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COMPARISON OF IMPES, SEQUENTIAL, AND FULLY IMPLICIT FORMULATIONS FOR TWO-PHASE FLOW IN POROUS MEDIA WITH THE ELEMENT-BASED FINITE VOLUME METHOD

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Abstract. This paper presents comparative results of IMPES (IMplicit Pressure, Explicit Saturation), sequential, and fully implicit solution schemes for isothermal, immiscible, incompressible two-phase flow reservoir simulation with the Element-based Finite Volume Method (EbFVM). The IMPES method solves pressure implicitly and saturation explicitly, as the acronym suggests. As a result of this explicit calculation its stability is subjected to a restriction of the time step. Nevertheless, this scheme reduces the computational effort and facilitates implementation. The sequential method is a modified IMPES with the aim of improving stability of explicit formulations. The Fully Implicit Method (FIM) solves the system of equations that models the problem simultaneously with the Newton-Raphson method. This formulation implies larger system of equations with many nonlinearities and thus higher computational cost. Regardless the difficulties related to the numerical scheme and its implementation it is a more stable method. Furthermore, in this work it is also presented a variable time step strategy in order to accelerate the performance of the methods. This strategy consists basically in modifying the time step according to the current solution. In this paper, IMPES, sequential and fully implicit methods are compared in terms of stability, computational time and accuracy of their results.

Keywords: Reservoir simulation, Two-phase flow, EbFVM, unstructured grids, Newton-Raphson method

1 INTRODUCTION

Multiphase flow in porous media is modeled by nonlinear, coupled, and time-dependent sets of differential equations. A variety of approaches can be used for solving these equations, such as IMPES (IMplicit Pressure, Explicit Saturation), sequential and fully implicit or simultaneous solution schemes.

The IMPES (IMplicit Pressure Explicit Saturation) method was originally developed by Sheldon et al. (1959) and Stone and Garder (1961). Its fundamental idea is to split the coupled set of differential equations and solve the pressure equations implicitly and the saturation equations explicitly (Chen, 1962). This explicit calculation simplifies IMPES implementation and reduce its computational costs. On the other hand, this explicit treatment of the saturation equations is also the cause of one of its great disadvantages: for it to be stable, small time steps are required. This condition is sometimes expensive and prohibitive, particularly for long time integration problems and for small control volumes problems, such as reservoir simulations with local grid refinement (LGR) in the near well-reagion. Further developments were presented in Coats (1982), Watts (1985) and Young and Stephenson (1983) and other IMPES-based methodologies were proposed in Buchwalter and Miller (1993), Coats et al. (1995), and Cao and Aziz (2002). Later, Chen and Li (2004) and Hurtado (2005) proposed a modified IMPES in which different time steps were used to solve the pressure and the saturation equations. In order to improve IMPES stability, MacDonald and Coats (1970) suggested a modified IMPES known as sequential method. In this formulation, after saturation is calculated explicitly, pressure is calculated again with updated coefficients until both pressure and saturation values variate less than a specified tolerance.

Alternatively, the FIM (Fully Implicit Method) or simultaneous approach solves pressure and saturation simultaneously. Although it requires solving a nonlinear set of differential equations -e.g. with the Newton-Raphson method - and thus is more computationally expensive, it is a more stable and robust method, as stated in Aziz and Settari (1979), Farnstrom and Erte-kin (1987), Peaceman (1977) e Watts (1985).

In this paper, IMPES, sequential, and fully implicit solution formulations are applied to isothermal, immiscible, incompressible two-phase flow reservoir simulation. In order to discretize the governing equations on unstructured grids the Element-based Finite Volume Method (EbFVM) (Hurtado, 2005, 2011, Maliska, 2004) is applied. With the aim of reducing the computational effort, a variable time step strategy was implemented. The main idea of this scheme is to use the variation of the saturation field to decide if the time step value could be set as a higher value or if it should be decreased. It is important to stress that applying this adaptive time step is not a common practice to accelerate explicit method calculations. This sort of strategy is usually applied to implicit formulations but will be used here in order to compare all three methods behavior with respect to that criterion. In this paper, IMPES, sequential, and fully implicit solution schemes are compared in terms of stability, computational time and accuracy of their results.

