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PHASE FIELD MODEL FOR THE NUMERICAL SIMULATION OF SALT TECTONICS

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Abstract. *The study of the salt tectonics has received much attention in recent times. Geologists and reservoir engineers have devoted great effort to quantitatively understand this phenomenon that has a strong impact on the oil and gas exploitation offshore Brazil, specifically in the so-called pre-salt layer. In this work, we applied the residual-based Allen-Cahn phase field model to numerically simulate diapirs motion. It is assumed that the main driven force arises from buoyancy since the salt is lighter than the overburdening sedimentary material. So the diapiric growth may be recast in the Rayleigh-Taylor theory to describe the evolution of the gravity instability among fluids or media layers. The phase field model is able to track the interface between the two media as well to minimize volume losses. The numerical formulation is based on a pure Eulerian approach including mesh adaptivity which aims to track the interface between different layers. Due the materials high viscosity, the incompressible Navier-Stokes equations are reduced to the Stokes problem coupled with the transport of the phase-field. It is assumed that the rheology of salt and surrounding rocks in geological time scale behave as Newtonian fluids. The implementation has been performed using the libMesh finite element library, which provides support for AMR/C and parallel computations. Example computations illustrate the good properties of the present simulation capabilities.*

Keywords: *salt tectonics, finite element, mesh refinement, phase field, parallel computation*

1. INTRODUCTION

The term salt will be used in this work as a generic name for rock bodies composed essentially by halite (NaCl). According to Hudec and Jackson (2007), salt is mechanically weak and flows like a fluid. The formation of diapirs plays a major role in the evolution of geological structures in the Earth's crust. Initially, interest in salt tectonics came from the petroleum industry since oil and gas traps are often associated with salt domes (Ramberg (1981)). This can be related to the lower permeability of salt with respect to the sedimentary rocks. In the past few years, the research effort has been focused on establishing the conditions, which apart from the basic Rayleigh-Taylor instability, may influence and promote the formation of salt diapirs. Due to difficulties in establishing the in situ conditions, with obvious implications on uncertainties of the mathematical problem in terms of the boundary and initial conditions, and material properties, a debate has been open, with respect to the conditions that may affect salt deformations.

Perić and Crook (2014) have compiled, mostly analog models based studies, a wide number of different mechanisms influencing salt movement. They include compression and folding of overburden (Waltham, 1997), thick- and thin-skinned extension (Koyi, 1998), differential loading of overburden including progradation due to sedimentation (Waltham, 1997), falting (Koyi, 1998), flexural buckling of overburden (Waltham, 1997), and other mechanisms including sediment accumulation, erosion and dissolution. The additional difficulty is that a number of the above mechanisms can be active simultaneously (Perić and Crook, 2014). Besides these difficulties, seismic profiles and drilling demonstrate that salt diapirs feature a broad variety of shapes, that reflects the variety of modes in which salt diapirs interact with their overburden as they grow (Massimi *et al.*, 2007).

From the computational point of view, the deformation of the geological structures, salt diapirs due salt tectonics in

our case, may be addressed by Eurelian, Lagrangian or Arbitrary Lagrangian-Eulerian (ALE) formulations. The standard Eulerian formulation is normally based on a fixed grid covering the problem domain. For some problems, however, localised mesh refinement may be necessary. The critical aspect of the Eulerian approach is modelling the moving boundaries and interfaces. Second Shyy *et al.* (1986), among a number of different interface tracking techniques the most widely used are marker/string methods, volume-of-fluid (VOF) techniques, and techniques based on the level set (LS) method. Recently, the phase field approach with adaptive mesh refinement/coarsening (AMR/C) is also used to solve problem with moving interfaces (Vasconcelos *et al.*, 2014) as well fault problems (Duda *et al.*, 2015).

The main advantages of the Lagrangian methodology, which is based on the reference configuration that moves with particles (Bach and Hassager, 1985) are the intrinsic modelling of the interfaces between different phases of the system, direct modelling of material properties, which is important for complex material behaviour and faults. The main disadvantage of the Lagrangian approach is that it suffers from excessive mesh distortion due to often very large particle displacements, requiring frequent remeshing during the simulation.

