Three dimensional and thermal transient analysis of sedimentary rocks

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Abstract

This work presents the implementation of a finite element code for the thermal transient analysis of sedimentary rocks. This analysis provides a means to assess the thermal history in sedimentary rocks, assisting the studies of hydrocarbon generation and migration processes. The unstructured 3D mesh of tetrahedral elements provides the discrete model. An iterative driver using an edge-by-edge data structure solves the resulting system of equations at each time step. This strategy provides considerable improvements in terms of CPU time and memory demand. This combination enables the study of complex 3D problems, a key issue to basin analysis.

1 Introduction

In recent years, oil companies have made prediction a priority. The modeling of the process of generation, migration and accumulation of petroleum has occurred through a better understanding and basic quantifying of how petroleum systems function and also helping lower exploration costs.

The need for renewal requires significant investments in exploration that the large oil companies nowadays almost systematically integrate basin modeling into their exploration strategy, making the numerical simulation of those process one of the most computationally intensive engineering activities.

The simulations of thermal events have a great importance in exploration because they have influence in the thermal stratification of sedimentary basin, therefore also affecting the generation and migration process from the source
rock (Allen and Allen [1] and Barbosa [3]. In some of those events, such as intrusive igneous bodies, the temperature is very high and in others, like salt domes, the high value of thermal conductivity may result in anomalous isotherm contours lines (Turcotte and Schubert [11]).

Geological structures have complex geometry and boundary conditions, as well as heterogeneous lithology properties. Consequently the need for three-dimensional and unstructured grids provides a consistent analysis of the problem, as studied by Cavalcanti and Mello [5]. The utilization of finite element approximations instead of finite difference has been a renewed interest, mainly due to their ability to handle complex geometries.

The most important computational kernel of finite element analysis is the solution of the system of linear equations, basically due to the unstructured nature of finite element grids. For most problems of practical interest, especially in three-dimensions, solution methods based on direct methods, such as Gaussian elimination, lead to massive storage demands and large computer times (Hughes et al [7,8]). Iterative methods, on the other hand, present comparatively low storage requirement and, when associated with suitable preconditioners, provide a powerful computational strategy.

In this work we employ iterative techniques in combination with edge-by-edge data structure to solve transient problems derived by Martins et al [6]. In these strategies the matrix-vector multiplication, operation used in the iterative method of pre-conditioner conjugated gradient (PCG), is done at the edge level. The transition from an element-by-element data structure to an edge-by-edge data structure provides high computational performance as well as a decrease of total floating point operations (flops) and indirect addresses.

This paper is organized as follows. In the next Section we review the mathematical model. The resulting finite elements equations are presented in Section 3. The Section that follows describes the edge-by-edge data structure in combination with iterative techniques. Section 5 presents a numerical example of thermal history. Finally, we gather the main conclusions of this work in the last Section.

2 Problem statement

The governing equation for thermal transfer by conduction at an instant \( t \in [0, t_f] \) in \( \Omega \subseteq \mathbb{R}^3 \) with boundary \( \Gamma \), can be described by the following equation (Incropera et al [9]),

\[
\frac{\partial}{\partial x} \left( k_x \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial u}{\partial z} \right) + f = \rho c \frac{\partial u}{\partial t}
\] (1)

where the spatial coordinates are denoted by \( x, y \) and \( z \), \( u (x, y, z, t) \) is the temperature, \( k \) is the thermal conductivity tensor, \( \rho \) and \( c \) are respectively density and specific heat and \( f \) is the thermal source.
The initial conditions assumed that thermal distribution in t=0 is given by:

\[ u(x, y, z, 0) = 0 \]  

(2)

The respective essential and natural boundary conditions used to solve eqn (1) are:

\[ u(x, y, z, t) = T_1 \text{ on } \Gamma_q \]  

(3)

\[-k \frac{\partial u}{\partial y} = q \text{ on } \Gamma_h \]  

(4)

\[ \Gamma_g \cup \Gamma_h = \Gamma \]  

(5)

where \( T_1 \) is the temperature at surface and \( q \) is the basal heat flow entering the basin.

In this work we are considering isotropic materials which means \( k_{xx} = k_{yy} = k_{zz} \).

Eqn. (1) can be expressed as:

\[ \nabla \cdot k \nabla u + f = \rho c \frac{\partial u}{\partial t} \]  

(6)

2.1 Thermal properties

Analysing thermal history of sedimentary basins we need to take into account the different litologies. The relevant litology properties are solid grain thermal conductivity, porosity at surface, porosity decay rate, solid grain density, specific heat, fluid thermal conductivity, pore fluid density and sedimentary layer depth.

