FCUBED

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1 Introduction

FCubed=FFF=Fluid Fracturing Flow

2 Physics & Equations

2.1 Basic equations

2.1.1 Stokes flow

$$\vec{\nabla} \cdot \boldsymbol{\sigma} + \rho\vec{g} = \vec{0} \quad (1)$$
$$\vec{\nabla} \cdot \vec{\mathrm{v}} = 0 \quad (2)$$

The full stress tensor is given by

$$\boldsymbol{\sigma} = -p\mathbf{1} + \boldsymbol{\tau}$$

where $\mathbf{1}$ is the unit matrix, p is the pressure and $\boldsymbol{\tau}$ is the deviatoric stress tensor which can be written as

$$\boldsymbol{\tau} = 2\eta\dot{\boldsymbol{\varepsilon}}(\vec{\mathrm{v}})$$

where η is the viscosity, $\vec{\mathrm{v}} = (u, v)$ is the velocity vector, and $\dot{\boldsymbol{\varepsilon}}(\vec{\mathrm{v}})$ is the (deviatoric) strain rate tensor.

Putting it all together we obtain:

$$-\vec{\nabla}p + \vec{\nabla} \cdot (2\eta\dot{\boldsymbol{\varepsilon}}(\vec{\mathrm{v}})) + \rho\vec{g} = \vec{0} \quad (3)$$
$$\vec{\nabla} \cdot \vec{\mathrm{v}} = 0 \quad (4)$$

In what follows we assume the buoyancy forces are negligible, i.e. the term $\rho\vec{g}$ is neglected.

2.1.2 Rheology

In the case of a dislocation creep rheology, we have (REF?)

$$\dot{\varepsilon} = A\sigma^n \exp -\frac{Q}{nRT}$$

In practice, this is expressed in the form of an effective viscosity that is a function of strainrate and temperature:

$$\eta_{dsl} = \frac{1}{2}A^{-1/n}\dot{\varepsilon}_e^{1/n-1} \exp \frac{Q}{nRT}$$

where $\dot{\varepsilon}_e$ is the effective strain rate defined as

$$\dot{\varepsilon}_e = \sqrt{\frac{1}{2}(\dot{\varepsilon}_{xx}^2 + \dot{\varepsilon}_{yy}^2) + \dot{\varepsilon}_{xy}^2}$$

We also wish to take plastic deformation and we therefore consider a Drucker-Prager yield criterion:

$$\sigma_{yield} = p\sin\phi + c\cos\phi$$

where c is the cohesion and ϕ is the angle of friction. Likewise, we end up defining a so-called 'plastic effective viscosity':

$$\eta_{pl} = \frac{\sigma_{yield}}{2\dot{\varepsilon}_e}$$

2.1.3 Darcy flow

Following chapter 10 of Guy Simpson's book Simpson [11] the equations governing the evolution of the fluid pressure and fluid flow velocities are[1]

$$\varphi\beta\frac{\partial p_f}{\partial t} = -\vec{\nabla} \cdot \vec{v} + H - \frac{\partial\varphi}{\partial t} \quad (5)$$
$$\vec{v} = -\frac{K}{\eta_f}\vec{\nabla}p_f \quad (6)$$

is this the equation we want to use ? other ref ? what are other ppl using ?

where

[1] I have slightly changed the notations.

- p_f is the pore fluid pressure,
- $\vec{v}$ is the fluid velocity vector,
- φ is the porosity (-). Wikipedia[2]: "Porosity or void fraction is a measure of the void (i.e. "empty") spaces in a material, and is a fraction of the volume of voids over the total volume, between 0 and 1, or as a percentage between 0% and 100%".
- β is the bulk compressibility(Pa^{-1}),

typical va for rocks?

we find online multiple compressbilities in the context of rocks. Which are we to use?

- K is the permeability (m^2). Wikipedia[3]: "Permeability is a property of porous materials that is an indication of the ability for fluids (gas or liquid) to flow through them. Fluids can more easily flow through a material with high permeability than one with low permeability. The permeability of a medium is related to the porosity, but also to the shapes of the pores in the medium and their level of connectedness. Fluid flows can also be influenced in different lithological settings by brittle deformation of rocks in fault zones; the mechanisms by which this occurs are the subject of fault zone hydrogeology. Permeability is also affected by the pressure inside a material."