Three types of problems are exploit in order to compare the methods. The first one is the so called Buckley-Leverett problem. It is a one-dimensional displacement case in which there exists a well known analytic solution. The second problem is a two-dimensional classical case of secondary recovery known as quarter five-spot. The third and last example presented is a secondary recovery case simulated with a three-dimensional hybrid grid.

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2 MATHEMATICAL MODEL AND DISCRETIZATION

Let ϕ and \mathbb{K} denote the porosity and the permeability of a porous media, S^p , ρ^p and k_r^p be the saturation, the density and the relative permeability of the p phase, p = w, o, respectively. Neglecting any influence of capillary pressure and considering an isothermal, immiscible, incompressible two-phase flow in a porous media, the mass conservation equations are represented by the equation

$$\frac{\partial}{\partial t} \left(S^p \phi \right) + \nabla \cdot \left(-\lambda^p \mathbb{K} \nabla \Phi^p \right) - f^p = 0 \tag{1}$$

for p = w, o, where the potencial Φ^p of the phase p is given by $\nabla \Phi^p = \nabla P - \rho^p \mathbf{g}$, P represents the pressure and \mathbf{g} the gravitational acceleration vector. Also, λ^p is the mobility of the phase p, given by $\lambda^p = k_r^p / \mu^p$. The fact that the two phases will jointly fill the porous volume is given by the equation

$$S^w + S^o = 1. (2)$$

The Element-based Finite Volume Method (EbFVM) will be the chosen approach in order to discretize the system of differential equations. It follows the basic guidelines of conventional finite volume method (FVM), since the procedure goes through the integration of differential equations over the control volumes and thus the conservation is automatically enforced. EbFVM considers the element as the basic geometrical entity for spacial discretization. As a consequence, the method provides a significant improvement in representing complex geometries and facilitates local grid refinement (LGR).

The main geometrical entities considered in EbFVM are ilustrated in Fig. 1. The unknowns are calculated at the nodes, which are located at the element vertices. The control volume is built around each node gathering the portions of the elements – subelements – which share the node to which the control volume is associated. The contour of a control volume, known as control surface, is then composed by a certain number of faces. In two dimensions, faces are line segments that connect the element centroid to the midpoints of its two sides that share the node associated to the control volume. More details about EbFVM can be found in Maliska (2004), Hurtado (2005) and Hurtado (2011).



Figura 1: Main geometrical entities considered in EbFVM

After integrating the water and the oil conservation equations and adding these two discretized equations the global or total conservation equation is obtained. Hence, the discretized water mass and total mass conservation for an arbitrary control volume associated a node \mathcal{P} are, respectively, given by

$$\frac{\phi_{\mathcal{P}}\Delta V_{\mathcal{P}}}{\Delta t} \left[S_{\mathcal{P}}^{w} - (S_{\mathcal{P}}^{w})^{\text{old}} \right] + \sum_{e \in \mathscr{E}^{\mathcal{P}}} \left(-\lambda^{w} \mathbb{K} J^{-1} D \ \Phi_{e} \right) \cdot \Delta \mathbf{A}_{f} = q_{\mathcal{P}}^{w} \Delta V_{\mathcal{P}}, \tag{3}$$

$$\sum_{e \in \mathscr{E}^{\mathfrak{P}}} \left(-\lambda^t \mathbb{K} J^{-1} D \ \Phi_e \right) \cdot \Delta \mathbf{A}_f = q_{\mathfrak{P}}^t \Delta V_{\mathfrak{P}},\tag{4}$$

where the superscript old indicates that the value is calculated in the last time level, Φ_e is a vector with the values of Φ at the element (e) nodes and $\mathscr{E}^{\mathcal{P}}$ is the set of elements that share the node \mathcal{P} . Moreover, $\Delta V_{\mathcal{P}}$ is the control volume, Δt is the time step, $\Delta \mathbf{A}_f$ is the area vector of a face limiting the control volume and $J^{-1}D$ is the EbFVM discrete gradient operator. Combining equations (2), (3), and (4), there exist three equations and three unknowns – S^w , $S^o \in P$.