The ALE method is also often employed for flow problems with moving boundaries and interfaces. However, depending on the formulation, the ALE method inherits features of both Eulerian and Lagrangian methodologies. For instance, for large deformations problems the ALE reduces but does not completely remove the need for remeshing.

Besides the classical volume of fluid (VOF) and level-set (LS) methods to deal with interface tracking, the phase field model considers a different approach to this problem. The phase field model assumes a (thin) diffuse transition where the interface is specified by a scalar variable (the phase field) defined in the range $\phi(\mathbf{x}, t) \in [-1, 1]$. In this model, a continuous transition zone among phases is introduced, defined by this additional field variable describing the evolution and shape of the interface. The interface is then represented by a slim thickness with continuously varying properties. See Anderson *et al.* (1998) and Vasconcelos *et al.* (2013, 2014) for a brief review of phase-field models.

The remainder of this paper is organized as follows. In the next section the free energy functional for the phase field model will be presented as well the dimensionless governing equations for the coupled viscous flow and transport followed by the correspondent stabilized finite element formulation section. Section 3 shows the numerical results for some test problems: a formation of a salt diapir in a two layer case. The paper ends with our main conclusions.

2. MATHEMATICAL FORMULATION

2.1 Governing Equations

2.1.1 Phase field model

Phase field models are based on a free energy functional that aims to describe the process of phase change taking into account the hydrophilic and hydrophobic contribution to the total (elastic) mixing energy (Yang et al., 2006). The Ginzburg-Landau energy functional (Chen, 2004) is widely used in many phase field models and it may be written as follows:

$$W = \int_{\Omega} \left(\frac{1}{2} \left| \overrightarrow{\nabla \phi} \right|^2 + F(\phi) \right) \mathrm{d}\Omega \tag{1}$$

where $\phi(\mathbf{x}, t) \in [-1, 1]$ is the phase field variable, Ω is the physical domain and F is a double-well potential function which carries the thickness of the diffusive region η as follows:

$$F(\phi) = \frac{1}{\eta^2} \left(\phi^2 - 1\right)^2 \mathrm{d}\Omega \tag{2}$$

The phase field model may be obtained from the classical sharp interface models known as VOF and LS and takes into account the first variation of elastic mixing energy functional as follows:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = -\gamma \frac{\delta W}{\delta \phi} \tag{3}$$

where $\mathbf{u}$ is the fluid (or media) velocity and γ is the elastic relaxation time.

The Allen-Cahn phase field model to deal with the dynamics of $\phi(\mathbf{x}, t)$ results in:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \left(\nabla^2 \phi - F'(\phi) \right) \tag{4}$$

The constant γ is a physical parameter that describes the damping applied to the Allen-Cahn's model. It is important to notice that the effects of the hydrophilic and hydrophobic contributions occurs only within the mixture thickness.

It can be shown (Vasconcelos et al. (2013, 2014) and Anderson et al. (1998)) that the first variation of the Ginzburg-Landau energy functional with respect to the phase field variable is identical to the chemical potential ψ of the mixture.

Therefore, Eq. (3) may be written as

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \psi. \tag{5}$$

Combining Eq. (3) and (4) it is possible to define the chemical potential in terms of the field variables as given below

$$\psi = \nabla^2 \phi - f(\phi) = \frac{R(\phi)}{\gamma}, \tag{6}$$

where

$$R(\phi) = \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi \tag{7}$$

is the residual of the sharp interface model. This will allow us to express the elastic relaxation γ as a function of the phase field ϕ, which is our goal.

2.1.2 Physical problem

The typical geological time scale of the diapiric growth is of the order of millions years. As an example, offshore Brazil, its assumed that diapirism started around 112 My (million years) ago and ended near 65 My ago, a total duration around 50 My (Corrêa, 2015)[1]. The most active tectonic time was the Late Cretaceous, as a response to the load of progradational wedges over the thick salt layer (Garcia *et al.*, 2012).

Neglecting temperature effects, on this time scale the sedimentary rocks and the halite may be modelled as Newtonian fluids characterized by high viscosities (Massimi *et al.* (2007). Therefore it is possible to adopt the Rayleigh-Taylor theory to describe the displacement evolution driven by the gravitational instability among different (incompressible) media layers.