  In the code it is assumed to be given by Skarbek and Rempel [12] and Bernaudin and Gueydan [1]

$$K = K_0 \left(\frac{\varphi}{\varphi_0} \right)^3$$

  where K_0 is the permeability at a reference porosity φ_0. See eq 10 of Walder and Nur [14]
- η_f is the fluid viscosity ($\mathrm{Pa\,s}$), typically water[4]
- ρ_f is the water density ($\mathrm{kg\,m^{-3}}$),
- g is acceleration due to gravity ($\mathrm{m\,s^{-2}}$),
- H accounts for any fluid pressure sources or sinks (e.g., due to devolatilization reactions)

substituting (6) into (5) lead to a single parabolic equation for the excess fluid pressure as follows:

$$\varphi\beta\frac{\partial p_f}{\partial t} = \vec{\nabla}\cdot\left(\frac{K}{\eta_f}\vec{\nabla}p_f\right) + H - \frac{\partial\varphi}{\partial t} \tag{7}$$

Note that once the excess pressure is computed one can recover the fluid velocity via $\vec{v} = -\frac{K}{\eta_f}\vec{\nabla}p_f$.

Also, assuming all coefficients to be constant in space (and therefore neglecting the $\partial\varphi/\partial t$ term), we can write the equation above as

$$\frac{\partial p_f}{\partial t} = \underbrace{\frac{K}{\eta_f\varphi\beta}}_{\kappa}\Delta p_f + H$$

which is a diffusion equation.

Following Walder and Nur [14], we can define a characteristic time for the diffusion as

$$t_s = \frac{H^2}{\kappa}$$

2.1.4 Coupling

Remark1: when using tectonic dt (which is $\mathcal{O}(10^5)$ year, we find that $\frac{\partial\varphi}{\partial t} \simeq \frac{\varphi^n - \varphi^{n-1}}{\delta t} \to 0$ so that the contribution of this term to the equation is virtually inexistant.

Remark2: Likewise the characteristic Darcy time is probably about $\mathcal{O}(10^0)$ year so that when carrying out tectonic time steps the Darcy diffusion process has the time to reach steady state. Since we are currently not relying on an operator splitting approach, we might as well directly solve the steady state Darcy equation, i.e. $\partial p_f/\partial t \to 0$.

Remark: I have serious doubts about our approach here concerning the coupling. Reading the short chapter in Ismail-Zadeh and Tackley [8] on this topic there seems to be quite some work done in the 90s and I suspect we should first consider this literature rather than blindly couple Stokes and Darcy.

[2] https://en.wikipedia.org/wiki/Porosity
[3] https://en.wikipedia.org/wiki/Permeability_(Earth_sciences)
[4] https://en.wikipedia.org/wiki/Water

3 Numerical aspects

The domain is a 2D Cartesian box of size $L_x \times L_z$ with the lower left corner at $(x, y) = (0, 0)$. The partial differential equations above are discretised and solved by means of the Finite Element method. In the case of the Stokes equation the $Q_2 \times Q_1$ pair is used Thieulot and Bangerth [13] while Q_2 elements are used for the Darcy equation.

Both finite element matrices are assembled using lil_matrix, converted to CSR format and then passed to a direct solver.

Node that the code is based on the codes available in the educational Fieldstone project and is therefore not optimised for performance.

3.1 FE formulation of the equations

3.1.1 Stokes equations

Following a standard approach, the discretised Stokes equations yield the following linear system

$$\begin{pmatrix} \mathbb{K} & \mathbb{G} \\ \mathbb{G}^T & 0 \end{pmatrix} \cdot \begin{pmatrix} \vec{\mathcal{V}} \\ \vec{\mathcal{P}} \end{pmatrix} = \begin{pmatrix} \vec{f} \\ \vec{h} \end{pmatrix}$$

where $\vec{\mathcal{V}}$ is the vector containing all velocity degrees of freedom (size NfemV=NV*ndofV) and $\vec{\mathcal{P}}$ is the vector containing all pressure degrees of freedom (size NfemP=NP*ndofP).

3.1.2 Darcy equations

Applying standard FE methodology to what is essentially a diffusion equation, we arrive at:

$$\mathbb{M} \cdot \vec{\mathcal{P}}_e + \mathbb{K}_d \cdot \vec{\mathcal{P}}_e = rhs$$

with

$$\mathbb{M} = \int_\Omega \varphi \beta \vec{\mathcal{N}}^T \vec{\mathcal{N}}$$

$$\mathbb{K}_d = \int_\Omega \boldsymbol{B}^T \boldsymbol{B} \frac{K}{\eta_f}$$

$$rhs = \int_\Omega \vec{\mathcal{N}}^T H$$

Using a simple first order time discretisation yields

$$(\mathbb{M} + \mathbb{K}_d \delta t) \cdot \vec{\mathcal{P}}_e^n = \mathbb{M} \cdot \vec{\mathcal{P}}_e^{n-1} + rhs \delta t$$

3.2 Rheological parameters

include here data for A,n,Q of different materials

specify c,phi for plasticity

3.3 Specific algorithms

3.3.1 computing time step

The time step δt is limited by a CFL condition and implemented as follows:

$$\delta t = C \frac{h}{\max |\vec{\mathbf{v}}|_\Omega}$$

where h is the element size and $C \in [0, 1[$.

