Flexible Multi-Physics Solvers for Magma Dynamics

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1 Introduction:

Magmatism, the flow of partially molten rock in the Earth's interior, is an essential feature of global plate boundaries and may be critical for maintaining the structure of global mantle convection. Melting and melt transport also has fundamental controls on the chemical evolution of the planet. For all of these reasons, understanding the dynamics and observable consequences of magma dynamics is of considerable interest to geodynamicists and geochemists.

From a computational mathematics point of view, Magma Dynamics also provides one of the more dramatic examples of coupled multi-physics problems in the Solid Earth sciences. In its simplest form, it describes the inter-penetrating flow of a low-viscosity fluid in a *viscously deformable* permeable medium and is a consistent coupling of Darcy flow of the fluid with Stokes flow for the solid matrix. More complex formulations also couple multi-component thermodynamics and reactive flow to these deforming systems.

Considerable work has been done to explore and understand models of magma migration, and has demonstrated a rich array of behavior ranging from non-linear magma waves, to chemical and mechanical localization instabilities (see below). Computation has played a major part in these studies, but principally through a series of carefully crafted "Hero Codes" each designed to explore a specific aspect of the dynamics or a specific coupling. These studies show that small changes in assumptions of coupling (for example in constitutive relationships) can cause significant changes in physical behavior which may require concomitant changes in computational methods/solvers. For traditional codes, many of the computational "bets" (choice of discretization, mesh, solver) are made well in advance and hardwired into these codes making the codes fragile to change and or difficult to reuse. Given the general complexity of multi-physics problems, it would be preferable to provide more flexibility up front so that many of the critical bets can be deferred closer to run time. In addition, however, it is critical to preserve much of the hard won insight into solvers, variable ordering and iterative schemes that have been shown to work, while allowing easy substitution of other schemes. Fortunately, there have been some recent innovations in computational science that appear to make much of this possible.

Here we will briefly review the basic formulation and behavior of magma-dynamics, illustrate the computational issues and present new results that demonstrate a more unified framework for composing, solving and exploring the sort of multi-physics problems common in solid earth geophysics.

2 PDE's for Magma Migration

2.1 Formulation

There are several formulations available for magma dynamics , but McKenzie, 1984 [1] is probably the simplest and best understood. We have recently reformulated it [2] as a consistent coupling of compressible Darcy flow and Stokes to make it more tractable and more easily integrated with computational methods for mantle convection. The key is to split the fluid pressure P into three components

$$P = P_l + \mathcal{P} + P^* \tag{1}$$

where $P_l = \rho_s^0 gz$ is the reference background "lithostatic" pressure, $\mathcal{P} = (\zeta - 2\eta/3)\boldsymbol{\nabla}\cdot\mathbf{V}$ is the "compaction" pressure due to expansion or compaction of the solid and P^* includes all remaining contributions to the pressure including dynamic pressure due to viscous shear of the matrix.

With these definitions we rewrite the equations for mass and momentum conservation as

$$\frac{D\phi}{Dt} = (1-\phi)\frac{\mathcal{P}}{\xi} + \Gamma/\rho_s \tag{2}$$

$$-\boldsymbol{\nabla}\cdot\frac{K}{\mu}\boldsymbol{\nabla}\mathcal{P} + \frac{\mathcal{P}}{\xi} = \boldsymbol{\nabla}\cdot\frac{K}{\mu}\left[\boldsymbol{\nabla}P^* + \Delta\rho\mathbf{g}\right] + \Gamma\frac{\Delta\rho}{\rho_f\rho_s} \tag{3}$$

$$\boldsymbol{\nabla}\cdot\mathbf{V} = \frac{\mathcal{P}}{\xi} \tag{4}$$

$$\boldsymbol{\nabla}P^* = \boldsymbol{\nabla}\cdot\eta\left(\boldsymbol{\nabla}\mathbf{V} + \boldsymbol{\nabla}\mathbf{V}^T\right) - \phi\Delta\rho\mathbf{g} \tag{5}$$