Thus, assuming an unsteady incompressible viscous flow of immiscible fluids/media subjected to gravitational effects due the difference in their densities, the dimensionless Navier-Stokes and continuity equations can be written in a non-conservative form following a pure Eulerian description as

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \frac{\tilde{\mu}}{Re} \nabla \cdot \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}} \right) + \frac{1}{Fr^2} \nabla p = \mathbf{l}, \\ \nabla \cdot \mathbf{u} = 0 \end{aligned} \tag{8}$$

defined in the domain Ω, equipped with the smooth boundary Γ, in the time interval $[0, T]$.

In system (8) Re is the Reynolds number, p is the hydrostatic pressure and the its right hand side stands for the dimensionless body force defined as

$$\mathbf{l} = \frac{\tilde{\rho}}{Fr^2} \mathbf{e} \tag{9}$$

where Fr is the Froude number and $\mathbf{e}$ is an unit vector aligned with the gravity field.

We adopt the overburden physical values as reference to compute the non-dimensional viscosity $\tilde{\mu}$ and density $\tilde{\rho}$ which are defined by means of the phase field parameter ϕ as follows:

$$\begin{aligned} \tilde{\mu} &= \frac{1}{2}(1+\phi)\mu_{+1} + \frac{1}{2}(1-\phi)\mu_{-1}, \\ \tilde{\rho} &= \frac{1}{2}(1+\phi)\rho_{+1} + \frac{1}{2}(1-\phi)\rho_{-1} \end{aligned} \tag{10}$$

where the sub-indices $+1$ and -1 stand for each one of the two different fluids or media.

The essential and natural boundaries conditions of the nonlinear coupled system (4) and (8) are

$$\begin{aligned} \mathbf{u} &= \mathfrak{g} \quad \text{on } \Gamma_{\mathfrak{g}}, \\ \mathbf{n} \cdot \boldsymbol{\sigma} &= \mathfrak{h} \quad \text{on } \Gamma_{\mathfrak{h}}, \\ \mathbf{n} \cdot \nabla \phi &= 0 \quad \text{on } \Gamma. \end{aligned} \tag{11}$$

where $\mathbf{n}$ is the boundary outward unit normal vector and $\mathfrak{g}$ and $\mathfrak{h}$ are given functions. The initial conditions are:

$$\begin{aligned} \mathbf{u}(\mathbf{x}, 0) &= \mathbf{u}_0, \\ \phi(\mathbf{x}, 0) &= \phi_0 \end{aligned} \tag{12}$$

[1] Personal communication with geologist Luís Mauirício êa.

where the initial velocity field $\mathbf{u_0}$ is divergent free.

Due to the huge geological time scale, the inertial terms from the system (8) may be dropped. Therefore the evolution of the diapirs can be described by the following Stokes system:

$$\begin{aligned} -\tilde{\mu}\frac{Fr^2}{Re}\nabla\cdot\left(\nabla\mathbf{u}+\left(\nabla\mathbf{u}\right)^{\mathrm{T}}\right)+\nabla p &= \mathbf{l}, \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned} \tag{13}$$

together with the same boundary and initials conditions given by (11) and (12). In system 13 we handle the dimensionless parameters. Consequently the body force vector becomes:

$$\mathbf{l}=\tilde{\rho}\mathbf{e}. \tag{14}$$

Following Massimi *et al.* (2007), assuming constant rheological properties within each layer we can reduce the system time-dependence exclusively to the dynamics of the interface between layers which, in our case, is obtained by the solution of the residual-based Allen-Canh model, given by Eq. (5).

2.2 Stabilized Finite Element Formulation

Given a suitably defined finite-dimensional trial solution and weight functions spaces for velocity, pressure and phase field variable

$$\begin{aligned} S_{\mathbf{u}}^h &= \left\{\mathbf{u}^h \mid \mathbf{u}^h\in\left[H^{1h}\left(\Omega\right)\right]^3,\ \mathbf{u}^h\doteq\mathfrak{g}^h\ \text{ on }\ \Gamma_{\mathfrak{g}}\right\}, \\ V_{\mathbf{w}}^h &= \left\{\mathbf{w}^h \mid \mathbf{w}^h\in\left[H^{1h}\left(\Omega\right)\right]^3,\ \mathbf{w}^h\doteq 0\ \text{ on }\ \Gamma_{\mathfrak{g}}\right\}, \\ S_p^h &= V_p^h=\left\{q^h \mid q^h\in H^{1h}\left(\Omega\right)\right\}, \\ S_\phi^h &= V_\phi^h=\left\{w^h \mid w^h\in H^{1h}\left(\Omega\right)\right\}, \end{aligned} \tag{15}$$

