ARES: a crude but efficient approach to adaptive time integration for stiff Differential-Algebraic Equations

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Outline

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3. Why it works in theory
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In many industrial or natural configurations, involving heat and reactive transport we face :

Stiff Nonlinear Differential-Algebraic Equations

$\longrightarrow$ *Chemical processes, Nuclear PWR clogging, Radioactive waste recycling or disposal, Hydrogeology,* CO_2 *underground storage...*

Stiffness of a solution curve may result from chemical reactions depending on temperature, catalytic processes or complex fluxes etc...

When looking for the **steady state** of a system, through a transient simulation with stiff phenomena, **adaptive time integration** then becomes a necessity, to adapt the timestep to local stiffness.

2 broad categories of time integrators are often used :

- BDF (backwards differentiation formula) and MEBDF (modified extended backwards differentiation formula) approaches (Gear, DASSL or MEBDFDAE algorithms)
- Runge-Kutta approaches

High order time discretization $\Rightarrow$ costly additional operations at each iteration of the nonlinear solver

What if you **only care for a precise evaluation of the steady state**, however precise the transient way to get there may be ?

$\longrightarrow$ **ARES** may be of service.

You are the god(dess) of war aiming at a swift victory over your nonlinear foe !

$\longrightarrow$ Let $F : (\mathbb{R}, \mathbb{R}^p, \mathbb{R}^p) \longrightarrow \mathbb{R}$ be a continuously differentiable nonlinear function. A typical DAE solution $y : \mathbb{R} \longrightarrow \mathbb{R}^p$ writes :

$$F\left(t, y, \frac{dy}{dt}\right) = 0$$

$$\forall t, \forall i \in [\![1, p]\!],\ l_i \leq y_i(t) \leq u_i$$

$\longrightarrow$ Euler implicit time integration scheme means that we solve at every t_n :

$$F(t_n, y_n, \frac{y_n - y_{n-1}}{h_n}) = 0$$

$\longrightarrow$ Implicit Euler time schemes with an adaptive timestep differ mainly by the strategy governing the choice of the next timestep $h_n = t_n - t_{n-1}$.

$\longrightarrow$ As is done very often in adaptive time schemes, we use a predictor to propose a prediction of y_n, noted as $y_n^*(o)$, based upon a Taylor evaluation of order $o = 1$ or $o = 2$

$$\begin{cases} y_n^*(1) &= y_{n-1} + d_{n-1} h_n \text{ with } d_{n-1} = \dfrac{y_{n-1} - y_{n-2}}{h_{n-1}} \\ y_n^*(2) &= y_n^*(1) + \dfrac{1}{2} d_{n-1}^2 h_n^2 \text{ with } d_{n-1}^2 = \dfrac{d_{n-1} - d_{n-2}}{h_{n-1}} \end{cases}$$

$\longrightarrow$ $y_n^*(o)$ is used as the initial guess for a classical Newton method.
$\longrightarrow$ We monitor the behaviour of the solution using the number of iterations used by the Newton method (noted henceforth I_n) to converge towards the solution. This value is a direct product of the Newton solver and **needs no further calculation.**

A very basic and simple idea :

$\longrightarrow$ The Newton solver's number of iterations is viewed here as an indicator of the gap between y_n and the predicted value $y_n^*(o)$.

$\longrightarrow$ This gap between y_n and $y_n^*(o)$ is informally related to the stiffness of the solution.

$\longrightarrow$ We allow the timestep to increase when this number is low, because the solution should be smooth enough between t_{n-1} and t_n. Conversely, we decrease the timestep when this number is high.

$\longrightarrow$ Since we aim only for the steady state : $F(t, y, 0) = 0$, high order time discretization of $\dfrac{dy}{dt}$ is nullified in the end and order 1 is sufficient.

I_n	: number of iterations needed to compute y_n
I_u	: a user-defined "ideal" number of iterations
$\gamma_a > 1$	: acceleration rate
$0 < \gamma_d < 1$	: deceleration rate

At first, we take $h_n = h_{n-1}$ and then we apply the following choices, naming h_n^* the previous value of h_n :

- Convergence fails $\longrightarrow h_n = \gamma_d h_n^*$
- Convergence succeeds in I_n iterations :
  - $I_n = I_u \longrightarrow$ next timestep with $h_{n+1} = h_n^*$
  - $I_n > I_u \longrightarrow$ treated as failure
  - $I_n < I_u \longrightarrow$ next timestep with $h_{n+1} = max(\gamma_a h_n^*, h_{max})$

Delayed version : $I_n > I_u$ is not treated as a failure, but the timestep is nevertheless reduced : $h_{n+1} = \gamma_d h_n^*$.

