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**Implementation of Richardson extrapolation in an
efficient adaptive time stepping method: applications
to reactive transport and unsaturated flow in porous
media**

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1 **Abstract**

2 Environmental studies are commonly carried out through numerical simulations, which have
3 to be accurate, reliable and efficient. When transient problems are considered, the validity of
4 the solutions requires the calculation and management of the temporal discretization errors.
5 This paper describes an adaptive time stepping strategy based on the estimation of the local
6 truncation error via the Richardson extrapolation technique. The time marching scheme is
7 mathematically based on this *a posteriori* error estimation that has to be gauged. General
8 optimisations are also suggested making the control of both the temporal error and the
9 evolution of the time step size very efficient. Furthermore, the algorithm connecting these
10 methods is all the more interesting as it could be implemented in many computational codes
11 using different numerical schemes. In the hydrogeochemical domain, this algorithm
12 represents an interesting alternative to a fixed time step as shown by the various numerical
13 tests involving reactive transport and unsaturated flow.

14

15 **Key words:** Richardson extrapolation, adaptive time stepping, reactive transport, unsaturated
16 flow.

17

18 **1. Introduction**

19 Even if it can never replace experiments and field studies, modelling is of interest in many
20 science and engineering applications for scientific understanding and/or technological
21 management. In such an approach, Ordinary- or Partial Differential Equations (ODE and
22 PDE) are commonly used to develop mathematical models describing unsteady phenomena.

1 The resolution of these equations through numerical approximation leads to temporal, and
2 often spatial discretizations, that invariably introduce numerical errors.

3 Because analytical solutions of the problem are often not known, the error may not be
4 determined exactly and must be approximated in some way. The classical *a priori* theory
5 provides or tries to determine a bound on the discretization error before the computation of
6 the solution. It can become a challenge to obtain this bound with a sufficient accuracy. In fact,
7 this depends on the convergence rate and on the derivatives of the function, which are both
8 related to the particularities of the numerical scheme and the problem. Nevertheless *a priori*
9 methods have been developed in various numerical schemes implemented in problems
10 dealing with porous media. Recent applications are available (Schneid *et al.*, 2004 ; Bause
11 and Merz, 2005 ; Sun and Wheeler, 2005). *A posteriori* techniques give an estimation of the
12 error, as a function of the results just obtained. Either the error estimation is in accordance
13 with the numerical scheme (Babuska and Rheinboldt, 1978; Zienkiewicz and Zhu, 1992;
14 Bank and Smith, 1993), or it can be based on extrapolation techniques. In the last category
15 can be found order- or grid-extrapolation error estimators. Predictor corrector approach or
16 embedded Runge Kutta formulas are classical and efficient methods based on order
17 extrapolation. However, it can be difficult to program these methods, which need very
18 specific modifications depending on the complexity of the problem. Perhaps less adapted for
19 specific problems with nonlinearities or complex geometries, an interesting aspect of the
20 extrapolation-based error estimator is the possibility of its implementation in a wide variety
21 of calculation codes. From our point of view, this advantage justifies the attention we will
22 confer to the Richardson extrapolation method. Many papers deal with the Richardson
23 extrapolation, which is also referred to as the doubling method or h^2 - / h^4 -extrapolation.
24 Hence, considerations for using the doubling method can be for instance, the mathematical
25 convergence aspects (Ayati and Dupont, 2004; Aïd, 1999), the increase of accuracy order

1 (Abbasian and Carey, 1997) or the applicability to both time and spatial grids (Richards,
2 1997).

3 Focusing on the temporal approximation, a natural connection for error estimation is its
4 management through an optimal adaptive step size strategy. For the grid adaptation process, *a*
5 *priori* methods relate the truncation error to the step size evolution coefficient. Nonetheless
6 this relation is not necessary mathematically based, i.e., heuristic parameters are included to
7 increase or decrease the time step. Otherwise, the error estimation and the time marching
8 scheme are simply dissociated. Actually, an adaptive time stepping algorithm can also be
9 developed by means of heuristic methods. This means for instance that the number of
10 iterations achieved by an iterative solver can be used to define the next time step size. This
11 kind of procedure requires a good appreciation on both the physical problem solved and the
12 numerical method used.

13 In the view of temporal discretization error that invariably arises in numerical
14 approximations, control of the temporal error and optimisation of the time step are of great
15 importance. Consequently, our main contribution consists in showing the efficiency of the
16 Richardson extrapolation when combined with an *a priori* mathematical-based time stepping
17 strategy, which really differs from fixed or heuristic control. The principle and demonstration
18 of the Richardson extrapolation can be found in Richardson (1910 and 1927), Shampine
19 (1985) or in Hairer *et al.* (2000). The main results of this grid extrapolation technique are
20 depicted at the beginning of the paper to present the time stepping algorithm we focus on.
21 Then, several techniques dealing with the estimated error, the choice of the initial time step,
22 or the initialisation in an iterative process are proposed in the part entitled “optimisation of the
23 method”. The general formulation of the algorithm allows treatment of a large variety of
24 nonlinear physical processes with very different time scales. They also involve rather
25 different mathematical models and specific numerical solutions. Consequently, the proposed

1 time marching scheme and optimisations have been incorporated in different codes describing
2 reactive transport and unsaturated flow in porous media. Several test cases are performed to
3 illustrate the interest of monitoring both the local error and the time step size.

4

5 **2. Presentation of the method**

6 The main idea of the Richardson extrapolation is to solve the same problem first in one large
7 time step and secondly in two half time steps. These approximations are used to estimate the
8 local truncation error. This estimation can be used to define the length of the next time step
9 and therefore allows the development of an efficient automatic and adaptive time stepping
10 algorithm.

11

12 2.1. EXTRAPOLATION

13 Let equation (1) be the general form of an ODE, a system of ODE, a PDE or a system of
14 PDE.

$$15 \quad \frac{dy}{dt} = f(t, y(t)) \quad (1)$$

16 Assuming that the numerical method used is of p order in time, the difference between the
17 exact value of the variable, y_{Ex}^{n+1} , and the approximate one obtained in a single step, $\tilde{y}^{n+1,*}$,
18 at $t = n + 1$, is the error given by the approximation (Shampine, 1985 ; Hairer *et al.*, 2000):

$$19 \quad y_{Ex}^{n+1} - \tilde{y}^{n+1,*} = A \Delta t^{p+1} + O(\Delta t^{p+2}), \quad (2)$$

20 where A depends on the size of the derivatives of the solution in the interval.

1 For a sufficiently smooth function f , the local error of the two steps viewed as a single step
 2 can be expressed as follow (Shampine, 1985 ; Hairer *et al.*, 2000):

$$3 \quad y_{\text{Ex}}^{n+1} - \tilde{y}^{n+1,**} = 2 A \left(\frac{\Delta t}{2} \right)^{p+1} + O(\Delta t^{p+2}), \quad (3)$$

4 where $\tilde{y}^{n+1,**}$ is the variable obtained in two steps.