3.3.2 Generating weak seeds

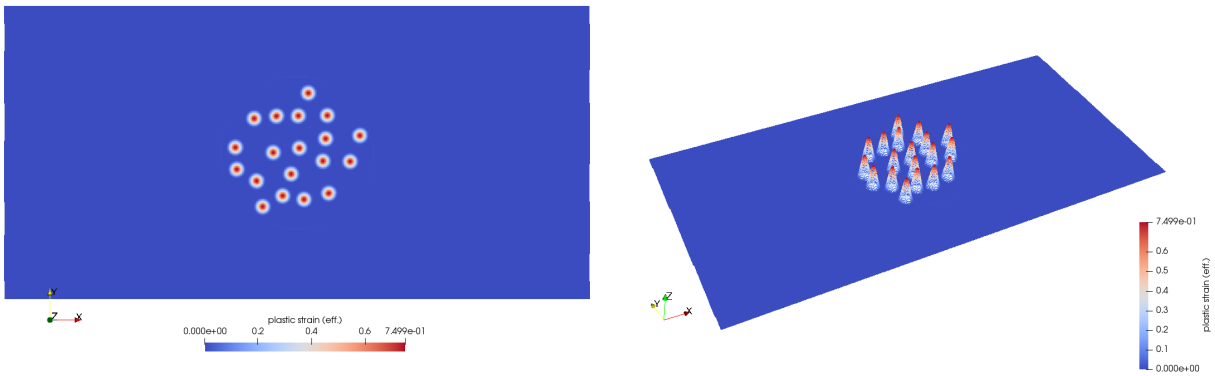
Poisson disc distribution seeds generated in square.

Notes that seeds which are kept are those inside circle or size ainclusion-w

For each marker im we test whether it is at a distance of w or less of seed is and the prescribed strain is then parameterised as follows

$$A\frac{1}{2}\left(\cos(\pi\frac{\sqrt{(x_{im}-x_{is})^2+(y_{im}-y_{is})^2}}{w})+1\right)$$

where w is the radius of the seed, and A its maximum amplitude



Example of about 20 seeds placed in the domain

3.3.3 Time dependent b.c.

At the moment these are parameterised by t_1, t_2 and velofact.

```
       +-----------------+ -- velofact
       |                 |
-------|-----------------|------> time
       t1                t2
```

3.3.4 Dealing with nonlinearities

Picard iterations

Nonlinear residual

3.4 Numerical parameter values and meaning

3.4.1 Marker in cell technique

The code implements the marker in cell technique to track materials/fluids. The ensemble of markers is called a swarm[5]. At the beginning of the simulation marker_per_dim^2 markers are placed regularly inside each element. In total there are then nmarker=nel*marker_per_dim^2 markers.

Each marker carries a variety of fields:

- swarm_x,swarm_y:
- swarm_mat: type of material
- swarm_paint paint to show the virtual deformation of the grid
- swarm_r,swarm_s reduced coordinates s
- swarm_u,swarm_v velocity y
- swarm_exx,swarm_exy,swarm_eyy strain rate xy
- swarm_ee: effective strain rate

[5] https://en.wikipedia.org/wiki/Swarm_behaviour

- swarm_total_strainxx, swarm_total_strainxy, swarm_total_strainyy
- swarm_total_strain_eff
- swarm_plastic_strainxx, swarm_plastic_strainxy, swarm_plastic_strainyy
- swarm_plastic_strain_eff
- swarm_plastic_strain_eff0
- swarm_tauxx, swarm_tauxy, swarm_tauyy:
- swarm_tau_eff
- swarm_iel: element containing the marker
- swarm_eta: (effective) viscosity of the marker
- swarm_rho: density of the marker
- swarm_p_dyn
- swarm_yield
- swarm_is_plastic
- swarm_tau_angle
- swarm_sigmaxx, swarm_sigmaxy, swarm_sigmayy: components of the full stress tensor
- swarm_sigma_angle: principal angle full stress
- swarm_sigma1, swarm_sigma2: principal stresses
- swarm_sw_level: level of strain weaking betw. 0 and 1

Before the FEM can be built we need to project density and viscosity onto the mesh so that these quantities can be used in the matrix and right hand side. We have opted here for the very simple elemental approach. All markers inside an element are taken into account and their harmonic average is used for the viscosity while the arithmetic average is used for the density.

advection, periodic pc, painting

3.5 Code parameters

Global parameters common to all experiments only:

- Lx,Ly: domain size
- nelx,nely: number of elements in x,y direction
- nstep:
- niter:
- tol:
- CFL_nb:
- marker_per_dim:
- eta_ref:
- tfinal:
- output_folder:
- linear: boolean flag to indicate whether the rheology is linear or not.
- every_vtu:
- every_png:
- use_fluid:
- etc ...

