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

Keywords Richardson extrapolation · Adaptive time stepping · Reactive transport · Unsaturated flow

1 Introduction

Even if it can never replace experiments and field studies, modelling is of interest in many science and engineering applications for scientific understanding and/or technological management. In such an approach, ordinary- or partial-differential equations (ODE and PDE) are commonly used to develop mathematical models describing unsteady phenomena. The resolution of these equations through numerical

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approximation leads to temporal, and often spatial discretizations, that invariably introduce numerical errors.

Since analytical solutions of the problem are often not known, the error may not be determined exactly and must be approximated in some way. The classical a priori theory provides or tries to determine a bound on the discretization error before the computation of the solution. It can become a challenge to obtain this bound with a sufficient accuracy. In fact, this depends on the convergence rate and on the derivatives of the function, which are both related to the particularities of the numerical scheme and the problem. Nevertheless a priori methods have been developed in various numerical schemes implemented in problems dealing with porous media. Recent applications are available (Schneid et al. 2004; Bause and Merz 2005; Sun and Wheeler 2005). A posteriori techniques give an estimation of the error, as a function of the results just obtained. Either the error estimation is in accordance with the numerical scheme (Babuska and Rheinboldt 1978; Zienkiewicz and Zhu 1992; Bank and Smith 1993), or it can be based on extrapolation techniques. In the last category can be found order- or grid-extrapolation error estimators. Predictor corrector approach or embedded Runge Kutta formulas are classical and efficient methods based on order extrapolation. However, it can be difficult to programme these methods, which need very specific modifications depending on the complexity of the problem. Perhaps less adapted for specific problems with non-linearities or complex geometries, an interesting aspect of the extrapolation-based error estimator is the possiblility of its implementation in a wide variety of calculation codes. From our point of view, this advantage justifies the attention we will confer to the Richardson extrapolation method. Many papers deal with the Richardson extrapolation, which is also referred to as the doubling method or h^2-/h^4-extrapolation. Hence, considerations for using the doubling method can be for instance, the mathematical convergence aspects (Ayati and Dupont 2004,Aïd 1999), the increase of accuracy order (Abbasian and Carey 1997) or the applicability to both time and spatial grids (Richards 1997).

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

In the view of temporal discretization error that invariably arises in numerical approximations, control of the temporal error and optimization of the time step are of great importance. Consequently, our main contribution consists in showing the efficiency of the Richardson extrapolation when combined with an a priori mathematical-based time stepping strategy, which really differs from fixed or heuristic control. The principle and demonstration of the Richardson extrapolation can be found in Richardson (1910; 1927), Shampine (1985) or in Hairer et al. (2000). The main results of this grid-extrapolation technique are depicted at the beginning of the article to present the time stepping algorithm we focus on. Then, several techniques dealing with the estimated error, the choice of the initial time step, or the initialization in an iterative process are proposed in the part entitled "optimization of the method".

The general formulation of the algorithm allows treatment of a large variety of non-linear physical processes with very different time scales. They also involve rather different mathematical models and specific numerical solutions. Consequently, the proposed time-marching scheme and optimizations have been incorporated in different codes describing reactive transport and unsaturated flow in porous media. Several test cases are performed to illustrate the interest of monitoring both the local error and the time step size.

2 Presentation of the method

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

2.1 Extrapolation

Let Eq. 1 be the general form of an ODE, a system of ODE, a PDE or a system of PDE.

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f\left(t, y\left(t\right)\right). \tag{1}$$

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

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

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

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

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

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

Hence, neglecting terms of order higher than $p + 1$ and combining Eqs. 2 and 3 gives:

$$A = \frac{2^p}{\Delta t^{p+1}} \frac{\tilde{y}^{n+1,**} - \tilde{y}^{n+1,*}}{2^p - 1}. \tag{4}$$

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

$$y_{\mathrm{extrap}}^{n+1} = \tilde{y}^{n+1,**} + \frac{\tilde{y}^{n+1,**} - \tilde{y}^{n+1,*}}{2^p - 1}. \tag{5}$$

2.2 Time step size adaptation

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

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

where NN refers to the dimension of the solution vector.