where $\xi = (\zeta - 2\eta/3)$ and $\Delta\rho = \rho_s - \rho_f$. Equations (2–3) form a non-linear evolution equation for porosity and compaction pressure (and allow non-linear porosity waves), while Eqs. (4–5) solve principally for the creeping, compressible Stokes flow of the solid. These equations couple through the pressure terms $\mathcal{P}$, and P^* and through constitutive equations. In the limit $\phi \to 0$, the equations reduce to incompressible Stokes. In the limit $\eta \to \infty$ they reduce to Darcy flow in a rigid medium. Most of the behavior in these equations is controlled by an intrinsic length scale, the compaction length

$$\delta = \sqrt{\frac{K(\zeta + 4\eta/3)}{\mu}} \tag{6}$$

depends on both permeability and bulk viscosity.

2.1.1 Closure

To close these equations requires constitutive relationships for the permeability K, mantle shear and bulk viscosities η, ζ and functional relationships for the melting rate Γ. Many calculations assume both permeability and bulk-viscosity are non-linear functions of porosity (i.e. $K \propto \phi^n$ and $\zeta \propto 1/\phi^m$ with $n \sim 2 - -3$, $m \sim 0 - 1$).

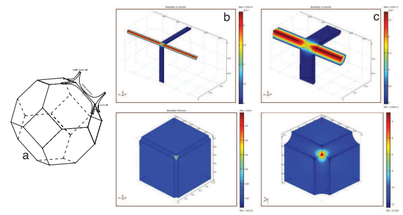
Melting rate can be closed for simple problems assuming parameterized melting. However, to solve consistent, reactive open systems require additional conservation equations for energy, composition, phase equilibria and/or reaction kinetics.

2.2 A more rigorous derivation via Homogenization

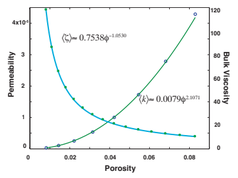
The original derivation of McKenzie[1] (and others [3, 4]) was purely macroscopic multi-phase approach, based on conservation principles and physical intuition. It assumed a microstructure consisting of a low viscosity melt in a porous deformable network, however, the details of that microstructure are not maintained at larger scales beyond simple volume averaging. Moreover, critical constitutive relationship (K, ζ which are emergent properties that must depend on that microstructure remained poorly constrained.

Recently, however Gideon Simpson [5, 6], has used homogenization techniques (e.g. [7]) to derive a consistent set of macroscopic equations for the homogenized conservation of momentum for two coupled Stokes problems at the microscale.

His results **1)** show that McKenzie's equations are consistent with two coupled stokes problems at the microscale for specific scaling regimes **2)** provide a rigorous machinery for computing consistent macroscopic constitutive relationships for (K and $zeta$) from the microstructure via Cell Problems.



Example cell problems for homogenization (G.Simpson) **(a)** Idealized micro structure for a network of low viscosity melt-tubules on a viscously deformable grain. **(b,c)** 3-D FEM calculations for pressure and stress in the fluid and solid phases for the simplest cubic lattice of cylindrical tubes. **b** $\phi = 3\%$ porosity. **c** $\phi = 10\%$



Homogenization results for effective permeability K and bulk viscosity ζ for homogenization of the "tubes on cubes" geometry above. Results and least-squares fits suggest that, for this geometry, $K \propto \phi^2$ and $\zeta \propto \eta/\phi$ thus the compaction-length approaches zero as $\phi \to 0$

The intrinsic length-scale in all magma-dynamics problems is the compaction length, Eq. (6), which depends on the product of the permeability and the bulk-viscosity. Homogenization gives a general method for calculating both constitutive relations for a common micro-structure. For the simplest geometry shown here the compaction length scales as $\delta \propto \sqrt{\phi}$ which predicts that the equations become singular in the limit that $\phi \to 0$. Fundamental mathematical and physical questions remain in this limit.