3 IMPES AND SEQUENTIAL METHODS

The discretized equations which correspond to implicit calculation of P and explicit calculation of S^w are, respectively,

$$\sum_{e \in \mathscr{E}^{\mathfrak{P}}} \left(-\lambda^t \mathbb{K} J^{-1} D \ \Phi_e \right) \cdot \Delta \mathbf{A}_f = q_{\mathfrak{P}}^t \Delta V_{\mathfrak{P}},\tag{5}$$

$$S_{\mathfrak{P}}^{w} = (S_{\mathfrak{P}}^{w})^{\text{old}} + \frac{\Delta t}{\phi_{\mathfrak{P}} \Delta V_{\mathfrak{P}}} \sum_{e \in \mathscr{E}^{\mathfrak{P}}} \left(-\lambda^{w} \mathbb{K} J^{-1} D \Phi_{e} \right) \cdot \Delta \mathbf{A}_{f} - \frac{\Delta t q_{\mathfrak{P}}^{w}}{\phi_{\mathfrak{P}}}.$$
 (6)

The classical IMPES iterative procedure to determine the primary unknowns is:

- 1. Specify P and S^w initial values in each grid node;
- 2. Calculate λ^p in each grid node and interpolate its values in elements faces;
- 3. Solve pressure implicitly with the linear system composed by Eq. (5) for each CV;
- 4. With the calculated pressure, calculate S^w explicitly with Eq. (6) for each CV;
- 5. Advance in time and return to item 2 until final simulation time is reached.

The sequential method follows a similar procedure. The difference between IMPES and sequential method is that the latter returns to item 2 after after item 4 until saturation and pressure fields variate less than a specified tolerance. The explicit calculation does not require solving a linear system and thus, IMPES and sequential are easier to implement computationally. On the other hand, as already discussed, it introduces severe limitations for the time step value.

4 FULLY IMPLICIT METHOD

The fully implicit method or simultaneous approach solves all unknowns concurrently. Despite its time step value limitations are less significant, it is a more complex formulation, which will be briefly explained here. Arises from this formulation the necessity of solving a non linear set of partial differential equations. With the aim of solving this set, the Newton-Raphson method for multiple variables was employed. The main goal of this method is to simultaneously solve roots of several equations, which are called residual equations. The water and total residual equations are, then:

$$R^{w} = \frac{\phi_{\mathbb{P}} \Delta V_{\mathbb{P}}}{\Delta t} \left[S_{\mathbb{P}}^{w} - (S_{\mathbb{P}}^{w})^{\text{old}} \right] + \sum_{e \in \mathscr{E}^{\mathbb{P}}} \left(-\lambda^{w} \mathbb{K} J^{-1} D \ \Phi_{e} \right) \cdot \Delta \mathbf{A}_{f} - q_{\mathbb{P}}^{w} \Delta V_{\mathbb{P}}, \tag{7}$$

$$R^{t} = \sum_{e \in \mathscr{E}^{\mathcal{P}}} \left(-\lambda^{t} \mathbb{K} J^{-1} D \Phi_{e} \right) \cdot \Delta \mathbf{A}_{f} - q_{\mathcal{P}}^{t} \Delta V_{\mathcal{P}}, \tag{8}$$

since the root of these functions is the solution of the set of equations. R^w denotes the residual associated to water mass conservation and R^t denotes the residual associated to the total mass conservation. Both are functions of S^w and P – the primary unknowns of the problem. The Newton-Raphson iterative procedure is executed as follows:

- 1. Construct a vector \mathbf{X} with the estimates of P and S^w in each CV;
- 2. Calculate mobilities in each CV and interpolate the mobility values in elements faces;
- 3. Compute R^w and R^t in each control volume;
- 4. Compute the partial derivatives of the residuals in each node using truncated Taylor series expansion $\partial R^i / \partial X = [R^i(X + dX) R^i(X)] / dX;$
- 5. Solve the linear system $J\Delta \mathbf{X} = -\mathbf{R}$ where J is the jacobian matrix composed by the partial derivatives of the residuals, $\Delta \mathbf{X}$ is the correction vector and \mathbf{R} is the residual vector.
- 6. Correct the unknowns values contained in X using the equation $X^{k+1} = X^k + \Delta X$;
- 7. Return to item 2 and iterate until a specified criterion for convergence is achieved;
- 8. Return to item 2 and advance in time until final simulation time is reached.