5 Hence, neglecting terms of order higher than $p + 1$ and combining equations (2) and (3)
 6 gives:

$$7 \quad A = \frac{2^p}{\Delta t^{p+1}} \frac{\tilde{y}^{n+1,**} - \tilde{y}^{n+1,*}}{2^p - 1} \quad (4)$$

8 An extrapolated solution, y_{extrap}^{n+1} , of order $p + 1$ can be calculated as follow:

$$9 \quad y_{\text{extrap}}^{n+1} = \tilde{y}^{n+1,**} + \frac{\tilde{y}^{n+1,**} - \tilde{y}^{n+1,*}}{2^p - 1} \quad (5)$$

10

11 2.2. TIME STEP SIZE ADAPTATION

12 The error of this method corresponds to the difference between the exact value of the variable,
 13 y_{Ex}^{n+1} , and the approximate one:

$$14 \quad \text{Err}_i(\Delta t) = \left| y_{\text{Ex},i}^{n+1} - y_{\text{extrap},i}^{n+1} \right|, i = 1, \dots, \text{NN}, \quad (6)$$

15 where NN refers to the dimension of the solution vector.

16 Because y_{extrap}^{n+1} is a local extrapolation of order $p + 1$, the following inequality is proposed:

$$17 \quad \text{Err}_i(\Delta t) \leq \left| y_{\text{Ex},i}^{n+1} - \tilde{y}_i^{n+1,**} \right|, i = 1, \dots, \text{NN} \quad (7)$$

18 Due to the fact that the accuracy of the extrapolated solution is unknown, inequality (7) is
 19 assumed to be correct and an estimated error, $\text{Err}_{\text{est}}(\Delta t)$, is then calculated. Hence, equations

1 (3) and (4) can be combined and then inserted in expression (7) to define the estimated error,
 2 which has to be gauged using the following inequality:

$$3 \quad \text{Err}_{\text{est},i}(\Delta t) = \left| \frac{\tilde{y}_i^{n+1,**} - \tilde{y}_i^{n+1,*}}{2^p - 1} \right| \leq \varepsilon_i = \varepsilon_a + \varepsilon_r \left| y_{\text{extrap},i}^{n+1} \right|, \quad i = 1, \dots, \text{NN} \quad (8)$$

4 In the previous equation, ε_i is the precision criterion we want to respect by adjusting the time
 5 step length. This mixed type of error control includes an absolute, ε_a , and a relative, ε_r ,
 6 truncation error tolerance.

7 Assuming that a calculation is performed with the time step $\Delta t_{\text{current}}$, an estimation of the
 8 error for this time step, $\text{Err}_{\text{est}}(\Delta t_{\text{current}})$, is calculated. This estimation can be smaller or
 9 greater than ε_i . Independently of the result obtained in equation (8), a new time step Δt_{new}
 10 must be calculated, either to estimate the variable y at time $n+2$ or to improve the accuracy at
 11 time $n+1$. Equation (4) and the definition of the estimated error give:

$$12 \quad A_i = \frac{2^p}{\Delta t_{\text{current}}^{p+1}} \text{Err}_{\text{est},i}(\Delta t_{\text{current}}), \quad i = 1, \dots, \text{NN} \quad (9)$$

13 Assuming that A is unchanged, i.e., f is considered (sometimes by extension) as smooth, the
 14 respect of the criterion (8) implies that the new time step should fulfill the equation (10):

$$15 \quad A_i = \frac{2^p}{\Delta t_{\text{new}}^{p+1}} \varepsilon_i, \quad i = 1, \dots, \text{NN} \quad (10)$$

16 Simplifying A in both equations (9) and (10) provides an estimation of the new time step:

$$17 \quad \Delta t_{\text{new}} = \sqrt[p+1]{\min_{i=1, \dots, \text{NN}} \left| \frac{\varepsilon_i}{\text{Err}_{\text{est},i}(\Delta t_{\text{current}})} \right|} \Delta t_{\text{current}} \quad (11)$$

18 If the current time step is sufficiently small, then the estimated error is smaller than the
 19 truncation error tolerance, so that the factor multiplying the current time step is greater than

1 one and the new time step consequently increases. Otherwise the calculation of y_{extrap}^{n+1} is then
2 rejected and should be repeated with a smaller time step.

3 An algorithm is also implemented to avoid large changes in the time step evolution around
4 output times (Kavetski *et al.*, 2001).

5

6 2.3. OPTIMISATION OF THE METHOD

7 Some adjustments should be made to increase the efficiency of the method. They deal with
8 the control of the time step size. Specifications due to the implementation of the Richardson
9 extrapolation for the resolution of nonlinear system or for the initialisation strategy are also
10 reported.

11

12 2.3.1. Relative test and tolerance on the precision criterion

13 For many applications described with PDE or systems of ODE, the variable y is a vector in
14 which component values can vary over several orders of magnitude. In this case, a strictly
15 relative test ($\epsilon_a=0$) can be attractive and has been kept in the examples performed in the next
16 section.

17 To avoid too many failed steps, a safety factor can be introduced to relax the time step size
18 evolution (Hairer *et al.*, 2000). An other possibility consists in relaxing the truncation error
19 test with a factor Tol:

$$20 \quad \text{Err}_{\text{est},i}(\Delta t) \leq \epsilon_i \times \text{Tol}, i = 1, \dots, NN \quad (12)$$

21 where Tol refers to a tolerance on the precision criterion, which lies between two and ten
22 (Tol = 5 in this paper).

1 Practically, this tolerance means that the calculation can be accepted even if the estimated
 2 error is Tol times larger than the precision criterion. The time step size control formula (11)
 3 does not change. Therefore, it may be noticed that even if a calculation is accepted with an
 4 estimated error higher than ε due to the tolerance, the next time step size is determined to give
 5 an estimated error equal to ε . This leads then to a reduction of the time step size.
 6 If the computing time of one time step is great, for PDE over a large domain for instance, this
 7 procedure avoids too many failed steps, which are CPU time consuming.

8

9 *2.3.2. Selection of the first time step*

10 The choice of the first time step is the most empirical decision for such a method. It can be
 11 selected from previous experiences in computation of similar problems or from other
 12 considerations such as stability conditions of the numerical method (Courant or Péclet number
 13 for example in the case of PDE).

