3-D Numerical Modeling of Coupled Crustal Deformation and Fluid Pressure Interactions

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Program Element II

ABSTRACT

This report summarizes the results from a project aimed at investigating the interrelationships of crustal deformation and pore fluid pressures. The project had three main goals: (1) to develop an algorithm for simulating crustal deformation and fluid flow processes, (2) to implement and validate numerical models based on selected benchmark hydrogeophysical problems related to specified boundary conditions, and (3) to use the numerical simulations to explore poroelastic processes in realistic geologic domains. The results of the project should be useful for reducing seismic hazard by increasing our understanding of fluid pressures in postseismic deformation and by providing a coupled crustal deformation and pore pressure propagation modeling tool available to others for use in exploring the poroelastic response of brittle crustal rocks and sedimentary basins to strong earthquakes. The codes developed as part of this grant, referred to herein as PFLOW, are described in this report. PFLOW is a 3-D time-dependent pore-pressure diffusion model developed to investigate the response of pore fluids to the crustal deformation generated by strong earthquakes in heterogeneous geologic media. Given crustal strain generated by changes in Coulomb stress, this MATLAB-based code uses Skempton's coefficient to calculate resulting initial change in fluid pressure (initial condition). Pore-pressure diffusion can be tracked over time in a user-defined model space with user-prescribed Neumann or Dirichlet boundary conditions and with spatially variable values of permeability. PFLOW employs linear or quadratic finite elements for spatial discretization and explicit or implicit first order, or implicit second order, finite difference discretization in time. PFLOW is easily interfaced with output from deformation modeling programs such as Coulomb (Toda et al., 2005) or 3D-DEF (Gomberg and Ellis, 1993). The code is useful for investigating, to first-order, the evolution of pore pressure changes induced by changes in Coulomb stress and their possible relation to water-level changes in wells or changes in stream discharge. We offer it to users as a possible research and educational tool, for non-commercial use.

INTRODUCTION

Field evidence suggests a causal relationship between hydrologic changes and earthquakes. For instance, pore-pressure increases due to deep-well injection, increased stream discharge, groundwater recharge, and the filling of reservoirs have been linked to earthquake triggering (e.g., Costain et al., 1987). Conversely, moderate to large earthquakes have generated significant hydrologic changes, such as fluctuations of stream discharge and groundwater levels (e.g., Muir-Wood and King, 1993; Roeloffs, 1998), variations in groundwater geochemistry (e.g., Claessen et al., 2004), and soil liquefaction (Tuttle et al., 2002). Several mechanisms have been proposed on the origin and evolution of hydrologic changes associated with strong earthquakes. Sibson (1994) examined how crustal fluids can be drawn into fractured rocks as tectonic stresses or strains increase, and then “pumped out” when the strain energy is released during an earthquake. Several case studies provide field evidence for hydrologic changes that are consistent with measured coseismic strains (e.g., Muir-Wood and King, 1993; Quilty and Roeloffs, 1997). Others hypothesized that tectonically induced fracturing, faulting, or unclogging can change the permeability in the shallow crust, thus initiating changes in streamflow, groundwater discharge or water levels (Manga, 2001, Rojstaczer and Wolf, 1992; Sato et al., 2000; Brodsky et al., 2003; Wang et al., 2004). Still others invoke sediment compaction or consolidation from strong ground shaking or dynamic strain as a mechanism for overpressure development in alluvial sediments (Wang et al., 2001, Wolf et al., 2006). Coseismic and postseismic events such as streamflow increase, overpressure development, liquefaction, and aftershocks can be sustained from days to years, indicating that these time-dependent changes are influenced strongly by rates of overpressure relaxation and fluid flow. Although the interplay between seismicity and hydrologic phenomena are intriguing, few tools exist to explore coupled media deformation and hydrologic processes operating in the earth's crust. In this project, we present a 3-D time-dependent pore pressure diffusion code developed to investigate the response of pore fluids to the crustal deformation generated by strong earthquakes in heterogeneous geologic media.

