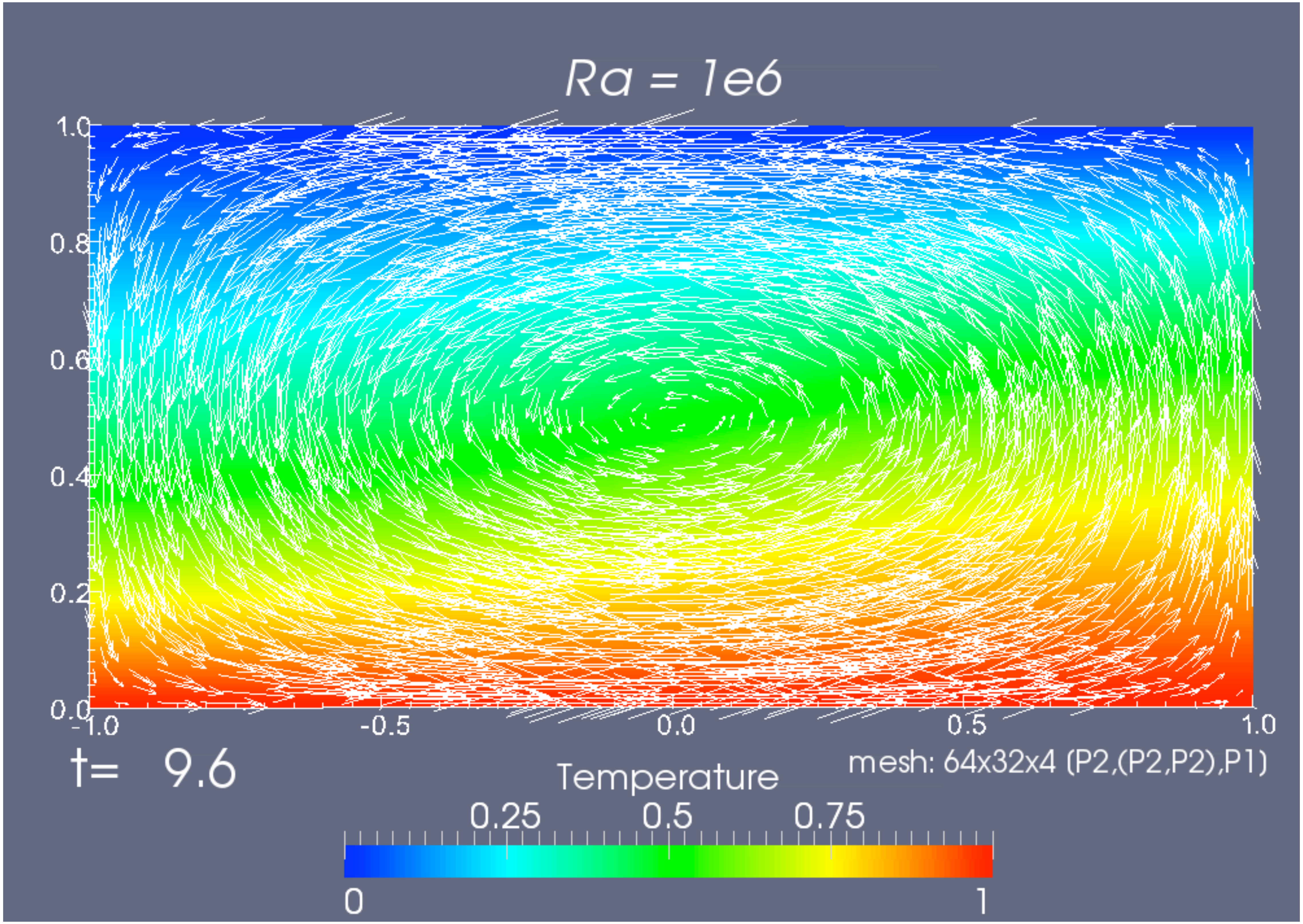
-fieldsplit_1_ksp_rtol 1.e-4
-fieldsplit_1_ksp_type fgmres
-fieldsplit_1_ksp_monitor
-fieldsplit_1_pc_fieldsplit_type multiplicative

# pressure split (1,0)
-fieldsplit_1_fieldsplit_0_ksp_type cg
-fieldsplit_1_fieldsplit_0_pc_type sor
-fieldsplit_1_fieldsplit_0_ksp_max_it 2

# Velocity split (1,1)
-fieldsplit_1_fieldsplit_1_ksp_type preonly
-fieldsplit_1_fieldsplit_1_pc_type hypre
```

It actually works:

A hybrid FEniCS/PETSc code for Infinite Prandtl Number Thermal Convection



Results: Convergence

FS_direct_preonly	FS_direct	FS_Nested
(64x32x4 triangles, cfl=1, n=1) 0 SNES norm 1.440775725816e-04 1 SNES norm 1.121163685700e-05 2 SNES norm 8.684216284984e-07 3 SNES norm 6.724036897955e-08 4 SNES norm 5.206153641239e-09 5 SNES norm 4.030909787299e-10	0 SNES norm 1.440775934047e-04 0 KSP norm 1.440775934047e-04 1 KSP norm 2.180436488650e-07 2 KSP norm 8.082898217229e-11 1 SNES norm 4.501827567666e-07 0 KSP norm 4.501827567666e-07 1 KSP norm 8.111259702458e-09 2 KSP norm 1.591023715205e-11 2 SNES norm 3.448948297201e-10	0 SNES norm 1.440775934702e-04 0 KSP norm 1.440775934702e-04 1 KSP norm 8.547666994358e-05 2 KSP norm 5.143221835930e-06 3 KSP norm 1.625345646434e-06 4 KSP