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

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

Due to the fact that the accuracy of the extrapolated solution is unknown, inequality (7) is assumed to be correct and an estimated error, $\text{Err}_{\text{est}}\left(\Delta t\right)$, is then calculated. Hence, Eqs. 3 and 4 can be combined and then inserted in expression (7) to define the estimated error, which has to be gauged using the following inequality:

$$\text{Err}_{\text{est},i}\left(\Delta t\right) = \left| \frac{\tilde{y}_i^{n+1,**} - \tilde{y}_i^{n+1,*}}{2^p - 1} \right| \leq \varepsilon_i = \varepsilon_{\text{a}} + \varepsilon_{\text{r}} \left| y_{\text{extrap},i}^{n+1} \right|, \quad i = 1, \ldots, \text{NN}. \tag{8}$$

In the previous equation, ε_i is the precision criterion we want to respect by adjusting the time step length. This mixed type of error control includes an absolute, ε_{a}, and a relative, ε_{r}, truncation error tolerance.

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

$$A_i = \frac{2^p}{\Delta t_{\text{current}}^{p+1}} \text{Err}_{\text{est},i}\left(\Delta t_{\text{current}}\right), \quad i = 1, \ldots, \text{NN}. \tag{9}$$

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

$$A_i = \frac{2^p}{\Delta t_{\text{new}}^{p+1}} \varepsilon_i, \quad i = 1, \ldots, \text{NN}. \tag{10}$$

Simplifying A in both Eqs. 9 and 10 provides an estimation of the new time step:

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

If the current time step is sufficiently small, then the estimated error is smaller than the truncation error tolerance, so that the factor multiplying the current time step is greater than one and the new time step consequently increases. Otherwise the calculation of y_{extrap}^{n+1} is then rejected and should be repeated with a smaller time step.

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

2.3 Optimization of the method

Some adjustments should be made to increase the efficiency of the method. They deal with the control of the time step size. Specifications due to the implementation of the Richardson extrapolation for the resolution of non-linear system or for the initialization strategy are also reported.

2.3.1 Relative test and tolerance on the precision criterion

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

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

$$\mathrm{Err}_{\mathrm{est},i}\,(\Delta t) \leq \varepsilon_i \times \mathrm{Tol}, \quad i = 1, \ldots, \mathrm{NN}, \tag{12}$$

where Tol refers to a tolerance on the precision criterion, which lies between 2 and 10 (Tol = 5 in this article).

Practically, this tolerance means that the calculation can be accepted even if the estimated error is Tol times larger than the precision criterion. The time step size control formula (11) does not change. Therefore, it may be noticed that even if a calculation is accepted with an estimated error higher than ε due to the tolerance, the next time step size is determined to give an estimated error equal to ε. This leads then to a reduction of the time step size.

If the computing time of one time step is great, for PDE over a large domain for instance, this procedure avoids too many failed steps, which are CPU time consuming.

2.3.2 Selection of the first time step

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

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

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

Equation 10 is supposed to be valid for the first time step and assuming that the derivative of Eq. 13 and can be evaluated, the first time step is given by

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

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

$$\Delta t_{\text{first}} = \left(2^p - 1\right) \cdot \sqrt{\min_{i=1,\ldots,\text{NN}} \left| \frac{\varepsilon_{\text{a}} + \varepsilon_{\text{r}} \left| y_{i,t=0} \right|}{f\left(t, y_i\right)_{t=\Delta\widetilde{t}} - f\left(t, y_i\right)_{t=0}} \right| \times 2^p \Delta\widetilde{t}}, \tag{15}$$

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

In the case of the first order method, the derivative is also easier to evaluate numerically with Eq. 15.

2.3.3 Implementation for non-linear ODE or PDE

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

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

3 Examples

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

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

The ability of the proposed time-marching scheme to control temporal errors is assessed using two kinds of error measurements. The first one, which could be called cumulated relative error measure versus the reference solution ($\mathrm{CREM_{ref}}$), collects the relative error produced at each time step until the end of simulation:

$$\mathrm{CREM_{ref}} = \sum_{t=1}^{\text{Nb time steps}} \left| \frac{y_{\mathrm{NN},t} - y_{\mathrm{ref,NN},t}}{y_{\mathrm{ref,NN},t}} \right|, \tag{16}$$

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

The differences between the profiles of the computational results and the reference solution can be integrated along the spatially discretized domain at any observation time where the reference is known. This relative error measure ($\mathrm{REM_{ref}^{n+1}}$) is defined at time $n+1$ with:

$$\mathrm{REM_{ref}^{n+1}} = \sum_{i=1}^{\mathrm{NN}} \left| \frac{y_i^{n+1} - y_{\mathrm{ref},i}^{n+1}}{y_{\mathrm{ref},i}^{n+1}} \right|, \tag{17}$$