3 Basic Behavior of the Magma Dynamics Equations

Coupling Darcy Flow for the fluid and Stokes flow for the solid, gives rise to a much richer range of behavior than either sub-problem alone. In general, the introduction of the small lengthscale, δ allows for the spontaneous formation of small-scale structure that can have important implications for melt transport and observable geochemistry. Here we illustrate this behavior with three specific computations.

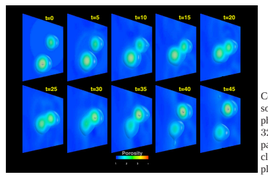
3.1 Magmatic Solitary Waves

In the limit of no solid shear deformation or melting, small porosity ($\phi_0 << 1$) and the simplifications $K \propto \phi^n$, $\zeta = \eta\phi^{-m}$, then Equations (2)–(5) can be reduced to a coupled hyperbolic/elliptic system for pressure and porosity

$$-\boldsymbol{\nabla}\cdot\phi^n\boldsymbol{\nabla}\mathcal{P} + \phi^m\mathcal{P} = \boldsymbol{\nabla}\cdot\phi^n\mathbf{k} \tag{7}$$

$$\frac{D_s\phi}{Dt} = \phi^m\mathcal{P} \tag{8}$$

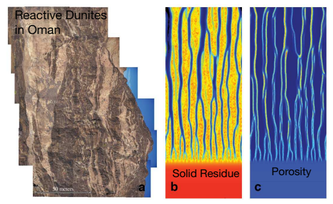
Which is a degenerate, dispersive, non-linear wave equations for the porosity that have been shown to admit solitary waves in 1,2 and 3 dimensions (e.g. [8, 9, 10, 11]. More recent analysis of these equations by G. Simpson [12, 13, 5], demonstrates global existence and well-posedness of solutions for small data for all parameter values (n, m), global well-posedness of solutions for arbitrary initial data for a range of parameters (n, m), and non-linear asymptotic stability of the solitary waves. These equations are singular in the limit $\phi \to 0$ and important open questions remain as to the behavior of this system in this limit (although for global $\phi = 0$, the overall equations reduce to incompressible Stokes.



Computation illustrating the collision of two 3-D magmatic solitary waves for the parameters $n = 3, m = 0$ showing phase shift plus radiation on collision [14]. The domain is $32 \times 32 \times 32$ compaction lengths with 2 grid-points per compaction length, finite volume discretization with light weight classical Geometric Multi-Grid for the elliptic solve and explicit time stepping.

3.2 Melt Localization by Reactive Instabilities

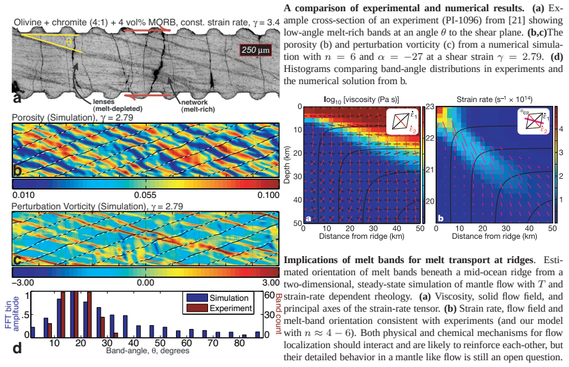
Solitary waves exist for fluctuation in melt flux that occur on scales larger than the compaction length. However, there are other instabilities in this system that occur on scales smaller than δ and lead to the localization of porosity into high-permeability channels. One mechanism for flow localization is the reactive infiltration instability [15, 16, 17] initially hypothesized as a mechanism for producing replacive-dunites observed in ophiolites.