14 A proposition for efficiently choosing the first time step is developed in the following
 15 part. Similar methods can be found in Hairer *et al.* (2000). Using a Taylor's expansion in the
 16 function f makes it possible to express A as:

17
$$A = \frac{\partial^p f}{\partial t^p} \tag{13}$$

18 Equation (10) is supposed to be valid for the first time step and assuming that the derivative
 19 of equation (13) and can be evaluated, the first time step is given by:

20
$$\Delta t_{\text{first}} = \sqrt[p+1]{2^p \min_{i=1, \dots, NN} \frac{\varepsilon_a + \varepsilon_r |y_{i,t=0}|}{\left| \frac{d^p f}{dt^p} \right|_{y_{i,t=0}}} } \tag{14}$$

1 For high order methods (fourth order Runge-Kutta for example), it seems that the best way to
 2 estimate the p derivative of f is to do this analytically. Nevertheless, if the p derivative is not
 3 known, we propose the following empirical relation to calculate the first time step length:

$$4 \quad \Delta t_{\text{first}} = (2^p - 1) \cdot \sqrt{\min_{i=1, \dots, NN} \left| \frac{\varepsilon_a + \varepsilon_r |y_{i,t=0}|}{f(t, y_i)_{t=\Delta \tilde{t}} - f(t, y_i)_{t=0}} \right|} \times 2^p \Delta \tilde{t}, \quad (15)$$

5 where $\Delta \tilde{t}$ has to be chosen sufficiently small depending on the characteristic time of the
 6 simulation and the precision criterion.

7 In the case of the first order method, the derivative is also easier to evaluate numerically with
 8 equation (15).

9

10 2.3.3. Implementation for nonlinear ODE or PDE

11 The algorithm based on Richardson extrapolation can also be used for nonlinear problem. The
 12 linearization with iterative methods requires an initial guess, which can be estimated with a
 13 predictor technique for the first big step and trapezoidal rules for the two half steps.

14 Difficulties can be observed when secondary variables or mass balance have to be calculated
 15 with the extrapolated solution, which does not necessary respect the convergence criterion
 16 checked by $\tilde{y}^{n+\frac{1}{2}}$, $\tilde{y}^{n+1,*}$ and $\tilde{y}^{n+1,**}$. The examples developed in the next section provide
 17 interesting illustrations of this kind of problem and the specific ways to solve them. The first
 18 idea consists in solving again the system with the extrapolated solution as an initial guess and
 19 especially with a higher order method. If a first order Euler discretization is initially used, it
 20 means that a Crank-Nicolson scheme should be implemented. This strategy maintains the
 21 accuracy's order of y_{extrap}^{n+1} . A technique, that has also been tested, is a generalization of the
 22 extrapolation for all the variables used.

23

1 **3. Examples**

2 Two examples are solved with the optimised algorithm. They deal successively with reactive
3 transport and unsaturated flow. Reactive transport modelling leads to a differential and
4 algebraic system representing the coupled solution of chemical reaction and solute transport
5 equations. On the one hand, the advective-dispersive solute transport equation behaves as
6 hyperbolic when transport is advection dominated, or parabolic when dispersion dominates.
7 On the other hand, instantaneous equilibrium chemistry is described by a nonlinear algebraic
8 system. The first test case includes field observations published by Valocchi *et al.* (1981) and
9 serves subsequently as a benchmark problem for testing reactive transport codes. It deals with
10 an advection dominated transport associated with nonlinear cation-exchange reactions.
11 Besides, unsaturated flow is described with a highly nonlinear parabolic equation, which is
12 really challenging to solve when sharp infiltration fronts are simulated. Therefore, the
13 classical benchmark scenario described by Celia *et al.* (1990) is used to check the robustness
14 of the numerical method.

15 In each part, after a short presentation of the method developed to treat the problem, we
16 specify the model traditionally used in the context, the implementation of the algorithm, and
17 the test case with its conclusions.

18 The ability of the proposed time marching scheme to control temporal errors is assessed
19 using two kinds of error measurements. The first one, which could be called Cumulated
20 Relative Error Measure versus the reference solution (CREM_{ref}), collects the relative error
21 produced at each time step until the end of simulation:

$$22 \quad \text{CREM}_{\text{ref}} = \sum_{t=1}^{\text{Nb time steps}} \left| \frac{y_{\text{NN},t} - y_{\text{ref},\text{NN},t}}{y_{\text{ref},\text{NN},t}} \right|, \quad (16)$$

1 where $y_{\text{ref},\text{NN},t}$ refers to the reference solution at node NN and time t. It corresponds to elution
2 curve.

3 The differences between the profiles of the computational results and the reference solution
4 can be integrated along the spatially discretized domain at any observation time where the
5 reference is known. This Relative Error Measure ($\text{REM}_{\text{ref}}^{n+1}$) is defined at time $n + 1$ with :

$$6 \quad \text{REM}_{\text{ref}}^{n+1} = \sum_{i=1}^{\text{NN}} \left| \frac{y_i^{n+1} - y_{\text{ref},i}^{n+1}}{y_{\text{ref},i}^{n+1}} \right|, \quad (17)$$

7 where $y_{\text{ref},i}^{n+1}$ is the reference solution at time $n + 1$ and node i .

8

9 3.1. REACTIVE TRANSPORT WITH OPERATOR SPLITTING

10 The Richardson extrapolation is usually applied to steady state problems to estimate the
11 spatial truncation error and to adapt the grid size. Also, it has been carried out for advection
12 diffusion problems (Natividad and Stynes, 2003) and for advection-diffusion-reaction
13 problems describing laminar flames (Claramunt *et al.*, 2004). Richardson extrapolation has
14 also been used to increase the temporal accuracy of reaction-diffusion equations solved by a
15 global approach (Liao *et al.*, 2002). Nevertheless, these authors did not use the ability of
16 Richardson extrapolation to provide adaptive time stepping. Therefore, the algorithm
17 combining the time step selection and the error estimated with the Richardson extrapolation
18 could be originally developed in the context of transient flow for hydrogeochemical
19 calculations. The control of the error is all the more important because the standard non
20 iterative operator splitting approach used in this work can introduce some temporal error due
21 to the discretization (Carrayrou *et al.*, 2003).

22

1 *3.1.1. Presentation of the model*

2 The reactive transport equation for porous media is written, under the instantaneous
3 equilibrium assumption (Rubin, 1983; Steefel and Mcquarrie, 1996):

4
$$\frac{\partial(\omega T_d + \rho_s T_f)}{\partial t} = \nabla \cdot [D \cdot \nabla(T_d)] - U \cdot \nabla(T_d), \quad (18)$$

5 where T_d is the total mobile (dissolved) component concentration, T_f is the total immobile
6 (fixed) component concentration, ω is the porosity of the media, ρ_s is the density of the solid
7 matrix, U is the Darcy velocity, and D is the dispersion coefficient.