ARES fully solves at each timestep the equation $F(t_n, y_n, \frac{y_n - y_{n-1}}{h_n}) = 0$, through the Newton method, at any requested precision.

Stationary time : $y_n - y_{n-1} = 0 \Longrightarrow F(t_n, y_n, 0) = 0$

$\longrightarrow$ y_n solves the exact equation of the steady state equation (provided of course that this solution remains within the boundaries).

ARES can also be used for a transient calculation, with $h < h_{max}$ to ensure a minimal precision, since the order of the time scheme remains 1.

Let $G : \mathbb{R}^p \longrightarrow \mathbb{R}^p$ be the following function :

$$G(y) = F(t_n, y, \frac{y - y_{n-1}}{h_n}) \tag{1}$$

At every timestep t_n, we search for y_n as the solution of $G(y) = 0$ through the Newton method. Let $J(y)$ be the jacobian of G for y. One Newton iteration (step k) verifies :

$$J(y^k)(y^{k+1} - y^k) = -G(y^k) \tag{2}$$

If we decompose $y = [y_A, ..., y_p]$ and $G(y) = [g_1(y), ..., g_p(y)]$ accordingly for a p-sized system, we have :

$$\sum_{j=1}^{p} (y_j^{k+1} - y_j^k) \frac{\partial g_i}{y_j}(y_A^k, ..., y_p^k) = -g_i(y_A^k, ..., y_p^k) \quad \forall i \in [1, p] \tag{3}$$

Let $z : \mathbb{R} \longrightarrow \mathbb{R}^p$ be solution of the following differential equation :

$$\frac{d}{dt}[g_i(z(t))] = -g_i(z(t)) \tag{4}$$

$\longrightarrow \forall i \in [1, p]$ (3) can be seen as an **implicit Euler time discretization** of (4), with a constant timestep=1.

The solution $z(t)$ ("Newton flow") verifies :

$$g_i(z(t)) = g_i(z(0))\exp^{-t} \tag{5}$$

If the Newton iterations run by (3) converge towards the solution y_n, there is by construction a discret solution of (4) $\forall i \in [1, p]$.
The values of $z(t)$ form then a trajectory towards y_n, with a constant timestep.
According to (5), the trajectory depends only on the values of $g_i(z(0))$ or **the first iterate of the Newton method**.

$\longrightarrow$ Direct correspondence between the number of Newton iterations I_n and the overall closeness of $G(y_n^*(o))$ to zero.

$\longrightarrow$ Preserving a low I_n ensures then a relative smoothness of the solution between t_{n-1} and t_n.

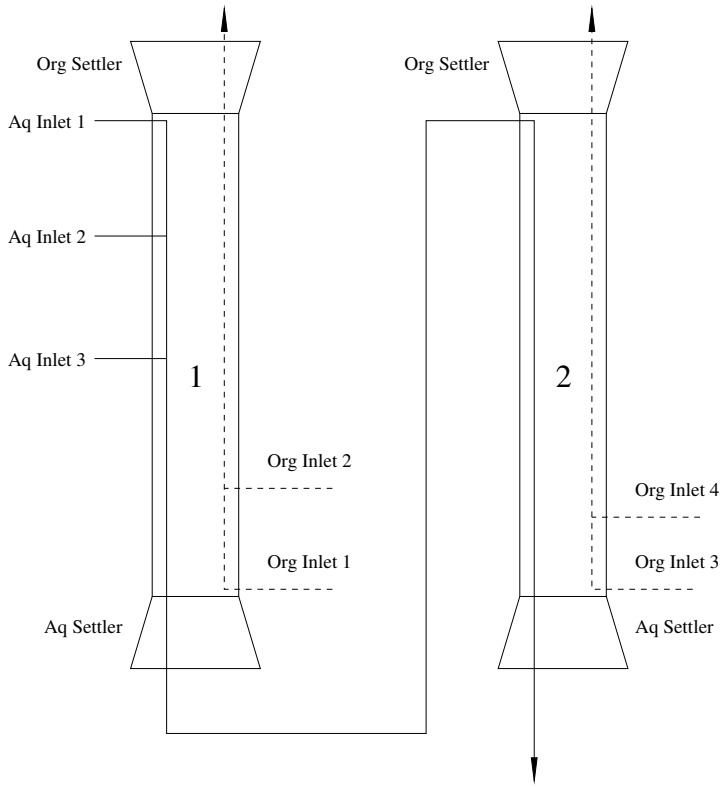
SIDES is a module of the open source platform TRUST, dedicated to thermohydraulics in the context of nuclear plant simulations :