where $H^{1h}\left(\Omega\right)$ is the finite-dimensional space function square integrable into the element domain, the PSPG FEM formulation (Tezduyar (1992), Bazilevs et al. (2013)) for the non-dimensional Stokes and continuity system (8) can be written as: Find $\mathbf{u}^h\in S_{\mathbf{u}}^h$ and $p^h\in S_p^h$ such as, $\forall\,\mathbf{w}^h\in V_{\mathbf{w}}^h$ and $\forall\,q^h\in V_p^h$,

$$\begin{aligned} &\frac{1}{Re}\int_\Omega\nabla\mathbf{w}^h\cdot\left(\nabla\mathbf{u}^h+\left(\nabla\mathbf{u}^h\right)^{\mathrm{T}}\right)\,\mathrm{d}\Omega-\int_\Omega\nabla\mathbf{w}^h p^h\mathbf{I}\,\mathrm{d}\Omega-\int_\Omega\mathbf{w}^h\cdot\mathbf{l}^h\,\mathrm{d}\Omega-\int_\Gamma\mathbf{w}^h\cdot\mathfrak{h}^h d\Gamma+\int_\Omega q^h\nabla\cdot\mathbf{u}^h\,\mathrm{d}\Omega+ \\ &+\sum_{e=1}^{n_el}\int_{\Omega^e}\tau_{PSPG}\nabla q^h\cdot\left(\nabla p^h-\mathbf{l}^h\right)\,\mathrm{d}\Omega^e=0. \end{aligned} \tag{16}$$

The first four integrals in (16) arise from the Galerkin weak formulation over the Stokes equation. The fifth integral represents the Galerkin formulation for the continuity equation. The summation over the elements is the pressure stabilizations (PSPG) over the pressure gradient and body force of Stokes equation. Finally, $\mathbf{l}^h$ is the discrete load vector and $\mathbf{I}$ is the identity matrix. One must notice that contributions emanating from the viscous terms are disregarded, since we use bilinear quadrilaterals and trilinear hexahedra.

The SUPS stabilization parameter, τ_{SUPS}, is obtained from Bazilevs et al. (2013) and defined as follows

$$\tau_{SUPS}=\left[\left(2\frac{\left\|\mathbf{u}^h\right\|}{l^e}\right)^2+9\left(\frac{4}{{l^e}^2Re}\right)^2\right]^{-\frac{1}{2}}. \tag{17}$$

The non-dimensional stabilization parameters are local (element level) then, the velocity modulus $\left\|\mathbf{u}^h\right\|$ is calculated for each element e and $\mathfrak{l}^e$ is an element length measure (see Bazilevs et al. (2013)).

For the non-dimensional Allen-Cahn model we adopt the same assumptions, taking again S_ϕ^h and V_ϕ^h as the finite-dimensional trial solution and weight functions spaces for ϕ as well $S_{\mathbf{u}}^h$ as the finite-dimensional trial solution for the velocity field, the stabilized FEM formulation can be written as: Find $\phi^h\in S_\phi^h$ such as, $\forall\,w^h\in V_\phi^h$,

$$\begin{aligned} &\int_\Omega w^h\left(\frac{\partial\phi^h}{\partial t}+\mathbf{u}^h\cdot\nabla\phi^h\right)\mathrm{d}\Omega+\int_\Omega\gamma\nabla w^h\cdot\nabla\phi^h\mathrm{d}\Omega+\int_\Omega\gamma w^h\left(f^h\right)\mathrm{d}\Omega+ \\ &\sum_{e=1}^{n_el}\int_{\Omega^e}\tau_{SUPG}\,\mathbf{u}^h\cdot\nabla w^h\left(\frac{\partial\phi^h}{\partial t}+\mathbf{u}^h\cdot\nabla\phi^h-\gamma\left(\nabla^2\phi^h-f^h\right)\right)\mathrm{d}\Omega^e=0. \end{aligned} \tag{18}$$