With those litology properties we can calculate three important thermal properties as follows.

2.1.1 Porosity

Porosity has an important role in the study of thermal history of sedimentary basin, due to the inverse proportionally relation with thermal conductivity. The porosity can be described by Athy’s [2] equation:

\[ \phi(z) = \phi_0 e^{-cz} \]  

(7)

where \( \phi \) is the porosity (%), \( \phi_0 \) is the porosity at surface, \( c \) is the porosity decay rate and \( z \) is the sedimentary layer depth.
2.1.2 Thermal conductivity
Thermal conductivity is a property that describes how well a material can transmit heat (Athy [2]). It can be expressed as:

\[ k(z) = k_r (1 - \phi(z)) k_w \phi(z) \]  
(8)

where \( k_r \) is the solid grain thermal conductivity and \( k_w \) is the fluid thermal conductivity.

2.1.3 Density
To calculate the sedimentary layer density, we should know the porosity \( \phi \), the solid grain density \( \rho_g \) and the pore fluid density \( \rho_w \) (Athy [2]):

\[ \rho(z) = \rho_w \phi(z) + \rho_g (1 - \phi(z)) \]  
(9)

3 Finite element formulation
The Finite Element Method (FEM) is a flexible numerical method due to the feature of solves any mathematical problem represented by a differential equation. In addition to that this method works well with refined and unstructured grids. Consequently it has the ability to handle complex geometries and discontinuities (such as faults).

The use of FEM to solve differential equations in engineering is more common, while in geology is not so frequent, due to the materials heterogeneity that result in stiff meshes.

However, to achieve high performance, we have employed the iterative technique of Precondition Gradient Conjugate (PCG) in combination with edge-by edge data structure to solve the resulting system of linear equations. For a review of such topics please see Hughes et al [7,8].

3.1 Space discretization
FEM has provided the spatial discretization, where discrete variables are replaced by continuous variables that are defined at the nodes of a mesh of finite elements.

Denoting the set of elements resulting from the finite element discretization of the computational domain \( \Omega \) into subdomains \( \Omega^e \), \( e=1, 2, \ldots, nel \), where \( nel \) is the number of elements of the mesh. Introducing a shape function associated with a node number, the temperature can be approximated by:

\[ u^h = \sum_{i=1}^{n} N_i u_i = Nu \]  
(10)
where $u^h$ represents the element finite approximation for the temperature, $u_i$ is the temperature at each node, $n$ is the number of nodes and $N_i$ is the shape function.

The semi-discrete formulation for heat transfer by conduction is given by:

$$M \dot{u} + Ku = f$$

(11)

where $M$ is the global capacity matrix (mass matrix, from now on), $K$ is the global thermal conductivity matrix and $f$ is the heat supply vector. $M$, $K$ and $f$ are the sums of elemental contributions, given by:

$$M = \sum_{e=1}^{nel} (m^e)$$

(12)

$$K = \sum_{e=1}^{nel} (k^e)$$

(13)

$$f = \sum_{e=1}^{nel} (f^e)$$

(14)

and $A$ is the finite element assembly operator and $nel$ is the number of elements.

3.2 Time discretization

In this work we used an implicit method called trapezoidal rule to time discretization. To solve eqn (11) we first calculate $\tilde{u}$ and then calculate $\dot{u}$ as follow:

$$\tilde{u}_1 = u_0 + (1 - \alpha)\Delta t \dot{u}_0$$

(15)

$$\dot{u}_1 = \left( M + \alpha \Delta t K \right)^{-1} \left( F_0 - K \tilde{u}_1 \right)$$

(16)

$$Mef = M + \alpha \Delta t K \quad \alpha = \frac{1}{2}$$

(17)

$$F = F_0 - K \tilde{u}_1$$

(18)

$$u_1 = \tilde{u}_1 + \alpha \Delta t \dot{u}_1$$

(19)

As memory is a very important limiting factor of current large-scale 3D analyses, in this work we employ the iterative method of the conjugate gradient with preconditioning to solve eqn. (16). This method in combination with edge-by-edge data structure provides high computational performance as well as a decrease of total floating point operations (flops) and indirect addresses, improving the computational efficiency (Martins et al [6]).
4 Edge-by-edge data structure

The conjugate gradient method used to solve eqn (16) makes repeated matrix-vector multiplication $A \cdot p$. The use of an edge data structured increases the velocity in these operations.

In spite of having the number of edges higher than the number of elements, a factor of 1.5, and still have to assembly this structure internally in the pré-processor, the efficiency in matrix vector operations is high.