Certainly, constructing the jacobian matrix is the most complex and computationally expensive part of the Newton-Raphson method. Furthermore its construction is very particular when the EbFVM is used, whereas that this method considers the element as the basic geometrical entity for spacial discretization.

Since it was chosen to put water and total mass conservation equations sequentially for each node in the residual vector, the linear system $J\Delta X = -R$ becomes

$$\begin{pmatrix} \frac{\partial R_1^w}{\partial S_1} & \frac{\partial R_1^w}{\partial P_1} & \cdots & \frac{\partial R_1^w}{\partial S_n} & \frac{\partial R_1^w}{\partial P_n} \\ \frac{\partial R_1^t}{\partial S_1} & \frac{\partial R_1^t}{\partial P_1} & \cdots & \frac{\partial R_1^t}{\partial S_n} & \frac{\partial R_1^t}{\partial P_n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial R_n^w}{\partial S_1} & \frac{\partial R_n^w}{\partial P_1} & \cdots & \frac{\partial R_n^w}{\partial S_n} & \frac{\partial R_n^w}{\partial P_n} \\ \frac{\partial R_n^t}{\partial S_1} & \frac{\partial R_1^t}{\partial P_1} & \cdots & \frac{\partial R_n^t}{\partial S_n} & \frac{\partial R_n^t}{\partial P_n} \\ \end{pmatrix} \begin{bmatrix} \Delta S_1 \\ \Delta P_1 \\ \vdots \\ \Delta S_n \\ \Delta P_n \end{bmatrix} = - \begin{bmatrix} R_1^w \\ R_1^t \\ \vdots \\ R_n^w \\ R_n^t \end{bmatrix}.$$
(9)

CILAMCE 2016 Proceedings of the XXXVII Iberian Latin-American Congress on Computational Methods in Engineering Suzana Moreira Ávila (Editor), ABMEC, Brasília, DF, Brazil, November 6-9, 2016 Organizing the conservation equations in this order, each line of the jacobian matrix contains derivatives of only one residual equation $-R^w$ or R^t – and each column contains derivatives with respect to only one variable $-S^w$ or P. Figure 2 shows an example of a jacobian matrix structure for an arbitrary control volume. It is interesting to notice that its structure is the same as the structure that corresponds to IMPES pressure linear system matrix. The difference between them is that in the jacobian matrix presented in Fig. 2 is a block matrix in which the entries are 2x2 matrices with partial derivatives of R^w and R^t with respect to S^w and P, as illustrated in the figure. On the other hand, IMPES pressure linear system matrix would have only one entry per block in the same figure.



Figura 2: Exemplo de estrutura da matriz jacobiana

5 VARIABLE TIME STEP STRATEGY

In order to avoid unnecessary computational effort and excessive large time step specification, it was implemented an adaptive time step scheme that modifies the time step value according to the variation in saturation field through time. This scheme is explained in Fig. 3. The parameters used in this paper are listed in Table 1.

The only part of the flowchart that has to be adapted according to the method (IMPES, sequential or FIM) is the convergence verification. For the IMPES method it is enough to check if the pressure linear system has converged. For the sequential formulation, not only that has to be done, but also it has to be assured that the specified maximum number of sequential iterations has not been reached. Lastly, for the fully implicit method, linear and non-linear system convergence have to be checked.

Tabela 1: Parameters corresponding to the variable time step strategy

ΔS_{\max}	ΔS_{\min}	$\alpha_{\rm inc}$	$\alpha_{\rm red}$
0.1	0.05	1.01	0.5



Figura 3: Adaptive time step strategy flowchart

6 **RESULTS**

6.1 The Buckley-Leverett problem

There only exists an analytic solution for a two-phase immiscible displacement if it is assumed unidirectional and incompressible macroscopic flow with homogeneous porous media and uniform initial phase distribution. Also, the effects due to capillarity and gravity should be neglected. This analytic solution is presented in Dullien (1979) and will be used in this paper with the aim of verification.

Despite the unidirectional flow, two-dimensional grids were employed -430, 1961, and 7392 nodes. All these grids are composed only by triangular elements. Moreover, the chosen relative permeability model is a Corey model with unitary coefficient and exponential factor 2.

