Advances in Engineering Software 81 (2015) 17–29

Contents lists available at ScienceDirect

Advances in Engineering Software

journal homepage: www.elsevier.com/locate/advengsoft

Study of a Jacobian-free approach in the simulation of compressible fluid flows in porous media using a derivative-free spectral method

Nélio Henderson [a,c,*], Gisiane Simão [a,c], Wagner F. Sacco [b,c]

[a] Instituto Politécnico, Universidade do Estado do Rio de Janeiro, 28625-570 Nova Friburgo, RJ, Brazil
[b] Instituto de Engenharia e Geociências, Universidade Federal do Oeste do Pará, 68135-110 Santarém, PA, Brazil
[c] Thermodynamics and Optimization Group (TOG), Brazil

ARTICLE INFO

Article history:
Received 5 August 2014
Received in revised form 19 September 2014
Accepted 26 October 2014
Available online 25 November 2014

Keywords:
Compressible fluids
Miscible flows
Porous media
Jacobian-free approach
Derivative-free spectral method
Large-scale nonlinear systems

ABSTRACT

The development of Jacobian-free software for solving problems formulated by nonlinear partial differential equations is of increasing interest to simulate practical engineering processes. For the first time, this work uses the so-called derivative-free spectral algorithm for nonlinear equations in the simulation of flows in porous media. The model considered here is the one employed to describe the displacement of miscible compressible fluid in porous media with point sources and sinks, where the density of the fluid mixture varies exponentially with the pressure. This spectral algorithm is a modern method for solving large-scale nonlinear systems, which does not use any explicit information associated with the Jacobin matrix of the considered system, being a Jacobian-free approach. Two dimensional problems are presented, along with numerical results comparing the spectral algorithm to a well-developed Jacobian-free inexact Newton method. The results of this paper show that this modern spectral algorithm is a reliable and efficient method for simulation of compressible flows in porous media.

1. Introduction

The simulation of the flow of miscible fluids through porous materials takes place in several situations of interest in applied sciences and engineering, as in oil recovery, subsurface contaminant transport and remediation, supercritical extractions, chromatography processes, etc. In fact, after the initial stages of oil extraction, the enhanced oil recovery techniques use injections of fluids that seek to reduce the viscosity of the resident oil and improving the flow. In general, these fluids comprise gases or liquids that are miscible with oil, such as carbon dioxide, nitrogen, gels, polymer solutions, and other. A large number of chemical substances commonly used in the industrialized world have their fate in the environment. Such events that occur intentionally or accidentally include fertilizer and pesticide applications in agriculture, leaks in industrial (and residential) facilities used for the disposal of waste, and inappropriate choices of waste disposal sites. These chemicals often contaminate sources of subsurface water. Thus, to simulate such events, many of these processes are modeled as the flow of miscible fluids, water and a solute. Various processes for remediation of soil and ground water that use injections of solvents can also be described by these miscible models. In chemical engineering, the study of miscible flows in porous media is important in many practical situations, such as the simulation of supercritical processes used in the extraction of natural products. As an example, we can cite the extraction of caffeine from the injection of carbon dioxide in a supercritical state. In applied analytical chemistry, the flows in porous columns, used in chromatography processes, are in general miscible, where the injected fluid (eluent) can be in a supercritical state.

Generally, the mathematical models used to describe these complex processes are formulated by nonlinear partial differential equations [3,7], which can present solutions with singularities in the injection and production wells.

Thus, the discretization of these problems (governed by nonlinear differential equations) leads to large nonlinear systems of algebraic equations. These equations are commonly solved using the classical Newton method [1]. In spite of this, the convergence of the Newton method depend on the location of the starting point; this iterative method is attractive because it usually presents a local quadratic rate of convergence [9]. However, to simulate the dynamic evolution of the flow, at each time step the Newton method requires the solution of a number of linear systems, where the Jacobians of the nonlinear system evaluated at the current points are the coefficient matrices, which are generally large and sparse.

* Corresponding author at: Instituto Politécnico, Universidade do Estado do Rio de Janeiro, 28625-570 Nova Friburgo, RJ, Brazil. Tel./fax: +55 22 2533 2263.
E-mail address: nelio@iprj.uerj.br (N. Henderson).

http://dx.doi.org/10.1016/j.advengsoft.2014.10.005
0965-9978/

To minimize the computational cost spent on resolutions of such linear systems, in recent years some researchers in this area have used inexact Newton methods, [4,8,14,16]. Such inexact methods are variants of the Newton method, where linear systems are solved only approximately [10,12,13], what is commonly done using a Krylov method [15].

The Derivative-Free Spectral Algorithm for Nonlinear Equations (DFSANE) is a modern method for solving large-scale nonlinear systems, developed from the spectral gradient method [2,21], which does not solve linear systems, nor use any explicit information associated with the Jacobin matrix, being a Jacobian-free approach with a solid theoretical foundation [17].

The objective of this work is to study the performance of the DFSANE in the numerical simulation of miscible compressible fluid flows in porous media, where the model used considers point sources and sinks, possible large adverse mobility ratio and anisotropic dispersion in tensor form. Furthermore, in this model the density of the fluid mixture varies exponentially with the pressure. In addition, using a pseudo-language, all the algorithms discussed here will be presented in a clear and well-established form, in order to facilitate future applications to engineering problems.

For this, two dimensional problems are presented, along with numerical results comparing the DSANE to a Jacobian-free inexact Newton method.

The remainder of this paper is organized as follows. In Section 2, we describe the mathematical model for the miscible compressible fluid flows in porous media. Section 3 is devoted to the presentation of the DFSANE. In Section 4 we report the numerical results and comparisons. The conclusions are given in Section 5.