The first three integrals in (18) arise from the Galerkin weak formulation where f^h is the discrete form of the double-well function derivative. Note that the term corresponding to the hydrophilic forces has been integrated by parts in the usual manner. The integral into the summation over the elements is the SUPG stabilization. The non-dimensional stabilization parameter is computed similarly to (17), that is

$$\tau_{SUPG} = \left(\frac{\mathfrak{l}^e}{2 \left\| \mathbf{u}^h \right\|} \right). \tag{19}$$

2.3 Residual-based Allen-Cahn Model

Recently Vasconcelos et al. (2014) have modified the classic Allen-Cahn phase field model to make it less parameter dependent, exploring the similarities between $YZ\beta$ discontinuing capturing (DC) operator (Bazilevs et al. 2007) with the term stemming from the integration by parts of the hydrophilic forces in (18). Inspecting this term and assuming that the elastic relaxation time γ can be interpreted as a variable diffusive coefficient such that $\gamma = \gamma(\phi)$ and that the thickness η is related to the mesh resolution, it is possible to develop a less parameter dependent phase field model, as shown below.

The $YZ\beta$ DC operator requires the calculation of a parameter named δ which is a function of the transported scalar and its residual and it may be written as follows:

$$YZ\beta = \sum_{e=1}^{n_{el}} \int_{\Omega^e} \delta\left(\phi^h\right) \nabla w^h \cdot \nabla \phi^h \, \mathrm{d}\Omega. \tag{20}$$

The δ parameter can be calculated as follows:

$$\delta\left(\phi^h\right) = \left(\frac{\mathfrak{l}^e}{2} \right)^{\beta} \left| R^e\left(\phi^h\right) \right| \left(\sum_{i=1}^{n_{sd}} \left| \frac{\partial \phi^h}{\partial x_i} \right|^2 \right)^{\frac{\beta}{2}-1}. \tag{21}$$

The parameter β controls the nonlinearity of the discontinuity-capturing term, $R^e\left(\phi^h\right)$ is the element-level residual of the phase field advective-diffusive-reactive transport equation and n_{sd} stands for the spatial dimension. Thus, the second integral of Eq. (18) in the Allen-Cahn phase field model naturally considers a DC-like operator as follows:

$$AC_{DC} = \sum_{e=1}^{n_{el}} \int_{\Omega^e} \gamma \nabla w^h \cdot \nabla \phi^h \mathrm{d}\Omega. \tag{22}$$

Consequently, based on equations (20) and (22) it is natural to consider in the weak formulation that the hydrophilic term has a DC-like form where $\gamma = \gamma^e\left(\phi^h\right) = \delta\left(\phi^h\right)$ and, therefore, $\gamma^e\left(\phi^h\right)$ is the element-level dynamic elastic relaxation time. If the elastic relaxation time γ is taken as a local variable assumed to be equal to $\delta\left(\phi^h\right)$ in Eq. (4), then it can be shown that a local chemical potential ψ^e of the mixture of two different fluids is given by

$$\psi^e = \left(\frac{2}{\mathfrak{l}^e} \right)^{\beta} \frac{1}{\left(\sum_{i=1}^{n_{sd}} \left| \frac{\partial \phi^h}{\partial x_i} \right|^2 \right)^{\frac{\beta}{2}-1}}. \tag{23}$$

Applying Eq. (23) in Eq. (6) it can be easily deduced that the element-level dynamic elastic relaxation time $\gamma^e\left(\phi^h\right)$ is given by

$$\gamma^e\left(\phi^h\right) = \left(\frac{\mathfrak{l}^e}{2} \right)^{\beta} \left(\sum_{i=1}^{n_{sd}} \left| \frac{\partial \phi^h}{\partial x_i} \right|^2 \right)^{\frac{\beta}{2}-1} \left| R^e\left(\phi^h\right) \right| \tag{24}$$

which has exactly the same right rind side of the Eq.(21).

