

Original Paper

A novel unstructured-grid generator using upscaling applied to a compositional reservoir simulator

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ABSTRACT

This work introduces a novel unstructured grid generator using an upscaling technique and the Element-based Finite Volume Method (EbFVM). The proposed grid generator can either replicate the original structured Corner Point grid as an unstructured mesh or coarsen it by upscaling reservoir properties for computational efficiency. The proposed methodology enables flexible grid coarsening from structured geological models while preserving numerical accuracy in critical flow regions. The approach integrates a user-defined clustering algorithm with a Dykstra-Parsons coefficient to generate hybrid-resolution grids. A modified Cardwell-Parsons method is used for permeability upscaling and volumetric averaging for porosity. An unstructured grid option has been implemented into the UTCOMPRS simulator, and the grid generator is evaluated and validated through five case studies, including realistic reservoir models and industry benchmarks such as UNISIM-I, model 2 of the SPE10 case, and the Sleipner CO₂ storage project using the UTCOMPRS. Results demonstrate the approach's ability to significantly reduce computational costs while maintaining reliable production forecasts. This work presents a compelling and computationally efficient tool for reservoir simulation.

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1. Introduction

The exploration and production of oil and gas often require substantial investment due to the challenges associated with reaching deep reservoirs. Reservoir rocks located kilometers below the surface introduce uncertainties in the acquisition of essential reservoir data and fluid parameters. To mitigate uncertainties and propose an optimal oil production layout, engineers must integrate geological, production, and reservoir data using numerical simulation. Hence, when modeling fluid flow in porous media, different production and injection layouts can be evaluated to optimize oil and gas production. Commercial simulators commonly utilize Cartesian grids for discretizing reservoir geometries. However, Cartesian grids are not the ideal choice for representing complex reservoir geometries, such as faults and

complex reservoir boundaries, or for addressing the grid orientation effect. To overcome the limitations imposed by Cartesian grids, structured Corner Point grids were developed as described in Peaceman (1983). Corner Point grid blocks are defined by the eight vertices of the hexahedron, offering greater flexibility in representing reservoir geometry.

Alongside the evolution of computational performance, the use of unstructured grids presents itself as an alternative to structured grids. When geometries are discretized by unstructured grids, elements are arbitrarily defined by the coordinates of their nodes. For that reason, unstructured grids offer greater flexibility compared to traditional Corner Point grids. One of the early applications of unstructured grids in the oil and gas industry addressed the reservoir simulation problem using the Finite Element Method (FEM). Despite being developed for structural analysis, the FEM approach started to gain popularity due to its generality and capability of dealing with irregular geometries (Dalen, 1979; Heinemann et al., 1998; Langsrud, 1976). Regarding traditional discretization techniques, the two-point flux approximation generally employed by commercial simulators reduces its

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accuracy when dealing with non-orthogonal grids (Chen et al., 2008). Multipoint flux approximation (MPFA) methods have been studied in the literature to overcome this issue. MPFA methods were initially proposed for Corner Point geometries as they are the standard approach adopted by the oil industry (Aavatsmark et al., 1996; Edwards and Rogers, 1998). Due to the flexibility of the MPFA technique, its application was extended to unstructured grids, changing from a cell-center approach to a cell-vertex approach (Aavatsmark et al., 1998; Samier and Masson, 2017).

Beyond MPFA formulations, several advanced techniques have been developed for unstructured grids, including Discrete Duality Finite Volume (DDFV) (Njifenjou et al., 2013), Hybrid Mimetic Mixed (HMM) approaches (Droniou and Nataraj, 2018), the Vertex-Approximate Gradient (VAG) method (Brenner et al., 2015), and ROUND schemes (Deng, 2023).

Another important multipoint scheme is the use of unstructured grids with the Element-based Finite Volume Method (EbFVM). The method was initially referred to as the Control Volume Finite Element Method (CVFEM) (Baliga and Patankar, 1980). However, the term CVFEM gives the wrong impression of having an FEM based on a Finite Volume Method (FVM). Because the EbFVM approach is still an FVM that only borrows the concept of elements and shape functions from the FEM, the EbFVM nomenclature proposed in (Maliska, 2023) will also be adopted in the present work. The EbFVM has been extensively discussed in the literature over the past decades (Araújo et al., 2016; da Silva et al., 2012; Ding and Lemonnier, 1995; Fernandes et al., 2017; Forsyth, 1990; Fung et al., 1991; Honório et al., 2018; Marcondes et al., 2013; Rozon, 1989; Sepehrnoori et al., 2020; Verma and Aziz, 1997).

In the context of modern reservoir simulation, unstructured grid formulations have emerged as essential tools for accurately representing complex geological structures. These formulations have been extensively applied in various advanced modeling approaches, including multiscale flow simulations, adaptive time-step and mesh refinement strategies (de Souza et al., 2022; Mehrdoost, 2024; Solovský and Firoozabadi, 2025; Teixeira et al., 2021), fractured reservoir representations (Guo et al., 2019), and embedded discrete fracture model (EDFM) applications (Cavalcante et al., 2024). Despite their versatility, much of the existing research has focused on simplified grid configurations, such as Cartesian or radial geometries, limiting their direct applicability to field-scale problems.

As highlighted by Sadykov et al. (2018) and de Figueiredo et al. (2023), realistic reservoir models, particularly those incorporating geomechanical coupling, often consist of millions of grid blocks. This large number of grid blocks contributes to a significant increase in computational costs, both in terms of memory requirements and simulation time. Consequently, there is a growing need for numerical schemes capable of reducing grid resolution without significantly compromising the accuracy of the numerical solution. As presented in (Farias et al., 2019), the EbFVM enables coarsening of unstructured grids while preserving the accuracy of the numerical solution, offering a promising approach to reduce computational cost.

Coarsening and upscaling techniques have been addressed in the literature over the past years. Upscaling methods in unstructured grids typically rely on static pre-simulation methods, where a fine-scale geological or flow model is simulated to enable the construction of a coarser geometry. MPFA approximation (Manchuk et al., 2012), averaging techniques (Mourlanette et al., 2020), wavelet transformation (Rezapour et al., 2019), dual-grid

approach (Prévost et al., 2005), and the Eikonal equation (Ahmadov et al., 2025) are a few techniques available in the literature for unstructured grids.

This work presents a novel unstructured grid generator based on a coarsening approach that enables an unstructured flexible generation of grids from structured Corner Point geometries. The proposed method preprocesses a structured grid to identify regions of interest that will maintain their original level of refinement, while the remaining sections of the reservoir are coarsened. Upscaled permeabilities are calculated using a modified Cardwell-Parsons formulation, and porosity is obtained through a weighted mean. Compared to traditional flow-based techniques, this method optimizes reservoir layout testing since it eliminates the need for fine-scale simulations. This method is implemented in an in-house grid generator, and simulations are performed in the UTCOMPRS simulator.

2. Governing equations

This section presents the main equations and assumptions adopted by the compositional simulator UTCOMPRS. The combination of equations describes the flow in porous media for an isothermal, multicomponent, and multiphase simulation. The equation that represents the material balance, neglecting dispersion terms, is given by

$$\frac{\partial N_i}{\partial t} + \nabla \cdot \left(\sum_{j=1}^{n_p} \xi_j x_{ij} \vec{u}_j \right) + \frac{q_i}{V_b} = 0 \quad (1)$$

where N_i is the number of moles of each component. In the mass conservation equation, V_b is the bulk volume, ξ_j is the molar density of the phase j , x_{ij} is the molar fraction of component i in phase j . The q_i refers to the injection or the production flow rate for a given grid block that has a well perforated and is equal to zero when there is no well in that grid block. The parameter $\vec{u}_j$ is the velocity of phase j and is calculated from the multiphase version of Darcy's law, defined as

$$\vec{u}_j = - \vec{k} \lambda_{rj} (\nabla P_j - \gamma_j \nabla D) \quad (2)$$

where $\vec{k}$ is the absolute permeability tensor, λ_{rj} is the relative mobility of phase j , P_j is the pressure of phase j , γ_j is the specific weight of phase j , and D is the depth, which is positive in the downward direction.

The criterion of phase equilibrium states that fugacity is only a function of pressure and phase composition at a given temperature. To obtain this parameter, a thermodynamic equation of state must be used. The present work utilizes the equation proposed by Peng and Robinson (Robinson et al., 1985). In this work, the correlations proposed in Lohrenz et al. (1964) are used to calculate the viscosities of oil and gas phases. All cases in the present work assume constant water viscosity during the simulation. Initially, the viscosity of a pure component at low pressures is calculated using the correlation proposed in Yoonm and Thodos (1970). For relative permeability, the Stone II model (Stone, 1973) is used to calculate three-phase relative permeabilities. Regarding well equations, the model proposed by Peaceman (Peaceman, 1978, 1983) is employed.

The pressure equation, which is derived from the volume material balance in the UTCOMPRS, is defined by

$$\left[V_p^o C_f - \left(\frac{\partial V_t}{\partial P} \right)_{N_i} \right] \frac{\partial P}{\partial t} = \sum_{i=1}^{n_c+1} \left\{ \bar{V}_{Ti} \bar{\nabla} \cdot \left[\sum_{j=1}^{n_p} \xi_{ij} x_{ij} \frac{\vec{\nabla} k_{rj}}{\mu_j} (\nabla P - \gamma_j \nabla D) \right] \right\} - \sum_{i=1}^{n_c+1} \bar{V}_{Ti} q_i \quad (3)$$

$i = 1, \dots, n_c$

where C_f is the compressibility factor, V_p^o is the porous volume, and $\bar{V}_{Ti}$ is the derivative of the total volume of fluid with respect to the number of moles of a specific component i .

In this study, IMPEC and fully implicit (FI) formulations are chosen. In the IMPEC approach, the pressure is evaluated implicitly, while the compositions and saturations are explicitly solved throughout the simulation. For more complex cases that require stability in time-step selection, the FI formulation is used. This approach solves both pressure and compositions implicitly in time. In addition to mass conservation and pressure equations, a set of constraints and equations for phase behavior and fluid/rock properties calculation must be defined. For further details on these correlations and other aspects of the IMPEC and FI formulations, readers are referred to (Chang, 1990; Fernandes et al., 2016).

3. Structured formulations

The structured formulation is briefly presented here since it will be used as a benchmark for unstructured formulation results. Corner Point geometries are widely adopted as the standard approach used by most commercial simulators in the industry. When applying the mass conservation equation using Corner Point geometries, it is better to apply a transformation from the physical domain to a regular computational domain. The Cartesian coordinates x , y , and z are converted to a computational domain with coordinates ξ , η , and γ . The coordinates of the computational domain are functions of the coordinates from the physical domain, defined by

$$\xi = \xi(x, y, z); \quad \eta = \eta(x, y, z); \quad \gamma = \gamma(x, y, z) \quad (4)$$

The transformed mass equation in the computational plane is given by

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\phi N_i \right) + \frac{\partial}{\partial \xi} \left(\sum_{j=1}^{n_p} D_{11ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \xi} \right) \\ & + \frac{\partial}{\partial \xi} \left(\sum_{j=1}^{n_p} D_{12ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \eta} \right) + \frac{\partial}{\partial \xi} \left(\sum_{j=1}^{n_p} D_{13ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \gamma} \right) \\ & + \frac{\partial}{\partial \eta} \left(\sum_{j=1}^{n_p} D_{21ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left(\sum_{j=1}^{n_p} D_{22ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \eta} \right) \\ & + \frac{\partial}{\partial \eta} \left(\sum_{j=1}^{n_p} D_{23ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \gamma} \right) + \frac{\partial}{\partial \gamma} \left(\sum_{j=1}^{n_p} D_{31ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \xi} \right) \\ & + \frac{\partial}{\partial \gamma} \left(\sum_{j=1}^{n_p} D_{32ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \eta} \right) + \frac{\partial}{\partial \gamma} \left(\sum_{j=1}^{n_p} D_{33ij} x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \frac{\partial \phi_j}{\partial \gamma} \right) \\ & + \frac{q_i}{V_{bT}} \\ & = 0 \end{aligned} \quad (5)$$

where ϕ_j is the potential of the phase, J_t is the determinant of the Jacobian of the transformation, and D is a tensor that contains

fluid, reservoir, and geometric information. The D tensor is always symmetric and is represented as a full tensor with nine terms. The parameters ξ_x , ξ_y , ξ_z , η_x , η_y , η_z , γ_x , γ_y , and γ_z are the direct metrics of the transformation, defined as the derivatives of the coordinate in the computational plane with respect to its subscript. Further details of the method and how to obtain the metrics can be found in (Fernandes et al., 2014; Marcondes et al., 2008).