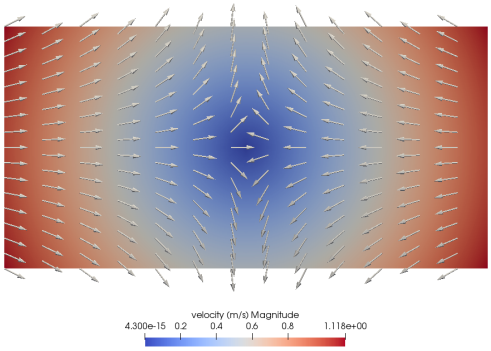
4 Benchmarks

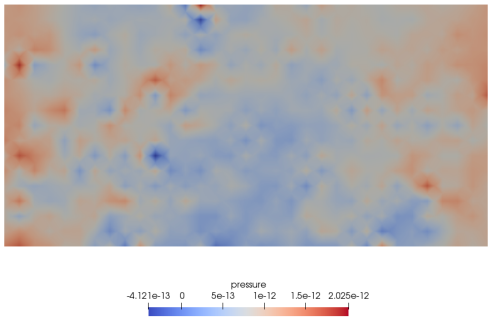
4.1 Pure shear

The domain is a Cartesian box of size 2×1. Pure shear kinematical boundary conditions are prescribed: $u = v_{ref}/L_y$ on the left boundary, $u = -v_{ref}/L_y$ on the right boundary, $v = -v_{ref}/L_x$ on the bottom boundary, $v = v_{ref}/L_x$ on the top boundary. This is such that one can change either L_x or L_y at will and the in/out-fluxes balance each other out.

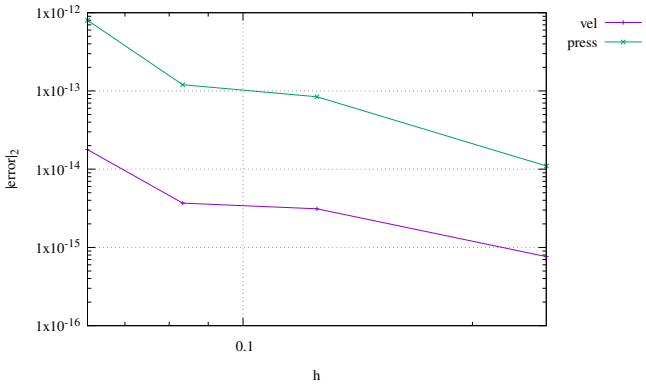
The analytical solution is then

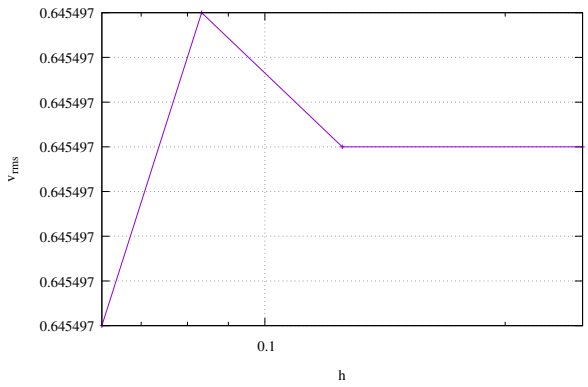
$$u(x,y) = 1 - x \qquad v(x,y) = -0.5 + y \qquad p(x,y) = 0$$





As such the analytical solution can be represented exactly with the basis functions of the code. We therefore recover errors that are machine precision:



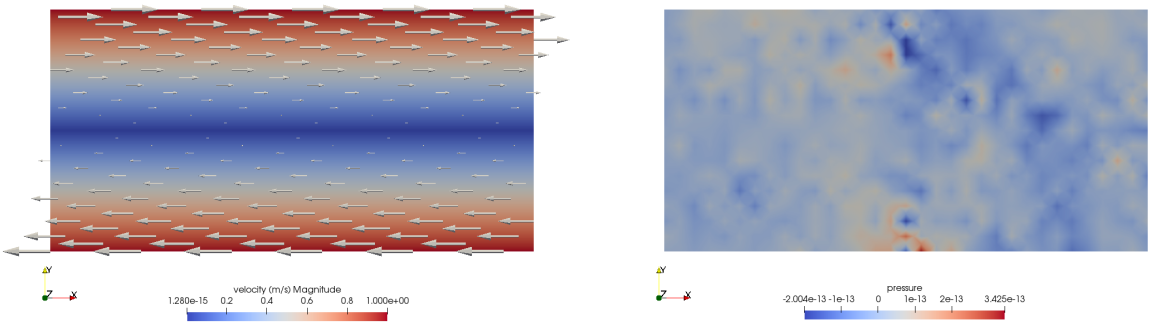


4.2 Simple shear

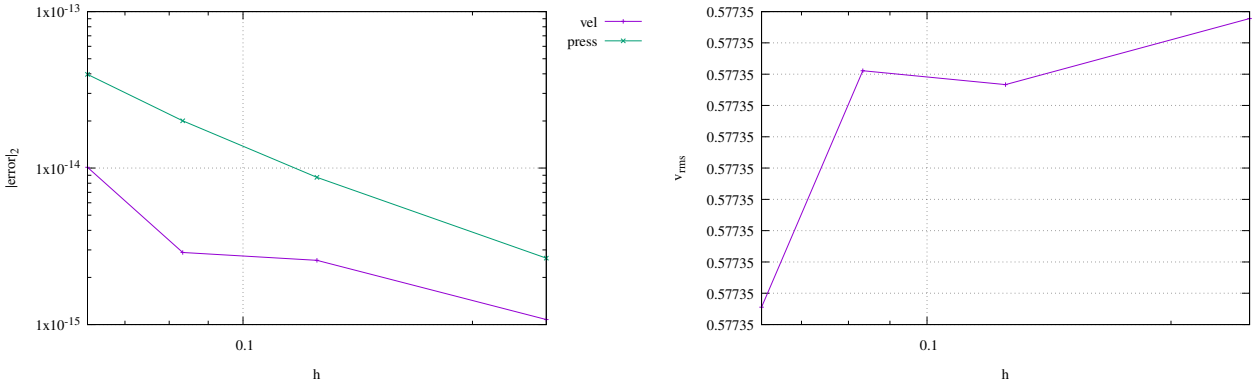
The domain is a Cartesian box of size 2×1. Boundary conditions are as follows: Left and right sides: $v = 0$; top: $u = 1$, bottom: $u = -1$.

The analytical solution is then

$$u(x,y) = 2(y - 1/2) \qquad v(x,y) = 0 \qquad p(x,y) = 0$$



Here too the analytical solution can be represented exactly with the basis functions of the code and we therefore recover errors that are machine precision:



4.3 SolVi

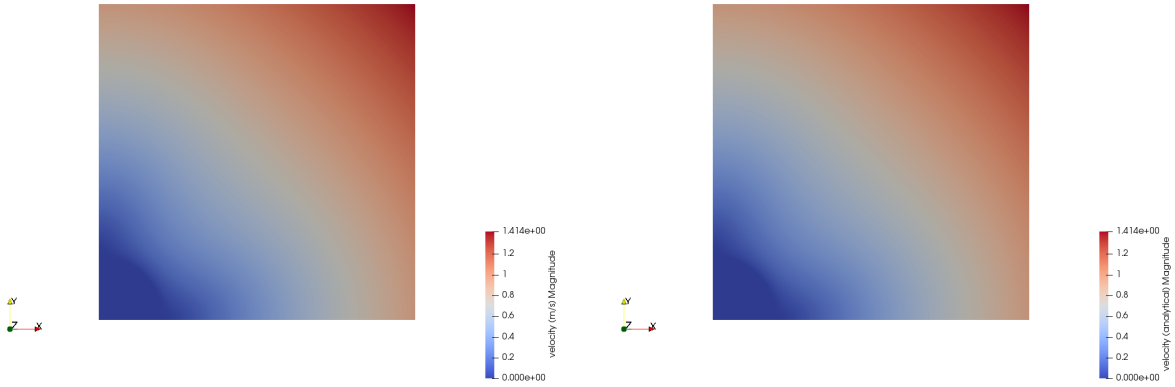
SolVi is another very common benchmark carried out in the computational geodynamics literature.

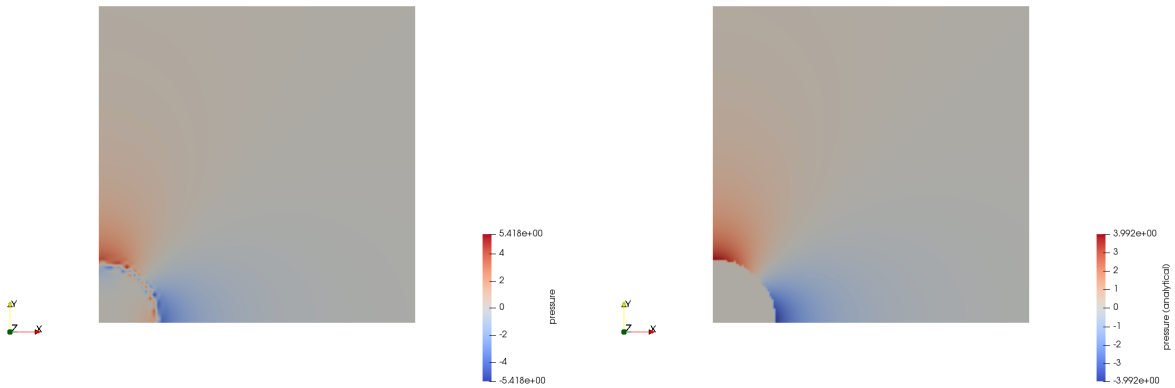
This inclusion benchmark solves a problem with a discontinuous viscosity, which is chosen in such a way that the discontinuity is a circle. Given the regular nature of the used by a majority of codes, this ensures that the discontinuity in the viscosity never aligns to cell boundaries. This in turns leads to almost discontinuous pressures along the interface which are difficult to represent accurately.