2. The mathematical model

In this section, we describe the differential equations that model the isothermal compressible fluid flows in porous media. In addition, we include a discretized form of this mathematical model, which was used to test the spectral method for nonlinear systems of interest here.

We consider flows of binary mixtures (an invading fluid plus a resident fluid) through porous materials associated with processes where the invading fluid and the resident fluid are fully miscible, and flow together as one-phase fluid. Here, these processes are described by the mass conservation equations for the invading fluid and for the mixture, Darcy's law, and an equation of state, which will provide the thermodynamic properties of the binary mixture [3,7].

Let w be the mass fraction of the invading fluid in the mixture, and t the time. Then, the mass conservation equations of this species is given by

$$\phi\frac{\partial(\rho w)}{\partial t}+\nabla.(\rho w u)-\nabla.(\rho D\nabla w)=wq, \tag{1}$$

where ϕ is the porosity of the porous material, ρ is the mass density of the fluid mixture, q is the source (or sink) term that represents the mass flow rate per unit volume injected into (or produced from) the porous medium, D denotes the tensor of the mass diffusive-dispersive flux of the invading fluid, and u is the velocity of the fluid mixture. Here, this velocity is described using a differential form of Darcy's law,

$$u=-\frac{k}{\mu}\nabla P, \tag{2}$$

which disregards gravity effects. In Eq. (2) k is the permeability of the porous medium, μ and P are, respectively, the viscosity and pressure of the binary mixture. The governing differential equation that describes the conservation of mass for the total fluid mixture is given by

$$\phi\frac{\partial\rho}{\partial t}+\nabla.(\rho u)=q. \tag{3}$$

The viscosity of binary mixture depends on the mass fraction w, being described by the following mixing rule [22],

$$\mu(w)=\frac{\mu_r}{\left[(1-w)+w(\mu_r/\mu_i)^{1/4}\right]^4} \tag{4}$$

where μ_i and μ_r are, respectively, the viscosities of the invading and resident fluids.

The density ρ depends only on the pressure of the fluid, and obeys the equation of state [7],

$$\rho(P)=\rho_{ref}e^{c_f(P-P_{ref})}, \tag{5}$$

where ρ_{ref} is the value of ρ at a reference pressure P_{ref}, and c_f is the compressibility of the fluid.

For a two-dimensional velocity field of the type $u=u_1\,i+u_2\,j$ (where i and j are the unit vectors in x-direction and y-direction, respectively), the diffusion–dispersion tensor D takes the form shown in [19],

$$\underbrace{\begin{pmatrix}D_{11}&D_{12}\\D_{21}&D_{22}\end{pmatrix}}_{D}=\phi d_M\begin{pmatrix}1&0\\0&1\end{pmatrix}+\alpha_T\sqrt{u_1^2+u_2^2}\begin{pmatrix}1&0\\0&1\end{pmatrix}+\frac{(\alpha_L-\alpha_T)}{\sqrt{u_1^2+u_2^2}}\begin{pmatrix}u_2^2&u_1u_2\\u_1u_2&u_1^2\end{pmatrix}, \tag{6}$$

where, from Eq. (2), we have

$$u_1=-\frac{k}{\mu(w)}\frac{\partial P}{\partial x}, \tag{7}$$

$$u_2=-\frac{k}{\mu(w)}\frac{\partial P}{\partial y}. \tag{8}$$

In Eq. (6), the scalar d_M is the coefficient of molecular diffusion, and α_T and α_L are, respectively, the transverse dispersivity and longitudinal dispersivity of the invading fluid. The coefficient d_M has dimension of area per unit time, while α_T and α_L have dimensions of length.

Let Ω be the spatial domain representing the porous medium, whose boundary is denoted by $\partial\Omega$. The boundary conditions are those that describe the absence of flow in the borders of Ω:

$$\rho u\cdot n=0,\quad \text{at}\quad \partial\Omega,\quad \text{for all}\quad t\geq 0, \tag{9}$$

$$(\rho w u-\rho D\nabla w)\cdot n=0,\quad \text{at}\quad \partial\Omega,\quad \text{for all}\quad t\geq 0, \tag{10}$$

where n is the unit vector normal to $\partial\Omega$.

Here, the spatial domain Ω is (essentially) two-dimensional. This rectangular domain (supposedly horizontal) will be denoted by $\Omega=[0,L_x]\times[0,L_y]$, where L_x and L_y are the lengths of the sides of this rectangular region in x-direction and y-direction, respectively. For the spatial discretization, we use a uniform block-centered grid. Thus, given two integers n_x and n_y, this grid will be described by $\widehat{\Omega}=\{(x_i,y_j)\in\mathbb{R}^2; i=1,\ldots,n_x \text{ and } j=1,\ldots,n_y\}$, with $x_i=(i-1/2)\Delta x$ and $y_j=(j-1/2)\Delta y$, such that $\Delta x=L_x/n_x$ and $\Delta y=L_y/n_y$. Each point $(x_i,y_j)\in\widehat{\Omega}$ represents a node of the block-centered grid, where the values of the unknown functions of the problem in question are effectively calculated. Given $x_{i+1/2}=x_i+\Delta x/2$, $y_{j-1/2}=y_j-\Delta y/2$, etc., the set $\widehat{\Omega}_{ij}=[x_{i-1/2},x_{i+1/2}]\times[y_{j-1/2},y_{j+1/2}]$ denotes a block of $\widehat{\Omega}$, whose node is the point (x_i,y_j). Thus, we have $n_x\times n_y$ discretization blocks. The temporal domain is represented by a closed interval $[t_0,t_f]$, where t_f denotes the final time and $t_0(=0)$ is the initial time. Given an integer n_t, this interval