The element matrices can be disassembled into their edge contributions, fig.1.

\[
\begin{bmatrix}
\bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet \\
\bullet & \bullet \\
\bullet \\
\end{bmatrix} = \begin{bmatrix}
x \times 0 0 0 \\
x \times 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
\end{bmatrix} + \begin{bmatrix}
0 0 0 0 \\
0 \times 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
\end{bmatrix} + \begin{bmatrix}
x 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
\end{bmatrix} + \begin{bmatrix}
0 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
\end{bmatrix} + \begin{bmatrix}
0 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
\end{bmatrix} + \begin{bmatrix}
0 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
0 0 0 0 \\
\end{bmatrix}
\]

Figure 1: Edges matrices from element matrix.

In the steady-state analysis, we need to store just one coefficient per edge, which corresponds the off diagonal.

In the transient analysis, after the time discretization, we need to store 2 coefficients per edge.
As we have an unstructured mesh, we deal with data by indirect address. Hence, to have an efficient data structure we should renumber strategically the nodes aiming that once data has been gathered, reuse them as much as possible.

Martins et al [6] have found that structures formed by gathering edges in spatial triangular and tetrahedral arrangements, the superedges, present a high data reutilization ratio and are simply to implement. The superedges are formed reordering the edge list, gathering edges with common nodes to form tetrahedral and triangles. To make a distinction between elements and superedges, we call a triangular superedge a superedge\(^3\) and a tetrahedral superedge a superedge\(^6\). The matrix-vector product for a superedge\(^3\) may be expressed as,

\[
Ap = \sum_{a=1}^{N_{edges,3}} \left( A_a p_a + A_{a+1} p_{a+1} + A_{a+2} p_{a+2} \right) \tag{20}
\]

and for a superedge\(^6\),

\[
Ap = \sum_{a=1}^{N_{edges,3}} \left( A_a p_a + A_{a+1} p_{a+1} + A_{a+2} p_{a+2} + A_{a+3} p_{a+3} + A_{a+4} p_{a+4} + A_{a+5} p_{a+5} \right) \tag{21}
\]

5 Numerical example

We analyse the heat transfer by conduction of a sedimentary basin presenting a sedimentary cover of shale (4Km) over a sandstone (2Km) with length of 15 Km and thickness of 6 Km. The model has an ancient fault between the two material layers, parallel to the right and left faces, with 500 m length and 60° of slope. Table 1 lists the relevant material properties. We assume that initial conditions are:

\[
T(x, y, z, 0) = 0°C \tag{22}
\]

and boundary conditions are:

\[
\dot{q}(x,0, z, t) = 0.05296 \text{ W/m}^2 \text{ and } T(x,6000, z, t) = 20°C \tag{23}
\]

Table 1: Material properties.

<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal Conductivity</th>
<th>Density</th>
<th>Specific Heat</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - Shale</td>
<td>1.93 W/(mK)</td>
<td>2,680 Kg/m³</td>
<td>900 J/(kg.K)</td>
</tr>
<tr>
<td>2 - Sandstone</td>
<td>5.57 W/(mK)</td>
<td>2,650 Kg/m³</td>
<td>850 J/(kg.K)</td>
</tr>
</tbody>
</table>
Figure 2: Scheme of the sedimentary basin.

Figure 3: View of the finite element mesh.

Figure 4: Thermal transient analysis of the sedimentary basin.
The finite element mesh comprises 25,001 tetrahedra, 5,257 nodal points and 32,133 edges. The number of edges grouped into superedges’s and superedges’s are 56.6 and 32,133 edges. Fig. 2 shows the scheme of the sedimentary basin and fig. 3 shows a view of the mesh.

Next sequence of fig. 4 shows the thermal transient analysis of the sedimentary basin. We may note that the maximum temperature was 367.15°C and the steady state was achieved at 1.42 Ma.

We solve this problem on a PC Pentium 4, with 2 GHz and 523,568 KB of RAM memory using operational system Windows 2000. The solution of the problem took only 33.43 seconds.

6 Conclusion

In this paper we have presented the implementation of edge-based finite element techniques in transient heat transfer by conduction. We observed that using this strategy the solution time and memory where reduced enabling the study in basin scale which has a large number of elements.

In this implementation an alternative manipulation and storage of elements matrix was done reducing the effects of indirect addressing.

In case of needing higher detail models the supercomputer Cray at COPPE/UFRJ is able to do this analysis as Martins [6] and Souza [10] concluded.

Therefore, the computational strategies presented herein provide a natural way to deal with more complex scenarios, particularly involving three-dimensional geological problems.

References