4. Unstructured formulations

In this study, unstructured grids are used in conjunction with the EbFVM. The foregoing approach integrates the concepts of elements and shape functions from FEM with the local conservative property of FVM. Due to the use of FVM, the EbFVM conserves mass both globally and locally, presenting a higher numerical accuracy. The EbFVM uses grids that are arbitrarily defined by a list of nodes, coordinates, and connectivities. For this reason, elements present greater geometric flexibility. Regarding the discretization of the EbFVM, Eq. (1) is integrated over sub-control volumes, which are constructed in a cell-vertex scheme. In this approach, the control volumes are built around the nodes of the grid. The elements are divided into sub-control volumes equal to the number of vertices. The sub-control volumes are defined by joining the barycenter of the element to its medians. Fluid flow is evaluated at integration points (IPs), which lie in the center of these sub-control volume faces. Fig. 1 illustrates how sub-control volumes are divided inside elements used by the EbFVM. Although prisms and pyramids are two possible elements, in this work, only hexahedral and tetrahedral elements will be used to match the hexahedrons of the Corner Point grid.

The gradient of properties on the IPs is calculated as follows:

$$\frac{\partial \phi}{\partial x} = \sum_{i=1}^{n_v} \frac{\partial \tilde{N}_i}{\partial x} \bigg|_{ip} \phi_i \quad (6)$$

$$\frac{\partial \phi}{\partial y} = \sum_{i=1}^{n_v} \frac{\partial \tilde{N}_i}{\partial y} \bigg|_{ip} \phi_i \quad (7)$$

$$\frac{\partial \phi}{\partial z} = \sum_{i=1}^{n_v} \frac{\partial \tilde{N}_i}{\partial z} \bigg|_{ip} \phi_i \quad (8)$$

where ϕ denotes any property on the nodes of the element, n_v is the number of vertices, and $\tilde{N}$ are the shape functions of elements. For more details of the discretization of the fluid flow equations using the EbFVM, readers are referred to (Marcondes and Sepehrnoori, 2010).

5. Grid generator

In reservoir simulation, computational optimization in terms of CPU time and memory allocation is highly desirable. Structured reservoirs are often presented as complex models with a high number of grid blocks. The construction of structured geometries results in a significant increase in memory requirements and CPU time, particularly when solving the linear system. In many situations, it becomes necessary to use parallel computing techniques to optimize and even enable this type of simulation. From an operational perspective, it is preferable to refine the grid only in specific regions of the reservoir where high gradients are expected, such as areas around the wells. With this approach, other regions

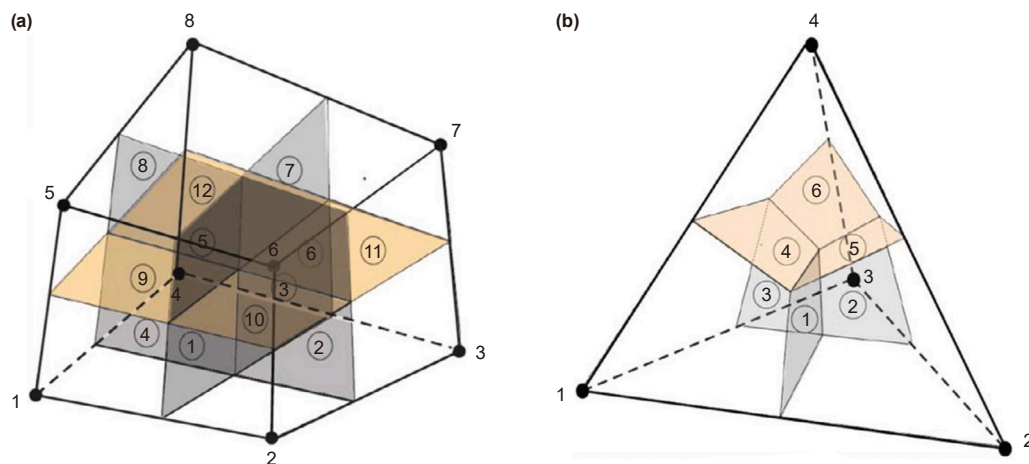


Fig. 1. EbFVM elements: (a) hexahedron, (b) tetrahedron (Marcondes et al., 2015).

of the grid model could be coarsened without compromising the numerical solution. Additionally, it is desirable to employ mathematical methods that can provide reliable numerical solutions in these coarsened regions. Keeping the above observations in mind, the EbFVM emerges as a viable alternative for addressing these challenges. The EbFVM offers a geometric advantage over traditional structured formulations, and it is also locally conservative.

The lack of a standard format for unstructured grids in reservoir simulation motivated the development of a grid generator to be used alongside UTCOMPRS. Previous works based on the EbFVM were limited to Cartesian geometries or distorted synthetic models. To obtain more realistic simulations, an in-house grid tool was developed to obtain unstructured grids from a standard Eclipse COORD/ZCORN file. This converter offers two main capabilities: converting the structured geometry into a hexahedral or tetrahedral grid and coarsening the structured grid into a tetrahedral unstructured grid. This section will present further details of the implementation of grid conversion and upscaling methods.

Initially, the structured reservoir grid is preprocessed and treated by our in-house grid generator. The EbFVM input format contains information regarding nodes and element connectivity. This approach supports only the hexahedral, tetrahedral, prisms, and pyramidal elements, imposing strict geometric constraints.

However, structured grids derived from geological models frequently contain collapsed edges and pinched-out layers. This effect causes the appearance of degenerate grid blocks, which are not supported by the EbFVM. To address this issue, a Laplacian smoothing (Field, 1988) technique based on the works of Wen et al. (2003) is implemented herein. The Laplacian smoothing is applied on the top and bottom interfaces of pinched-out layers, eliminating invalid or collapsed elements while preserving the reservoir characteristics. Different from the classical Laplacian smoothing, an adapted version is implemented here. The adapted method defines boundaries in the active elements above and below the pinched-out layers to preserve characteristics of the reservoir. This procedure ensures that the resulting grid contains only hexahedral elements, maintaining compatibility with the EbFVM. Fig. 2 presents an example of how the adapted Laplacian smoothing is applied.

The grid generator employs a hierarchical set of rules (CMG, 2023) to determine whether a grid block is treated as pinched-out, allowing vertical fluid flow, or as completely inactive. The guideline is presented below:

1. Pinch-out flag: If the block has a value of zero in the pinch-out input file, it is treated as pinched-out, allowing vertical fluid communication through its volume.

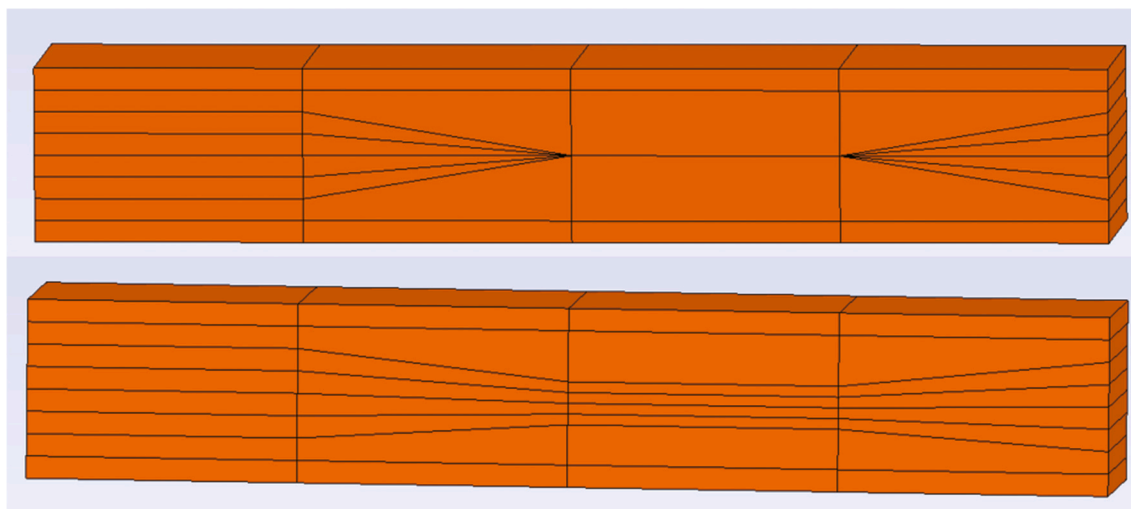


Fig. 2. Adapted Laplacian smoothing.

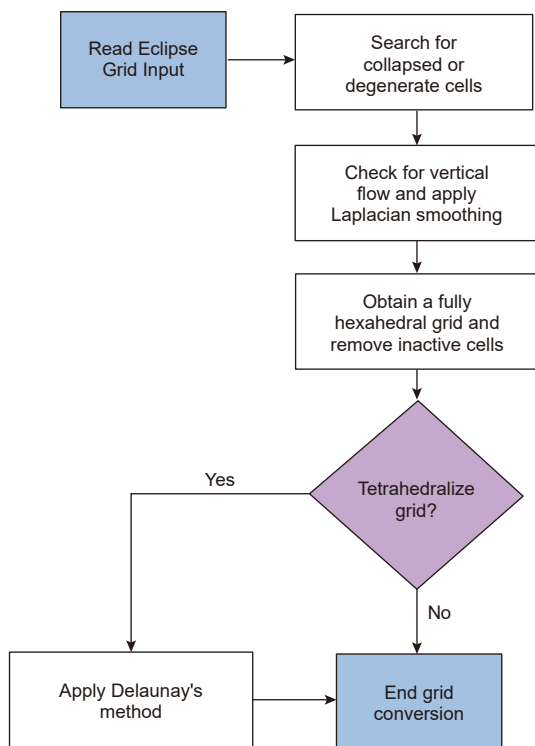


Fig. 3. Flow chart for unstructured grid conversion for the EbFVM.

2. Inactive flag: If the block is flagged as inactive with a zero in the inactive cells array, it is treated as completely inactive, blocking all fluid flow.
3. Near-zero thickness: If the block has near-zero vertical thickness, it is treated as pinched-out, allowing vertical flow.
4. Zero-value properties: If the block has zero pore volume or permeability, it is considered inactive by default, preventing any fluid flow.

Reservoir geometries commonly exhibit large areal extents combined with thin vertical layering. In this context, challenges related to the aspect ratio of grid blocks may arise. Tetrahedralization algorithms can fail to generate valid elements in regions with fine vertical resolution. To mitigate this issue, Z coordinates are scaled by a user-defined factor, improving element quality during mesh generation. After completion of the tetrahedralization process, the coordinates are rescaled to their original dimensions to preserve geometric fidelity.

Once the structured grid is evaluated, inactive cells are identified and removed from the hexahedral mesh. At this point of grid generation, it is possible to convert the mesh directly to a hexahedral geometry or to a tetrahedral grid through triangulation and tetrahedralization using Delaunay's method (Si, 2015). To simplify the understanding of the grid conversion process, Fig. 3 presents a flow chart of the algorithm adopted here.

To coarsen the mesh and upscale reservoir properties, the following approach is adopted. A user-defined 3D hexahedral clustering algorithm scans the entire domain and classifies it into three distinct regions: refinement, transition, and coarsening zones. The size of each cluster is determined by the number of Corner Point blocks and their corresponding (i, j, k) indices, rather than their actual geometric dimensions. This index-based definition simplifies the identification of regions for selective upscaling. Refinement zones correspond to areas of interest that must retain the original level of resolution. In the current implementation of

the grid generator, three types of regions are automatically designated as refinement zones: vicinity of wells, where flow behavior is highly sensitive to grid resolution; areas containing non-active cells, to maintain specific characteristics of the reservoir; and regions exhibiting high permeability heterogeneity. The latter is quantified using Dykstra-Parsons coefficient (Dykstra and Parsons, 1950), which provides a statistical measure of heterogeneity within a given cluster. The Dykstra-Parsons (DP) coefficient is calculated for a given direction as

$$DP = 1 - \exp \left[- \sqrt{\ln \left(K_A / K_H \right)} \right] \quad (9)$$

where K_A and K_H are respectively the arithmetic and harmonic means of all grid blocks within a cluster. For every user-defined cluster, the DP coefficient is computed separately, corresponding to the x, y, and z directions of the reservoir model. If any of the three directional coefficients exceed the specified threshold, the corresponding cluster is automatically flagged as a refinement zone.

Regions surrounding refinement zones are marked as transition zones. In the transition zone, vertices of the grid are adjusted to ensure a consistent interface between coarsened and refined regions. Only the bounding vertices of the scanning cluster are preserved, and then new vertices are inserted within the transition region, ensuring that the faces of coarse blocks align consistently with those of the neighboring fine-scale grid blocks. This is done by initially triangulating the faces of refinement and coarsening clusters. In transition clusters, faces of the hexahedral are triangulated by joining the vertices of triangles from both regions.