That is, each phase relative permeability is the square of its saturation. Besides, the viscosity ratio is $\mu^o/\mu^w = 4$, the porosity is unitary and the fluid velocity in the left boundary is 1 m/s.

Figure 4 shows the saturation profile calculated with IMPES, sequential and fully implicit formulations with and without adaptive time step in the coarsest grid for 0.8, 1.2, 1.6, and 2.0 seconds. With the other two finer grids the results were very similar to those presented in Fig. 4, but closer to analytic solution as it was expected. Besides, Fig. 5 shows how much CPU time was spent simulating the problem in all three grids and with all three methods.



Figura 4: Water saturation profile calculated with a 430 nodes grid for 0.8, 1.2, 1.6, and 2.0 seconds



Figura 5: CPU time spent with 430, 1961, and 7392 nodes

The results shows that all three methods solutions are physically consistent despite the presence of numerical diffusion caused by discontinuity of the saturation profile and space discretization. Furthermore, Fig. 4 shows that when a constant time step is specified the three methods provide practically identical solutions. However, when the adaptive time step strategy is utilized IMPES method provides a more accurate saturation profile. It can be shown for a one-dimensional situation that there exists a time step value (that satisfies the condition of unitary CFL) for which IMPES gives precisely the analytic solution. This result suggests that this behavior also occurs with a two-dimensional unstructured grid.

Figure 5 shows that IMPES formulation uses less CPU for this problem with all three grids.

Also, it shows that CPU time spent by the fully implicit method can be significantly reduced for refined grids when the adaptive time step scheme is used.

6.2 The quarter five-spot problem

The classical quarter five-spot is a standard porous media problem that simulates injection of water into a square oil-filled reservoir. Water is injected through a well at the lower left corner of the computational domain at a constant rate, and fluid is produced at the same rate through a well located in the upper right corner.

It is considered a 300 m x 300 m reservoir with absolute permeability 10^{-11} m² and porosity 0.2. Water and oil viscosity are 10^{-3} and 10^{-2} Pa.s, respectively. Water is injected with a 2 10^{-5} m³/s flow rate and 5000 days are simulated. Once more, the chosen relative permeability model is a Corey model with unitary coefficient and exponential factor 2. Three grids with different levels of refinement were used – 425, 1483, and 5985 nodes. Again, all grids are composed only by triangular elements. Figures 6 and 7 show the results obtained with the finest grid with constant and adaptive time step, respectively. The well index value is 6.18471 10^{-11} . In these results – figures 6 and 7 – average pressure builds to a peak after the breakthrough and then drops. This peak is due to to a pressure increase in the well control volume, which occurs because with a quadratic relative permeability model total mobility achieves its lowest value when oil saturation is less than 1 in the well control volume. Figure 8 shows how much CPU time was spent simulating the problem in all three grids and with all three methods. Lastly, Fig. 9 shows the saturation field for 500, 1500, 3000 and 5000 days.

Figure 6 shows that when a constant time step is considered, all methods provide practically identical solutions. On the other hand, Fig. 7 shows that when the adaptive time step scheme is used, only the fully implicit and sequential methods are stable. In this case, IMPES numerical solution is unstable after the breakthrough, that is, where the water injected to maintain reservoir pressure via injection wells breaks through to the producing well. This unstable solution occurs because IMPES uses an old saturation value to calculate the well flow rate. In order to reduce IMPES oscillations, instead of only reducing the time step when any saturation value exceed ΔS_{max} , the solution corresponding to that time level could be calculated again with this reduced time step value. It is important to notice, though, that this approach would only diminish the oscillations. One possible way of avoiding them would be using an iterative procedure, *i.e.*, the sequential method. Indeed, Fig. 7 shows that sequential method solution is stable in this case. This severe IMPES time step limitation is the main reason why the common approach is not using an adaptive time step strategy with this method, but finding its maximum value that provide a stable solution.

In addition, it is interesting to notice from figures 6, 7, and 8 that for all three grids with the constant time approach IMPES is the less costly method and, as well as the others, provides a stable solution. Besides, when the adaptive time step scheme is employed the fully implicit method is not the only method capable of providing stable solutions but it is faster stable method. Furthermore, fully implicit method with adaptive time step scheme has a computational cost of the same order of IMPES formulation with constant time step. Lastly, it can be easily noticed that the time step variation scheme is responsible for a significant reduce of computational cost. Nevertheless it should evidently be used with parsimony with explicit methods in order to guarantee stability.