Making $\beta = 1$, $\gamma^e\left(\phi^h\right)$ vanishes where the gradient of the phase field is null what is consistent with the free surface boundary condition applied to regions outside the transitional zone. The resulting weak formulation for the residual-based Allen-Cahn model is written as:

$$\begin{aligned} &\int_{\Omega} w^h \left(\frac{\partial \phi^h}{\partial t} + \mathbf{u}^h \cdot \nabla \phi^h \right) \mathrm{d}\Omega + \sum_{e=1}^{n_{el}} \int_{\Omega} \gamma^e\left(\phi^h\right) \nabla w^h \cdot \nabla \phi^h \mathrm{d}\Omega + \sum_{e=1}^{n_{el}} \int_{\Omega} \gamma^e\left(\phi^h\right) w^h f^h \mathrm{d}\Omega + \\ &\sum_{e=1}^{n_{el}} \int_{\Omega^e} \tau_{SUPG} \, \mathbf{u}^h \cdot \nabla w^h \left(\frac{\partial \phi^h}{\partial t} + \mathbf{u}^h \cdot \nabla \phi^h - \gamma^e\left(\phi^h\right) \left(\nabla^2 \phi^h - f^h \right) \right) \mathrm{d}\Omega^e = 0. \end{aligned} \tag{25}$$

Again, following Vasconcelos et al (2014), one must notice that the local dynamic elastic relaxation time renders the residual-based Allen-Cahn's phase field model more general, since outside the transition region it behaves as a classical sharp interface model and within the transition region it acts as a phase field model. The contributions from the second-order derivatives in the phase-field element residua are disregarded too.

The above semi-discrete weak formulation for the residual-based Allen-Cahn model (25) and the Stokes equation (16) are discretized in time by the Euler backward scheme. We adopt a fixed point linearisation and a segregate method to advance in time, solving first the Stokes problem for velocity and pressure and then updating the phase-field.

Both the residual-based Allen-Cahn model and the Stokes equation are implemented in `libMesh` (Kirk *et al.*, 2006). Mesh refinement in `libMesh` can be accomplished by element subdivision (h-refinement), increasing the local polynomial degree (p-refinement) as well a combination of both methods (hp-refinement). `libMesh` uses a statistical refinement/coarsening scheme based on the ideas presented in Carey (1997) in which the mean and the standard deviation of the error indicator "population" are computed. This scheme is suitable for evolution problems where, in the beginning, a small error is evenly distributed. Throughout the simulation the error distribution spreads and the AMR/C process starts. If the solution approaches its steady state, the distribution of error also reaches the steady state, stopping the AMR/C process.

3. NUMERICAL RESULTS

In this section we present the results of a numerical simulation of a two layer problem. The 2D non-dimensional physical domain has width 10 and height 3. The salt layer is completely covered by a heavier material. In the center of the horizontal domain we create a small geometric perturbation over the salt top surface starting at $x = 4.5$ given by the following sinusoidal function $y(x) = h_s 0.5 \sin(\pi x / l_s)$ where $h_s = 0.75$ is the salt layer thickness and $l_s = 1$ the the perturbation length.

The Fig 1 shows the geometric domain for the initial configuration. The material and reference parameters are summarized in Tab. 1

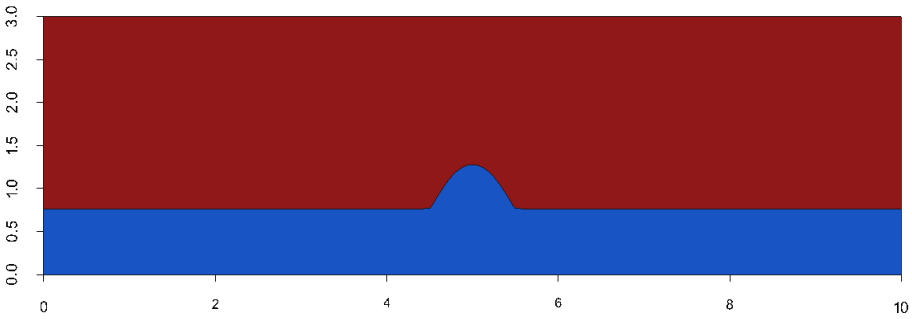

Figure 1. Initial domain: salt (blue) and overburden (red) layers.