norm 1.066985886044e-07 1 SNES norm 3.882662679061e-07 0 KSP norm 3.882662679061e-07 1 KSP norm 1.179958777726e-07 2 KSP norm 1.040916620187e-08 3 KSP norm 6.871221156164e-09 4 KSP norm 1.060162940204e-09 5 KSP norm 2.618492833850e-10 2 SNES norm 9.208414734450e-10

FS_direct_preonly	FS_direct	FS_Nested
(128x64x4 triangles, cfl=2, n=1) 0 SNES norm 7.209390761755e-05 1 SNES norm 5.610105695322e-06 2 SNES norm 4.345432491886e-07 3 SNES norm 3.364588778704e-08 4 SNES norm 2.605064460130e-09 5 SNES norm 2.016992518469e-10	0 SNES norm 7.209390761755e-05 0 KSP norm 7.209390761755e-05 1 KSP norm 1.090781352139e-07 2 KSP norm 4.037606468691e-11 1 SNES norm 2.252626498074e-07 0 KSP norm 2.252626498074e-07 1 KSP norm 4.060434945128e-09 2 KSP norm 7.945568136744e-12 2 SNES norm 1.726435313005e-10	0 SNES norm 7.209390763950e-05 0 KSP norm 7.209390763950e-05 1 KSP norm 4.302281006644e-05 2 KSP norm 2.575155542825e-06 3 KSP norm 8.172703781034e-07 4 KSP norm 5.354585680104e-08 1 SNES norm 1.942724998785e-07 0 KSP norm 1.942724998785e-07 1 KSP norm 5.946234196409e-08 2 KSP norm 5.243563962848e-09 3 KSP norm 3.441167666531e-09 4 KSP norm 5.364061333279e-10 5 KSP norm 1.317802056418e-10 2 SNES norm 4.603579469808e-10