Figura 6: Quarter five-spot results with constant time step and a 5985 nodes grid



Figura 7: Quarter five-spot results with adaptive time step and a 5985 nodes grid



Figura 8: CPU time spent with 425, 1483, and 5985 nodes



Figura 9: Saturation field for 500, 1500, 3000, and 5000 days

6.3 Three dimensional displacement with a three-dimensional hybrid grid

This last application example consists in a secondary recovery case simulated with a threedimensional hybrid grid which has Brazilian territory approximate shape. This grid represents a reservoir with three injector and two producer wells, as illustrated in Fig. 10.

Injector wells are vertical and producer wells are directional. Reservoir maximum dimensions are 200 m (length and width) and 130 m (thickness). The grid is composed by 8073 nodes, 35286 tetrahedra, 544 hexahedra, 544 prisms and 576 pyramids. Besides, there is a cylindrical portion of the grid in the near well region. It is considered a reservoir with absolute permeability $4 \ 10^{-14} \ m^2$ and porosity 0.1. Water and oil viscosity are 10^{-3} and 10^{-2} Pa.s, respectively. As before, it is used a Corey model with unitary coefficient and exponential factor 2 to model relative permeability. Moreover, Table 2 shows the water injection rate in each well.



Figura 10: Three dimensional displacement problem configuration

Tabela 2:	Water	injection	rate
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Injector well 1	Injector well 2	Injector well 3
$1.1 \ 10^{-4} \ \mathrm{m^{3/s}}$	9 10 ⁻⁵ m ³ /s	$8 \ 10^{-5} \ \mathrm{m^{3}/s}$

Figure 11 shows the results obtained with FIM method and adaptive time step and with IMPES and sequential formulations with constant time step. CPU time spent obtaining the results were 16,914.3 s, 219,877 s and 571,286 s with fully implicit, IMPES, and sequential methods, respectively.

Notwithstanding all three methods provide consistent and stable solutions IMPES and sequential methods require excessive computational cost – FIM spent only 7.69% of IMPES and 2.96% of sequential CPU time. It is interesting to notice that the time step curve associated to the fully implicit method is monotonically crescent, which means the time step value only did not need to be set as a lower value in any time. Only the final time step value was decreased but the reason for that was because the final simulation time was specified.

With the aim of exploiting the fully implicit method robustness, the same problem was simulated with this method for 10000 days. CPU time spent in that simulation was 18,908.8 seconds, only 11.79% higher than the time spent in simulating 3000 days. All things considered, this result shows a great computational effort reduction once that due to the adaptive time step strategy it was possible to increasedays of simulation more than three times only with an addition of 11.79% of CPU time. The results are shown in Fig. 12. Besides, Fig. 13 shows time evolution of water saturation in the reservoir, predicted using the fully implicit method.



Figura 11: Three-dimensional displacement results with a hybrid grid for 3000 days



Figura 12: Three-dimensional displacement FIM results with a hybrid grid for 10000 days



Figura 13: Predicted water saturation field

7 CONCLUDING REMARKS

Comparative results of IMPES (IMplicit Pressure, Explicit Saturation), sequential, and fully implicit solution schemes were presented for isothermal, immiscible, incompressible twophase flow reservoir simulation with the Element-based Finite Volume Method (EbFVM). The methods were compared in terms of stability, computational time and accuracy of their results. It was also presented an adaptive time step strategy that modifies time step value according to how much saturation field variate through time. Even though applying this adaptive time step is not a common practice to accelerate explicit method calculations, it was applied in order to compare all three methods behavior with respect to that criterion.

As seen in three application examples, one of the main advantages of the fully implicit method is it robustness. The method requires less prohibitive time step values and thus has a better performance with the implemented adaptive time step scheme specially in the threedimensional displacement problem that were presented, in which reservoir domain was geometrically complex and there were local grid refinement near the wells. Certainly, these advantages should encourage further developments in reservoir simulation applying the fully implicit method and the element-based Finite Volume Methodology jointly.

8 PERMISSION

The authors are the only responsible for the printed material included in this paper.

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