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Algebraic dynamic multilevel method with local time-stepping (ADM-LTS) for sequentially coupled porous media flow simulation

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Abstract

This paper presents an algebraic dynamic multilevel method with local time-stepping (ADM-LTS) for transport equations of sequentially coupled flow in heterogeneous porous media. The method employs an adaptive multilevel space-time grid determined on the basis of two error estimators, one in time and one in space. More precisely, at each time step, first a coarse time step on a coarsest space-grid resolution is taken. Then, based on the error estimators, the transport equation is solved by taking different time step sizes at different spatial resolutions within the computational domain. In this way, the method is able to use a fine grid resolution, both in space and in time, only at the moving saturation fronts. In order to ensure local mass conservation, two procedures are developed. First, finite-volume restriction operators and constant prolongation (interpolation) operators are developed to map the system across different space-grid resolutions. Second, the fluxes at the interfaces across two different time resolutions are approximated with an averaging scheme in time. Several numerical experiments have been performed

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to analyze the efficiency and accuracy of the proposed ADM-LTS method for both homogeneous and heterogeneous permeability field. The results show that the method provides accurate solutions, at the same time it reduces the number of fine grid-cells both in space and in time.

Keywords: Local time-stepping strategies, Conservative multirate methods, Algebraic Multilevel methods, Multiphase flow, Porous media

1. Introduction

Simulation of multiphase flow in natural porous media is challenging due to the variety of time and length scales involved in the process. In fact, geological formations extend for several hundreds of meters whereas physical and chemical phenomena which are of interest for many geoscientific applications (e.g., renewable energy and greenhouse gas storage, hydrocarbon production and geothermal energy extraction), occur at much smaller scales (cm and below). Moreover, fast process (e.g., high velocity flow in highly permeable rocks and fractures) and slow process (e.g., flow in low permeable porous rock) processes coexist, which have to be correctly represented to obtain reliable numerical simulations. Additionally, at the continuum (or Darcy) scale, porous media present highly heterogeneous properties (e.g., permeability). Thus, accurate numerical models require very high resolution grids both in space and time to capture all relevant physics. However, the size of the domains and the large number of simulations, required for uncertainty reduction [1, 2], make field scale simulations on such high resolution grids impractical.

Traditionally, the computational cost is reduced by employing upscaling methods [3] which define effective rock and fluid properties to represent the physics at a much coarser resolution. However, in presence of highly heterogeneous permeability fields and whenever a clear scale separation is not present, excessive upscaling may not give accurate results [4]. For this reason, advanced and scalable algorithms have to be developed to allow for efficient simulation on high resolution grids without having to define upscaled quantities.

Multiscale methods [5, 6, 7, 8, 9] and dynamic local grid refinement technique [10, 11] are among these advance simulation strategies. The first ones were developed to efficiently solve the elliptic (or parabolic) pressure equation on a coarser grid resolution, without losing the influence of the fine-

30 scale permeability distribution. The latter takes advantage of the locality
31 of transport processes by dynamically adapting the grid resolution so to al-
32 low for accurate transport simulations even in presence of complex physics
33 (e.g., [12, 4]). Recently, the Algebraic Dynamic Multilevel (ADM) method
34 [13, 14] has been developed to combine the consistent multilevel mapping
35 of the pressure field throughout different grid resolutions with an adaptive
36 grid refinement technique. In ADM simulation the discrete governing equa-
37 tions on a high resolution grid (referred to as fine-scale) are obtained. Then,
38 they are mapped and solved on a dynamically defined multilevel spatial grid
39 system. The final solution can be provided both at the dynamic multilevel
40 and fine-scale resolutions, through a sequence of prolongation and restriction
41 operators.

42 Along with the advancements in the space-grid aspect of simulation, in
43 order to reduce the overall simulation time, an implicit time integration
44 scheme is usually employed which allows for much larger time step sizes
45 (compared with the explicit alternative). Adaptive Implicit Methods (AIM)
46 [15, 16, 17, 18, 19, 20], which are able to combine explicit and implicit integra-
47 tion schemes, have also been proposed in the literature. Despite the use of im-
48 plicit integration, in presence of strong non-linearities, the Newton-Raphson
49 method fails to converge for large time steps. As a consequence, several
50 remedies have been proposed to enhance non-linear convergence [21, 22, 23];
51 these allow for the use of very large time steps and considerably improve sim-
52 ulation time. However, the excessive numerical dispersion introduced by the
53 use of large time steps can significantly impact the accuracy of the solution,
54 by, for example, smearing the advancing saturation front. Thus, multirate or
55 local time-stepping (LTS) approaches are of great interest for porous media
56 flow simulation. These methods employ different time step sizes within the
57 domain based on the local flow characteristics. In earlier multirate methods,
58 the fast and slow region were characterized a priori, based on the knowl-
59 edge of the problem [24]. In a more recent work, a self-adjusting, recursive
60 time-stepping strategy has been proposed [25]. The fast regions are detected
61 using a time error estimator after a tentative global time step and then re-
62 fined. In [26], an explicit adaptive conservative time integration techniques
63 is presented, where the sizes of the local time steps are imposing by the CFL
64 restriction. Very recently, a conservative implicit multirate method has been
65 developed and analyzed for hyperbolic equations [27], and also applied to
66 multiphase flow in heterogeneous porous media [28].

67 In this paper, an algebraic dynamic multilevel approach is combined with

68 a mass conservative local time-stepping strategy for the solution of the trans-
69 port equation. The proposed simulation strategy (ADM-LTS) employs an
70 adaptive multilevel grid both in space and in time. The dynamically de-
71 fined grid resolution is chosen based on two error estimators, one in time
72 and one in space. As a consequence, the method is able to use a fine grid
73 resolution only at the location of the moving saturation fronts. In particular,
74 the method first performs a global time step on the coarsest possible grid
75 resolution. Then, thanks to the error estimators, a multilevel grid resolution
76 is defined. On this new grid, the solution is recomputed with smaller time
77 steps only in a fraction of the domain.

78 ADM-LTS is applied to homogeneous and heterogeneous 2D and 3D test
79 cases. Systematic studies of the performance (i.e., accuracy and system com-
80 plexity) have been conducted. Numerical test cases show that the ADM-LTS
81 approach provides an accurate solution reducing the number of active cells
82 both in space and in time.

83 The paper is organized as follows. The equations describing multiphase
84 flow in porous media are presented in section 2 along with the fine-scale
85 discrete systems for transport equation. The ADM-LTS method is explained
86 in detail in section 3 whereas numerical experiments are presented in section
87 4. Finally, conclusions are provided in section 5.

88 2. Sequential implicit formulation for flow in porous media

89 Mass conservation for the flow of N_p incompressible phases in d -dimensional
90 porous domain $\Omega \subset \mathbb{R}^d$ reads

$$\frac{\partial}{\partial t} (\phi S_\alpha) - \nabla \cdot (\boldsymbol{\lambda}_\alpha \cdot \nabla p) = q_\alpha \quad \forall \alpha \in \{1, \dots, N_p\}, \quad (1)$$

91 where capillary and gravitational effects are neglected. Here, S_α , $\boldsymbol{\lambda}_\alpha$ and
92 q_α are the α -phase saturation, mobility and source term. Additionally, p is
93 the fluid pressure. The phase mobility $\boldsymbol{\lambda}_\alpha$ is $\boldsymbol{\lambda}_\alpha = \mathbf{K}k_{r\alpha}/\mu_\alpha$, where \mathbf{K} , $k_{r\alpha}$ and
94 μ_α are rock absolute permeability, phase relative permeability, and viscosity,
95 respectively. Remark that the constrain $\sum_{\alpha=1}^{N_p} S_\alpha = 1$ holds, which can be
96 used to eliminate one saturation unknown. By summing all the phase balance
97 equations [29], a global pressure equation is obtained, i.e.

$$-\nabla \cdot (\boldsymbol{\lambda}_t \cdot \nabla p) = q_t \quad \text{in } \Omega, \quad (2)$$

98 where $\boldsymbol{\lambda}_t = \sum_{i=1}^{N_p} \boldsymbol{\lambda}_i$ is the total mobility and $q_t = \sum_{i=1}^{N_p} q_i$ is the total source
 99 term. The total velocity, defined as $\mathbf{u}_t = \sum_{i=1}^{N_p} \mathbf{u}_i$, can be computed as

$$\mathbf{u}_t = -\boldsymbol{\lambda}_t \cdot \nabla p \quad \text{in } \Omega. \quad (3)$$

100 Thus, the $(N_p - 1)$ saturation equations can be rewritten as

$$\frac{\partial}{\partial t} (\phi S_\alpha) + \nabla \cdot (f_\alpha \mathbf{u}_t) = f_\alpha q_t \quad \forall \alpha \in \{1, \dots, N_{p-1}\}, \quad (4)$$

101 where f_α is the fractional flow function $f_\alpha = \boldsymbol{\lambda}_\alpha / \boldsymbol{\lambda}_t$. Equations (2), (3)
 102 and (4) are coupled by the total velocity and the (nonlinear) phases relative
 103 permeability $k_{r\alpha}$.