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

3.1 Reactive transport with operator splitting

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

3.1.1 Presentation of the model

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

$$\frac{\partial \left(\omega T_{\mathrm{d}} + \rho_{\mathrm{s}} T_{\mathrm{f}}\right)}{\partial t} = \nabla \cdot \left[D \cdot \nabla \left(T_{\mathrm{d}}\right)\right] - U \cdot \nabla \left(T_{\mathrm{d}}\right), \tag{18}$$

where T_{d} is the total mobile (dissolved) component concentration, T_{f} is the total immobile (fixed) component concentration, ω is the porosity of the media, ρ_{s} is the density of the solid matrix, U is the Darcy velocity and D is the dispersion coefficient.

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

$$\begin{cases} T_{\mathrm{d}} = f_{\mathrm{d}}\left(\omega T_{\mathrm{d}} + \rho_{\mathrm{s}} T_{\mathrm{f}}\right) \\ T_{\mathrm{f}} = f_{\mathrm{f}}\left(\omega T_{\mathrm{d}} + \rho_{\mathrm{s}} T_{\mathrm{f}}\right) \end{cases}, \tag{19}$$

where f_{d}, respectively f_{f}, represent the non-linear algebraic systems describing chemistry in aqueous and solid phases, respectively.

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

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

$$\omega \frac{T_{\mathrm{d}}^{n+1,T} - T_{\mathrm{d}}^{n}}{\Delta t} = \nabla \cdot \left[D \cdot \nabla \left(T_{\mathrm{d}}\right)\right] - U \cdot \nabla \left(T_{\mathrm{d}}\right). \tag{20}$$

This leads to an intermediate solution $T_{\mathrm{d}}^{n+1,T}$, which is used as an initial condition for the chemistry operator:

$$\begin{cases} T_{\mathrm{d}}^{n+1} = f_{\mathrm{d}}\left(\omega T_{\mathrm{d}}^{n+1,T} + \rho_{\mathrm{s}} T_{\mathrm{f}}^{n}\right) \\ T_{\mathrm{f}}^{n+1} = f_{\mathrm{f}}\left(\omega T_{\mathrm{d}}^{n+1,T} + \rho_{\mathrm{s}} T_{\mathrm{f}}^{n}\right) \end{cases} \tag{21}$$

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

3.1.2 Implementation of the time stepping method with the Richardson extrapolation

As presented previously, the overall system (20) and (21) is solved three times for each time step leading to $T_{\mathrm{d}}^{n+1,*}$, $T_{\mathrm{d}}^{n+1,**}$, $T_{\mathrm{f}}^{n+1,*}$ and $T_{\mathrm{f}}^{n+1,**}$. The extrapolation (5) is done for both variables T_{d}^{n+1} and T_{f}^{n+1} at each cell of the space discretization and for each chemical component. Estimated errors are calculated for both the total dissolved and the total fixed concentrations for each component and at each cell of the mesh. All of them have to verify Eq. 12 and the smallest time step coming from Eq. 11 is used. Therefore, the required precision for all the variables is ensured at the current time and should be at the next step.

Table 1 Physico-chemical parameters for the reactive transport test-case

	Cl^-	Na^+	Ca^{2+}	Mg^{2+}
Initial ($mg\,l^{-1}$)	5,700	1,990	444	436
Injected ($mg\,l^{-1}$)	320	216	85	12
Cation exchange capacity ($meq\,g^{-1}$)		0.1		
Bulk density ($g\,l^{-1}$)		1,875		
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		

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

$$\begin{aligned} T_{\mathrm{d}_i}^{n+1} &= 2T_{\mathrm{d}_i}^{n+1,**} - T_{\mathrm{d}_i}^{n+1,*}, \\ T_{\mathrm{f}_i}^{n+1} &= 2T_{\mathrm{f}_i}^{n+1,**} - T_{\mathrm{f}_i}^{n+1,*}. \end{aligned} \tag{22}$$

3.1.3 Test case and discussion

An experiment described by Valocchi et al. (1981) has been tested numerically. It presents the injection of water into the aquifer at the Palo Alto Baylands Field site. The chemical phenomena concern ion exchange, described by Eq. 23. Physico-chemical conditions of the test case are given in Table 1. Cl^- appears in this table to ensure electroneutrality.