Coarsened zones are adapted by defining the eight vertices that define the hexahedral cluster. After coarsening the mesh, the same procedure of triangulation and tetrahedralization is adopted to obtain the final grid. Fig. 4 presents an example of grid conversion with upscaling with all three types of refinement zones. In this example, a $15 \times 15 \times 1$ hexahedral grid is evaluated by $3 \times 3 \times 1$ clusters, dividing the mesh into three distinct zones. Grid is adapted to generate the unstructured tetrahedral mesh. The clustering process is controlled by the DP threshold, the presence of inactive cells, and well perforations. Altogether, these parameters define whether a cluster is preserved or coarsened.

After clustering and adaptation of the vertices of the grid, the resulting geometry is evaluated for consistency before mesh generation. If the geometry is valid, the grid is directly tetrahedralized. However, when invalid configurations are detected or the tetrahedralization algorithm is not capable of delivering a concise geometry, additional processing is required to ensure mesh conformity and element quality. Due to the non-orthogonality of reservoir grid blocks, arising from depth differences between vertices, the generation of transition clusters can lead to overlapping surfaces. Surfaces generated in transition clusters may lose their resolution, causing intersections between faces within refinement zones. To deal with this issue, Steiner points are used (Bern and Eppstein, 1992). Steiner points are auxiliary vertices that are not part of the original geometry but are inserted during the meshing process to improve element quality or to solve inconsistencies in the geometry. Steiner points may be used to either refine triangles or to resolve face intersections. Fig. 5 presents an example of grid processing with Steiner points. In this case, the transition region is coarsened by maintaining the bounding vertices of the cluster. This adaptation results in overlapping surfaces between refinement and transition regions. A Steiner point is inserted in the overlapping surface to fix this issue, and the valid resulting geometry may be triangulated to obtain the final mesh.

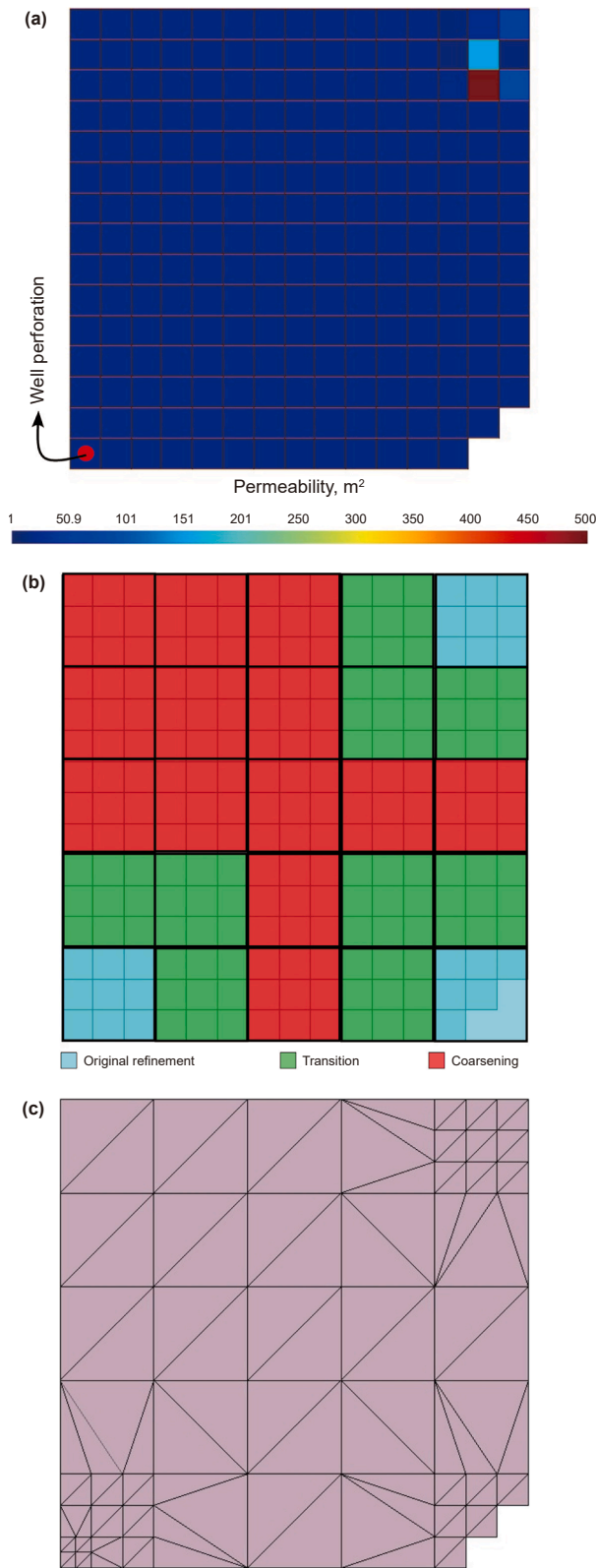


Fig. 4. Example of grid processing with clustering upscale: (a) Original structured grid; (b) division of zones in the clustering process; and (c) final unstructured grid.

Permeability undergoes an upscaling process inside the hexahedral cluster with a modified Cardwell-Parsons technique (Renard and de Marsily, 1997), given by

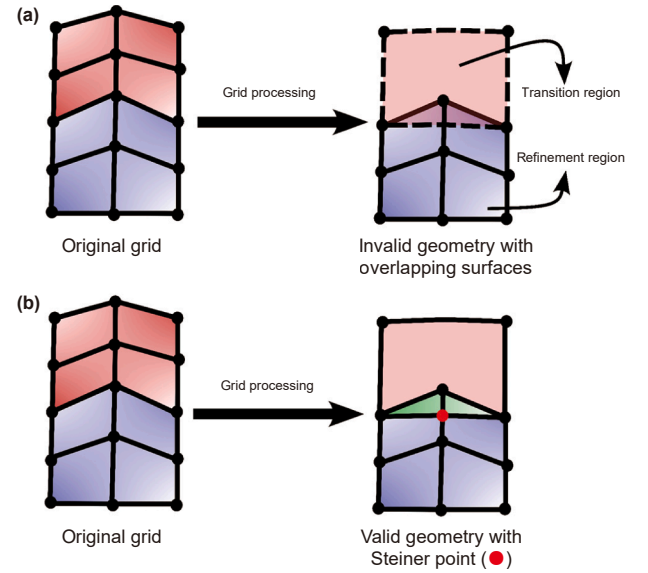


Fig. 5. Example of grid preprocessing: (a) with invalid geometry; and (b) valid geometry with the use of Steiner points.

$$k_{\text{ups}}^- = \frac{N_i}{N_j N_k} \sum_{j,k} \left(\sum_i \left(k_x^{i,j,k} \right)^{-1} \right)^{-1} \quad (10)$$

$$k_{\text{ups}}^+ = \frac{N_i}{N_j N_k} \left(\sum_i \left(\sum_{j,k} \left(k_x^{i,j,k} \right)^{-1} \right)^{-1} \right)^{-1} \quad (11)$$

$$k_{\text{ups}} = \sqrt{k_{\text{ups}}^+ k_{\text{ups}}^-} \quad (12)$$

where k_{ups}^- is the lower bound permeability, given by the arithmetic mean of the harmonic mean for a given direction, k_{ups}^+ is the upper bound permeability calculated as the harmonic mean of the arithmetic mean and k_{ups} is the upscaled property. Parameters N_i , N_j , and N_k are the number of grid blocks in each direction of the cluster. Upscaled porosity is calculated using a weighted volumetric mean inside the user-defined clusters. The grid converter then generates a tetrahedralized grid with upscaled properties for the EbFVM.

Adaptive mesh refinement (AMR) techniques (Cant et al., 2022; Hatami and Walsh, 2023; Mesri et al., 2013; Williamschen and Groth, 2013) represent another approach in the literature that optimizes grid resolution in key flow regions. Unlike AMR, which dynamically refines or coarsens cells during runtime based on error indicators or flow gradients, the method proposed in this work applies a static coarsening procedure prior to simulation, focusing on efficiency and geometric consistency rather than adaptive refinement. While AMR provides greater adaptability, it also introduces significant algorithmic complexity. The proposed method offers a simpler and efficient alternative, which can be readily used with existing simulators. Moreover, the proposed approach can be also integrated with AMR strategies in future works to combine static upscaling with dynamic refinement. The whole algorithm of upscaling discussed in this section is illustrated in Figs. 6 and 7.

6. Results and discussion

In this section, the results of five case studies are presented. The first two cases are designed for the verification of the grid

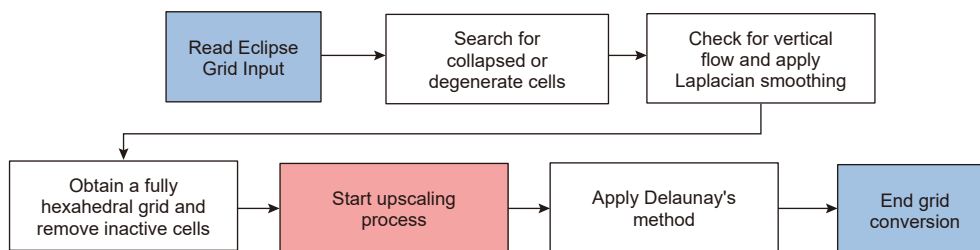


Fig. 6. General flow chart for grid generation with upscaling.

generator using real reservoir geometries and the validation of the unstructured numerical formulation. The last three cases aim to evaluate the EbFVM's performance in three different scenarios with the developed upscaling technique. Herein, two fluids are used throughout the case studies: a 2Comp and an 8Comp. The compositions and thermodynamic properties of the in-place fluids are presented in Tables 1–4.

Simulations were performed on the supercomputer Santos Dumont at the LNCC (National Laboratory of Scientific Computation). The LNCC supercomputer contains 1134 nodes, and

simulations were performed on one of the 504 thin nodes (B710). Each node has 2 CPU Intel Xeon E5-2695v2 Ivy Bridge (12c @2.4 GHz) and 64 GB RAM. Except for the case study in Section 6.4, all the other case studies are evaluated using an IMPEC formulation. The present work uses the GMRES (Saad and Schultz, 1986) solver with ILU(0) preconditioning (Meijerink and van der Vorst, 1977). Convergence tolerances for FI and IMPEC formulations are presented in Tables 5 and 6.

6.1. Verification case: UNISIM-I

The first case study presents a homogeneous reservoir model based on the UNISIM-I benchmark. It is a benchmark made

Table 1
Initial reservoir composition of 2Comp.

Components	Reservoir fluid composition
C ₁	0.2
NC ₁₆	0.8

Table 2
Thermodynamic properties of 2Comp.

Components	Critical pressure, kPa	Critical temperature, K	Critical volume, m ³ /mol	Acentric factor	Volume shift
C ₁	4601.5	190.61	0.008961	0.0255	0.0
NC ₁₆	1738.6	734.67	0.7327	0.683728	0.0

Table 3
Initial reservoir composition and injection composition of 8Comp.

Components	Reservoir fluid composition	Injection fluid composition
CO ₂	0.10	0.12
PC1	0.50	0.8
PC2	0.12	0.05
PC3	0.06	0.02
PC4	0.07	0.01
PC5	0.06	0.0
PC6	0.06	0.0
PC7	0.03	0.0

Table 4
Thermodynamic properties of 8Comp.

Components	Critical pressure, kPa	Critical temperature, K	Critical volume, m ³ /mol	Acentric factor	Volume shift
CO ₂	7376.0	304.2	0.094	0.225	0.257
PC1	4620.0	198.8	0.098	0.0098	−0.234
PC2	4630.5	343.7	0.171	0.123	−0.158
PC3	3597.0	545.15	0.305	0.199	−0.079
PC4	2735.8	677.91	0.507	0.465	−0.013
PC5	1925.2	785.36	0.793	0.698	0.025
PC6	1226.1	800.00	1.370	1.195	0.087
PC7	729.5	1064.10	2.120	1.40	0.165

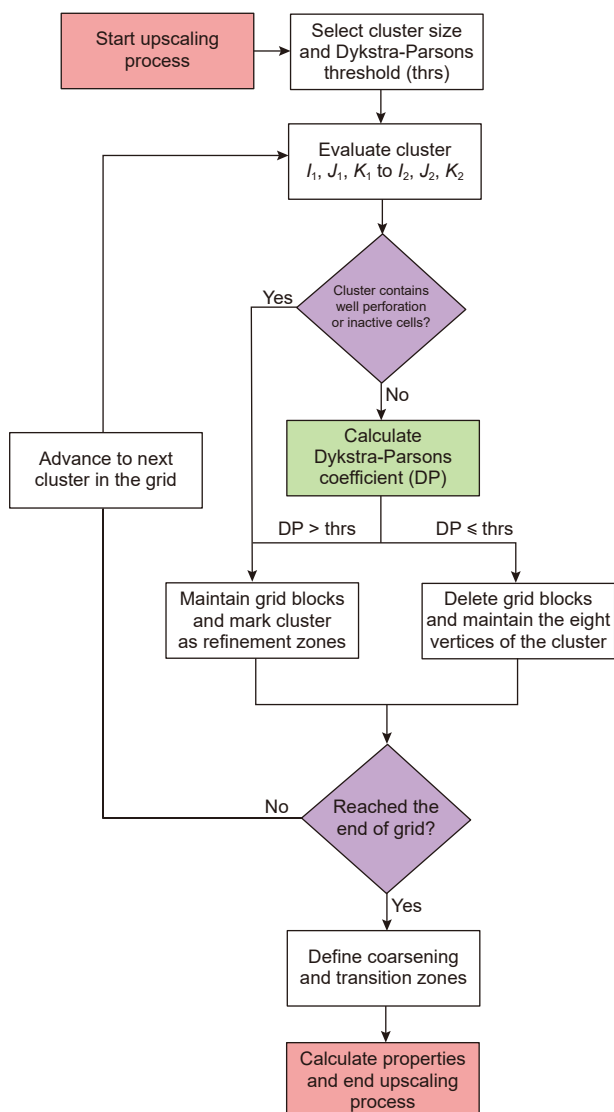


Fig. 7. Flow chart for the upscaling with clustering algorithm.