104 Sequential implicit simulation (SIM) consists of decoupling the pressure
 105 and the transport equation and solve them implicitly in time. Given the
 106 state at a current time t^n , the solution at time t^{n+1} is found by first solving
 107 Eq. (2), freezing all saturation dependencies, i.e.,

$$\nabla \cdot (\boldsymbol{\lambda}_t(S_\alpha^n) \cdot \nabla p^{n+1}) = q_t \quad \text{in } \Omega. \quad (5)$$

108 Then, given the pressure field, the total velocity is computed as

$$\mathbf{u}_t^{n+1} = -\boldsymbol{\lambda}_t(S_\alpha^n) \cdot \nabla p^{n+1} \quad \text{in } \Omega. \quad (6)$$

109 Finally the transport equations are solved, i.e.

$$\phi \frac{S_\alpha^{n+1} - S_\alpha^n}{\Delta t} + \nabla \cdot (f_\alpha^{n+1} \mathbf{u}_t^{n+1}) - f_\alpha^{n+1} q_t = 0 \quad \forall \alpha \in \{1, \dots, N_{p-1}\}. \quad (7)$$

110 The saturation equations are non-linear functions. Thus, Eq. (7) is solved
 111 with a Newton-Raphson's method and at each Newton's iteration, a system
 112 of the form $\mathbf{J}^\nu \delta \mathbf{x}^{\nu+1} = -\mathbf{r}^\nu$ has to be solved. Here, $\delta \mathbf{x}$ is the vector of increment
 113 for α -saturation, \mathbf{J} is the Jacobian matrix and \mathbf{r} is the residual.

114 Let us now consider a two-phase system of a wetting (w) and a non
 115 wetting (nw) phase. For such a system, for cell K one can write

$$\mathbf{r}_{w_K}^{n+1} = (S_{w_K}^{n+1} - S_{w_K}^n) - \frac{1}{\phi|K|} \sum_{e_{KL} \in \mathcal{E}_K} e_{KL} F_{e_{KL}}^{n+1} (u_{t_{KL}}^{n+1} + q_t^{n+1}) = 0. \quad (8)$$

116 Here, $|K|$ is the volume of element K and e_{KL} is the interface area between
 117 cells K and L and \mathcal{E}_K is the set of faces e of the element K . Finally, $F_{e_{KL}}^{n+1} u_t^{n+1}$
 118 is the numerical flux computed using the first-order upwind method, i.e.,

$$F_{e_{KL}}^{n+1} = \begin{cases} \Delta t f_\alpha(S_{w_U}^{n+1}) & \text{if } u_{TKL} > 0 \\ \Delta t f_\alpha(S_{w_D}^{n+1}) & \text{otherwise,} \end{cases} \quad (9)$$

119 where, S_U and S_D denote the upstream and downstream saturation values,
 120 respectively.

121 The quality of the solution of Eq. (7) is highly influenced by the resolution
 122 of the spatial and time discretization scheme. The objective of this work is
 123 the development of an algebraic dynamic multilevel method with local time-
 124 stepping (ADM-LTS) to solve efficiently and accurately Eq. (7) by employing
 125 a refined grid both in time and in space around the moving saturation front.

126 3. ADM-LTS method

127 In this section, first, the original ADM method [13] is reviewed, then, the
 128 newly proposed ADM-LTS algorithm is presented in details.

129 3.1. The ADM method

130 The ADM method is employed to reduce the computational cost associ-
 131 ated with the solution of the linear system arising from the linearized Eq.
 132 (7).

133 Let us consider a domain discretized with a high resolution grid which is
 134 assumed to be fine enough to capture all relevant physics and to honour the
 135 heterogeneous distribution of the geological properties. Given this fine-scale
 136 discretization, a hierarchy of n_l nested coarse grids is constructed. Each grid
 137 is formed by $N_l = N_{lx} \times N_{ly} \times N_{lz}$ grid cells, where l is the resolution index
 138 and $l = 0$ represents the fine grid resolution.

139 The set of all grid cells belonging to resolution level l is called Π^l . At each
 140 time step ADM defines a multilevel grid by combining grid cells belonging to
 141 the hierarchy of grids previously defined. Given a multilevel ADM grid, let
 142 us define Ω^l as the set of grid cells belonging to all levels from 0 to l which
 143 are present in the ADM grid. Additionally, it is convenient to define the set
 144 Γ^l as $\Gamma^l = \Omega^l \cap \Pi^l$.

145 Given an ADM grid formed by the set of grid cells Ω^l , ADM assumes
 146 that the fine scale solution can be approximated by employing a sequence of
 147 prolongation operators, i.e.

$$\delta \mathbf{x}_{w_f} \approx \delta \mathbf{x}'_w = \hat{\mathbf{P}}_0^1 \dots \hat{\mathbf{P}}_{l-1}^l \delta \mathbf{x}_w. \quad (10)$$

148 Here, operator $\hat{\mathbf{P}}_{i-1}^i$ interpolates the solution at level i to the finer resolution
 149 level $(i - 1)$ and $\delta \mathbf{x}_w^{ADM}$ is the ADM solution on the adaptive multilevel grid.
 150 The fine-scale Jacobian system is mapped to the ADM grid by

$$\hat{\mathbf{R}}_l^{l-1} \dots \hat{\mathbf{R}}_1^0 \hat{\mathbf{J}}_0^1 \dots \hat{\mathbf{P}}_{l-1}^l \delta \mathbf{x}_w^{ADM} = -\hat{\mathbf{R}}_l^{l-1} \dots \hat{\mathbf{R}}_1^0 \mathbf{r}_f, \quad (11)$$

151 where $\hat{\mathbf{R}}_i^{i-1}$ is the restriction operator and it maps the solution from resolution
 152 at level i to coarser level $(i - 1)$. In order to ensure mass conservation at all
 153 level, a finite volume restriction operator is considered [6]. Thus, the entry
 154 (i, j) of a restriction operator reads

$$\hat{\mathbf{R}}_l^{l-1}(i, j) = \begin{cases} 1 & \text{if cell } i \in \Gamma^l \text{ and cell } j \in \Gamma^{l-1}, \\ \delta_{ij} & \text{otherwise.} \end{cases} \quad (12)$$

155 Additionally, constant interpolation is considered for saturation,

$$\hat{\mathbf{P}}_{l-1}^l = \left(\hat{\mathbf{R}}_l^{l-1} \right)^T. \quad (13)$$

156 3.2. ADM method with local time-stepping (ADM-LTS)

157 At each time step n , after having solved the pressure equation and after
 158 having computed the total velocity field, the transport equation is solved
 159 employing the ADM-LTS algorithm

160 First, Eq. (11) is solved over the whole domain on the coarsest grid
 161 resolution (l_{max}) formed by cells belonging to $\Pi^{l_{max}}$ and keeping refinement
 162 only around the wells, with time step Δt . Then, based on the coarse solution
 163 obtained, the proper ADM grid resolution is chosen according to a front-
 164 tracking criterion. Two alternative front-tracking strategies are considered
 165 in this work:

- 166 • a criterion based on the saturation difference between neighbouring
 167 cells. A cell i belonging to level l is refined whenever the saturation
 168 difference, as defined in [13], between i and one of its neighbours exceeds
 169 a user-defined tolerance ϵ_x .
- 170 • a time-dependent criterion is combined with the previous one to de-
 171 termine whether cells belonging to Π^0 should stay fine. Let us de-
 172 fine $\psi_S = S^{n+1} - S^n$. A fine cell i is kept at the fine resolution
 173 only if $\psi_{S_i} > \epsilon_t$, where ϵ_t is a user-defined tolerance. A similar time-
 174 based coarsening criterion has successfully been used in the literature
 175 for channelized heterogeneous problems where stationary gradients are
 176 present [30].

177 Once the ADM grid resolution has been defined, the solution is recom-
 178 puted for all cells belonging to $\Omega^{l_{max}-1}$ with a time step $\Delta t_{l_{max}-1} = \Delta t / \eta$
 179 imposing local boundary conditions as described in the following subsection.

180 Here η is the time refinement ratio. Then, the same operation is repeated
 181 for all resolution levels l until $l = 0$ has been reached. Thus, each resolu-
 182 tion level l (formed by the set of grid blocks Ω^l) is solved with a time step
 183 $\Delta t_l = \Delta t_{l+1}/\eta$. For the finest level ($l = 0$) ADM-LTS only recomputes the
 184 solution, with time step $\Delta t_0 = \Delta t/\eta^{l_{max}}$, for a subset, defined Ω_A^0 , of the cells
 185 belonging to Ω^0 . Only fine cells for which $\psi'_S = S^{n+\Delta t_1} - S^n > \epsilon_t$ are part of
 186 the set Ω_A^0 .

187 The method advances in time for the active cells in Ω_A^0 until they reach
 188 $t = t^n + \Delta t_1$. Once they are synchronized, cells in Ω^1 advance in time. At
 189 this point, a new set of cells Ω_A^1 is selected and these cells are advanced by
 190 Δt_1 performing $\eta \Delta t_0$ time steps. Once all cells in Ω^1 have reached time
 191 $t = t^n + \Delta t_2$ another time step Δt_2 can be performed for all cells belonging
 192 to Ω^2 . This is a recursive procedure which is performed for all levels until all
 193 cells have reached time $t^{n+1} = t^n + \Delta t$.