POROELASTICITY

Biot (1941), Wang (2000), and Showalter (2000), among others, summarized the physical and mathematical models for poroelastic problems. A system of partial differential and algebraic equations can be used to describe the relationships among four basic variables: stress (σ), strain (ε), pore pressure (P), and increment of fluid content (ξ) in deformed porous media. First, the force equilibrium equations can be written as

$$\frac{\partial \sigma_{ji}}{\partial x_j} = -F_i \tag{1}$$

where σ_{ji} is the total stress in the j-direction acting on the surface with normal in the i-direction and F_i is a body force per unit bulk volume in the i-direction. The stress σ is related to the strain, the pressure, and the poroelastic moduli by

$$\sigma_{ij} = 2G\varepsilon_{ij} + 2G\frac{v}{1-2v}\varepsilon_{kk}\delta_{ij} - \alpha P\delta_{ij} \tag{2}$$

where G is the shear modulus, v is the drained Poisson's ratio, α is the Biot-Willis coefficient, and δ_{ij} is the Kronecker delta. The strain components in (2) can be evaluated in terms of displacement derivatives

$$\varepsilon = \frac{1}{2}\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right) . \tag{3}$$

Substituting equation (2) into (1) and replacing strain terms ε by displacements $\boldsymbol{u}$, the general force equilibrium equation (1) can be expressed as

$$-G\nabla^2\mathbf{u} - \frac{G}{1-2v}\nabla(\nabla\cdot\mathbf{u}) + \alpha\nabla P = \mathbf{F} . \tag{4}$$

The governing mechanical equilibrium and fluid flow equations contain the displacement and fluid pressure as the primary variables.

The continuity equation yields the following equation that describes the diffusion of induced excess pore pressure,

$$S_s \frac{\partial P}{\partial t} - \nabla \cdot (\frac{k}{\mu} \nabla P) = Q \tag{5}$$

where S_s is the hydrogeologic specific storage of rock, k is the permeability, μ is the viscosity, and Q is a fluid source term, as induced by seismic faulting. In heterogeneous media, the hydrologic properties k and μ are allowed to have spatial dependence. According to equation (5), the net pressure change depends on the magnitude of fluid source term (Q), the viscosity (μ), and the permeability (k) and specific storage capacity (S_s) of the rocks between the faulting zone and a site of interest. The increment of fluid volume (ξ) released per unit bulk volume can be evaluated by $\xi = S_s P$. Equation (5) can thus be rewritten in terms of ξ,

$$\frac{\partial \xi}{\partial t} - \nabla \cdot (\frac{k}{\mu} \nabla P) = Q \quad . \tag{6}$$

Furthermore, the increment of fluid volume ξ is related to stress and pore pressure as

$$\xi = \frac{1}{H}\sigma_{kk} + \frac{1}{R}P = \frac{\alpha}{K}\sigma_{kk} + \frac{\alpha}{KB}P \quad , \tag{7}$$

where $1/H$ is the poroelastic expansion coefficient, $1/R$ is the unconstrained specific storage coefficient , K is the bulk modulus, and B is Skempton's coefficient, which varies between 0 and 1. Substitution of (7) into (6) yields an equation that relates mean stress and pore pressure

$$\frac{\alpha}{KB}\left[\frac{\partial P}{\partial t} - B\frac{\partial \sigma_{kk}}{\partial t}\right] - \nabla \cdot \left(\frac{k}{\mu}\nabla P\right) = Q \tag{8}$$

If displacement is chosen as the mechanical variable instead of stress, equation (8) can be re-written as

$$\frac{\partial}{\partial t}\left(S_\sigma P + \alpha \nabla \cdot \boldsymbol{u}\right) - \nabla \cdot \left(\frac{k}{\mu}\nabla P\right) = Q \tag{9}$$

Here S_σ (defined as $S_\sigma = \alpha/KB$) is the poroelastic storage coefficient. Equations (4) and (9) couple the standard theory of (steady) linear elasticity and Darcy's law (by the addition of the pore pressure field) and form the equations of quasi-static poroelasticity. The solution of this system of equations can be approximated by numerical methods, such as finite-element or boundary-element methods (Smith & Griffiths, 1988; Masterlark & Wang, 2000).