Table 5
FI convergence parameters.

Tolerance	Value
Residual pressure	1×10^{-4}
Pressure variation	0.1
Molar residual	1×10^{-4}
Number of moles variation	0.1
Maximum number Newton iterations	10

Table 6
IMPEC and FI linear solver convergence parameters.

Parameter	Value
Relative convergence tolerance	1×10^{-7}
Absolute convergence tolerance	1×10^{-30}
Divergence tolerance	100,000
Maximum number of iterations	1000

available by UNICAMP that uses real data from the Namorado Field in the Brazilian Campos Basin. More details regarding the UNISIM-I benchmark can be found in (Avansi and Schiozer, 2015). The reservoir grid contains 93,960 grid blocks, of which only 38,317 are active. Fig. 8 presents the geometry of the UNISIM-I grid model.

The results are presented in terms of production profiles. The structured formulation and the unstructured formulations implemented in UTCOMPRS are verified and compared to a commercial simulator widely used in the industry. The primary objective of this analysis is to demonstrate the capability of EbFVM to produce reliable solutions in comparison to traditional numerical approaches.

For this case, the structured grid is not converted into a hexahedral grid for the EbFVM. The UNISIM-I grid contains dislocated grid blocks in the vertical direction, which causes the appearance of hanging nodes between adjacent cells. Due to the cell-vertex nature of the EbFVM, control volumes are constructed around the grid nodes rather than the cell centers. In this context, a node on the edge or face of a neighboring element would result in a non-communicating interface. To overcome this issue, hexahedrons from the structured grid are preprocessed and converted into tetrahedrons. The use of tetrahedrons is particularly advantageous because tetrahedralization algorithms can generate elements that align all nodal connections.

The newly converted grid has 40,519 nodes with 215,201 elements. Each hexahedron, on average, is divided into six tetrahedrons, which explains the increase in the number of elements. Fig. 9 presents the adapted tetrahedron grid of the UNISIM-I benchmark.

For the present case, 25 wells have been completed, comprising 11 injection wells and 14 production wells. The present case uses the 8Comp fluid, and Table 7 presents the reservoir properties and operational constraints for the wells.

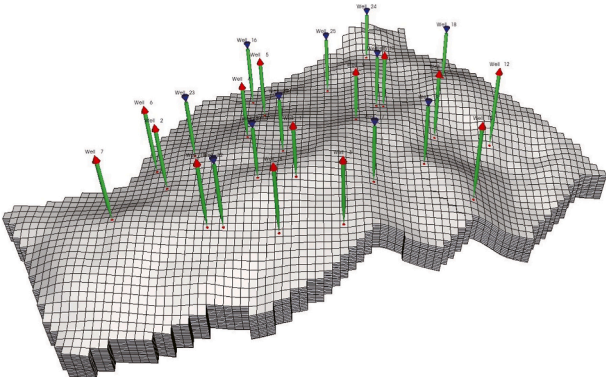


Fig. 8. UNISIM-I corner point grid.

Fig. 10 presents the production profile obtained for this case study. As observed, both structured and unstructured formulations implemented into the UTCOMPRS yielded reliable numerical solutions and showed good agreement with the commercial simulator. It is essential to highlight some notable differences between structured and unstructured formulations. Despite having the same number of control volumes, the unstructured formulation using tetrahedron has a much larger number of elements than the hexahedron; as we mentioned previously, each hexahedron is divided into six tetrahedral elements. Such a division will result in a significantly higher number of IPs around each control volume (node) compared to the hexahedral element.

6.2. Verification case: Proxy reservoir

The second case study uses a Proxy reservoir made available by PETROBRAS, which was developed to replicate a real Brazilian Pre-Salt reservoir. The structured Proxy reservoir grid contains 1,461,504 grid blocks, of which 767,336 are active. For the unstructured formulation, the Proxy model is directly converted into a hexahedral grid. This approach results in a mesh with the same number of elements and 800,513 nodes. Fig. 11 presents the geometry of the reservoir and configuration of well perforations. In total, 31 production wells and 29 injection wells were completed. Table 8 presents the reservoir properties of the Proxy model and the operational constraints of the wells. Here, the 8Comp fluid is used.

Herein, heterogeneous porosity and permeability fields are incorporated to assess the impact of reservoir heterogeneity on oil and gas production profiles. Fig. 12 presents the permeability and porosity fields used in the present case. Areal permeability is the same as shown in Fig. 12, and the vertical permeability is 10% of the permeability in X and Y directions.

Fig. 13 presents production profiles for the heterogeneous reservoir model. Again, UTCOMPRS presented a good agreement with the commercial simulator for both structured and unstructured formulations.

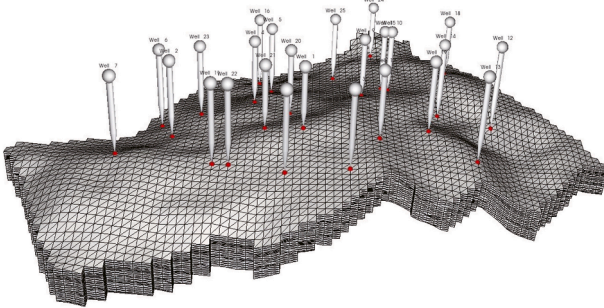


Fig. 9. Adapted UNISIM-I tetrahedral grid.

Table 7
Properties of UNISIM-I verification case.

Property	Value
Initial pressure	34,476 kPa
Temperature	310.93 K
Water saturation	0.30
Porosity	0.15
Permeability (i, j, k)	$1.974 \times 10^{-13} \text{ m}^2$, $1.974 \times 10^{-13} \text{ m}^2$, $1.974 \times 10^{-14} \text{ m}^2$
Production well BHP	33,650.3 kPa
Gas injection rate	141,584 m ³ /d

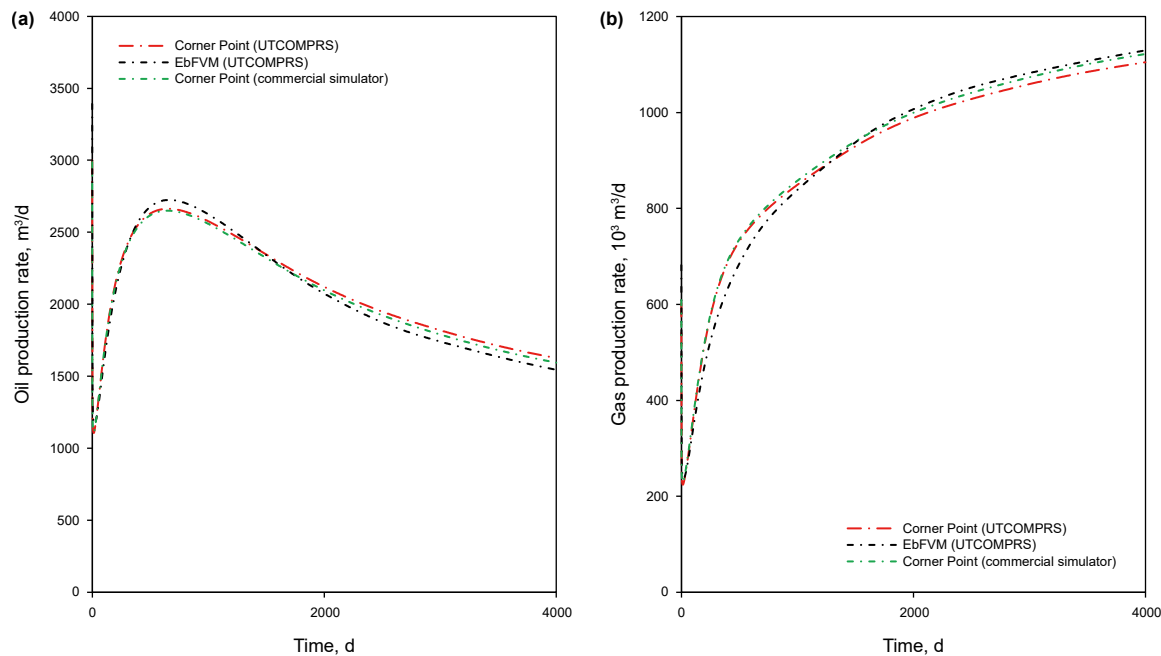


Fig. 10. UNISIM-I model: (a) oil production curves; (b) gas production curves.

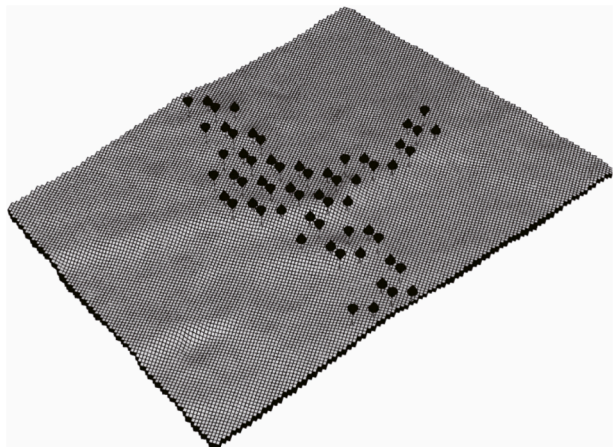


Fig. 11. Proxy model reservoir grid.

Table 8
Properties of Proxy verification case.

Property	Value
Initial pressure	50,000 kPa
Temperature	353.15 K
Water saturation	0.30
Production well BHP	47,579 kPa
Gas injection rate	1,415,840 m ³ /d

6.3. Upscaling of Sleipner’s Utsira L7

Previous case studies showed that the unstructured formulation can provide reliable numerical solutions for real reservoir grids. To investigate the impact of grid resolution on simulation accuracy and computational performance, Layer 7 (L7) of the Utsira formation is coarsened using different clustering dimensions. The Sleipner CO₂ storage project (Singh et al., 2010;

Sleipner Group, 2019; Zweigel et al., 2001) has become a relevant benchmark case for validating simulation strategies in carbon capture and storage (CCS). This study focuses on Layer 7 of the Utsira Formation, a region characterized by high porosity and homogeneity, making it suitable for testing grid coarsening techniques under simplified geological conditions. Since the aim is to evaluate the effect of grid resolution on pressure build-up of the reservoir, trapping mechanisms will be neglected. Fig. 14 presents the grid used in this case study. For better visualization, the aspect ratio of the grid is set to $X/Z = 1/10$. The reservoir geometry contains 120,832 grid blocks.

A DP threshold of 100% is used. Due to permeability homogeneity, only the region around the injection well will maintain its original level of refinement. Grid coarsening is performed using hexahedral clustering, with cell groupings of $2 \times 2 \times 2$, $3 \times 3 \times 3$, and $8 \times 8 \times 8$. Reservoir properties and operational constraints are presented in Table 9.

Fig. 15 presents the coarsened grids and the resulting number of vertices and elements.