8 For a given total mobile plus immobile concentration of components, solving the algebraic
9 system describing instantaneous equilibrium gives the concentration of each component, each
10 species, and then the distribution of the component between the mobile and immobile phases.
11 This is summarized as:

12
$$\begin{cases} T_d = f_d(\omega T_d + \rho_s T_f) \\ T_f = f_f(\omega T_d + \rho_s T_f) \end{cases}, \quad (19)$$

13 where f_d , respectively f_f , represent the nonlinear algebraic systems describing chemistry in
14 aqueous and solid phases, respectively.

15 Combining the transport equation (18) and the chemical laws (19) leads to a nonlinear
16 differential algebraic system. One of the simplest way to solve this system is to split it
17 between both transport and chemistry operator (Yeh and Tripathi, 1989; Carrayrou *et al.*,
18 2004). The standard non-iterative scheme has been used in this work. Because the error
19 introduced by this operator splitting approach depends on time discretization (Carrayrou *et*
20 *al.*, 2003), the Richardson extrapolation and the associated adaptive time marching scheme
21 provide an interesting means to control the error.

1 In this work, the transport operator includes an implicit first order time discretization and a
 2 finite volume method. The transport operator is first solved for all components assuming they
 3 are not reactive (20):

$$4 \quad \omega \frac{T_d^{n+1,T} - T_d^n}{\Delta t} = \nabla \cdot [D \cdot \nabla (T_d)] - U \cdot \nabla (T_d) \quad (20)$$

5 This leads to an intermediate solution $T_d^{n+1,T}$, which is used as an initial condition for the
 6 chemistry operator:

$$7 \quad \begin{cases} T_d^{n+1} = f_d \left(\omega T_d^{n+1,T} + \rho_s T_f^n \right) \\ T_f^{n+1} = f_f \left(\omega T_d^{n+1,T} + \rho_s T_f^n \right) \end{cases} \quad (21)$$

8 The chemistry operator is solved at each grid point using a combined algorithm associating
 9 the definition of the chemical allowed intervals, a preconditioning by positive continuous
 10 fraction method and a Newton-Raphson method (Carrayrou *et al.*, 2002). The solutions of the
 11 chemistry operator T_d^{n+1} and T_f^{n+1} are the solutions of the standard non iterative scheme at
 12 the time step $n + 1$. It is well known that this scheme increases the numerical diffusion, but is
 13 also useful to solve the convergence problems related to iterative schemes.

14

15 3.1.2. Implementation of the time stepping method with the Richardson extrapolation

16 As presented previously, the overall system (20) and (21) is solved three times for each time
 17 step leading to $T_d^{n+1,*}$, $T_d^{n+1,**}$, $T_f^{n+1,*}$ and $T_f^{n+1,**}$. The extrapolation (5) is done for
 18 both variables T_d^{n+1} and T_f^{n+1} at each cell of the space discretization and for each chemical
 19 component. Estimated errors are calculated for both the total dissolved and the total fixed
 20 concentrations for each component and at each cell of the mesh. All of them have to verify
 21 equation (12) and the smallest time step coming from equation (11) is used. Therefore, the

1 required precision for all the variables is ensured at the current time and should be at the next
 2 step.

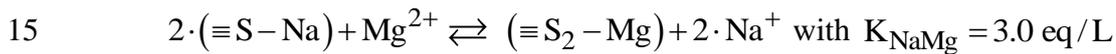
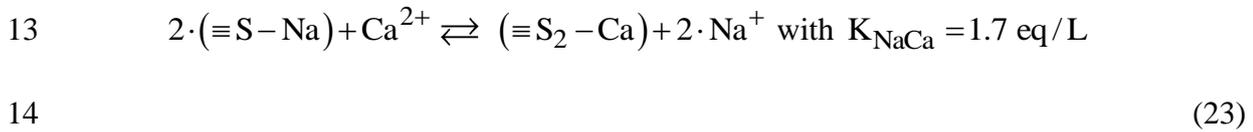
3 Because the extrapolated total concentrations calculated with equation (5) do not respect
 4 the chemical equilibrium condition, the instantaneous equilibrium system (21) is solved one
 5 more time after the extrapolated solution (22) is known.

$$6 \quad \begin{cases} T_{di}^{n+1} = 2T_{di}^{n+1,**} - T_{di}^{n+1,*} \\ T_{fi}^{n+1} = 2T_{fi}^{n+1,**} - T_{fi}^{n+1,*} \end{cases} \quad (22)$$

7

8 3.1.3. Test case and discussion

9 An experiment described by Valocchi *et al.* (1981) has been tested numerically. It presents the
 10 injection of water into the aquifer at the Palo Alto Baylands Field site. The chemical
 11 phenomena concern ion exchange, described by equation (23). Physico-chemical conditions
 12 of the test case are given in Table I. Cl⁻ appears in this table to ensure electroneutrality.



16 In Figure 1, elution curves for calcium and magnesium given by the adaptive time step
 17 with and without extrapolation are compared. A reference solution is obtained with a very
 18 small precision criterion and is validated by comparison with experimental data given by
 19 Valocchi *et al.* (1981). This figure illustrates clearly the increase of precision induced by the
 20 extrapolation explained in equation (5). The extrapolated elution curve is closer to the
 21 reference solution than the non extrapolated one.

22 Using the extrapolated solution (5) or (22) leads to a more accurate solution at the cost of
 23 one more solution of the instantaneous equilibrium. Although this involves additional

1 computation, the extrapolation with adaptive time stepping presented in this work is very
2 efficient, as can be seen in Figure 2. $CREM_{ref}$ has been calculated for each component and the
3 maximum value has been plotted. This figure shows that, as expected from the theory, a fixed
4 time step and an adaptive time step without extrapolation leads to a first order relation
5 between precision and CPU time. On the other hand, the combination of extrapolation and an
6 adaptive time step gives a second order relation between precision and CPU time.

7

8 3.2. UNSATURATED FLOW

9 The Richardson extrapolation has been studied for groundwater flow applications. Guarracino
10 *et al.* (2004) used the pressure head form of Richards' equation and associated the
11 extrapolation with a Crank-Nicolson scheme to reach a third order accurate temporal scheme.
12 The authors did not insert a time-marching scheme and verified principally the accuracy and
13 the mass conservation properties. Besides, Basombrio *et al.* (2006) developed a competitive
14 non-iterative algorithm combining Crank-Nicolson method, Richardson extrapolation and a
15 single Newton's iteration. However, the amplification or reduction factor for the time step is
16 quite heuristic.

17

18 3.2.1. Presentation of the model

19 The last example deals with the infiltration of water through an initially dry porous media.
20 The mathematical model used to describe this physical problem is given by equations (24)
21 and (25).

22 Darcy-Buckingham's law defines the water flux in the domain:

$$23 \quad \mathbf{q} = -\mathbf{K}(\mathbf{h}) \cdot \nabla(\mathbf{h} - z), \quad (24)$$

1 where q is the macroscopic fluid flux density, K is the hydraulic conductivity, h is the
 2 pressure head and z is the depth, taken to be positive downwards.