PFLOW MODELING SOFTWARE

Equations (4) and (9) describe the interplay among displacement and pressure as they evolve through time after a fault rupture. Numerical solutions to these coupled equations, however, are limited in the published literature. If the dilatation is constant in time (that is $\frac{\partial}{\partial t}\nabla \cdot \boldsymbol{u} = 0\partial\partial$) or if its derivative with respect to time is negligibly small, then equation (9) becomes

$$\frac{\partial}{\partial t}\left(S_\sigma P\right) - \nabla \cdot \left(\frac{k}{\mu}\nabla P\right) = Q \tag{10}$$

PFlow offers users a tool with which they can explore, to first-order, the effects of changes in Coulomb stress transfer on pore pressure over time through a one-way coupled model. The Coulomb failure stress change, ΔCFS, initiated by fault rupture is

$$\Delta CFS = \Delta\sigma_s - m\left(\Delta\sigma_n - \Delta P\right) \tag{11}$$

where $\Delta\sigma_s$ is the change in shear stress along a fault, m is the friction coefficient, ΔP is the change in pore pressure, and $\Delta\sigma_n$ is the change in normal stress (positive if the fault is unclamped). In areas where ΔCFS is positive, failure is encouraged, and where negative, failure is discouraged. In elastic deformation, stress (σ) is related to strain (ε) by Young's Modulus (E) as $\sigma = E\varepsilon$. The fractional volume change $\Delta V/V$ can be described as

$$\frac{\Delta V}{V} = \varepsilon\left(1 - 2\upsilon\right) = -\beta\sigma \tag{12}$$

where υ is Poisson's ratio and β is bulk compressibility. Coulomb strain (dilatation) calculated from the stress change provides the initial hydrologic disturbance, or induced excess pore pressure, which is then allowed to dissipate through a user-defined model space over time. In the one-way coupling, the pore pressure change induced by a stress change is calculated using Skempton's coefficient, B, (Skempton, 1954):

$$\Delta P = B\Delta\sigma \tag{13}$$

The propagation of induced excess pore pressures or heads, h $(P = \rho gh)$ can then be calculated using the well-known flow equation

$$S_s\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left[K_x\frac{\partial h}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_y\frac{\partial h}{\partial y}\right] + \frac{\partial}{\partial z}\left[K_z\frac{\partial h}{\partial z}\right] \tag{14}$$

where K_x, K_y, and K_z, are hydraulic conductivities (m/day), h is hydraulic head (m), and S_s is the hydrogeologic specific storage (m^{-1}). Thus the net pore pressure change over time depends on the volumetric strain produced from coseismic energy release and on the hydraulic conductivity of rocks between the rupture zone and a site of interest.

PFlow can be used to approximate solutions of Equation (10). Operationally, PFLOW codes utilize Matlab™ functions and a series of input files. Figure 1 contains a list of the functions that form the PFLOW program and a brief description of each file's functionality. The README file explains how to use *PFlow.m* to calculate the pressure (and fluid flow) induced by a strain field (deformation) and how to use *visP.m* in order to visualize the results. *PFlow.m* is a driver script for a finite-element code that performs the actual calculations. *PFlow.m*, in turn, relies on several Matlab™ functions (residing in Matlab m-files listed in Figure 1) and input files that provide boundary conditions, dilatation from which initial pressures are calculated, and information about the model space. Users can specify boundary conditions as either Neumann (no flow) or Dirichlet (drained or specified pressure) on the top, bottom, and sides of the model. In addition, users can specify hydrologic conductivity in three dimensions, either constant along a given axis direction, or variable. This flexibility is instructive for testing how rock permeabilities affect the dissipation of pore pressure and fluid flux over time. The script *visP.m* performs some basic post-processing and visualization of results and may serve as a basis for a program that provides additional post-processing. The script is easily modified to allow users the ability to examine calculation results in different regions of the model space and at specific time steps. Initial conditions for the calculations can be obtained from a deformation modeling program such as Coulomb (Toda et al., 2005) or 3D-DEF (Gomberg and Ellis, 1994). These programs calculate dilatational strain using a specified fault rupture model. The output values of strain become the initial conditions for pressure in the PFlow model.