Fig. 16 presents the average reservoir pressure for different coarsened grids with the unstructured formulation, and the original grid, using the Corner Point approach. All formulations presented comparable results, even with the loss of resolution in grid coarsening. Table 10 presents CPU time, number of time-steps and material balance error at 3200 days of simulations. Material balance error provides a numerical estimate of the discrepancy between the simulated mass inflows, outflows, and storage changes in the reservoir system over time. It helps to identify numerical inaccuracies or inconsistencies in the solution. Generally, values lower than 1% are desirable. All formulations presented acceptable values of material balance error, and as expected, the original grid presented the lowest value. Although the $2 \times 2 \times 2$ clustering reduces the total number of control volumes and elements relative to the original structured grid, lowering memory requirements, it resulted in comparable simulation times. While fewer elements reduce the time needed to solve the linear system, the assembly of the matrix and the calculation of advective terms become more computationally demanding due to the complexity of the

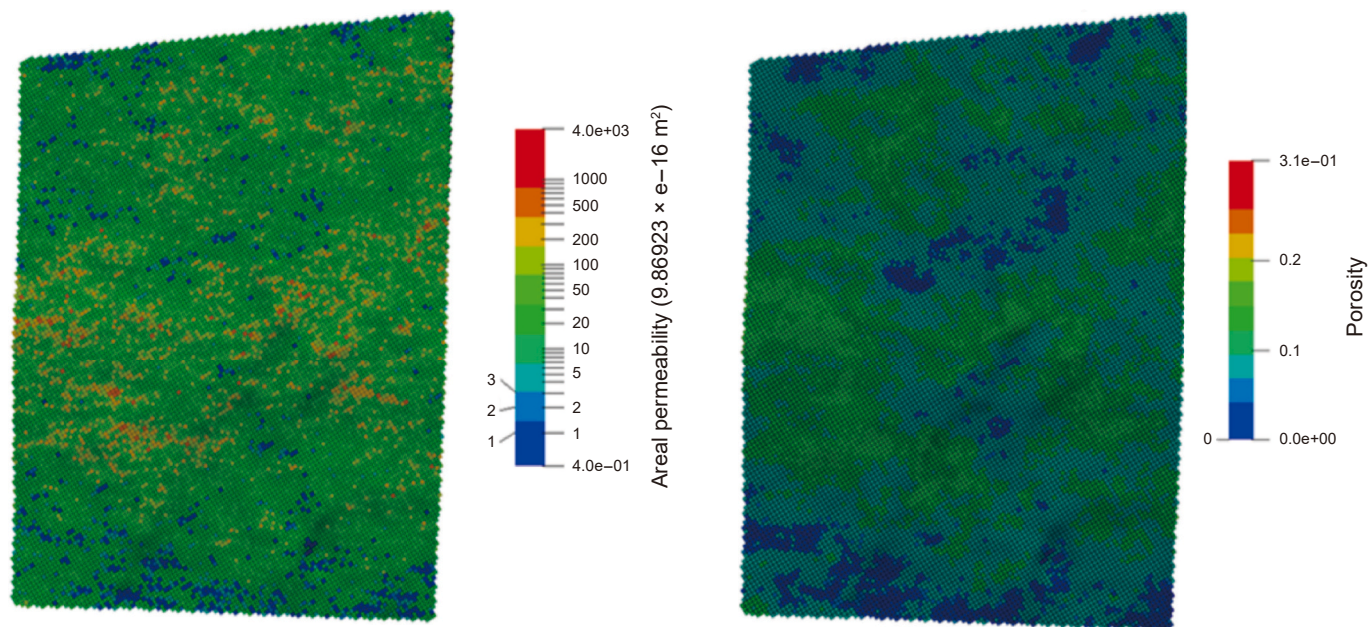


Fig. 12. Top layer permeability and porosity fields of the Proxy model.

unstructured formulation. To achieve the desired CPU time optimization, the grid must be further coarsened, as observed in the $3 \times 3 \times 3$ and $8 \times 8 \times 8$ clustering.

Linear solver and computing times are reported in Table 11. They respectively represent the time spent solving the Jacobian system and the time required for initialization, property calculation, matrix assembly, and output writing. The results show that the EbFVM reduced linear solver time compared to the Corner Point model due to the smaller number of control volumes and a reduced linear solver system. However, the $2 \times 2 \times 2$ coarsened case showed higher total computing time because the unstructured formulation adds overhead from complex data handling and

connectivity management. Despite this, the overall CPU time remained lower than that of the Corner Point formulation. Fig. 17 presents the speed-up curves for this case. They represent the relative improvement in computational time compared to the Corner Point model.

Table 12 presents the peak memory footprint and memory ratio for the different grid coarsening levels compared to the Corner Point formulation. The peak memory footprint is the maximum amount of RAM used by the simulation during execution. Memory ratio is defined as the peak memory footprint of the case divided by the Corner Point reference footprint. Despite presenting fewer elements, the $2 \times 2 \times 2$ coarsened grid presents memory

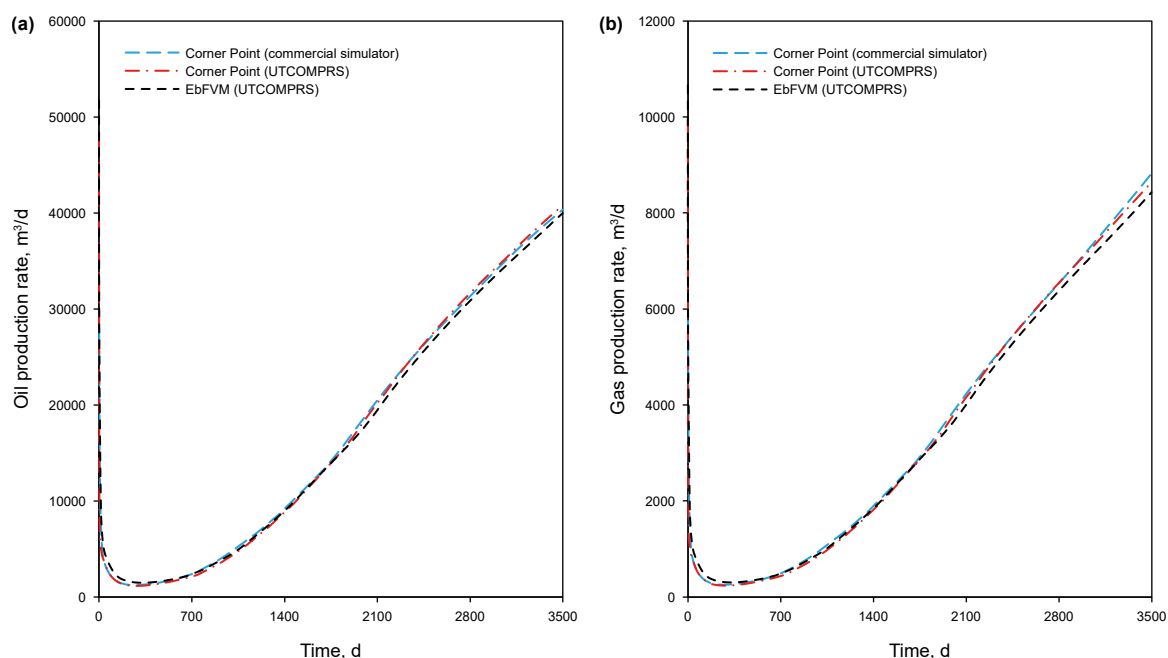


Fig. 13. Oil (a) and gas (b) production curves for the Proxy model.



Fig. 14. Reservoir grid of Utsira L7.

Table 9
Properties of Utsira L7 upscaling case.

Property	Value
$N_x/N_y/N_z$	64/118/16
$D_x/D_y/D_z$	15.24 m/15.24 m/0.6096 m
Initial pressure	10,342 kPa
Temperature	310.93 K
Water saturation	1.0
Porosity	0.34
Permeability (i, j, k)	$1.9738 \times 10^{-12} \text{ m}^2$, $1.9738 \times 10^{-12} \text{ m}^2$, $1.9738 \times 10^{-14} \text{ m}^2$
CO ₂ injection rate	28,316.8 m ³ /d

requirement comparable to the Corner Point model, as the unstructured formulation requires additional storage for auxiliary vectors and connectivity.

Although the $8 \times 8 \times 8$ clustering achieved the shortest simulation time, memory consumption increased due to challenges in maintaining smooth transitions between refinement and coarsening zones during the upscaling process. To preserve mesh quality, the grid conversion process introduced Steiner points. This step ensures conformity between nodes but also increases the number of neighboring elements. The increase in connectivity leads to greater memory allocation for auxiliary vectors associated with these connections. The $3 \times 3 \times 3$ clustering provided the best computational performance, both in terms of CPU time and memory requirement. Therefore, while larger clusters can reduce simulation time by decreasing the number of control volumes, they may also increase memory requirements due to the additional geometric complexity to maintain mesh quality.

6.4. Upscaling of SPE10 benchmark

The fourth case study presented in this section is based on Model 2 of the SPE10 benchmark. Herein, an adapted version of the SPE10 (Christie and Blunt, 2001) is used to verify the effect of the DP coefficient in a heterogeneous medium. For this case, only the Tarbert formation is considered. The adapted model contains 462,000 elements. This case follows the same well layout employed on the original SPE10 benchmark, where a water injection well is completed in the center of the reservoir, and four production wells are completed in the corners. The present case uses the 2Comp fluid, trying to reproduce a black oil fluid from the original benchmark. Table 13 presents the reservoir properties and

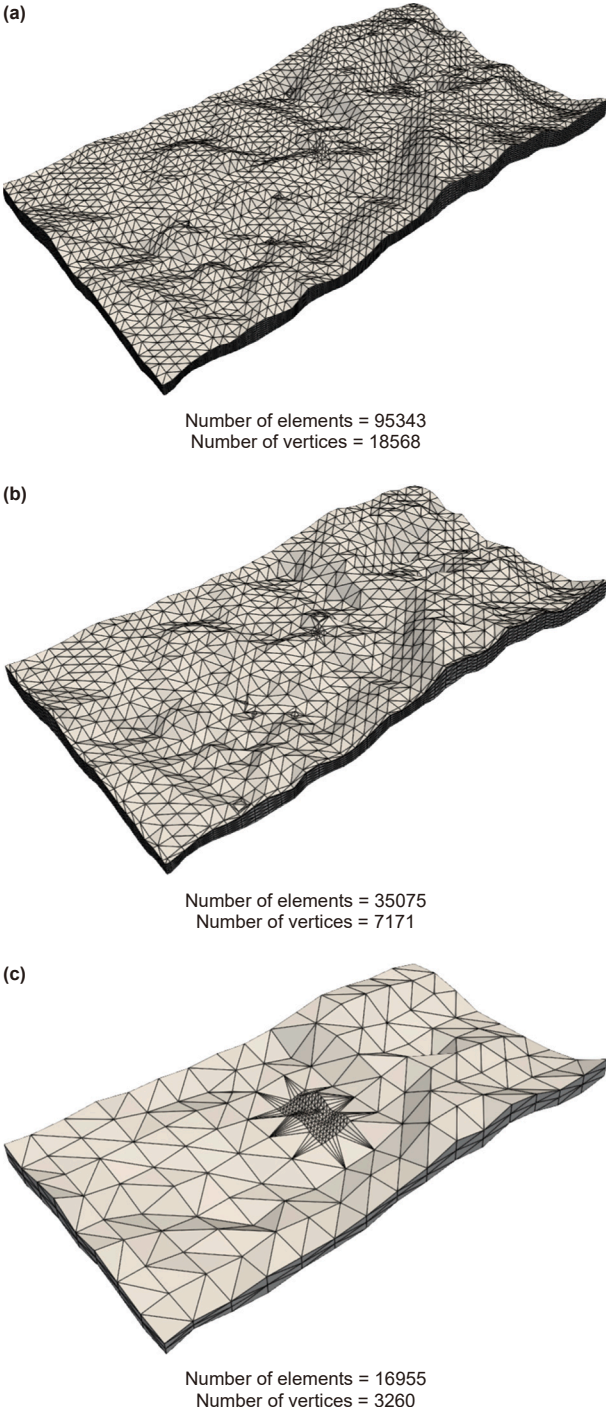


Fig. 15. Coarsened Utsira L7 grids for: (a) $2 \times 2 \times 2$; (b) $3 \times 3 \times 3$; (c) $8 \times 8 \times 8$ clusters.

the well operational constraints. This case study uses an FI approach for both structured and unstructured formulations. All simulations were performed using the same numerical and time-step selection parameters.

Two cluster configurations with different values of DP threshold were evaluated. Table 14 presents the clustering sizes, DP threshold values, number of control volumes (vertices) and elements resulting from the application of grid coarsening algorithm. It is important to reinforce that DP is calculated within a single cluster. If a cluster is marked as coarsened or transition

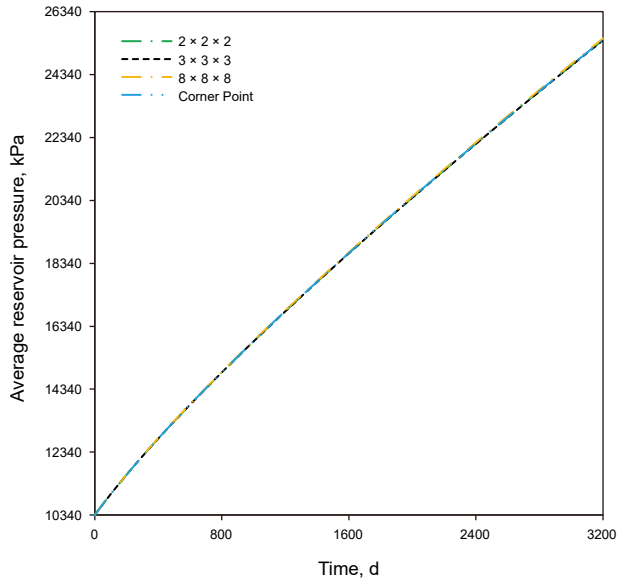


Fig. 16. Average reservoir pressure for Utsira L7.

zones, internal grid blocks of the original mesh will be used to calculate adapted properties.