3 The mixed form of Richards' equation represents the mass conservation of water:

$$4 \quad \frac{\partial \theta(h)}{\partial t} + \nabla \cdot q = f_v, \quad (25)$$

5 where θ is the volumetric water content, t is time, f_v is a source/sink term, and q is the water
 6 flux previously defined.

7 To complete this description, the interdependencies of the pressure head, the hydraulic
 8 conductivity and the water content must be characterized using constitutive relations. The
 9 standard Mualem - van Genuchten model (1980) is used :

$$10 \quad S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \begin{cases} \frac{1}{\left(1 + (\alpha|h|)^n\right)^{1-(1/n)}} & h < 0 \\ 1 & h \geq 0 \end{cases}, \quad (26)$$

$$K(S_e) = K_s S_e^{1/2} \left[1 - \left(1 - S_e^{(n/(n-1))}\right)^{1-(1/n)} \right]^2$$

11 where θ_s and θ_r are the saturated and residual volumetric water contents, respectively, α is a
 12 parameter related to the mean pore size and n a parameter reflecting the uniformity of the
 13 pore-size distribution ($n > 1$).

14 The numerical technique implemented is a traditional finite volume method for the spatial
 15 discretization and a backward Euler scheme for the temporal approximation. The interblock
 16 conductivities, which appear for the calculation of the flux between adjacent cells of the
 17 mesh, are calculated either with a geometric or an arithmetic mean. Due to the nonlinearities
 18 of the constitutive relationships, we have to solve nonlinear partial differential equations. The
 19 discretized system of PDE is linearized using the modified Picard (or fixed-point) method
 20 (Lehmann and Ackerer, 1998). Iterations proceed until the mixed absolute-relative
 21 convergence test is satisfied:

$$1 \quad \left| h_i^{n+1,k+1} - h_i^{n+1,k} \right| \leq \tau_r \left| h_i^{n+1,k} \right| + \tau_a, \quad i = 1, \dots, NN, \quad (27)$$

2 where k denotes the iteration number. τ_a and τ_r refer to absolute and relative convergence
3 criteria. They are hundred times smaller than the corresponding criteria on the truncation error
4 tolerance.

5

6 *3.2.2. Implementation of the time stepping method with the Richardson extrapolation*

7 After each time step, the pressure head and the water content are updated with the Richardson
8 extrapolation:

$$9 \quad \begin{aligned} h^{n+1} &= 2h^{n+1,**} - h^{n+1,*} \\ \theta^{n+1} &= 2\theta^{n+1,**} - \theta^{n+1,*} \end{aligned} \quad (28)$$

10 The temporal accuracy of the scheme has been considered as an important criterion.
11 However, the ability of the code to conserve good global mass balance is also essential. The
12 extrapolated solutions presented in (28) have no real physical meaning. To avoid a large mass
13 balance error, we suggested in a previous section to again solve the system with the
14 extrapolated solution at each time step with a higher order numerical scheme. Another
15 technique consists of extrapolating the flux.

16

17 *3.2.3. Test case and discussion*

18 We simulate a sharp infiltration front in a homogeneous dry porous media as proposed by
19 Celia *et al.* (1990). The initial, boundary conditions and the relevant material properties are
20 summarized in Table II.

21 Figure 3 displays pressure head profiles after a half day of infiltration. The dense grid
22 solution provided by Celia *et al.* (1990) has also been plotted to show the convergence of the
23 method when the nodal spacing decreases. The interblock conductivity is averaged using the

1 arithmetic mean. Figure 3 illustrates the interest of the extrapolation compared to fixed time
2 step, time stepping scheme without extrapolation, or a heuristic time marching scheme based
3 on the behaviour of the nonlinear iteration.

4 To investigate temporal aspects of the Richardson extrapolation in unsaturated water
5 movement, a surrogate “reference” solution is evaluated numerically using the adaptive
6 scheme with a relative error tolerance of $\varepsilon_r = 10^{-8}$ and a convergence criterion of $\tau_r = 10^{-10}$. An
7 identical fixed-grid with a nodal spacing of 1cm and a geometric interblock conductivity are
8 used for all simulations thus making it possible to neglect spatial errors and to focus only on
9 the temporal errors.

10 The proposed adaptive time stepping method allows the control of the temporal error with
11 the relative tolerance criterion ε_r . An improvement of the precision coincides with the
12 automatic decrease of the step size by the algorithm as depicted in Figure 4. It shows a very
13 classical evolution of the step size.

14 We observe that reducing the relative precision criterion by a factor of one hundred leads to a
15 decrease of ten times the mean step size. In fact, the mean length of the time step reaches 450
16 seconds for the worst precision considered and just above 1 second for the largest.

17 To analyse the efficiency of the method, the relative error has been plotted as a function of the
18 CPU time. Figure 5 is hence obtained by adjusting the criterion ε_r for the adaptive scheme or
19 varying the time step size for the fixed step method. As shown in the previous example,
20 Figure 5 clearly illustrates that the algorithm using the Richardson extrapolation leads faster
21 to a higher accuracy. Hence, the adaptive time stepping method becomes competitive when
22 associated to the extrapolation.

23 It is all the more interesting because the mass balance can be correctly managed when
24 some precautions are taken into account. With a constant nodal spacing, the formula
25 commonly used to calculate the global mass balance is (Celia *et al.*, 1990):

$$1 \quad \text{GMB}(\%) = \left| \frac{\left[\frac{1}{2} \times (\theta_1^{n+1} - \theta_1^0) + \sum_{i=2}^{N_e} (\theta_i^{n+1} - \theta_i^0) + \frac{1}{2} \times (\theta_{N_n}^{n+1} - \theta_{N_n}^0) \right] \times \Delta x}{\sum_{j=\text{time}_{\text{init}}}^{\text{time}_{\text{print}}} (q_1^j - q_{N_n}^j) \times \Delta t^j} - 1 \right| \times 100 \quad (29)$$

2 The fluxes that appear in the previous equation can be estimated using a variety of means. If
3 the extrapolation is used at each time step for the error estimation and the variable adaptation,
4 the flux can be calculated through a first (totally implicit formulation) or a second (Crank-
5 Nicolson formulation) order approximation. Nevertheless, Figure 6 shows that the best
6 technique is to also extrapolate the flux. If the variables obtained in two time steps are
7 retained, Figure 6 also illustrates that the flux can not be viewed as a general flux on this
8 period calculated with the last pressure. This must be calculated after each half time step.