Schmid & Podlachikov (2003) [10] derived a simple analytic solution for the pressure and velocity fields for such a circular inclusion under simple shear.

One important observation with this benchmark is the fact that the velocity is not zero even far away from the inclusion, so that the analytical solution must be imposed on the sides. Also, because of symmetry, it is often run on the top 1×1 quadrant $x > 0$, $y > 0$ with free slip imposed on the left and bottom boundaries.

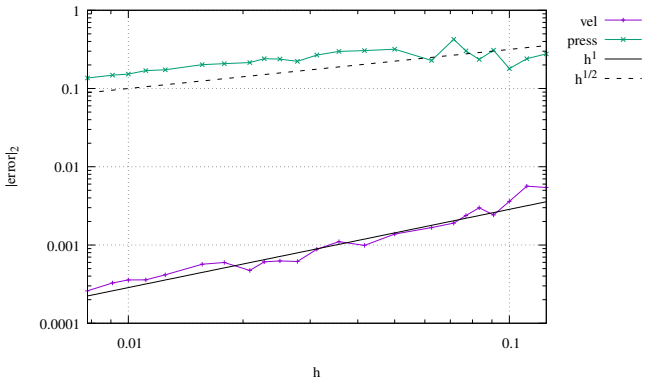
Results for this benchmarks are to be found in Kronbichler, Heister, and Bangerth [9] or Gerya, May, and Duretz [5] for example.