As expected, all grids presented a considerable reduction in the number of control volumes, particularly at higher coefficient values. However, a notable result is observed: for the coefficient of 85%, the number of elements increases compared to the original structured grid. This increase is attributed to the behavior of the tetrahedralization algorithm, which divides each hexahedron into multiple tetrahedra. Additionally, when comparing larger cluster sizes ($2 \times 4 \times 7$) to smaller ones ($2 \times 4 \times 5$) at the same DP coefficient, it is observed that larger cluster sizes may produce more elements and vertices, contrary to the expectation of higher coarsening. This occurs because larger clusters may overlap with more heterogeneous features, causing additional refinement regions to be flagged. Upscaled grids are presented in Fig. 18. Areal permeability fields for the original case and upscaled permeability fields are shown in Fig. 19. Permeability in the vertical direction is set to 30% of the areal permeability. Since the DP coefficient quantifies permeability heterogeneity rather than magnitude, the uniform anisotropy defined by $K_X = K_Y$ and $K_Z = 0.3K_X$ does not

Table 10

CPU time, number of time-steps and maximum material balance error for Utsira L7.

Formulation	CPU time, s	Number of time-steps	Maximum material balance error, %
Corner Point	14,063	32,186	0.0001
Coarsened grid – $2 \times 2 \times 2$	13,466	32,438	0.002
Coarsened grid – $3 \times 3 \times 3$	4770	32,414	0.001
Coarsened grid – $8 \times 8 \times 8$	3659	32,460	0.006

Table 11

Linear solver time and computing time for the Utsira L7 case study.

Formulation	Linear solver time, s	Computing time, s	Solver time/Total time ratio
Corner Point	2703.0	11,360.0	19.2%
Coarsened grid – $2 \times 2 \times 2$	745.0	12,701.0	5.5%
Coarsened grid – $3 \times 3 \times 3$	284.0	4486.0	5.9%
Coarsened grid – $8 \times 8 \times 8$	191.0	3467.0	5.2%

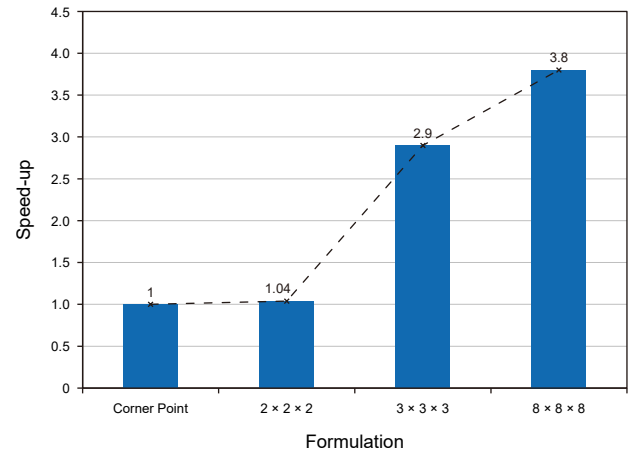


Fig. 17. Speed-up for Utsira L7 upscaling.

Table 12

Memory footprint for Utsira L7 case study.

Formulation	Peak memory footprint, Gb	Memory ratio
Corner Point	1.3	1.0
Coarsened grid – $2 \times 2 \times 2$	1.3	1.0
Coarsened grid – $3 \times 3 \times 3$	0.57	0.43
Coarsened grid – $8 \times 8 \times 8$	1.4	1.07

Table 13

Properties of SPE10 Tarbert upscaling case.

Property	Value
$N_x/N_y/N_z$	60/220/35
$D_x/D_y/D_z$	6.096 m/3.048 m/1.524 m
Initial pressure	41,368.6 kPa
Temperature	310.93 K
Water saturation	0.20
Porosity	0.30
Production well BHP	27,579 kPa
Water injection rate	794.94 m ³ /d
Maximum injection BHP	68,947.6 kPa

alter permeability variability within the cluster, leaving the coefficient unaffected in principal directions.

Fig. 20 presents oil production profiles and water cut for different upscaled grids and the original Tarbert formation with the structured formulation. All upscaled grids presented comparable solutions with the fine-scale model. Upscaling techniques may reduce the resolution of both geometric details and property fields. In the SPE10 benchmark, this leads to an increase in the

Table 14

Coarsened grids properties for Tarbert formation of SPE10 benchmark.

Clustering size	DP coefficient threshold	Number of vertices	Number of elements
$2 \times 4 \times 5$	85%	98,383	542,702
$2 \times 4 \times 5$	87.5%	59,304	321,193
$2 \times 4 \times 5$	90%	36,289	191,006
$2 \times 4 \times 5$	92.5%	26,086	132,456
$2 \times 4 \times 5$	95%	21,749	108,465
$2 \times 4 \times 7$	85%	124,566	697,219
$2 \times 4 \times 7$	87.5%	79,318	438,080
$2 \times 4 \times 7$	90%	50,909	276,157
$2 \times 4 \times 7$	92.5%	32,445	169,661
$2 \times 4 \times 7$	95%	20,570	101,554

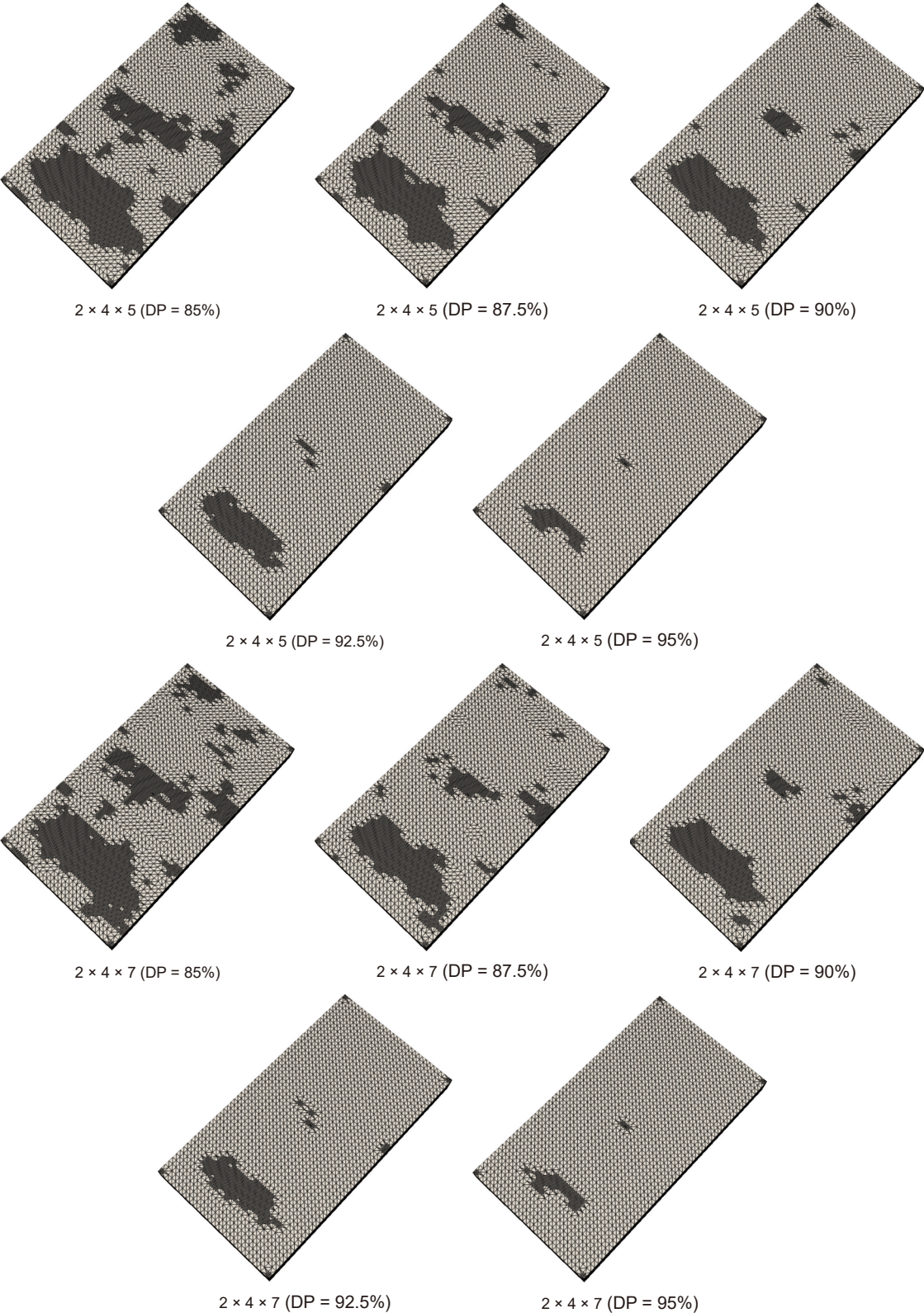


Fig. 18. Coarsened grids for SPE10 Tarbert.

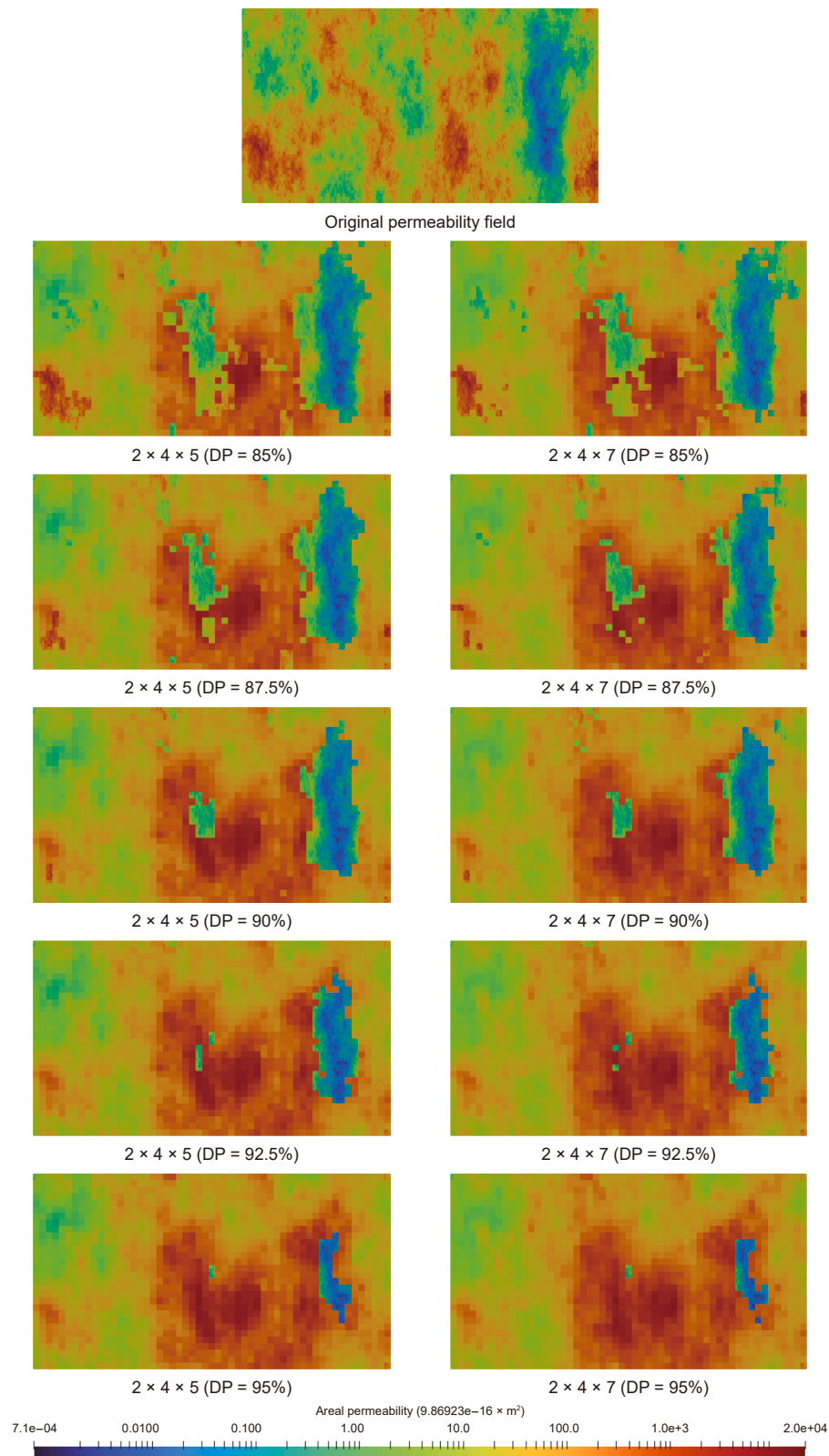


Fig. 19. Upscaled permeabilities for SPE10 Tarbert.