9

10 **4. Conclusion**

11 After a brief presentation of the Richardson extrapolation, this paper has described a general
12 way of taking into account the truncation error for an efficient management of the step size
13 evolution. The automatic time marching scheme is mathematically based and the user must
14 only define the accepted tolerance on the temporal discretization error. Another important
15 aspect of this work deals with optimisation strategies to estimate the first time step, to
16 implement the algorithm in a nonlinear system, or to introduce flexibility in the time
17 evolution, i.e., to avoid too many rejected time steps. The whole of our approach was
18 developed in a context that could allow its application to diverse numerical fields. This
19 algorithm can easily take into account specificities of a given problem.

20 In fact, all our propositions have been implemented in rather different codes that model
21 kinetic chemistry, reactive transport, or unsaturated flow. The global formulation of the

1 algorithm allows treatment of notably different mathematical models. The proposed method is
2 an efficient way of adapting the time step size and of estimating the error for many problems
3 frequently encountered in porous media.

4 The use of extrapolation technique appears advantageous. First, the examples show that the
5 accuracy has been improved. For a given error calculated with a reference solution, the
6 extrapolation of the variables yields a decrease in computation time compared to both a fixed
7 time step or an adaptive evolution without extrapolation. Second, although extrapolation may
8 not always have physical meaning, it can still conserve properties as illustrated in our
9 example mass balance calculation.

10 Future research could deal with a comparison of different time marching schemes, a spatial
11 adaptation coupled with the time stepping strategy, or a separate time stepping procedure for
12 the transport and reaction operators involved in the splitting method.

13

14

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17 CNRS Strasbourg) for their suggestions for improvements.

18

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Table I: Physico-chemical parameters for the reactive transport test-case.

3

	Cl ⁻	Na ⁺	Ca ²⁺	Mg ²⁺
Initial (mg.l ⁻¹)	5700	1990	444	436
Injected (mg.l ⁻¹)	320	216	85	12
Cation exchange capacity (meq.g ⁻¹)			0.1	
Bulk density (g.l ⁻¹)	1875			
Porosity	0.25			
Dispersivity (m)	2.96			
Length of the domain (m)	16			
Darcy velocity (m.s ⁻¹)	0.2525			
Spatial discretization (m)	0.1			

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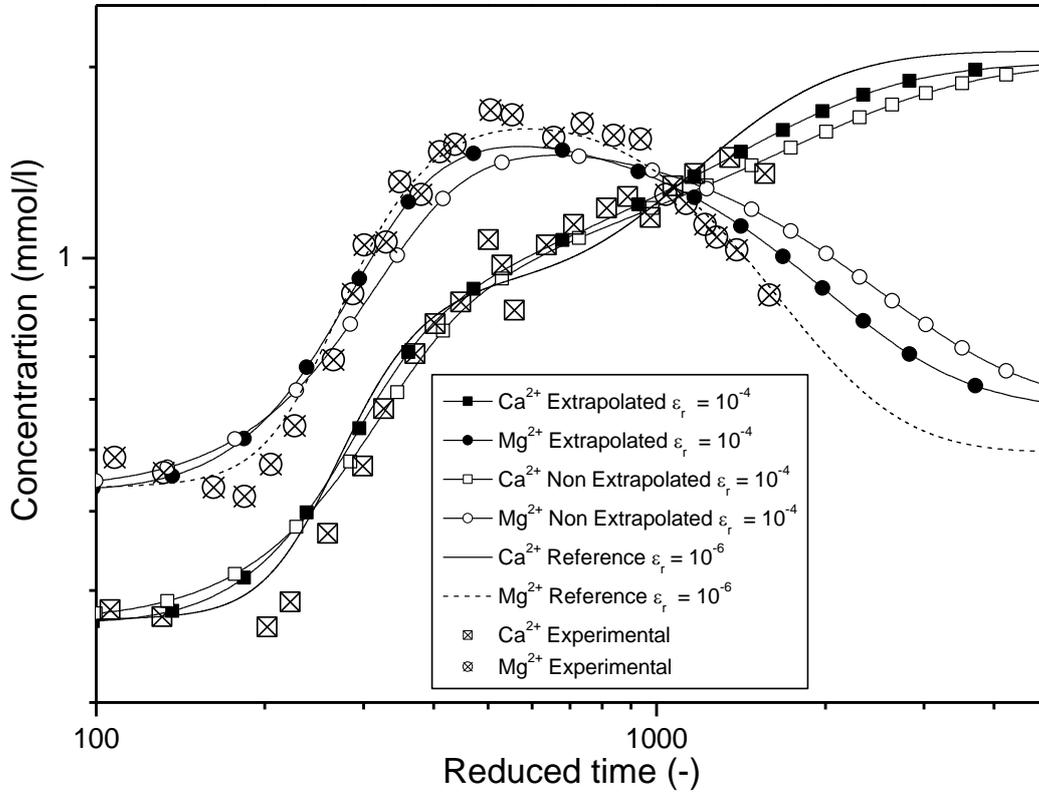
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Figure 1: Reactive transport test case: comparison of the elution curves.