Table 1. Physical parameters

Definition	Symbol	Value	Unit
Reference Length	L_∞	1000.0	m
Time scale	T_∞	1.0	$My\ (3.15576 \cdot 10^{13} s)$
Salt viscosity	μ_s	$1.0 \cdot 10^{18}$	$Pa.s$
Salt density	ρ_s	2000.0	kg/m^3
Overburden viscosity	μ_b	$1.0 \cdot 10^{18}$	$Pa.s$
Overburden density	ρ_b	2600.0	kg/m^3
Gravity acceleration	g	9.81	ms^{-2}

Reference values for viscosity and density are the data from the overburden material. Therefore the Reynolds number is $Re = \frac{\rho_\infty L_\infty^2}{T_\infty \mu_\infty}$ and the square of the Froude number is $Fr = \frac{L_\infty}{T_\infty^2 g}$. For both non-dimensional quantities we compute $Re \approx 8.245 \cdot 10^{-23}$ and $Fr^2 \approx 1.025 \cdot 10^{-25}$. To prevent numerical problems by using such small values, we compute the ratio between the square of Froude and Reynolds numbers, $Fr^2/Re \approx 1.243 \cdot 10^{-3}$ which multiplies the viscous terms of the Stokes equation.

The phase field variable is taken as $\phi = 1$ for the overburden layer $\phi = -1$ for the salt. The dimensionless time step size is $\Delta t = 0.001$, which gives a physical time interval of one thousand years. The nonlinear tolerance for both Stokes and transport solutions is set $ntol = 1.0 \times 10^{-3}$ and the linear solver tolerance is $ltol = 1.0 \times 10^{-6}$. Computations are

performed on the SGI Altix 8400 at the High Performance Computing Center of COPPE/UFRJ using 64 cores.

Figure 2 shows the evolution of the salt diapir after 1, 5, 10, 25, 50 and 60 My.