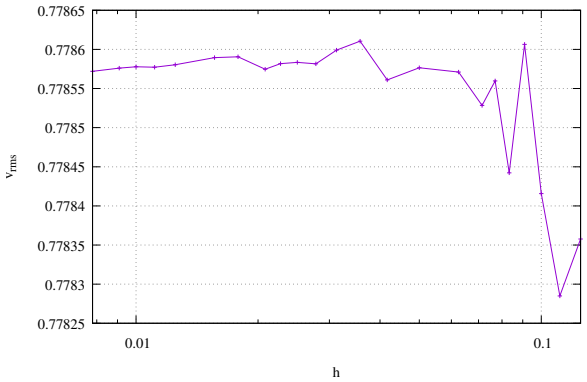


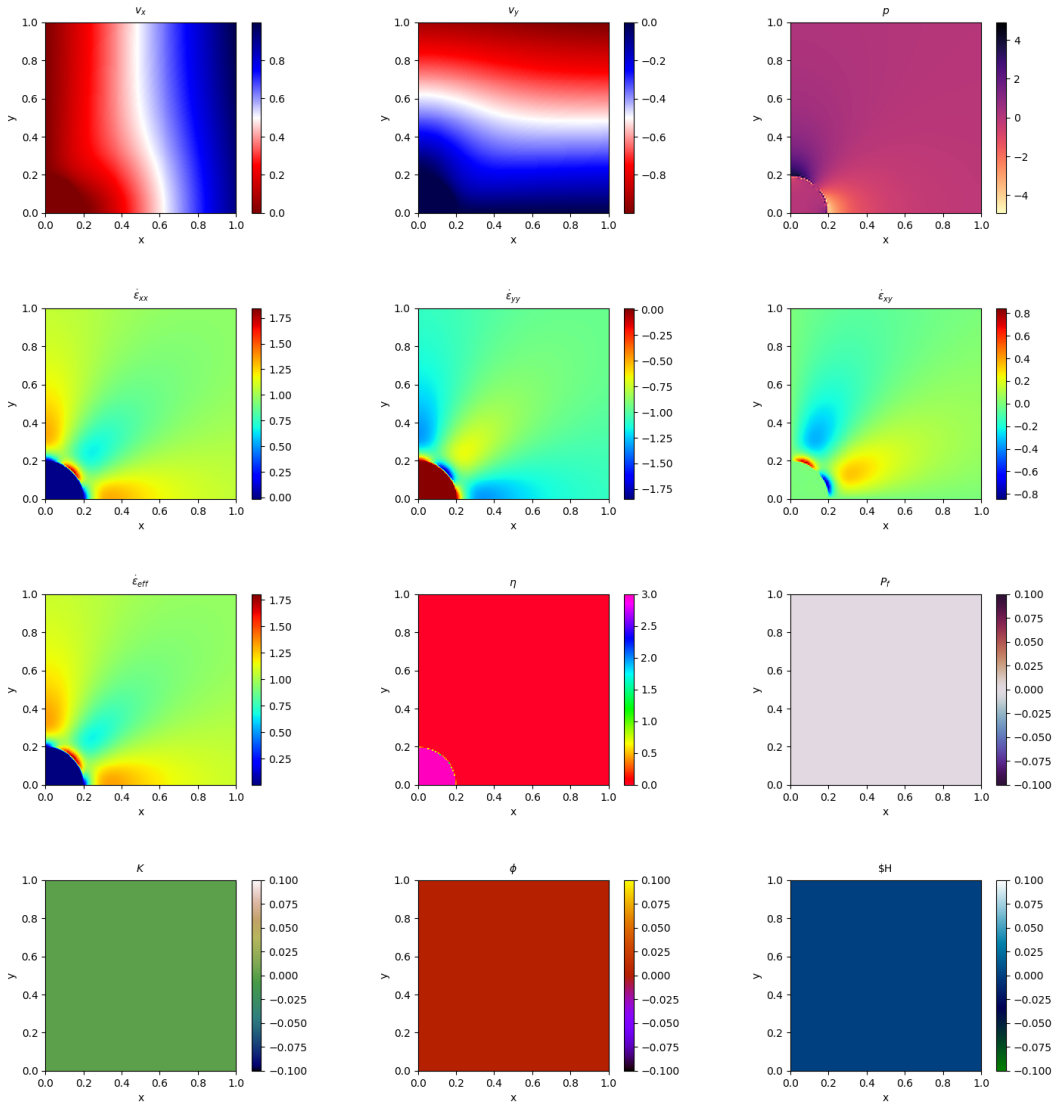


Top row: velocity, bottom row: pressure. Left column: computed field, right column: analytical solution.

We recover a linear convergence for the velocity error and a $h^{1/2}$ convergence for the pressure error as in REF:







4.4 SolKz

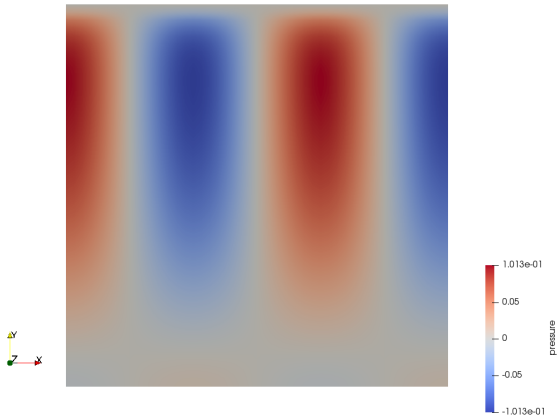
The viscosity is a function of the space coordinates and is given by

$$\eta(y) = \exp(2By) \quad \text{with} \quad B = 13.8155$$

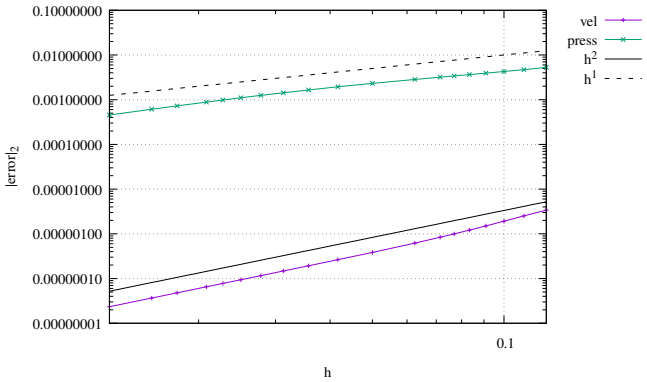
It is not a discontinuous function but grows exponentially with the vertical coordinate so that its overall variation is 10^6. The forcing is chosen by imposing a spatially variable density variation as follows:

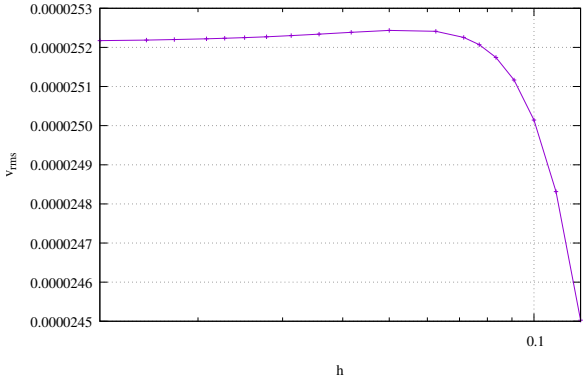
$$\rho(x, y) = \sin(2y)\cos(3\pi x)$$

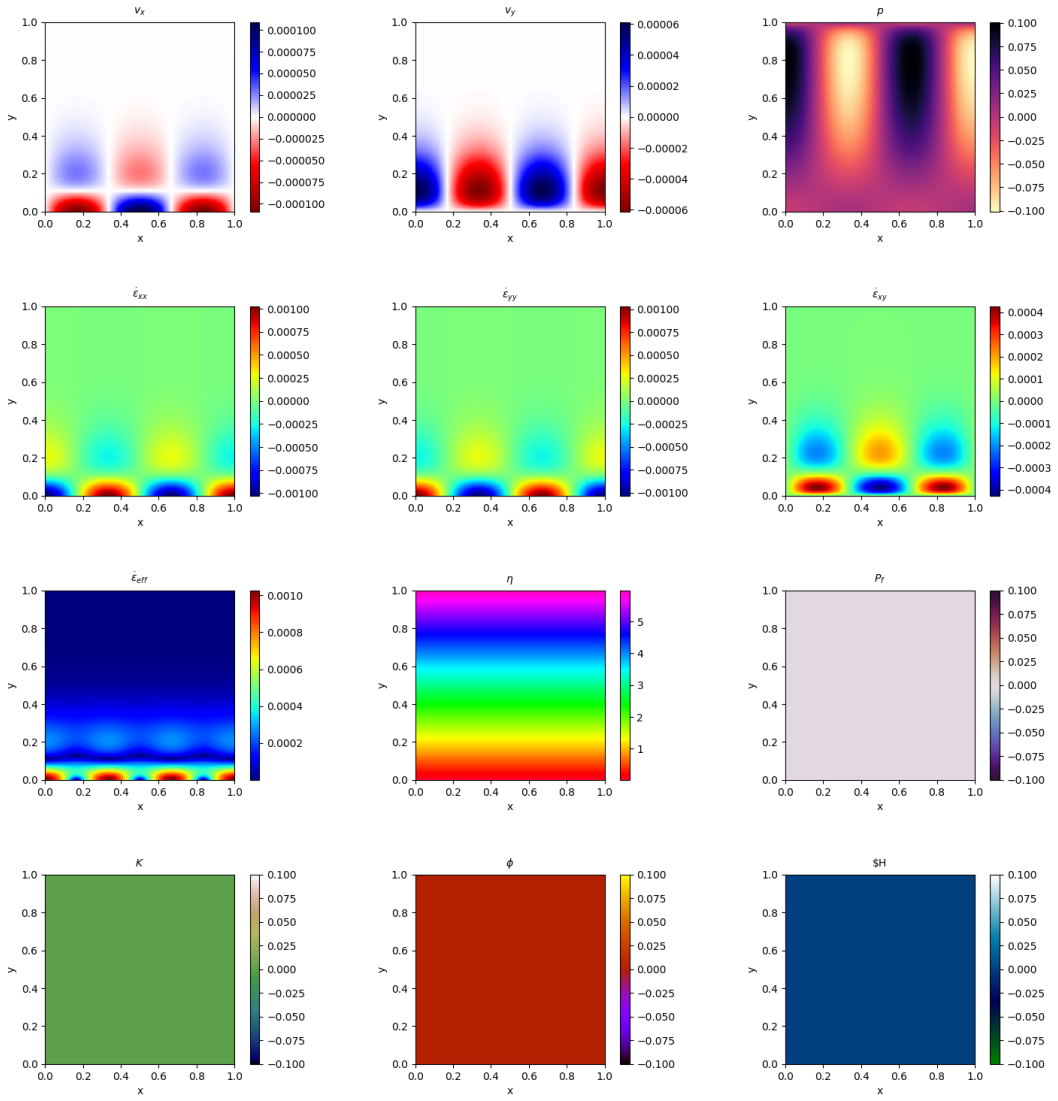
Free slip boundary conditions are imposed on all sides of the domain. This benchmark is presented in [15] and is studied in [2] and [5].



Despite an elemental averaging of the particle properties we recover a quadratic convergence for the velocity error and a linear convergence for the pressure error as expected:







4.5 Channel flow with stress-dependent rheology

This analytical benchmark is carried out in Gerya and Yuen [6], Fraters, Bangerth, Thieulot, Glerum, and Spakman [4], Gerya [7], and Elesin, Gerya, Artemieva, and Thybo [3].

It consists of a vertical flow of a non-Newtonian (with a power-law index n) viscous medium in a section of an infinite vertical channel of width L in the absence of gravity. The flow is driven by a pressure gradient $\partial P/\partial y$. along the channel and no-slip conditions at the walls. The viscosity of the non-Newtonian flow is defined by the following equation:

$$\eta_{eff} = \frac{1}{2} A^{-1/n} \dot{\varepsilon}_e^{-1+1/n}$$

I need to rederive it from scratch myself, write it all in fieldstone and then implement it here.

4.6 (E)VP experiment gerya 3 mats

4.7 darcy? simpson ?

4.8 gaussian pulse diffusion in time

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