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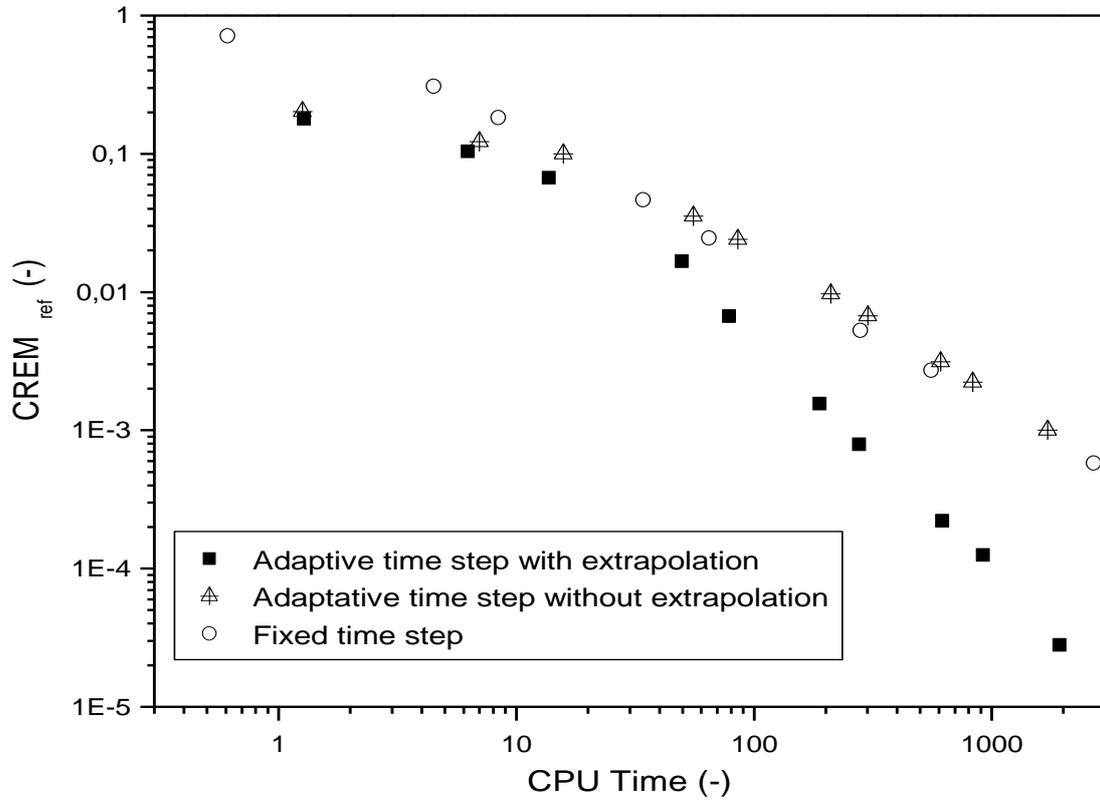
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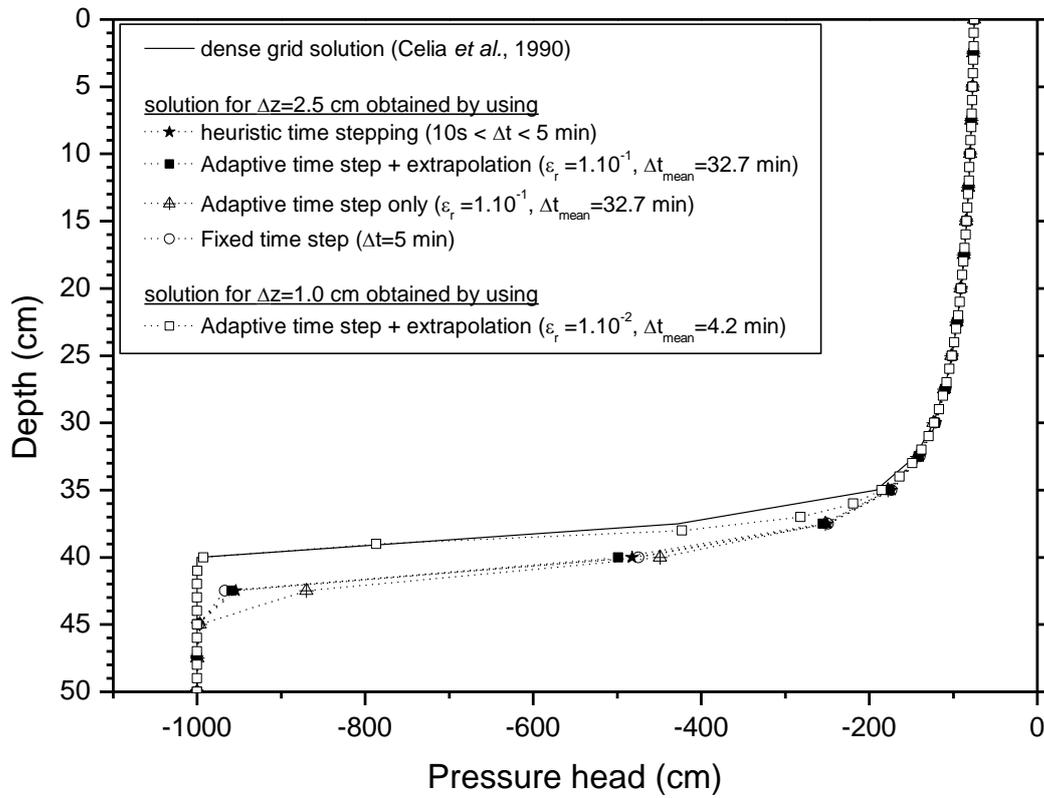
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4 **Figure 2:** Reactive transport test case: evolution of the Cumulated Relative Error Measure
5 (CREM_{ref}) versus the required CPU time.

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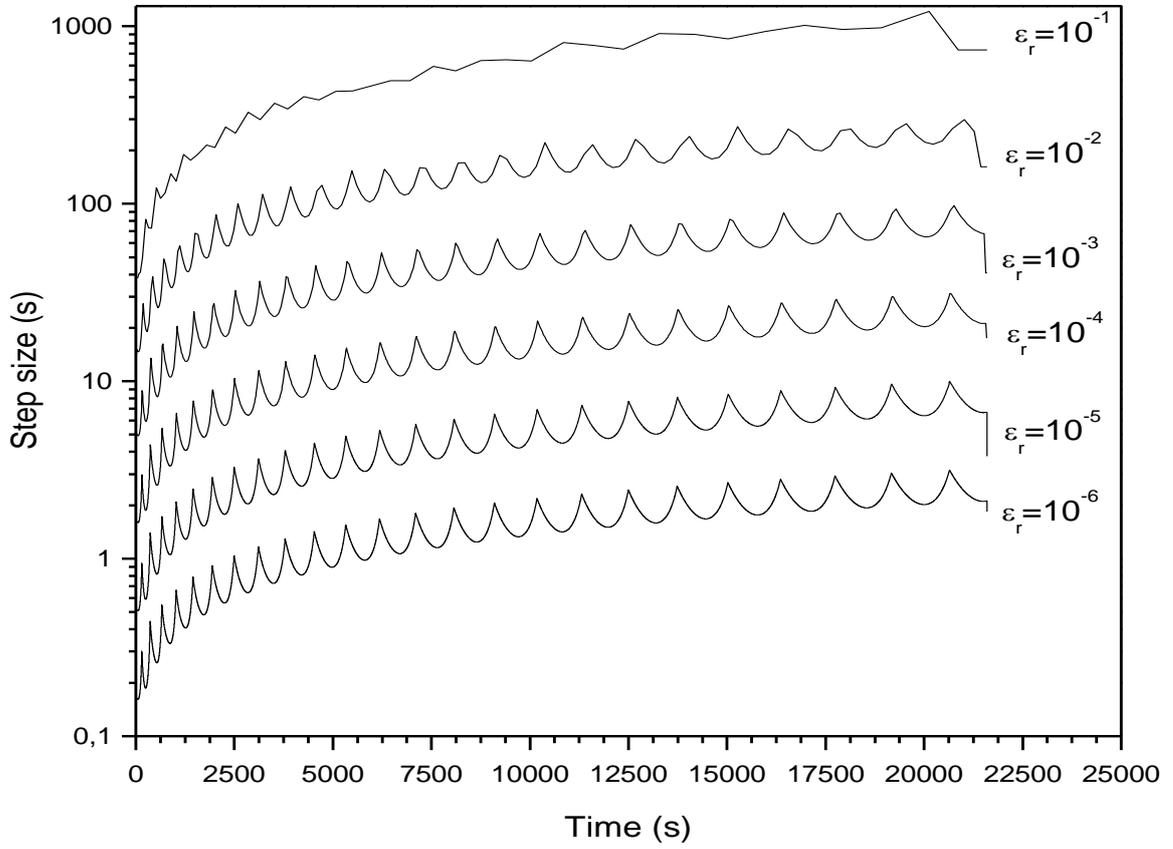


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3 **Figure 3:** Unsaturated flow test case: Pressure head profiles after 12 hours of infiltration.