Results: Convergence/performance

PC	KSP/SNES				time/FS_Direct_s	
(64x32x4 triangles, cfl=1, n=1)	n=1		n=230		n=1	n=230
FS_direct_preonly	1	5	1	8	2.17	3.34
FS_direct	2	2	4	4	1.00	1.89
FS_nested	4.5	2	6.5	4	1.00	2.18
Direct	1	2	1	4	1.09	1.89

PC	KSP/SNES				time/FS_Direct_s	
(128x64x4 triangles, cfl=2, n=1)	n=1		n=230		n=1	n=230
FS_direct_preonly	1	5	1	7	10.19	11.04
FS_direct	2	2	4	4	4.38	8.21
FS_nested	4.5	2	6	4	6.00	12.62
Direct	1	2	1	4	5.95	10.70

Magma Dynamics

(McKenzie Tutorial Notes (CIG), Katz et al, 2007 Pepi)

$$\frac{D\phi}{Dt} = (1-\phi)\frac{\mathcal{P}}{\xi} + \Gamma/\rho_s$$

Compressible Flow

$$-\boldsymbol{\nabla}\cdot\frac{K}{\mu}\boldsymbol{\nabla}\mathcal{P} + \frac{\mathcal{P}}{\xi} = \boldsymbol{\nabla}\cdot\frac{K}{\mu}\left[\boldsymbol{\nabla}P^* + \Delta\rho\mathbf{g}\right] + \Gamma\frac{\Delta\rho}{\rho_f\rho_s}$$

$$\boldsymbol{\nabla}\cdot\mathbf{V} = \frac{\mathcal{P}}{\xi}$$

"Incompressible" Flow

$$\boldsymbol{\nabla}P^* = \boldsymbol{\nabla}\cdot\eta\left(\boldsymbol{\nabla}\mathbf{V} + \boldsymbol{\nabla}\mathbf{V}^T\right) - \phi\Delta\rho\mathbf{g}$$

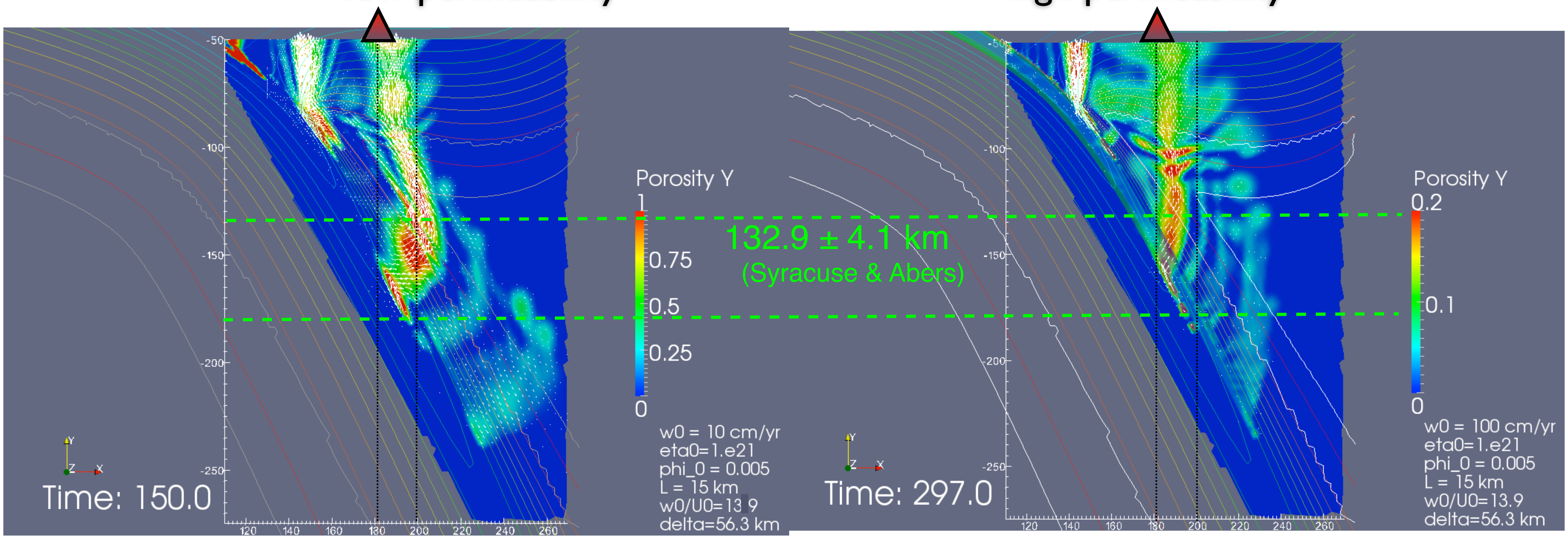
with

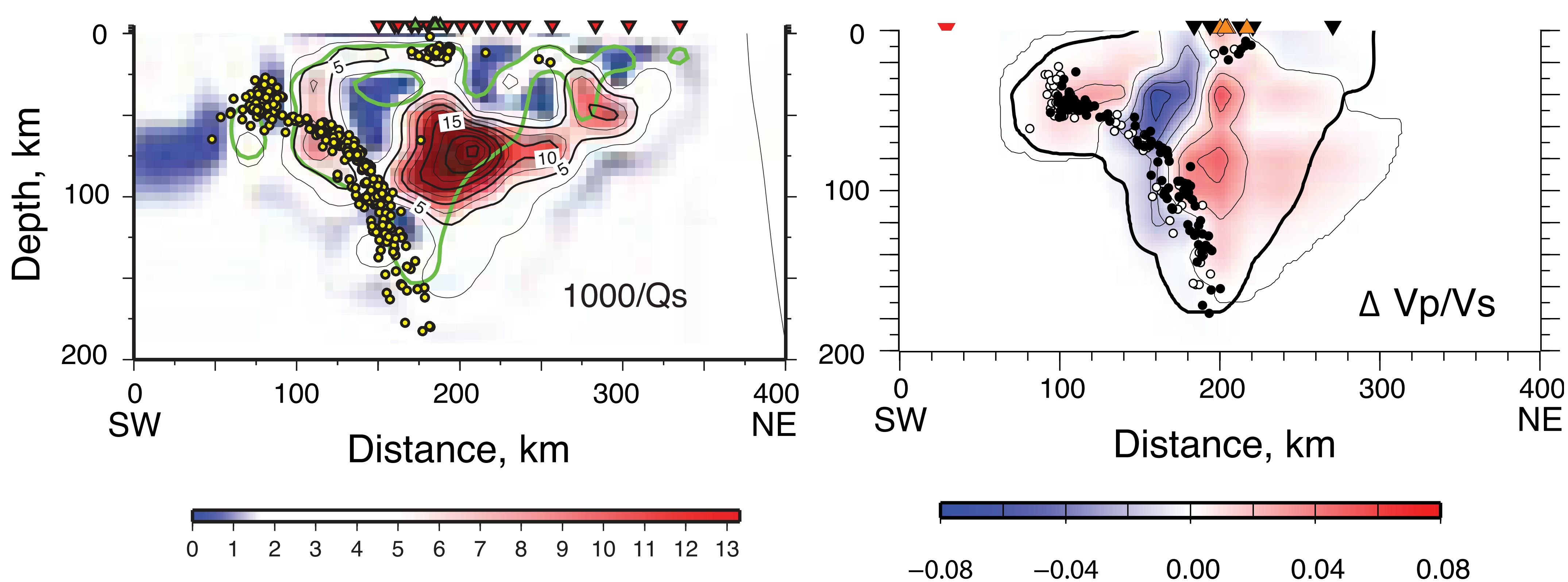
- $\xi = (\zeta - 2\eta/3) = \eta\left(\frac{1}{\phi} - \frac{2}{3}\right) \approx \eta/\phi$
- $\Delta\rho = \rho_s - \rho_f$

Comparison to TUCAN Data

low permeability

high permeability





Conclusions

- Advances in Software (FEniCS/PETSc) allows flexible and rapid composition of multi-physics models, discretization and block-preconditioners
- Allows choices of model coupling/solvers to be made at, or close to run time (but doesn't help you make those choices.)
- Newton with block pre-conditioners allows monitoring convergence of global non-linear problem.
- This approach has already led to working scientific codes.
- Physics based fieldsplit pre-conditioners are more efficient than Picard splitting, and comparable to sparse-direct (which is hard to beat in 2-D)

Ongoing Issues

- Performance tuning and profiling needs to be done to understand timing differences.
- Selective block assembly is needed for efficiency.
- Parallelism: Both FEniCS/PETSc are parallel (but need to implement parallel Semi-Lagrangian or choose a different advection scheme). Questions of performance and scaleability.
- Science Challenges: Full Magma Dynamics (RBConvection + fluids), 3-D, more non-linear couplings.
- Comparison to other multi-physics approaches
- But proof-of-concept exists.