$$\begin{aligned} 2 \cdot (\equiv \mathrm{S-Na}) + \mathrm{Ca}^{2+} &\rightleftarrows (\equiv \mathrm{S_2-Ca}) + 2 \cdot \mathrm{Na}^{+} \text{ with } \mathrm{K_{NaCa}} = 1.7\mathrm{eq/L} \\ 2 \cdot (\equiv \mathrm{S-Na}) + \mathrm{Mg}^{2+} &\rightleftarrows \left(\equiv \mathrm{S_2-Mg}\right) + 2 \cdot \mathrm{Na}^{+} \text{ with } \mathrm{K_{NaMg}} = 3.0\mathrm{eq/L} \end{aligned} \tag{23}$$

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

Using the extrapolated solution (5) or (22) leads to a more accurate solution at the cost of one more solution of the instantaneous equilibrium. Although this involves additional computation, the extrapolation with adaptive time stepping presented in this work is very efficient, as can be seen in Fig. 2. $\mathrm{CREM_{ref}}$ has been calculated for each component and the maximum value has been plotted. This figure shows that, as expected from the theory, a fixed time step and an adaptive time step without extrapolation leads to a first order relation between precision and CPU time. On the other hand, the combination of extrapolation and an adaptive time step gives a second order relation between precision and CPU time.

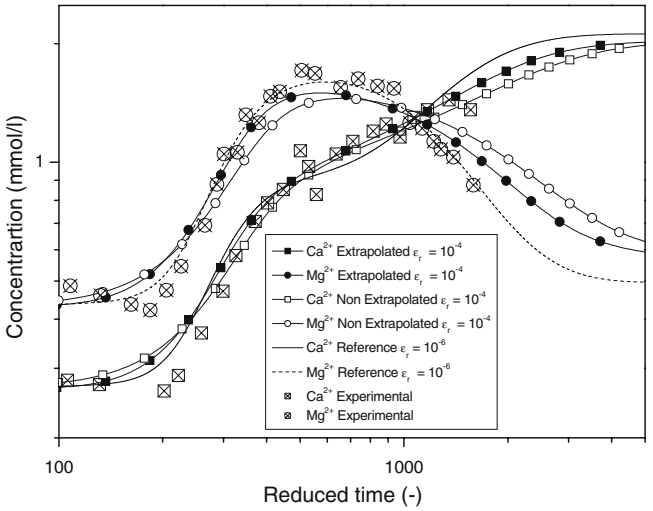

Fig. 1 Reactive transport test case: comparison of the elution curves

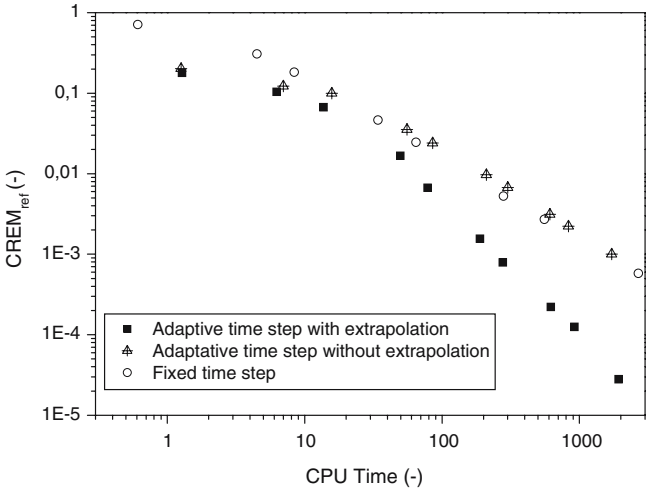

Fig. 2 Reactive transport test case: evolution of the Cumulated Relative error measure ($CREM_{ref}$) versus the required CPU time

3.2 Unsaturated flow

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

3.2.1 Presentation of the model

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

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

$$q = -K\left(h\right).\nabla\left(h - z\right), \tag{24}$$

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

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

$$\frac{\partial\theta\left(h\right)}{\partial t} + \nabla \cdot q = f_{\mathrm{v}}, \tag{25}$$

where θ is the volumetric water content, t is time, f_{v} is a source/sink term, and q is the water flux previously defined.