(a) Replacive dunites in Oman. **(b,c)** Calculations for reactive flow in compactible media suggests that fluid-flow up a solubility gradient will spontaneously produce high-porosity melt channels surrounded by low-permeability regions [16, 17]. Continued dissolution can exhaust the soluble phase leaving a record of melt flow in the residuum **b**. Stability analysis suggests that reactive channels will form wherever the solubility changes rapidly on a scale comparable to the compaction length. These channels form at scales smaller than δ.

3.3 Melt Localization by shear induced instabilities

An alternative instability occurs if the shear viscosity η is a decreasing function of porosity and the system is undergoing shear. These systems are unstable to localization instabilities [18, 19, 20] that form high-porosity melt bands on scales $<< \delta$. This effect has been demonstrated experimentally and these experiments provide important examples against which to validate the theory. Figures A–D, show experiments and calculations for flow bands in simple shear, showing the ubiquitous low angle of melt bands $\sim 20^\circ$ with respect to the shear plane. The other figure suggest that reoriented melt-bands could produce an anisotropic permeability that could also focus melt to the ridge axis.



A comparison of experimental and numerical results. (a) Example cross-section of an experiment (PI-1096) from [21] showing low-angle melt-rich bands at an angle θ to the shear plane. **(b,c)**The porosity (b) and perturbation vorticity (c) from a numerical simulation with $n = 6$ and $\alpha = -27$ at a shear strain $\gamma = 2.79$. **(d)** Histograms comparing band-angle distributions in experiments and the numerical solution from b.

Implications of melt bands for melt transport at ridges. Estimated orientation of melt bands beneath a mid-ocean ridge from a two-dimensional, steady-state simulation of mantle flow with T and strain-rate dependent rheology. **(a)** Viscosity, solid flow field, and principal axes of the strain-rate tensor. **(b)** Strain rate, flow field and melt-band orientation consistent with experiments (and our model with $n \approx 4 - 6$). Both physical and chemical mechanisms for flow localization should interact and are likely to reinforce each-other, but their detailed behavior in a mantle like flow is still an open question.

4 Open Problems/Computational Issues

These model problems illustrate some of the wide range of behavior inherent in the governing equations as demonstrate how small changes in assumptions about coupling or constitutive equations (e.g. constant η vs. $\eta(\phi)$), can lead to drastic changes in behavior and the introduction of multiple scales. All of these instabilities are likely to lead to a localized, dynamic melt transport network, however significant questions remain:

1. What is the interaction between mechanical and chemical localization phenomena?
2. How do the small scale structures interact with and affect the large scale mantle flow/effective properties of plate boundaries?
3. How do we incorporate consistent thermodynamic melting?
4. What are the observable consequences of these processes for geophysics and geochemistry?
5. Can we use available data to infer properties and processes at depth?

To answer these questions requires flexible, multi-physics codes and solvers (plus good theory, and data) that can rapidly explore a range of couplings, constitutive equations and additional processes/PDE's (such as energy conservation and thermodynamics). Given current codes, this is somewhat difficult as each code, is tailored to a specific problem and many of the critical computational choices (discretization, mesh, solvers, iterative strategy) are hard-wired in from the beginning. However, using recent advances in computational software, we are beginning to develop a new generation of codes that allow us to reuse much of our physical expertise, but defer many of the critical choices closer to run time.

5 Structure/Solution strategy for multi-physics problems

Equations (2)–(5) are typical of the systems of PDE's arising in solid earth dynamics, in that each of the equations (or subsystems of equations) can often be treated as linear equations if the other variables are frozen, leading to complicated (but efficient) operator splitting schemes based on careful ordering and lagging of variables, coupled with fast linear solvers and an overall functional iteration for the system. Infinite Prandtl number mantle convection provides a simpler example

$$\frac{DT}{Dt} = \nabla^2 T \tag{9}$$

$$-\boldsymbol{\nabla}\cdot\left[\eta\boldsymbol{\nabla}\mathbf{V} + \boldsymbol{\nabla}\mathbf{V}^T\right] + \boldsymbol{\nabla}P = \mathrm{Ra}T\hat{\mathbf{g}} \tag{10}$$

$$\boldsymbol{\nabla}\cdot\mathbf{V} = 0 \tag{11}$$

which is often solved by splitting an advection-diffusion equation for temperature (with known velocities) with a linear Stokes solver forced by T.