194 Figure 1 illustrates a schematic overview of the ADM-LTS method where
 195 η and l_{max} are both equal to 2. Figure 2 shows an example of the ADM
 196 grid at each step and the refining area. At the global time step Δt , the
 197 solution is computed on the coarsest resolution l_{max} . At the intermediate
 198 time step the ADM grid resolution is defined and the solution is recomputed
 199 with the intermediate time step everywhere except at the coarsest region
 200 (middle figure). At the end, the method checks the errors and defines the
 201 set of active cells Ω_A^0 (pink region on the right), the solution is recomputed
 202 with the smallest time step.

203 3.2.1. Local systems and local boundary conditions

204 For each resolution level l , the set of grid cells Ω^l is solved with the
 205 corresponding time step $\Delta t_l = \frac{\Delta t}{\eta^{(l_{max}-l)}}$. The number of active cells contained
 206 by Ω_l is N_A^l .

207 When solving for the cells belonging to Ω^l , the numerical flux at the inter-
 208 face between two cells K and L such that $K \in \Omega^l \wedge L \in \Gamma^{l+1}$ is approximated
 209 by

$$F_{KL}^{n+\beta(i)} = \frac{F_{KL}^{n+\gamma(j)}}{\eta} \quad (14)$$

210 where

$$\beta(i) = \frac{i}{\eta^{(l_{max}-l)}}, \quad i = \{1 \dots \eta^{(l_{max}-l)}\} \quad (15)$$

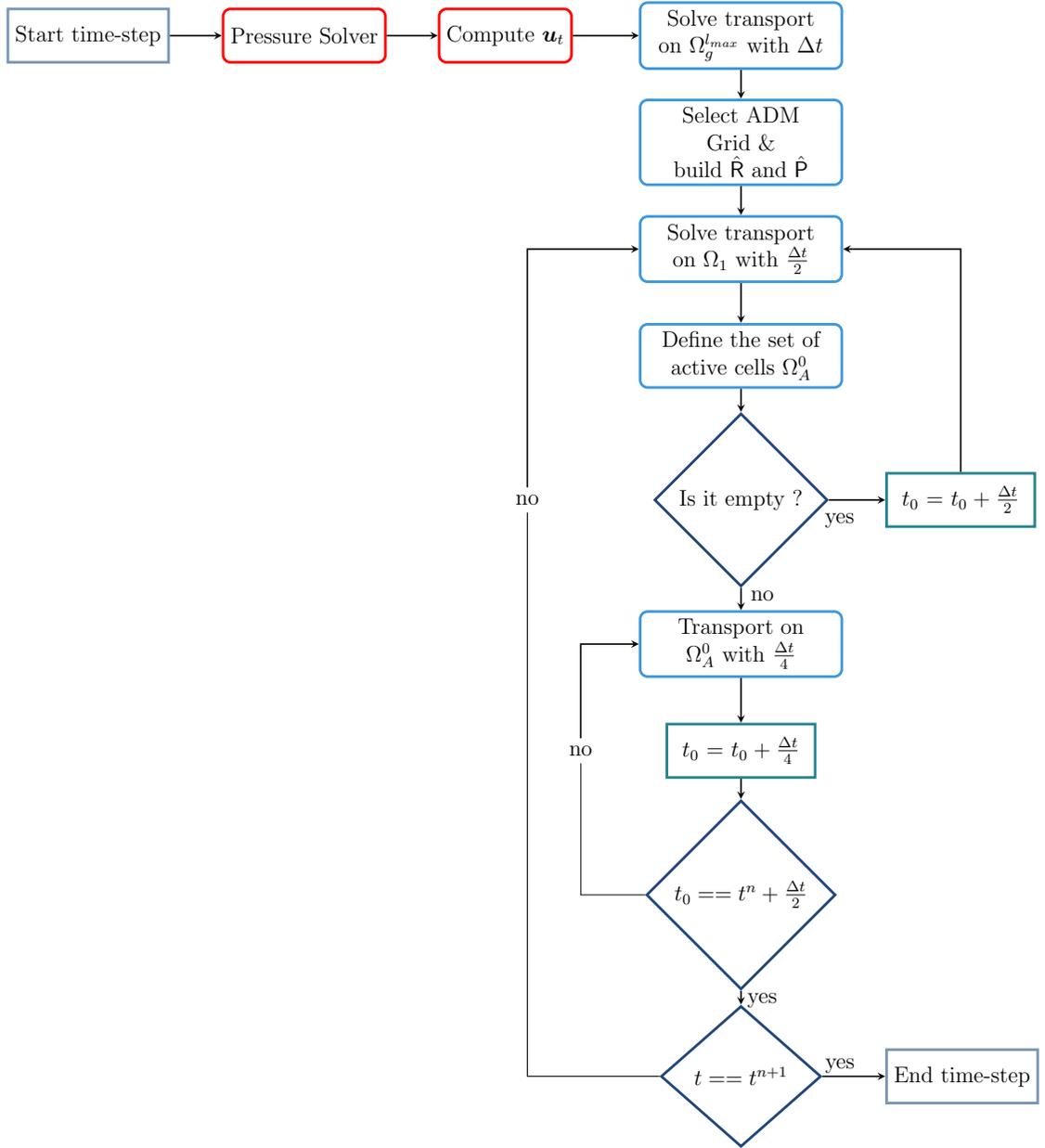


Figure 1: Schematic overview of a time step for the ADM-LTS strategy with $\eta = 2$ and $l_{max} = 2$.

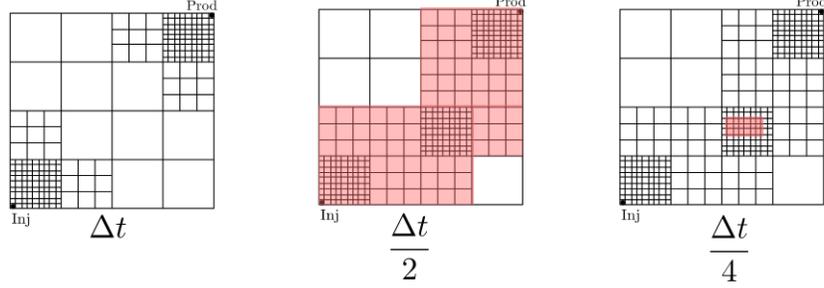


Figure 2: Example of ADM grid and active regions for the refinement time steps with $\eta = 2$ and $l_{max} = 2$.

211

$$\gamma(j) = \frac{j}{\eta^{(l_{max}-l-1)}}, \quad j = \{1 \dots \eta^{(l_{max}-l-1)}\}. \quad (16)$$

212 Thus, Eq. (8) can be modified to account for the presence of different time
213 levels,

$$\begin{aligned} r_K^{n+\beta(i)} &= (S_{w_K}^{n+\beta(i)} - S_{w_K}^{n+\beta(i)-1}) \\ &\quad - \frac{1}{\phi|K|} \sum_{e_{KL} \in \mathcal{E}_{KA}} e_{KL} F_{e_{KL}}^{n+\beta(i)} \left(u_{t_{KL}}^{n+\beta(i)} + q_t^{n+\beta(i)} \right) \\ &\quad - \frac{1}{\phi|K|} \sum_{e_{KL} \in \mathcal{E}_{KL}} e_{KL} \frac{F_{e_{KL}}^{n+\gamma(j)}}{\eta} \left(u_{t_{KL}}^{n+\gamma(j)} + q_t^{n+\gamma(j)} \right). \end{aligned} \quad (17)$$

214 Here, \mathcal{E}_{KA} is the set of interface fluxes exchanged between two cells K and L
215 both belonging to Ω^l . Additionally, \mathcal{E}_{KL} is the set of fluxes at the interface
216 between two cells K and L where $K \in \Omega^l$ and $L \in \Gamma^{l+1}$. Note that, for $l = 0$
217 the residual for the active cells is the same described by equation (8) but \mathcal{E}_{KL}
218 would be the set of fluxes at the interface between Ω_A^0 and $\Omega^1 \setminus \Omega_A^0$.

219 Remark that, for each level l , the linear system that has to be solved has
220 the size $N_A^l \times N_A^l$ which is significantly smaller than the full fine-scale system.

221 The above strategy allows for conservative multi-scale march in time
222 and space for transport equation within the sequentially implicit simulation
223 framework. Next, its performance is being studied for various test cases both
224 for 2D and 3D domains.

225 **4. Numerical results**

226 The performance the newly developed ADM-LTS strategy is thoroughly
 227 investigated for several challenging test cases. For all cases presented, quadratic
 228 relative permeability curves are considered. Additionally, all errors are com-
 229 puted with respect to a reference solution, obtained by employing a high
 230 resolution discretization both in space and in time.

231 *4.1. Test case 1: 2D homogeneous reservoir*

232 The first test case is a 100×100 [m²] homogeneous reservoir, with per-
 233 meability of 5×10^{-15} [m²]. A pressure-constrained wetting-phase injector
 234 well is positioned in the bottom-left corner of the domain with a pressure
 235 $p_{inj} = 10^8$ [Pa], whereas a production well is present in the top-right corner
 236 with a relative pressure of $p_{prod} = 0$ [Pa]. The phase viscosity values are
 237 $\mu_w = 10^{-3}$ [kg/m³] and $\mu_{nw} = 10^{-2}$ [kg/m³] for the wetting and non wetting
 238 phase, respectively. The final simulated time is 600 [days] after injection has
 239 started.