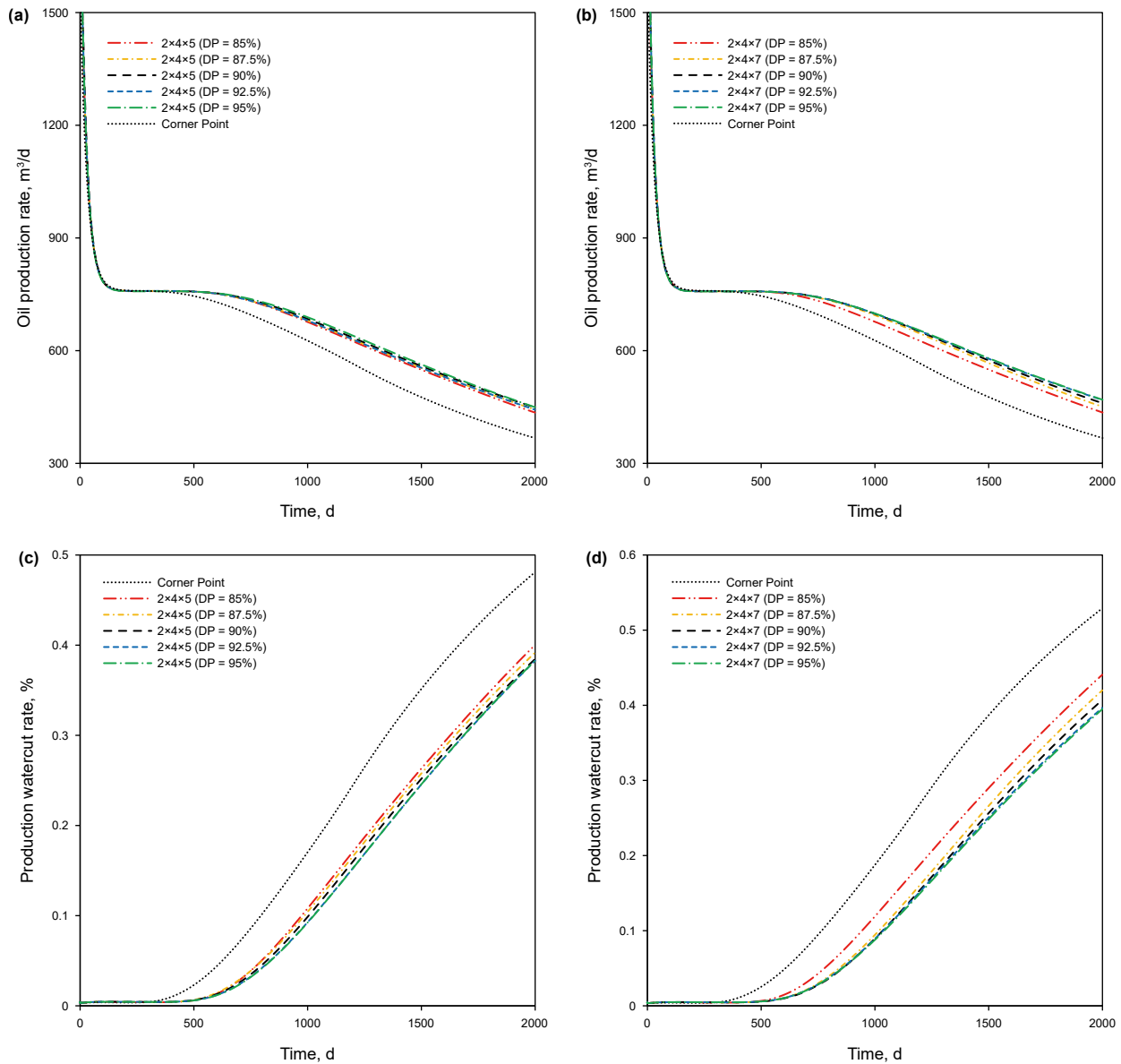


Fig. 20. Oil production and water cut curves for SPE10 Tarbert with: (a), (c) $2 \times 4 \times 5$ clustering; and (b), (d) $2 \times 4 \times 7$ clustering.

average value of the permeability field as observed in Fig. 19. The use of the Cardwell-Parsons method increases the average effective permeability, resulting in higher oil production rates in the coarsened models compared to the fine-scale. The resulting

effective permeability field improves intercell flow communication, leading to higher flow rates compared to the fine-scale model. Table 15 presents the number of time-steps, total CPU time, linear solver time, computing time, and solver time ratio for

Table 15

CPU time analysis and number of time-steps for the Tarbert formation of the SPE10 benchmark.

Formulation	Number of time-steps	Total CPU time, s	Linear solver time, s	Computing time, s	Solver time/Total time ratio
Corner Point	947	348,381.82	329,735.01	18,646.81	94.4%
$2 \times 4 \times 5$ (DP = 85%)	858	118,427.33	88,782.76	29,644.57	74.9%
$2 \times 4 \times 5$ (DP = 87.5%)	858	44,419.40	31,173.02	13,246.35	70.1%
$2 \times 4 \times 5$ (DP = 90%)	843	30,511.91	18,911.92	11,599.99	61.9%
$2 \times 4 \times 5$ (DP = 92.5%)	839	15,370.91	8469.31	6901.60	55.1%
$2 \times 4 \times 5$ (DP = 95%)	836	11,768.33	5460.38	6307.94	46.4%
$2 \times 4 \times 7$ (DP = 85%)	853	185,965.86	141,027.65	44,938.28	75.0%
$2 \times 4 \times 7$ (DP = 87.5%)	871	75,340.91	54,844.80	20,496.20	78.0%
$2 \times 4 \times 7$ (DP = 90%)	886	53,545.45	35,129.09	18,416.36	65.6%
$2 \times 4 \times 7$ (DP = 92.5%)	899	21,744.70	14,478.59	7266.11	66.5%
$2 \times 4 \times 7$ (DP = 95%)	931	16,967.65	10,505.28	6462.36	61.9%

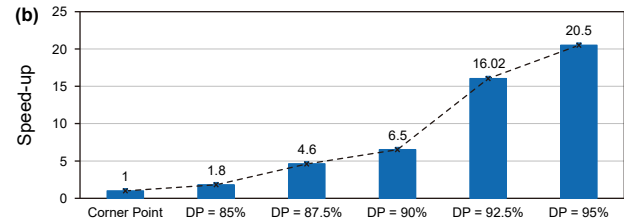
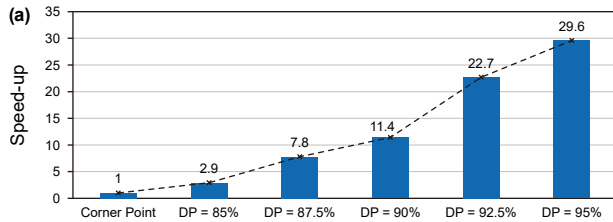


Fig. 21. Simulation time speed-up for: (a) $2 \times 4 \times 5$ clustering; and (b) $2 \times 4 \times 7$ clustering.

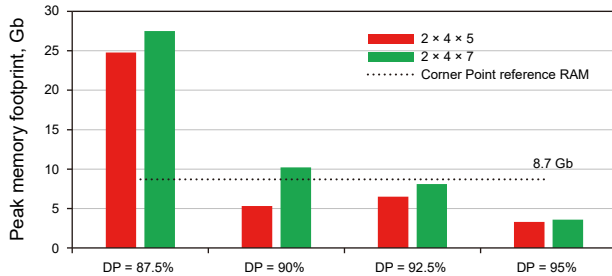


Fig. 22. Peak memory footprint for SPE10 Tarbert.

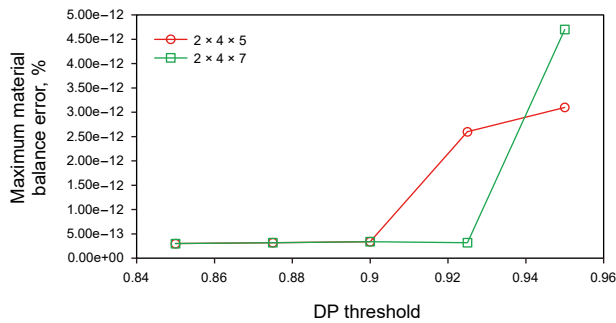


Fig. 23. Sensitivity plot of maximum material balance error as a function of DP threshold.

Table 16
Properties of Proxy upscaling case.

Property	Value
Initial pressure	50,000 kPa
Temperature	353.15 K
Water saturation	0.30
Production well BHP	47,578 kPa
Gas injection rate	12,831,680 m ³ /d

this case study. As discussed in Section 6.3, the EbFVM formulation reduced the linear solver time as the coarsening level increased, due to the smaller linear system to be solved. The time for solving the linear system/Total CPU Time ratio reduced from 94% for the Corner Point case to approximately 46% for the most coarsened grid. The total CPU time for the EbFVM presented lower results compared to the Corner Point formulation, reinforcing that the solver efficiency surpasses the added computational complexity.

The results presented in Figs. 21–23 illustrate the influence of DP thresholds on computational performance, material balance error, and memory usage for the present case study. The speed-up

plots show that the $2 \times 4 \times 5$ clustering achieved higher performance for all DP thresholds compared to the $2 \times 4 \times 7$ configuration. The sensitivity analysis of material balance error indicates that both cluster configurations maintain very low and similar errors for smaller DP thresholds. However, as the DP threshold increases, the error begins to rise as grids are coarsened. The peak memory footprint comparison highlights that mesh quality affects RAM usage. As previously discussed, larger clusters may require Steiner points to maintain mesh conformity between refinement and coarsening zones, which increases the number of neighboring connections and the associated memory allocation. Overall, in terms of computational efficiency, the results suggest that smaller clusters are more effective for handling a broader range of DP thresholds. In contrast, larger clusters tend to preserve more refinement zones, increasing the geometric complexity of the mesh and the RAM demand and CPU time.

6.5. Upscaling of Proxy reservoir

This case study utilizes the Proxy reservoir grid introduced in Section 6.2. Although the geometry looks like Cartesian, the structured grid includes inactive cells that result in diamond-shaped top and bottom surfaces. For that reason, when the clustering technique approaches the reservoir boundaries, it identifies these irregular edges as refinement regions. The case incorporates inactive cells, along with permeability and porosity heterogeneity. For this case, results are presented in terms of production profiles and CPU time. Table 16 presents the reservoir properties for the present case study. All reservoir properties defined in Section 6.2 are used here, except for an increased gas injection rate. This adjustment is done to enhance oil recovery while reducing the overall simulation time by limiting the number of days required for the analysis.

The grid converter was used to coarsen the mesh and upscale porosity and permeability fields. A DP coefficient threshold of 90% was applied. In this way, only regions around wells and highly heterogeneous zones maintained their original level of refinement. Fig. 24 presents the reservoir grids for the upscaled models of the Proxy reservoir. Two grids were generated for this case, using different cluster sizes. The grid with $2 \times 2 \times 2$ clusters contains 187,795 vertices and 988,481 elements, and the grid with the $3 \times 3 \times 3$ cluster presents 155,413 vertices and 794,660 elements. Again, properties will be evaluated inside the $2 \times 2 \times 2$ and $3 \times 3 \times 3$ cluster windows. The number of control volumes decreased drastically compared to the original number of grid blocks of the structured grid. Figs. 25 and 26 present the upscaled properties of the reservoir. Similar to the previous case study, DP coefficients are not affected by the choice of principal direction.

Production profiles for this case are presented in Fig. 27. As observed, the production curves for the upscaled models showed good agreement with the numerical solution obtained for the models with the original grid.

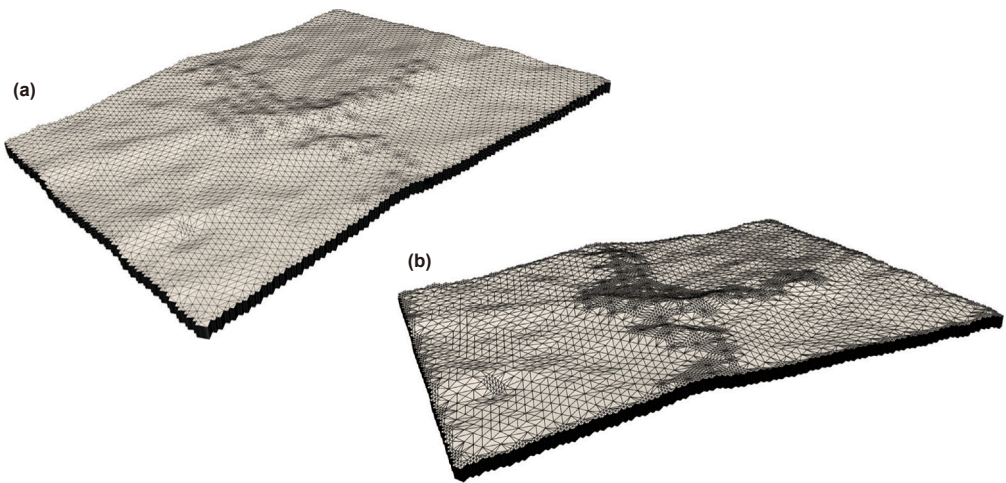


Fig. 24. Upscaled Proxy reservoir: (a) with $2 \times 2 \times 2$ cluster size; (b) with $3 \times 3 \times 3$ cluster size.