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

$$\begin{aligned} S_{\mathrm{e}}\left(h\right) &= \frac{\theta\left(h\right) - \theta_{\mathrm{r}}}{\theta_{\mathrm{s}} - \theta_{\mathrm{r}}} = \begin{cases} \frac{1}{\left(1+\left(\alpha|h|\right)^{n}\right)^{1-(1/n)}} & h < 0 \\ 1 & h \geq 0 \end{cases} \\ K\left(S_{\mathrm{e}}\right) &= K_{\mathrm{s}} S_{\mathrm{e}}^{1/2}\left[1 - \left(1 - S_{\mathrm{e}}^{(n/(n-1))}\right)^{(1-(1/n))}\right]^{2}, \end{aligned} \tag{26}$$

where θ_{s} and θ_{r} are the saturated and residual volumetric water contents, respectively, α is a parameter related to the mean pore size and n a parameter reflecting the uniformity of the pore-size distribution ($n > 1$).

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

$$\left|h_i^{n+1,k+1} - h_i^{n+1,k}\right| \leq \tau_{\mathrm{r}}\left|h_i^{n+1,k}\right| + \tau_{\mathrm{a}}, \quad i = 1, \ldots, \mathrm{NN}, \tag{27}$$

where k denotes the iteration number. τ_{a} and τ_{r} refer to absolute and relative convergence criteria. They are hundred times smaller than the corresponding criteria on the truncation error tolerance.

3.2.2 Implementation of the time stepping method with the Richarsdon extrapolation

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

$$\begin{aligned} h^{n+1} &= 2h^{n+1,**} - h^{n+1,*}, \\ \theta^{n+1} &= 2\theta^{n+1,**} - \theta^{n+1,*}. \end{aligned} \tag{28}$$

Table 2 Initial, boundary conditions and parameters values for the unsaturated flow test case

Parameters	Value
Material and/or	Sand
Reference	Celia et al. (1990)
$\theta_r(-)$	0.102
$\theta_s(-)$	0.368
α (cm^{-1})	0.0335
n (–)	2
K_s ($cm\,s^{-1}$)	9.22×10^{-3}
Initial conditions	
$h(z, t = 0)$ (cm)	−1,000
Boundary conditions	
$h(z = 0\ cm, t)$(cm)	−75
$h(z = 100\ cm, t)$(cm)	−1,000

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

3.2.3 Test case and discussion

We simulate a sharp infiltration front in a homogeneous dry porous media as proposed by Celia et al. (1990). The initial, boundary conditions and the relevant material properties are summarized in Table 2.

Figure 3 displays pressure head profiles after a half day of infiltration. The dense grid solution provided by Celia et al. (1990) has also been plotted to show the convergence of the method when the nodal spacing decreases. The interblock conductivity is averaged using the arithmetic mean. Figure 3 illustrates the interest of the extrapolation compared to fixed time step, time stepping scheme without extrapolation, or a heuristic time-marching scheme based on the behaviour of the non-linear iteration.

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

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

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

To analyse the efficiency of the method, the relative error has been plotted as a function of the CPU time. Figure 5 is hence obtained by adjusting the criterion ε_r for the adaptive scheme or varying the time step size for the fixed step method. As

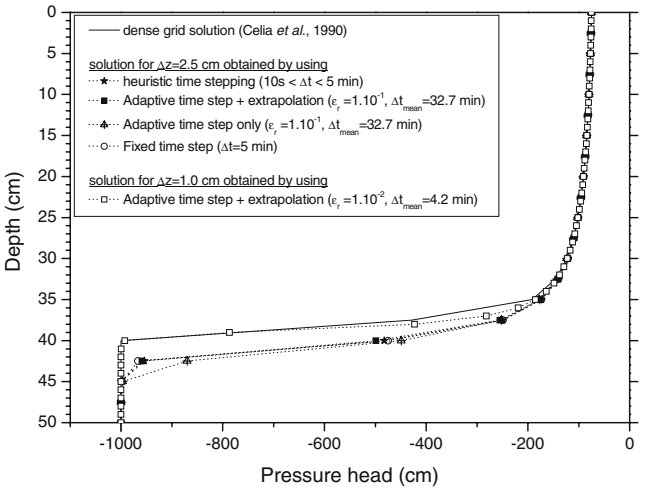

Fig. 3 Unsaturated flow test case: pressure head profiles after 12 h of infiltration