240 A fine-scale grid with 99×99 cells is imposed on the domain. ADM-LTS
 241 employs, a time refining ratio $\eta = 2$ and a space coarsening ratio equal to 3 in
 242 all directions. The user-defined tolerances for the coarsening and refinement
 243 criteria are $\epsilon_x = 0.07$ and $\epsilon_t = 5 \times 10^{-2}$.

244 Simulations are run employing three different time step sizes: 5, 10 and
 245 20 days. Figure 3 reports the CFL values at time $t = 500$ days for the three
 246 different time steps for fine-scale in space simulations.

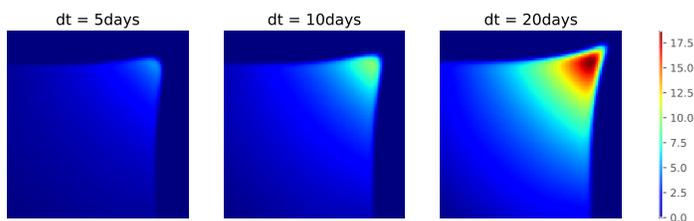


Figure 3: Test case 1 [99×99] - CFL values for different global time steps at time $t = 500$ days.

247 Figure 4 shows a comparison of the ADM-LTS solution with the reference
 248 solution at time $t = 500$ [days] using three different sizes of the global time
 249 steps.

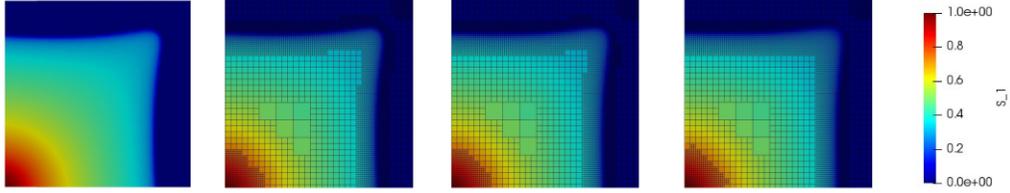


Figure 4: Test case 1 $[99 \times 99]$ - Reference solution (first column) and ADM-LTS solution using a global time step size: $\Delta t = 5, 10$ and 20 [days] at time $t = 500$ days for the second, third and fourth column, respectively.

250 Figure 5 reports the error for the saturation at time $t = 500$ days between
 251 a reference solution and the ADM method with fine time steps (first column)
 252 with the LTS approach (second column) and with the coarse time steps (third
 253 column) for the three different time steps sizes $\Delta t = 5$ (first row), $\Delta t = 10$
 254 ($\Delta t = 10$ (second row) and $\Delta t = 20$ (third row)). In all cases the AMD-LTS approach
 255 improves the errors of the coarse time step approach.

256 The complexity of the algorithm is shown in Fig. 6. In particular, each
 257 column represents the total amount of active cells multiplied by the number
 258 of Newton iterations involved to compute the solution, for the three
 259 approaches and for the three different global time step sizes. Note that, to
 260 obtain the solution at time $t=600$ [days], 120, 60 and 30 global time steps
 261 have been performed using the three analyzed time steps. Remark that the
 262 errors obtained by employing the original ADM method with a fine time step
 263 are comparable to those obtained with ADM-LTS.

264 Figure 7 shows the complexity per a single global time step. For the ADM
 265 method with fine time steps, the local steps are just the small steps applied
 266 at the domain. At the end of the local steps both the ADM-LTS method and
 267 the ADM fine step method reach the same time. For the ADM-LTS method,
 268 local step 1 indicates the global step on the coarsest grid, step 2 and 5 are the
 269 intermediate time steps performed on level 0 and 1 of the ADM grid, and the
 270 other local steps are the small time steps for the active cells detected by the
 271 error estimator in time. In particular, we can notice that the intermediate
 272 time steps have almost the same complexity of the small time steps of the
 273 ADM fine method, even if the size of the time step is two times bigger with
 274 almost the same number of active cells. This is due to the improvement of
 275 the initial guess for the Newton loop. In the intermediate time steps we use
 276 as initial guess a linear combination of the solution of the previous time t^n

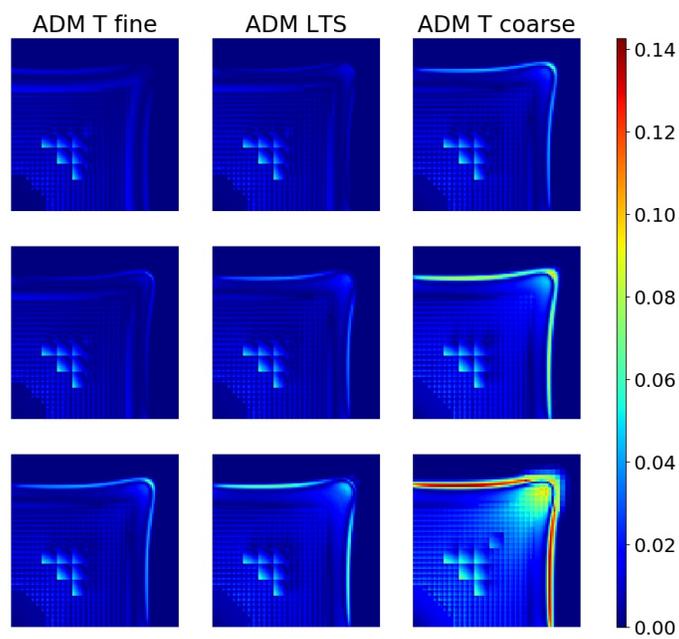


Figure 5: Test case 1 $[99 \times 99]$ - Saturation errors for the ADM method with fine time steps (first column), ADM-LTS method (second column) and ADM coarse time steps method (third column) for the three different global time step sizes.

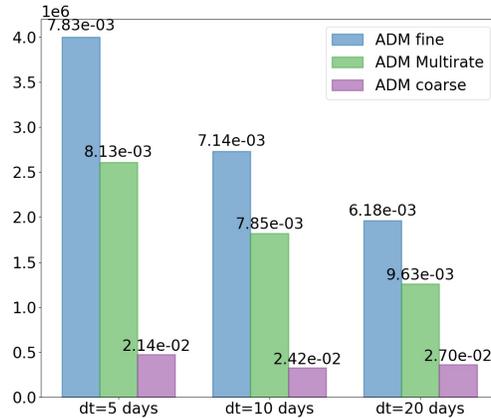


Figure 6: Test case 1 $[99 \times 99]$ - Total amount of active cells multiplied by number of Newton iterations for the three different time step sizes. On the top of each bar the mean in time of the averaged absolute difference respect to the reference solution for the saturation is displayed $E_s = \text{mean}|S(t_f) - S_{ref}(t_f)|$ where t_f is the final time 600 days.

277 and the solution obtained on the coarsest grid at the new global time t^{n+1} .
 278 In the small time steps is not necessary to perform this technique since a
 279 small step is used to advance in time.

280 The same test case is analyzed after performing a 2×2 refinement of the
 281 space fine-scale grid. In order to obtain a reasonable solution, using a global
 282 Δt equal to 20 [days], we need to compute more local time steps inside the
 283 global one, so a refining ratio equal to 4 has been taken into account.

284 Figure 8 reports the complexity for the entire simulation using ADM-
 285 LTS method and the ADM with fine time steps. To obtain the solution at
 286 final time $t = 600$ [days] with a global time step equal to 20 days, the same
 287 number of global time step are involved (30 time steps in total). Of course
 288 the number of local time step for both the LTS method and the fine time
 289 steps approach would be increased; but the ratio between active cells and
 290 total cells decreases.

291 Figure 9 shows the averaged number of active cells times the number of
 292 Newton iterations for each local time step within a global time step.

293 In Figure 10 we can see that the ADM-LTS approach reduces the errors
 294 obtained using a coarse grid in time.

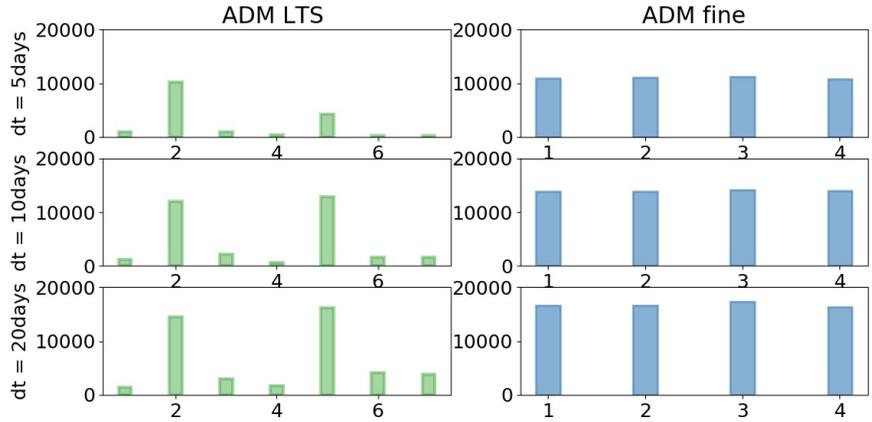


Figure 7: Test case 1 $[99 \times 99]$ - Computational complexity history at each local times step within a global step. The computation complexity is the number of active cells multiplied by the number of Newton iterations.