The problem with these schemes is that for larger systems, ordering, lagging and convergence control becomes unwieldy. An alternative approach is to discretize the entire system as a non-linear problem $\mathbf{F}(\mathbf{x}) = \mathbf{0}$ and use a suitable non-linear method such as Newton. For large systems, however, the Jacobians are large block matrices that can be difficult to both compute and solve. Nevertheless, the underlying "near linear" system of equations is preserved in the block structure and with suitable computational tools can be used to form efficient "physics based" or "PDE based" preconditioners based on existing or new splitting schemes. For example, the discrete linearized Jacobian for iso-viscous thermal convection can be written

$$\begin{bmatrix} A & \partial V & 0 \\ -RaI & K(\eta) & G \\ 0 & G^T & 0 \end{bmatrix} \begin{bmatrix} \delta_T \\ \delta\mathbf{V} \\ \delta_P \end{bmatrix} = \begin{bmatrix} \mathbf{r}_T \\ \mathbf{r}\mathbf{V} \\ \mathbf{r}_P \end{bmatrix}$$

where $A(\eta, \mathbf{V})$ is an advection diffusion operator, and Discrete Stokes exists in the lower 2×2 diagonal block. Coupling terms for temperature driven flow are in the $(2, 1)$ block and advection in $(1, 2)$ block. Additional coupling, for example a temperature dependent viscosity $\eta(T)$ would add additional terms to the $(2, 1)$ block and modify K. Likewise Equations (2)–(5), has the 4×4 block structure

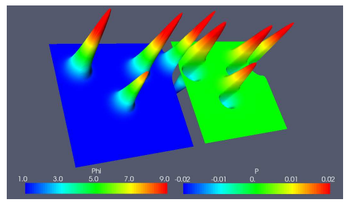
$$\begin{bmatrix} K(\eta) & G & 0 & -\beta M \\ G^T & 0 & M/\zeta & 0 \\ 0 & 0 & L(\phi) & f(\phi) \\ M_V & 0 & -\Delta t M & M \end{bmatrix} \begin{bmatrix} \delta_V \\ \delta_P^* \\ \delta\mathcal{P} \\ \delta\phi \end{bmatrix} = \begin{bmatrix} \mathbf{r}_V \\ \mathbf{r}_P^* \\ \mathbf{r}_\mathcal{P} \\ \mathbf{r}_\phi \end{bmatrix}$$

6 Computational Ingredients for Flexible multi-physics solvers

To explore and (efficiently?) solve these large block systems requires two critical software ingredients: 1) Efficient and flexible methods for assembling the discrete Jacobians 2) Flexible pre-conditioning schemes that allow arbitrary composition of the sub-blocks to reuse "physics based" recipes. Fortunately, several interoperable computational software projects (FEniCS and PETSc), have recently developed sufficient features to prototype such schemes easily. Here we demonstrate hybrid codes that utilize the following components

- FEniCS Form Compiler (FFC) (www.fenics.org): for automatic code generation of the weak form of analytic jacobians and residuals.
- Dolfin (www.fenics.org): for assembly of discrete block matrices and for a clean abstract interface for discrete functions on FEM spaces (used for Semi-Lagrangian schemes on unstructured meshes with GTS).
- PETSc non-linear solvers (SNES) with FieldSplit preconditioners (www-unix.mcs.anl.gov/petsc/petsc-2/): that allow arbitrary ordering and composition of sub-block pre-conditioners while preserving global convergence of the non-linear problem.