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4 **Figure 4:** Unsaturated flow test case: evolution of the time step size versus time for the
5 scheme with extrapolation.

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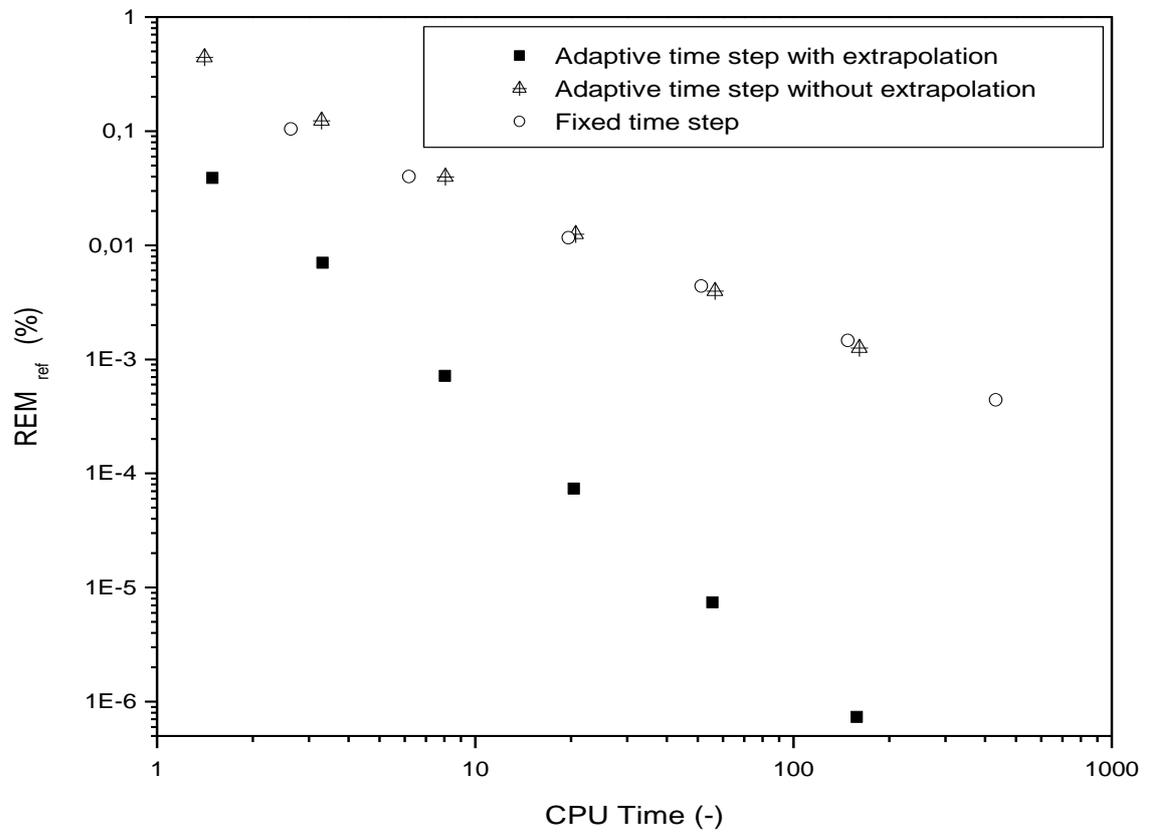
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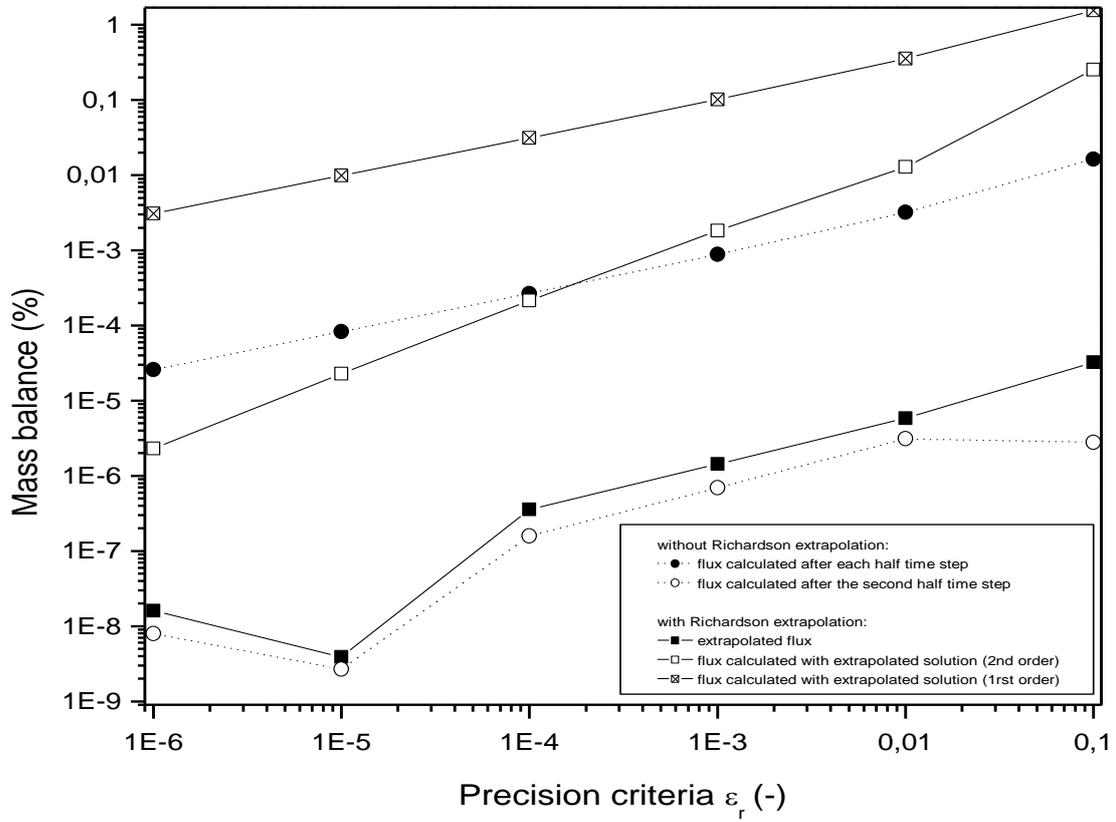
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4 **Figure 5:** Unsaturated flow test case: evolution of the relative error versus the required CPU
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5 relative precision criteria: comparisons of different techniques for the flux approximation.

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