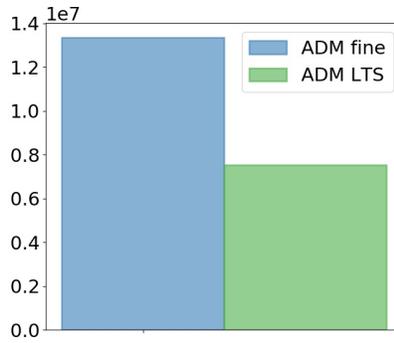


Figure 8: Test case 1 $[198 \times 198]$ - Total amount of active cells multiplied by number of Newton iterations for the ADM with fine time steps and the ADM LTS method.

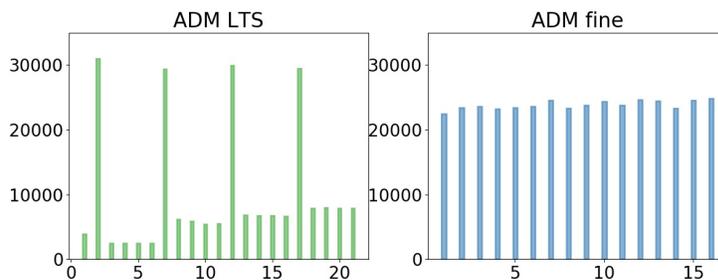


Figure 9: Test case 1 $[198 \times 198]$ - Computational complexity history at each local times step within a global step. The computation complexity is the number of active cells multiplied by the number of Newton iterations.

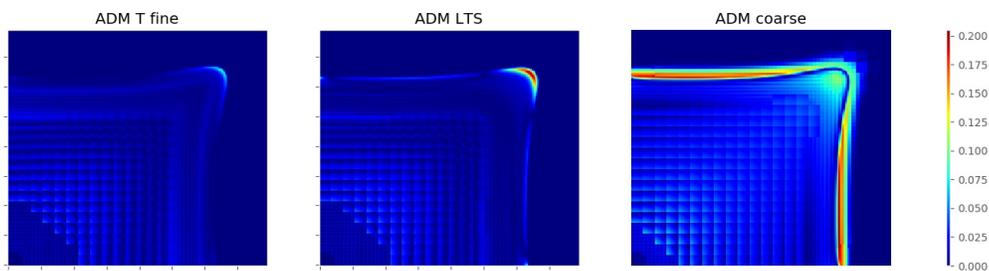


Figure 10: Test case 1 $[198 \times 198]$ - Saturation errors at time $t = 540$ [days] for the ADM method with fine grid in time (left), ADM-LTS method (center) and the ADM method with coarse grid in time (right).

295 *4.2. Test case 2: 3D homogeneous reservoir*

296 A 3D $108 \times 108 \times 108$ [m³] homogeneous reservoir is considered in this
 297 test case. The domain is discretized, at the fine-scale, with a $54 \times 54 \times 54$
 298 Cartesian grid for a total of 157464 cells. The physical parameters are the
 299 same of the first test case. The size of the global steps is equal to 125 days.
 300 The simulation ends after 70 global steps. The tolerances for the coarsening
 301 criteria in space and time are set to be $\epsilon_x = 0.2$ and $\epsilon_t = 5 \times 10^{-2}$.

302 Figure 11 reports the saturation maps at two different simulation times
 303 (on the top). For the first time the set of active cells Ω_A^0 (left, bottom) and
 304 also a section of the solution at final time $t = 8750$ days (right, bottom) are
 305 plotted. Note that ADM-LTS employs fine cells only around the advancing
 306 saturation front and that the active cells in time are only a fraction of them.
 307 Figure 12 shows the total complexity and the mean complexity per local time
 308 step for both the ADM-LTS method and the ADM method with fine time
 309 steps.

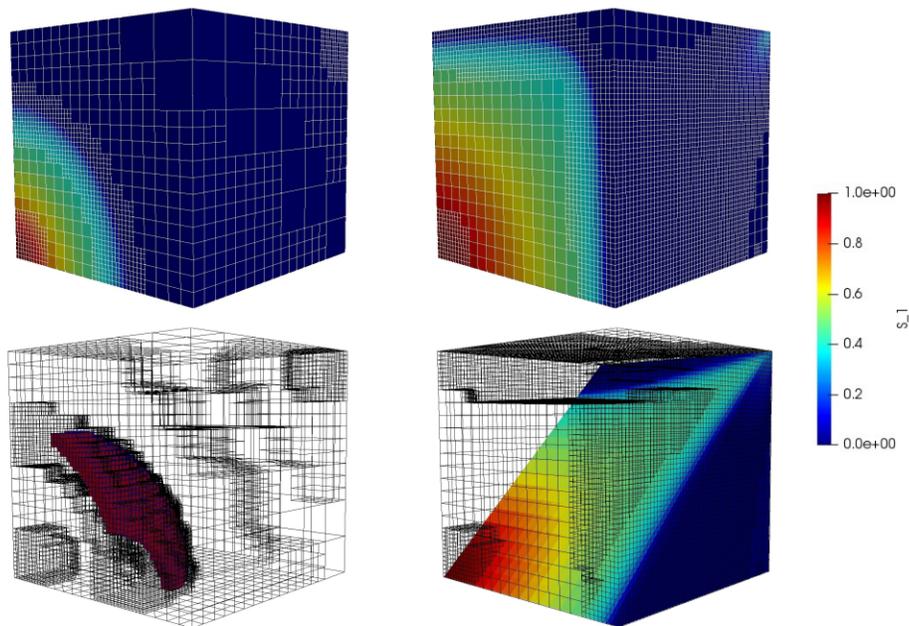


Figure 11: Test case 2 - Saturation profile (top row) at time $t = 1500$ days (left) and at time $t = 8750$ days (right). Active cells for the level $l_{ref=0}$ at time $t = 1500$ (bottom-left) and saturation profile inside the domain at time $t = 8750$ (bottom-right).

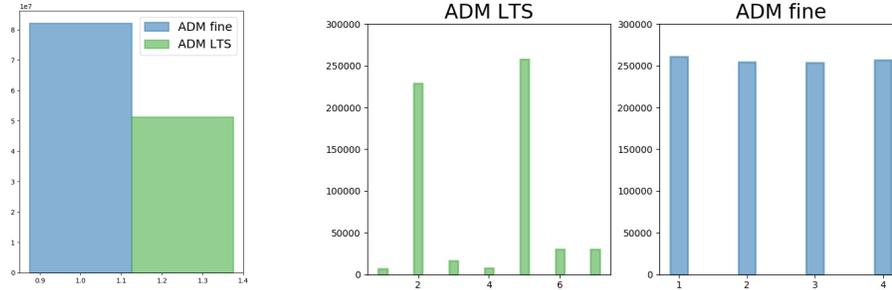


Figure 12: Test case 2 - Total amount of active cells multiplied by number of Newton iterations for the ADM with fine time steps and the ADM LTS method (left) and computational complexity history at each local times step within a global step (right).

310 *4.3. Test case 3: 2D homogeneous reservoir with barrier*

311 A 2D homogeneous reservoir with low permeability barriers is considered,
 312 as shown in Fig. 13. The same permeability field was presented in [30]. The
 313 domain dimensions and the physical parameters are the same of the first test
 314 case, the same 99×99 fine scale grid is imposed. The global time step is equal
 315 to 50 [days] and the simulation ends after 100 global time steps ($t = 5000$
 316 days).

317 Simulations are both with the original ADM method employing a global
 318 fine time-step and with ADM-LTS. The coarsening and the time-refinement
 319 criteria tolerances are set to $\epsilon_x = 0.05$ and $\epsilon_t = 0.005$.

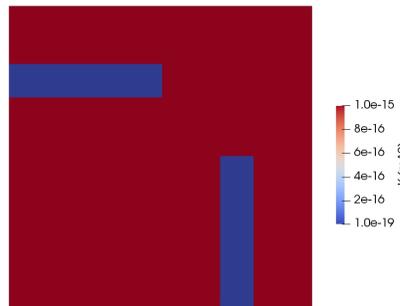


Figure 13: Test case 3 - Absolute permeability field.

320 Figure 14 shows a comparison of the saturation profile and the grid res-
 321 olution for the two different strategies. The original ADM method with a

322 saturation difference-based coarsening criterion (top row) employs a lot of
 323 fine grids wherever saturation gradients are present even if they are station-
 324 ary. On the other hand the newly proposed grid resolution criterion (bottom
 325 row) for the ADM-LTS approach uses fine cells only in those regions where
 326 the saturation gradient is moving, reducing the number of active cells.