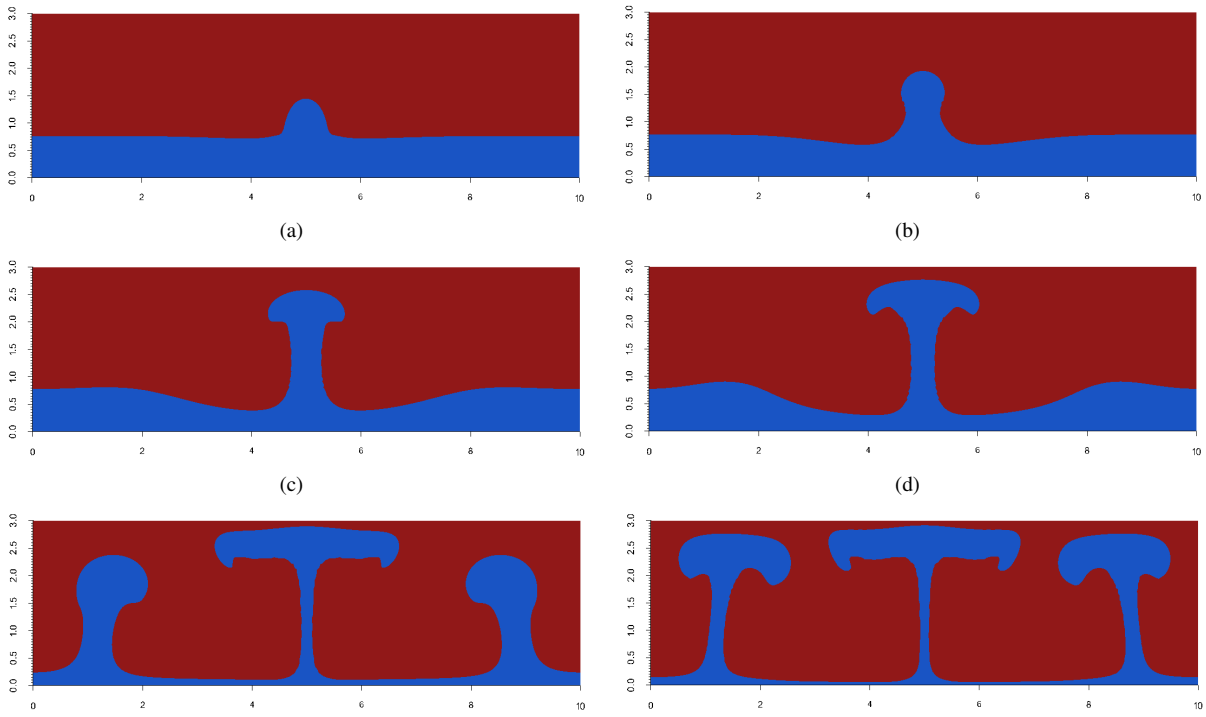

Figure 2. Single diapir evolution: (a) Geological time =$1My$, (b) Geological time =$5My$, (c) Geological time =$10My$, (d) Geological time =$25My$, (e) Geological time =$50My$ and (f) Geological time =$60My$.

4. CONCLUSIONS

We have implemented the residual-based AllenâĂŞCahn phase field stabilized finite element model for the simulation of the dynamics of a single salt. The salt layer is completed buried by an overburden layer. We considered constant rheological parameters for both materials. Neglecting temperature effects, the system evolution is modelled as a two-fluid Stokes system with a moving interface described by the Allen-Cahn phase-field model. Parallel adaptive simulations for a two-layer systems shows the effectiveness of the present approach. Future works include consideration of temperature effects and more complex physical rheologies and geometries.

5. ACKNOWLEDGEMENTS

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6. REFERENCES

Anderson, D.M., Mcfadden, G.B. and Wheeler, A.A., 1998. "Diffuse-interface methods in fluid mechanics". *Annual Review of Fluid Mechanics*, Vol. 30, pp. 139–165.

Bach, P. and Hassager, O., 1985. "An algorithm for the use of the lagrangian specification in newtonian fluid mechanics and applications to free-surface flow". *Journal of Fluid Mechanics*, Vol. 152, pp. 173–190.

Duda, F.P., Ciarbonetti, A., P.J., S. and Huespe, A., 2015. "A phase-field/gradient damage model for brittle fracture in elasticâĂŞplastic solids". *International Journal of Plasticity*, Vol. 65, pp. 269–296.

Garcia, S., Letouzey, J., Rudkiewicz, J. and Filho, A., 2012. "Structural modeling based on sequential restoration of gravitational salt deformation in the Santos Basin (Brazil)". *Marine and Petroleum Geology*, Vol. 35, pp. 337–353.

Hudec, M. and Jackson, M., 2007. "Terra infirma: Understanding salt tectonics". *Earth-Science Reviews*, Vol. 82, pp. 1–28.

Kirk, B.S., Peterson, J.W., Stone, R. and Carey, G.F., 2006. "Libmesh: a C++ library for parallel adaptive mesh refinement/coarsening simulations". *Journal Engineering with Computers*, Vol. 22, pp. 237–254.

Koyi, H., 1998. "The shaping of salt diapirs". *Journal of Structural Geology*, Vol. 20, pp. 321–338.

Massimi, P., Quarteroni, A., Saleri, F. and Scrofani, G., 2007. "Modeling of salt tectonics". *Computer Methods in Applied Mechanics and Engineering*, Vol. 197, pp. 281–293.

Perić, D. and Crook, A., 2014. "Computational strategies for predictive geology with reference to salt tectonics". *Computer Methods in Applied Mechanics and Engineering*, Vol. 193, pp. 5195–5222.

Ramberg, H., 1981. *Deformation and the Earth's Crust in Theory, Experiments and Geological Application*. Academic Press, London.

Shyy, W., Udaykumar, H., Rao, M. and Smith, R., 1986. *Computational Fluid Dynamics with Moving Boundaries*. Taylor & Francis.

Vasconcelos, D., Rossa, A. and Coutinho, A., 2013. "A globally conservative Allen-Cahn phase-field model for parallel adaptive simulation of moving boundary problems". In *Proceedings of the 34th Iberian Latin-American Congress on Computational Methods in Engineering - CILAMCE2013*. Pirenópolis, Brazil.

Vasconcelos, D., Rossa, A. and Coutinho, A., 2014. "A residual-based Allen-Cahn phase field model for the mixture of incompressible fluid flows". *International Journal for Numerical Methods in Fluids*, Vol. 75, No. 9, pp. 645–667.

Waltham, D., 1997. "Why does salt start to move?" Vol. 282, pp. 117–128.

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