7 Example: Block-preconditioners for non-linear magma wave equations



Solution of 2D non-linear wave equations using FFC generated Jacobians and PETSc FieldSplit preconditioners. Calculation includes

- FEM space: Mixed P1-P1 Lagrange for porosity and pressure
- Mesh: $128x128$ "UnitSquare Left"
- Domain: 64×64 compaction lengths
- Parameters: permeability $n = 2$, bulk viscosity $m = 1$

Full time-dependent calculation shows the instability of an initial 1-D Gaussian distribution of porosity into a family of 2-D solitary waves plus radiation (see the movie).

Choosing a finite element space, we compose the weak form of the Jacobian and residual of Eqs. (7)–(8) as

```
# choose Finite element space and compose mixed P1P1 elements
P1 = FiniteElement("Lagrange", "triangle", 1)
M = P1 + P1

(v,  u)  = TestFunctions(M)
(dp, df) = TrialFunctions(M) # deltas for pressure and porosity
(p, f)   = Functions(M)      # solution from last iteration

# set constants and auxiliary functions in form
dt = Constant("triangle")  # time step
hdt = 0.5*dt # half time step
hsquared = Constant("triangle") # (h/delta)^2: domain size in  compaction lengths
gStar = QuadratureFunction("triangle") # Semi-lagrangian source term
n = FacetNormal("triangle") # facet normal for surface integrals

# Permeability and its derivative with respect to porosity
def K(f):
       return f*f

def dKdf(f):
       return 2*f

# weak form of Jacobian (Bilinear Form)
a1 = (K(f)*dot(grad(v),grad(dp)) + hsquared*f*v*dp)*dx + ((dKdf(f)*dot(grad(v),grad(p))
     + hsquared*v*p - dKdf(f)*v.dx(1))*df)*dx + dKdf(f)*df*v*n[1]*ds
a2 = -u*hdt*hsquared*f*dp*dx + u*(1 - hdt*hsquared*p)*df*dx
a = a1 + a2

# weak form of non-linear residual Function -F(x): Linear Form
L1 = (K(f)*dot(grad(v),grad(p)) +hsquared*v*f*p - K(f)*v.dx(1))*dx + v*K(f)*n[1]*ds
L2 = u*(f - hdt*hsquared*(f*p) -gStar)*dx
L = -L1 - L2
```

Which upon assembly by dolfin produces a 2×2 block system

$$\begin{bmatrix} A(f) & B(f,p) \\ -\frac{\Delta t}{2}M & M \end{bmatrix} \begin{bmatrix} \delta p \\ \delta f \end{bmatrix} = -\begin{bmatrix} r_p \\ r_f \end{bmatrix} \tag{12}$$

Which is solved using a fieldsplit preconditioner defined by the PETSc options file

```
-ksp_type richardson # use Richardson on the full system
-pc_fieldsplit_type multiplicative
#
# set up fieldsplit preconditioner for Pressure (0) AMG on A block
#
-fieldsplit_0_ksp_type preonly
-fieldsplit_0_pc_type hypre
-fieldsplit_0_ksp_monitor
#
# set up fieldsplit preconditioner for Porosity(1) SOR on porosity Mass-Matrix
#
-fieldsplit_1_ksp_type preonly
-fieldsplit_1_pc_type sor
-fieldsplit_1_ksp_monitor
```

Other composite solver schemes are easily implemented by changing the options at run time. This algorithm gives quadratic convergence with performance comparable to AMG preconditioned GMRES for the entire 2x2 system (even with the memory overhead of computing sub-matrices). Initial results suggest the algorithm is optimal with grid size.

7.1 A ToDo list

- Parallel Assembly (coming in Dolfin, Sieve)
- Parallel Semi-Lagrangian methods (mesh partitioned GTS)
- Larger systems: Rayleigh-Benard Convection, Full Magma
- Improve interface for the educated geo-user (CIG)
- Integrate with other CIG Mantle/Convection/ Lithospheric deformation projects for plate boundary modeling