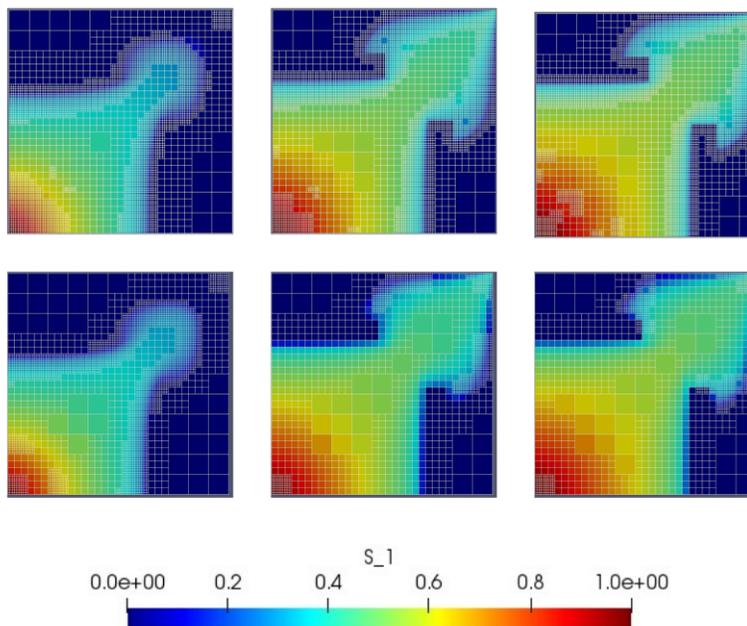


Figure 14: Test case 3 - Saturation profile and ADM grid at different time steps (columns) for ADM with coarse time steps and classical ADM grid resolution (first row) and for ADM-LTS method with the new ADM grid resolution (second row).

327 Figure 15 reports the evolution of the active grid cells percentage for the
 328 two different approaches (left) and the evolution of the relative saturation
 329 error in l^1 -norm (right). In the early steps, we can see that the ADM fine
 330 with just the gradient resolution approach employs almost the same number
 331 of active grid cells used by the ADM-LTS method. For the ADM with fine
 332 time steps at every small local time step we solve both the flow and the
 333 transport equations, instead for the ADM-LTS approach only the transport
 334 equation is solved for the local steps. This is the reason why in the first five
 335 steps the saturation errors for the ADM-LTS approach are bigger respect to
 336 the ADM fine steps approach. Instead, in the last steps the errors increase
 337 because a lower number of fine grid cells has been used.

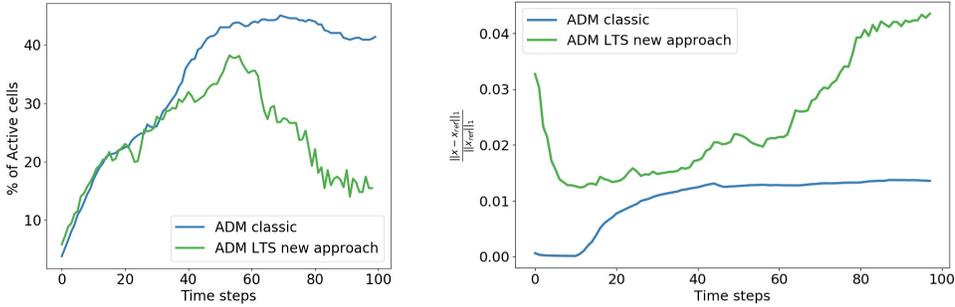


Figure 15: Test case 3 - number of active cells employed in ADM with fine grid in time and ADM-LTS simulations expressed as percentage of fine grid cells (left) and the saturation relative errors in l^1 -norm for the ADM fine and ADM-LTS method (right).

338 Figure 16 shows the total complexity (number of active cells multiplied by
 339 the number of Newton iterations) for the ADM with fine steps and the ADM-
 340 LTS approach. Remark that the local time steps of ADM-LTS method reduce
 341 the complexity of the system compared to the classical ADM approach.

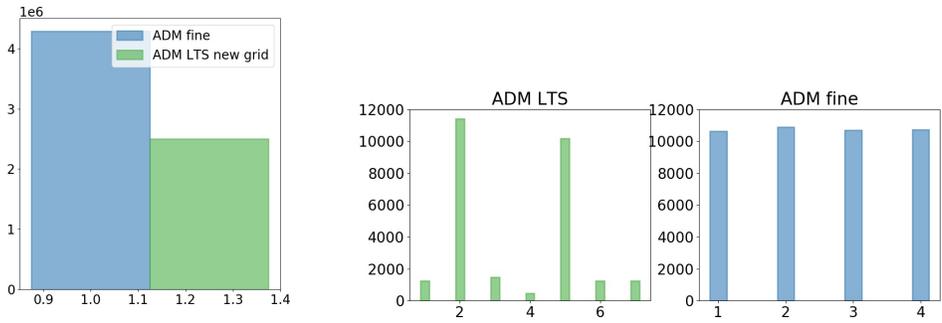


Figure 16: Test case 3 - Total amount of active cells multiplied by number of Newton iterations (left) and computational complexity history at each local times step within a global step (right) for the ADM with fine time steps approach and for the ADM-LTS method.

342 *4.4. Test case 4: Heterogeneous reservoir (SPE10 top layer)*

343 In this test case a heterogeneous reservoir is considered. The permeability
 344 map is the top layer of the SPE10 test case [31] and it is presented, in
 345 logarithmic scale, in Fig. 17. The size of the reservoir is 2200×600 [m²] and

346 a 216×54 grid is employed at the finest level. The injector is at the top
 347 left corner and has a constrained pressure 10^7 [Pa]. A producer is, instead,
 348 located at the bottom right corner of the domain with a pressure equal to
 349 0 [Pa]. The porosity of the reservoir ϕ is equal to 0.2. The viscosity for
 350 wetting phase is 10×10^{-5} [kg/m³], whereas, for the non-wetting phase, is
 351 10^{-4} [kg/m³]. The coarsening ratio for the space grid is equal to 2 as well as
 352 the time refining ratio. The error tolerance for the time estimator is equal
 to 5×10^{-2} .

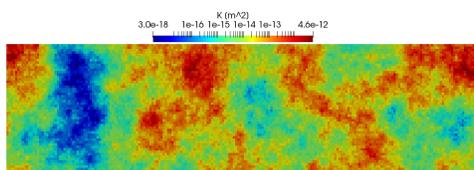


Figure 17: Test case 4 - Natural logarithm of the permeability.

353

354 Figure 18 reports the saturation map and the ADM grid for different
 355 threshold values of the ADM grid resolution criterion using the classical ADM
 356 approach with fine time steps and the ADM-LTS approach with the new grid
 357 resolution strategy. The classical approach uses, for small threshold values, a
 358 lot of fine grid cells. Relaxing the threshold parameter the method is not able
 359 to capture the fronts. Thanks to the new resolution approach, the method
 360 is able to apply the fine grid cells only where the front is moving fast (high
 361 permeability regions).

362 Figure 19 shows the active cells in time at the finest level $l_{ref} = 2$ for
 363 different global time steps. The method recomputes the solution with small
 364 time steps only for a few percentage of cells where the front pass high perme-
 365 ability regions. In fact, in the last snapshot, the saturation profile is almost
 366 evolved everywhere and so, the set of active cells, is very small.

367 In Figure 20 we compared the number of active cells and the saturation
 368 errors for the different simulations. Using the classical ADM approach with
 369 small values of the tolerance a lot of active grid cells are employed giving
 370 very small errors. The classical ADM approach with larger tolerance value
 371 and the ADM-LTS method are comparable in terms of active cells during all
 372 the simulation but the ADM-LTS approach gives better results in term of
 373 errors.

374 Figure 16 reports the complexity of the four simulations. The ADM ap-
 375 proach with fine grid in time and small threshold values are really expensive.

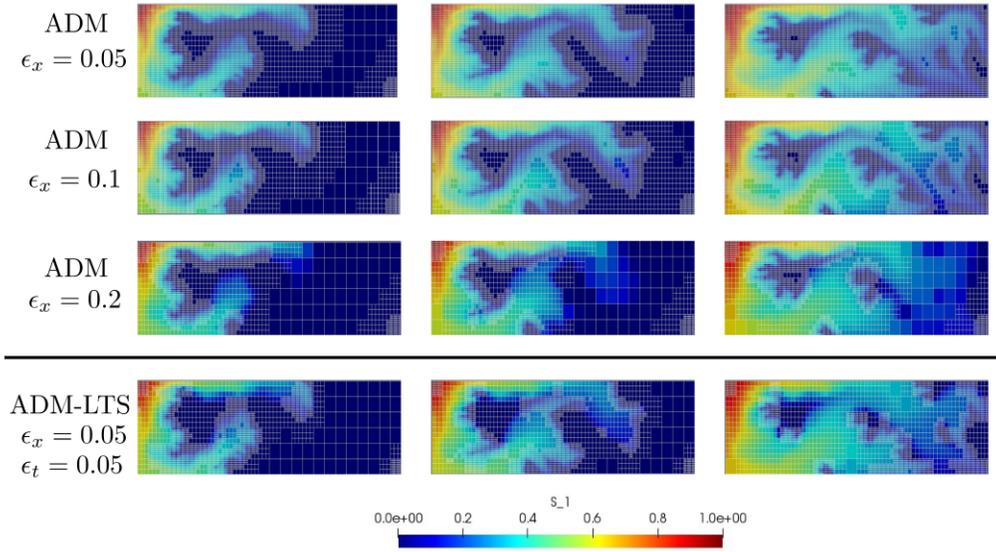


Figure 18: Test case 4 - Saturation map and ADM grid for the ADM with fine time step approach with classical grid criterion for different values of the threshold $\epsilon_x = 0.05, 0.1, 0.2$ (row 1, 2, and 3) and for the ADM-LTS method with the new grid criterion $\epsilon_x = 0.05$ and $\epsilon_t = 0.05$ (row 4) at time $t = 1200$ days (first column), $t = 15000$ days (second column) and $t = 20000$ days (third column).