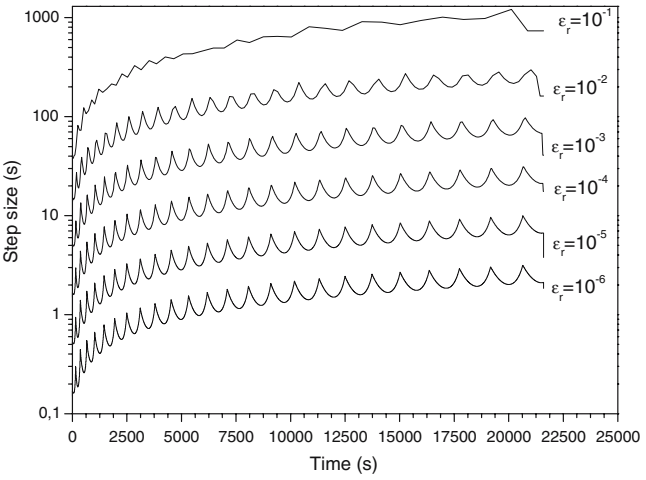

Fig. 4 Unsaturated flow test case: evolution of the time step size versus time for the scheme with extrapolation

shown in the previous example, Fig. 5 clearly illustrates that the algorithm using the Richardson extrapolation leads faster to a higher accuracy. Hence, the adaptive time stepping method becomes competitive when associated to the extrapolation.

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

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

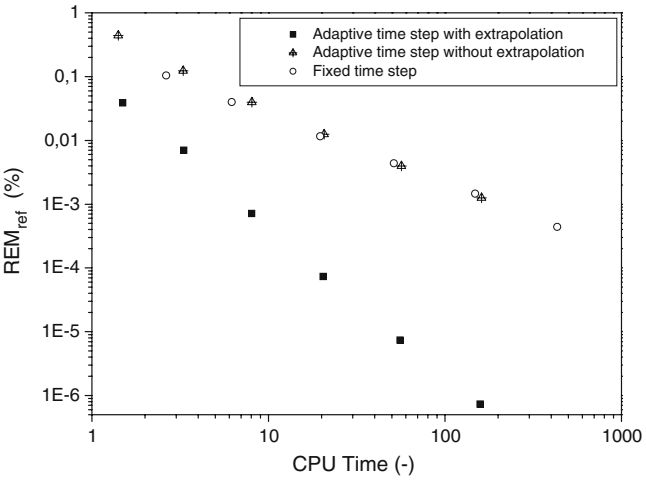

Fig. 5 Unsaturated flow test case: evolution of the relative error versus the required CPU time after 6 h of infiltration

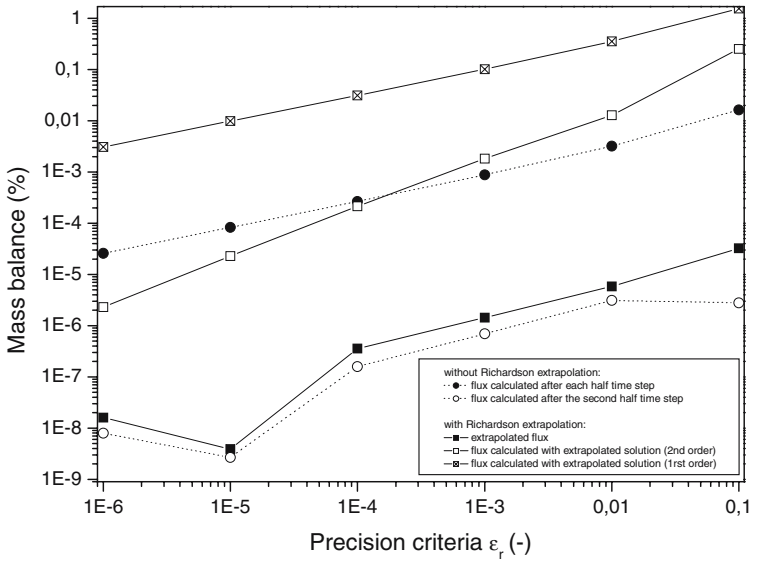

Fig. 6 Unsaturated flow test case: representation of the mass balance function of the relative precision criteria: comparisons of different techniques for the flux approximation

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

4 Conclusion

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

In fact, all our propositions have been implemented in rather different codes that model kinetic chemistry, reactive transport or unsaturated flow. The global formulation of the algorithm allows treatment of notably different mathematical models. The proposed method is an efficient way of adapting the time step size and of estimating the error for many problems frequently encountered in porous media.

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

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

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