Boundary and initial conditions

Equation (10) is posed on $\Omega \times (0,T)$, where $\Omega \subset R^3$ is a bounded spatial domain (in this case a cuboid) and $(0,T)$ is the time interval of interest. This equation must be supplemented by initial and boundary conditions. Assume that Γ the boundary of Ω, is divided into two disjoint parts Γ_d and Γ_f along which we have drained and flow boundary conditions, respectively. With these conventions we allow the following combinations of boundary conditions

$$P = 0 \text{ on } \Gamma_d \tag{15}$$

$$\frac{k}{\mu}\nabla P \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_f \quad . \tag{16}$$

Finally we have the initial conditions

$$S_\sigma P = v_0 \quad \text{on } \Omega \qquad \text{at } t = 0 \tag{17}$$

Numerical solutions

In PFlow, we numerically approximate the solution of Equation (10), subject to boundary conditions (eqns. 15 and 16) and initial condition (eqn. 17) using MATLAB™ code. Our programs employ the finite element method for first-order or second-order spatial discretization

(discretization of the spatial derivative) and explicit or implicit first-order, or implicit second order, finite difference discretization in time (discretization of the time derivative). After temporal discretization, equation (10) becomes

$$S_\sigma \frac{P^{n+1} - P^n}{\Delta t} - \theta \nabla \cdot \left(\frac{k}{\mu} \nabla P^{n+1}\right) = \theta Q^{n+1} + (1-\theta) Q^n + (1-\theta) \nabla \cdot \left(\frac{k}{\mu} \nabla P^n\right) \tag{18}$$

In the above semi-discrete (discrete in time, continuous in space) formulation, the superscript n denotes the discrete time level at which the function is evaluated and Δt is the time step. The parameter θ determines the discretization type (for $\theta = 0$, this yields Euler's method, explicit first-order; for $\theta = ½$, the Crank-Nicolson scheme, implicit second-order; and for $\theta = 1$, the backward Euler's method, implicit first-order). After spatial (finite element) discretization, the above becomes a system of linear algebraic equations, with sparse matrices. Once the initial pressure P^0 of seismic faulting is obtained from a crustal deformation modeling code, such as 3D-DEF (Gomberg and Ellis, 1993) or Coulomb (Toda et al., 2005), the system can be solved for P^n for $1 \leq n$. At each time step, the system is solved using a sparse direct solver, a built-in function of Matlab™.

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Figure 1. Description of files constituting the PFLOW suite of programs.

README.txt	Provides a overview of programs and instructions on how to use *PFLOW* and *visP.m*
PFlow.m*	Main driver script for the PFLOW suite of programs. Calculates pressure and resulting flow induced by Coulomb strain
VisP.m	Post-processing script that allows users to visualize results at specified time steps in the model space
Conductivity.txt	Example of hydraulic conductivity input file
Strain.txt	Example of dilatational strain input file
assemble.m	Assembly routine
boundaryCond.m	Calculates boundary conditions (needed for Dirichlet conditions; not currently used). Currently a zero vector is created directly in *setBC.m*
errors.m	Computes errors when exact solution is known for testing and diagnostics
exact.m	Calculates exact solution and its derivatives for error computation
initialCond.m	Computes initial condition
quadpts27.m	Gauss quadrature information for a 27-point Gauss quadrature rule on hexahedra
quadpts8.m	Gauss quadrature information on an 8-point Gauss quadrature rule on hexahedra

readIC.m	Reads initial dilatations from a file
readK.m	Reads hydraulic conductivities from a file
rhs.m	Calculates right-hand side
setBC.m	Sets boundary conditions, modifies matrices and right-hand side accordingly
setgrid3D.m	Generates a simple 3-D grid, with uniform hexahedral mesh for linear or quadratic elements
trilinear.m	Constructs trilinear basis functions on hexahedra
triquadratic.m	Constructs triquadratic basis functions on hexahedra

*All programs designated by ***.m*** are Matlab™-based programs.