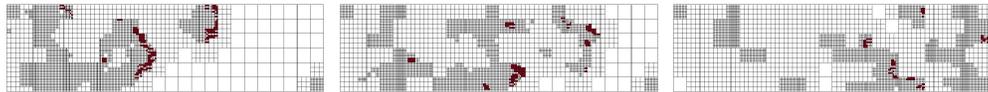


Figure 19: Test case 4 - Active cells for the refinement in time, at time $t = 1200$ days (left), $t = 15000$ days (center) and $t = 20000$ days (right).

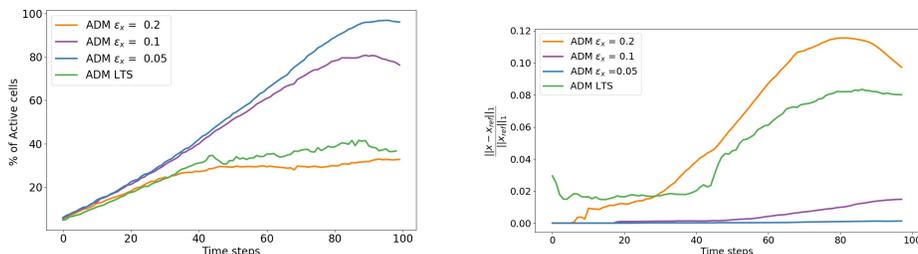


Figure 20: Test case 4 - Number of active cells expressed as percentage of fine grid cells (left) and saturation relative errors in l^1 -norm (right) for the ADM with fine grid in time with different values of the threshold and for the ADM-LTS simulation.

376 The ADM-LTS approach is comparable to the ADM with fine time step ap-
 377 proach and large value of ϵ_x but, as shown previously, the solution of the
 378 classic ADM, in this case, is not as accurate.

379 *4.5. Test case 5: Heterogeneous reservoir (SPE10 bottom layer)*

380 Permeability of SPE10 bottom layer is used for this test case, as show in
 381 Figure 22.

382 The global time step is equal to 10 days and the simulation ends after
 383 50 global time steps. The input parameters for the wells and the physical
 384 properties are identical to Test Case 4.

385 The top 2 rows of Fig. 23 shows the saturation distribution at simulation
 386 time of 150, 250 and 350 days obtained with $\epsilon_x = 0.15$ and $\epsilon_x = 0.2$. The
 387 bottom rows, instead, show the saturation map, at the same simulations
 388 times, obtained by employing the ADM-LTS method with $\epsilon_x = 0.05$ and
 389 $\epsilon_t = 5 \times 10^{-2}$ and $\epsilon_t = 5 \times 10^{-3}$.

390 Figure 24 shows the active cells for the refining in time for $l_{ref} = 2$ at
 391 time 150, 250 and 350 days. As expected, for smaller value of the threshold
 392 more cells are involved in the refining step.

393 The history of the percentage of active cells employed by the different
 394 simulation strategies for the various tolerances is shown in Fig. 25 (left),
 395 along with the l^1 norm of the saturation error (right). For both the ADM-
 396 LTS tolerance values less active cells are involved respect to the classical
 397 ADM approach. Since a smaller number of cells is employed, the saturation
 398 errors are higher but still of the same order of magnitude.

399 Figure 26 reports the complexity of the four simulations for different
 400 tolerance values.

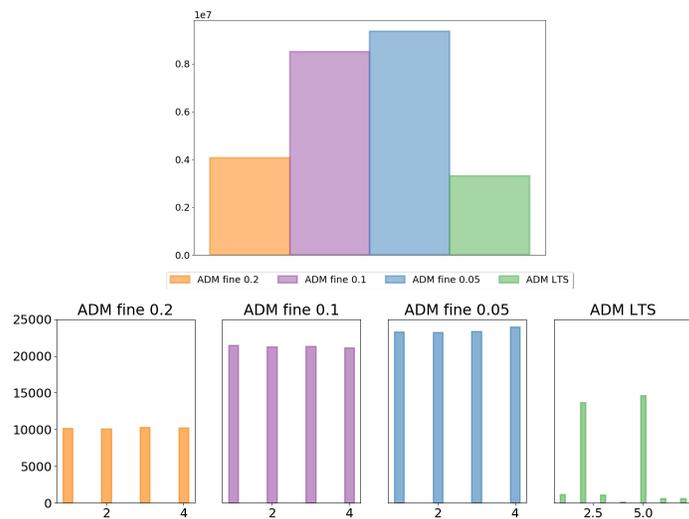


Figure 21: Test case 4 - Total amount of active cells multiplied by number of Newton iterations (top) and computational complexity history at each local times step within a global step (bottom) for the ADM approach.

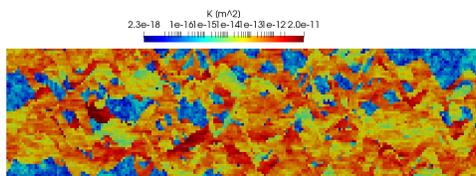


Figure 22: Test case 5 - Natural logarithm of the permeability.

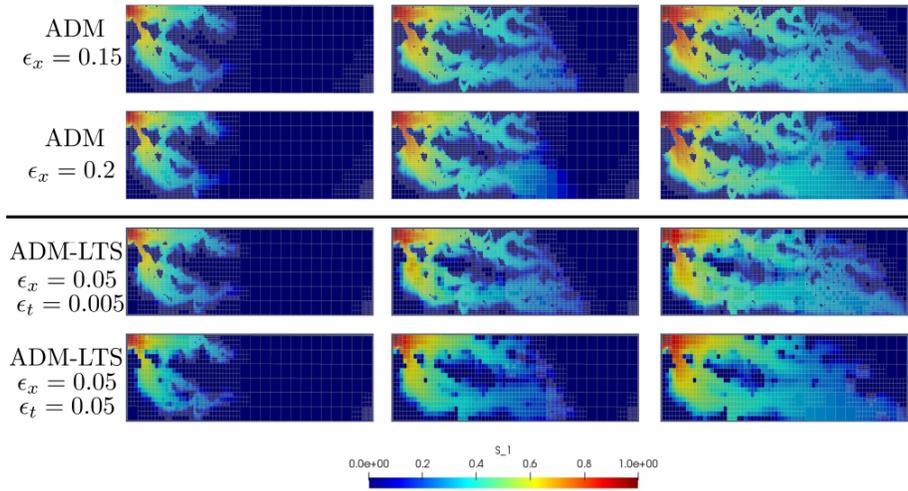


Figure 23: Test case 5 - Saturation map and ADM grid at 150, 250 and 350 days for the ADM approach with fine time steps and the ADM-LTS approach.

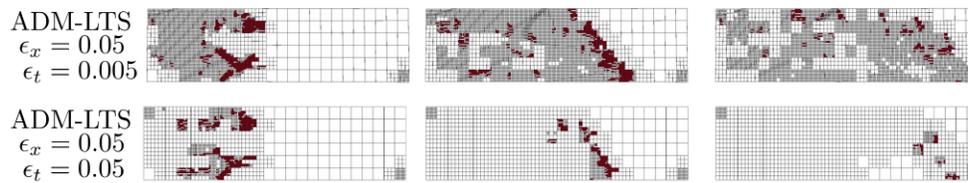


Figure 24: Test case 5 - Active cells for the refinement level $l_{ref} = 2$, at 150 (left), 250 (center) and 350 (right) days for the two threshold values.

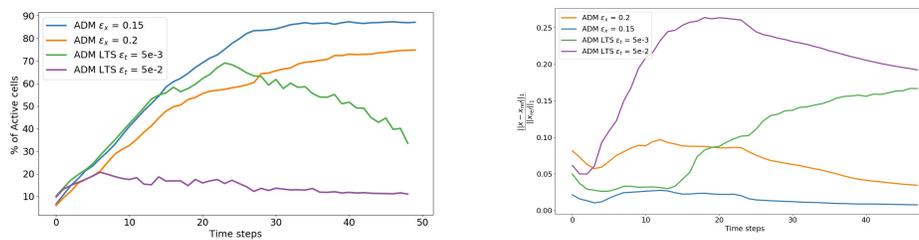


Figure 25: Test case 5 - Number of active cells expressed as percentage of fine grid cells (left) and saturation relative errors in l^1 -norm (right) for the ADM with fine grid in time and for the ADM-LTS simulations.

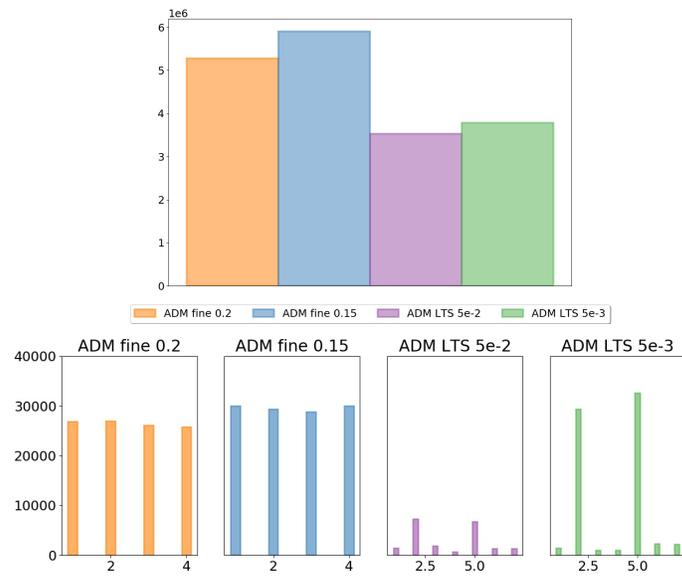


Figure 26: Test case 5 - Total amount of active cells multiplied by number of Newton iterations (top) and computational complexity history at each local times step within a global step (bottom) for the ADM approach.