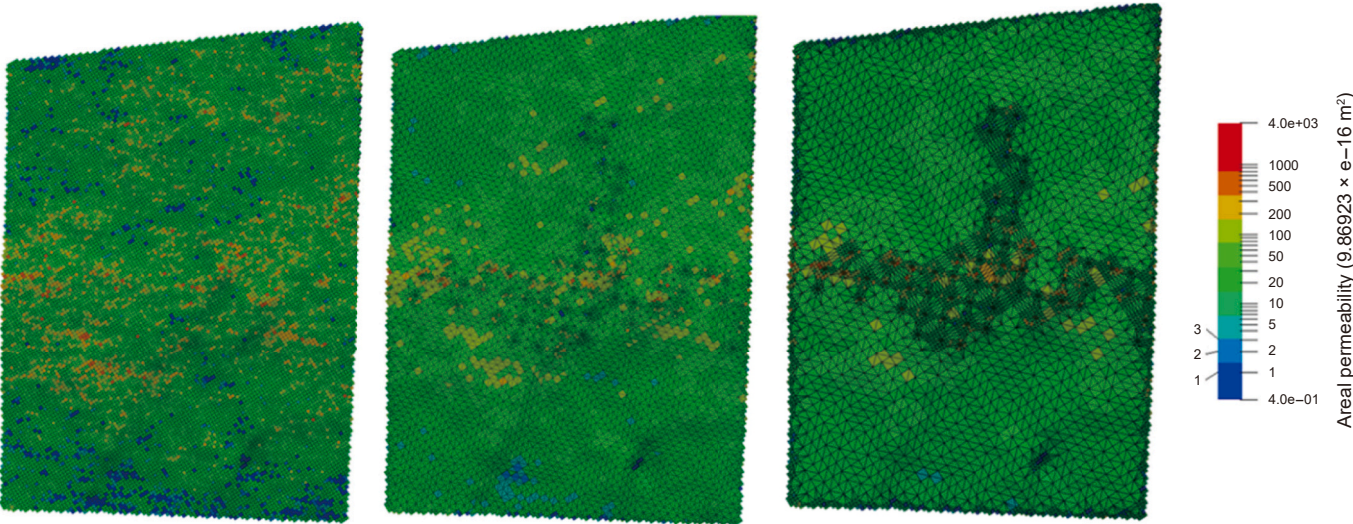


Fig. 25. Permeability fields in top layer with original grid, upscaled with $2 \times 2 \times 2$ cluster and upscaled with $3 \times 3 \times 3$ cluster.

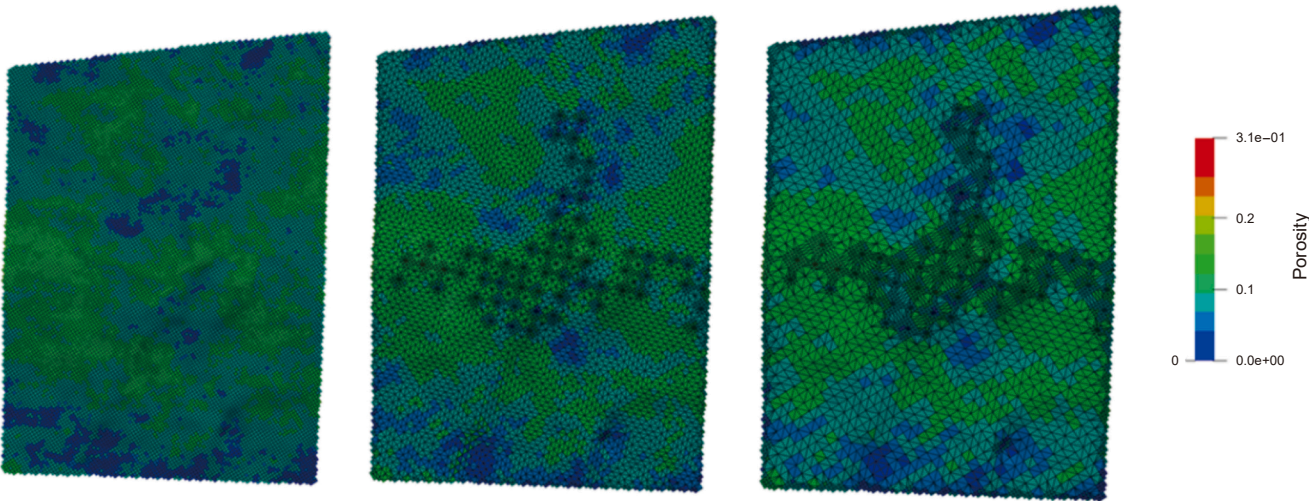


Fig. 26. Porosity fields in the top layer for the original grid, upscaled with $2 \times 2 \times 2$ cluster and upscaled with $3 \times 3 \times 3$ cluster.

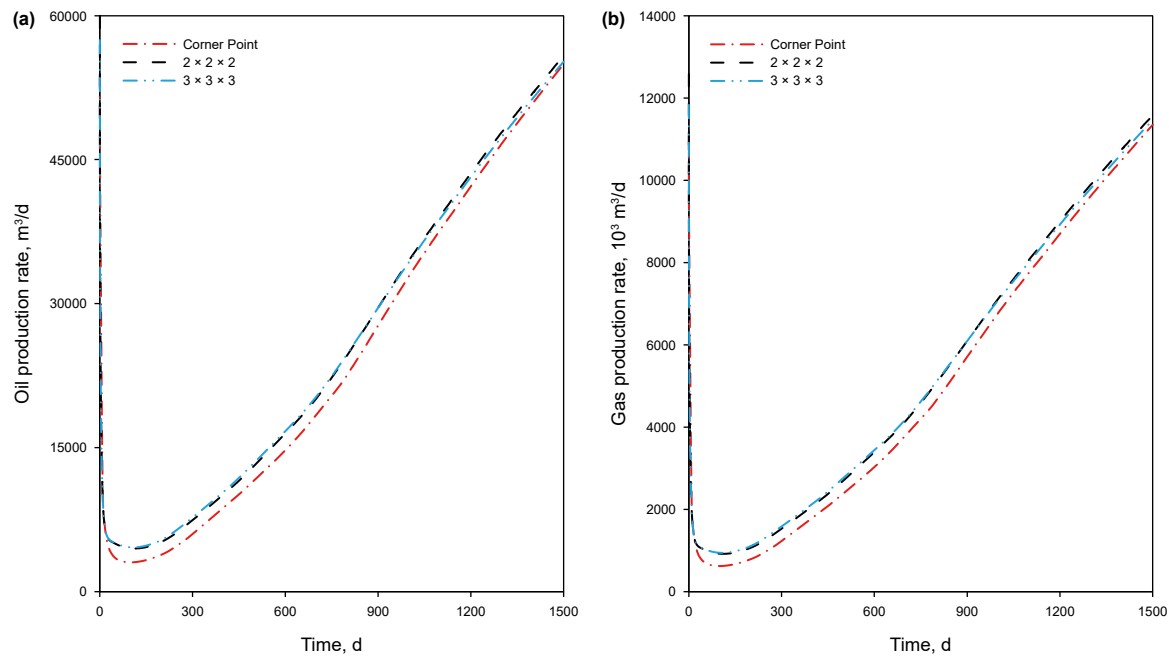


Fig. 27. Production profiles for the Proxy model with original and upscaled grids: (a) oil production curves; and (b) gas production curves.

Table 17
CPU time, number of time-steps, and maximum material balance error for the heterogeneous Proxy model.

Formulation	CPU time, s	Number of time-steps	Maximum material balance error, %
Corner Point	286,544.54	15,094	0.3700
Coarsened grid – $2 \times 2 \times 2$	132,636.59	15,972	0.0083
Coarsened grid – $3 \times 3 \times 3$	120,151.88	18,144	0.0720

Table 17 presents the CPU times for the simulations of this case study, the number of time-steps, and the maximum material balance error for the last time of each simulation. The original mesh with the Corner Point formulation presented the highest simulation time. The simulations performed with the adapted meshes once again showed the desired computational gain while maintaining reliable numerical solutions. The same trend is observed in the speed-up curves presented in Fig. 28.

Tables 18 and 19 summarize the memory usage and computational performance. Although the upscaling process reduced the

number of vertices for grids used in this case, the number of elements remains comparable for the $2 \times 2 \times 2$ coarsened grid and even increases for the $3 \times 3 \times 3$ configuration. This behavior results from the high number of wells and irregular reservoir boundaries, where the clustering scan identifies inactive cells. The high count of wells and complex boundaries increases the number of areas flagged for refinement, leading to a higher number of elements after conversion. These refinement regions increase the number of neighboring connections, resulting in higher memory consumption. Despite the increased memory requirements, both coarsened grids presented reductions in total computing time, achieving a considerable speed-up compared to the Corner Point case.

Table 18
Memory footprint for Proxy upscaling case study.

Formulation	Peak memory footprint, Gb	Memory ratio
Corner Point	23.8	1.0
Coarsened grid – $2 \times 2 \times 2$	36.0	1.51
Coarsened grid – $3 \times 3 \times 3$	33.2	1.39

Table 19
Linear solve time and computing time for upscaled Proxy reservoir case study.

Formulation	Linear solver time, s	Computing time, s	Solver time/ Total time ratio
Corner Point	4623	281,921	1.6%
Coarsened grid – $2 \times 2 \times 2$	1770	130,866	1.3%
Coarsened grid – $3 \times 3 \times 3$	1785	118,366	1.5%

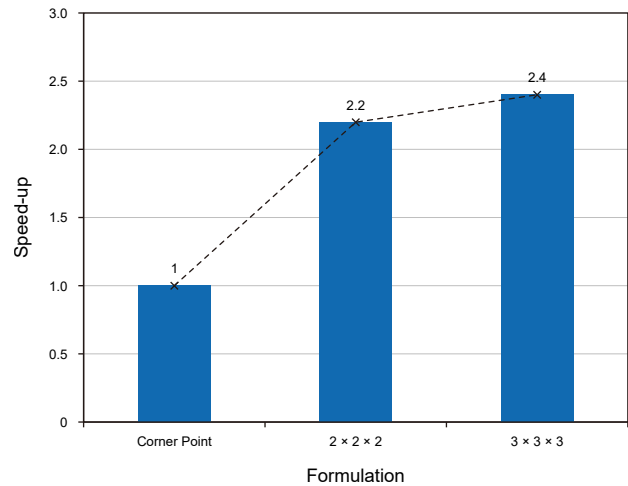


Fig. 28. Speed-up for Proxy upscaling case study.

7. Conclusions

This study presented a new unstructured grid generator method integrated with the EbFVM for compositional reservoir simulation, offering a compelling alternative to conventional structured grid formulations. By enabling selective grid coarsening through clustering and property upscaling techniques, the proposed methodology addresses the computational challenges of fine-scale reservoir models without compromising the numerical accuracy of simulations. The in-house grid generator allows for the conversion of standard Corner Point grids into hexahedral or tetrahedral unstructured meshes while dealing with pinched-out layers through an adapted Laplacian smoothing. The use of Dykstra-Parsons-based refinement ensures that heterogeneity is preserved within high-impact regions. Validation across five case studies showed that the unstructured formulation produces results comparable to commercial simulators, with substantial reductions in CPU time and memory usage, particularly in highly coarsened grids. Overall, this work advances reservoir simulation capabilities by combining numerical efficiency with the use of unstructured formulations, highlighting the EbFVM as a promising tool for future applications in reservoir management, CO₂ sequestration, and enhanced oil recovery.

CRedit authorship contribution statement

Marcelo Menezes Farias: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Conceptualization. **Pedro Salgueiro:** Visualization, Software, Methodology. **Ivens da Costa Menezes Lima:** Visualization, Validation, Methodology. **Francisco Marcondes:** Writing – review & editing, Supervision, Project administration, Methodology, Investigation. **Joaquim Bento Cavalcante-Neto:** Visualization, Supervision, Software, Investigation. **Kamy Sepehrnoori:** Writing – review & editing, Supervision, Software.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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