401 *4.6. Test case 6: Heterogeneous reservoirs with different layering orienta-*
402 *tions.*

403 A 500×500 m² 2D reservoir is considered on which a 99×99 grid is
404 imposed. The fluid properties, the location of the wells and their constraints
405 are the same as in the previous test cases. Five sets of permeability fields,
406 with different layering orientation and created using sequential Gaussian sim-
407 ulations with spherical variogram and dimensionless correlation lengths 0.5
408 and 0.02 [32], are considered. Each set consists of 20 statistically identical
409 realizations.

410 Figure 27 shows one realization for each set. Injection of the wetting
411 phase, for 560 days, is simulated for each realization. Simulations are run
412 both with the ADM-LTS method. For all runs, the spatial coarsening crite-
413 rion tolerance is $\epsilon_x = 0.008$. Two different values are instead considered for
414 the time-based criterion tolerance, ϵ_t : 5×10^{-2} and 5×10^{-3} .

415 Figure 28 shows a comparison, for one permeability realization of each
416 set, of the saturation map at the end of the simulation obtained with fine-
417 scale (time and space) simulation (top row), ADM-LTS employing a fixed
418 refined time-step.

419 Figure 29 displays the active cells in time for the last refinement level of
420 the last global time step. As expected, using bigger value of the tolerance
421 for the time error estimator, just few cells need to be computed with small
422 time steps, also the space grid changes and allow to use coarser grid cells.

423 Figure 30 represents the mean and the standard deviations of the com-
424 plexity for the ADM-LTS method using the two different time-based criterion
425 tolerances and for the solution computed with the fine grid resolution both
426 in space and in time. Note that the y-axis scale for the two pictures are
427 different.

428 Figure 31 shows the mean and the standard deviations of the satura-
429 tion errors respect to the reference solution for the ADM-LTS method using
430 the two different time-based criterion tolerances. From these studies, one
431 can conclude that the ADM-LTS performs robust when several equiproba-
432 ble realizations are considered. In other words, the error and computational
433 complexities for all 20 realizations are not much different compared with the
434 average values.

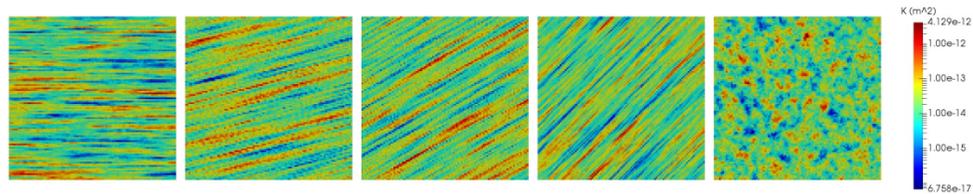


Figure 27: Test case 6 - One of the 20 realization of each of the 5 sets of permeability fields with different angles (0 deg, 15 deg, 30 deg, 45 deg and patchy from left to right).

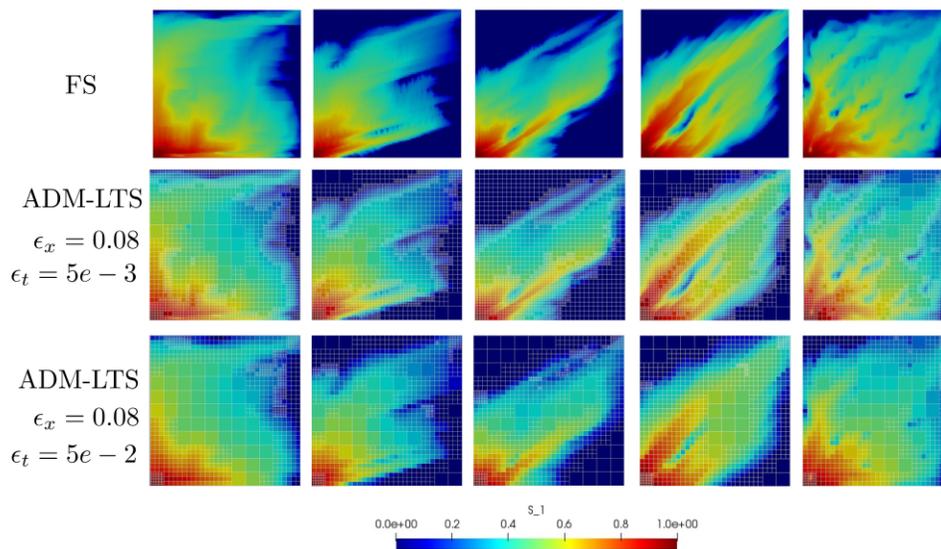


Figure 28: Test case 6 - Comparison of the saturation profile, for one realization of each set of permeability fields at time $t = 560$ days. Two different threshold values for the time error estimator are employed for the ADM-LTS simulation (center row and bottom row), the fine scale solution are also shown (top row).

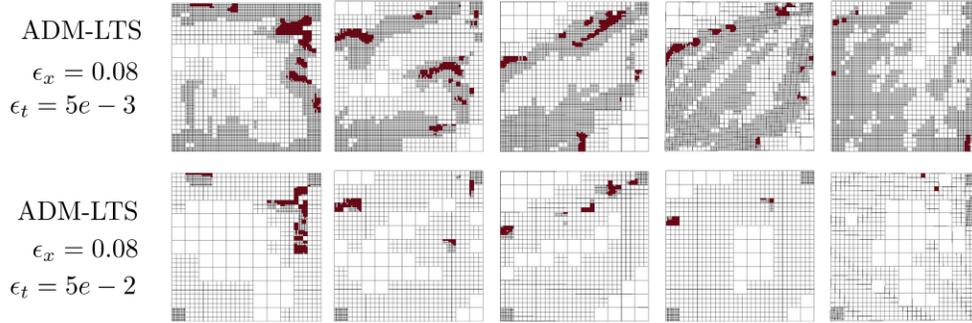


Figure 29: Test case 6 - Active calls at the last refinement level for the last global time step using two different threshold values for the error estimator in time.

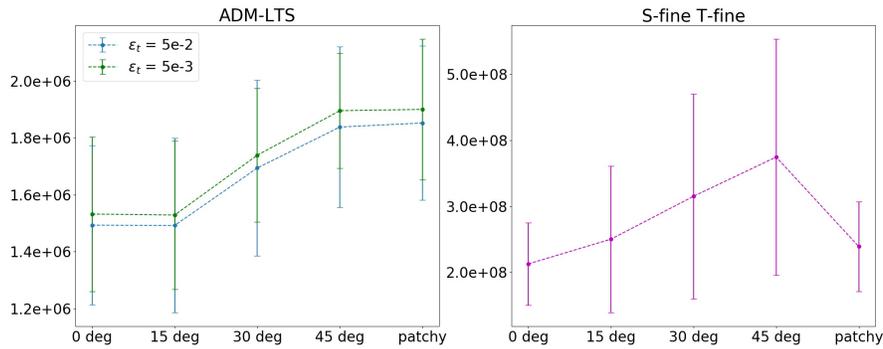


Figure 30: Test case 6 - Mean and standard deviation of complexity over 20 realization for the ADM-LTS method (left) and for the reference solution computed with fine grid resolution both in space and time (right).

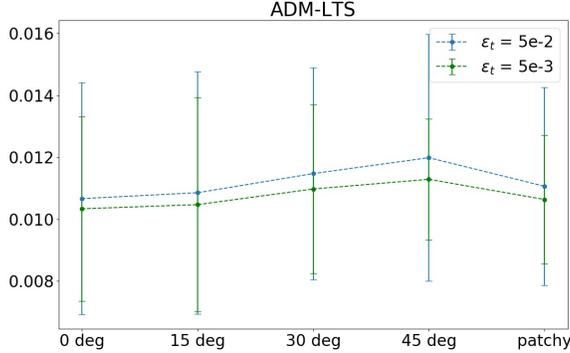


Figure 31: Test case 6: Mean and standard deviation errors of the saturation errors over 20 realization for the ADM-LTS method with different time threshold values respect to the reference solution $E_S = \text{mean}_{t=1}^{N_t} (\text{mean}|S_f(t) - S(t)|)$.

435 5. Conclusions

436 In this paper, a dynamic multilevel approach with a local time-stepping
 437 strategy for the solution of the transport equation in heterogeneous porous
 438 media was presented. The ADM-LTS method enables to capture the moving
 439 fronts. Particularly, it combines, at each global time step, a dynamic multi-
 440 level grid in space with a local time-stepping strategy that is able to use small
 441 time step only where the front is moving fast. Compared with the classical
 442 ADM approach, the newly developed method allows to use more coarsening
 443 regions where the high gradients do not evolve in time. This method is a
 444 promising way to reduce the size of the system in the nonlinear loop without
 445 loss of accuracy.

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 450 under Contract DE-AC52-07NA27344.

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