- C++ platform providing many numerical tools, such as PETSc linear solvers, pre- and postprocessing tools etc...
- Basis for TrioCFD, Genepi+, Cathare...
- SIDES aggregates objects associated with numerical methods : being given a nonlinear function of multipe variables, its jacobian and a set of bounds, it may be used to solve any $F\left(t, y, \frac{dy}{dt}\right) = 0$

$\longrightarrow$ ARES was used in SIDES for an industrial code dedicated to Liquid-Liquid-Extraction :

- reactive and heat transport between an organical and an aqueous phase countercurrently,
- both intra- and interphasic chemical reactions,
- chemical reactions under kinetics or at equilibrium,
- retroaction of chemistry on temperature.

2 Pulsed Colums, 2 chemical phases with 11 fictitious species



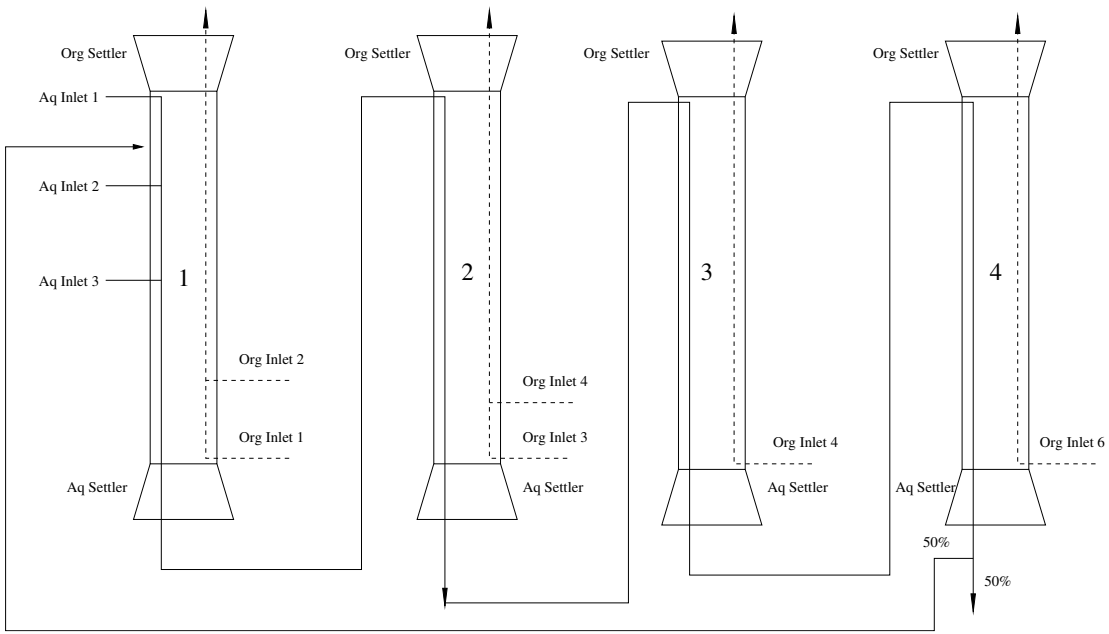
$$A_{aq} \rightarrow B_{aq} \qquad \lambda = 10 x_A$$
$$A_{aq} + C_{aq} \rightarrow D_{aq} \qquad \lambda = 8 x_A x_C$$
$$A_{org} \rightarrow B_{org} \qquad \lambda = 10 y_A$$
$$C_{org} + D_{org} \rightarrow B_{org} + E_{org} \qquad \lambda = 200 y_C y_D^2$$

$$A_{aq} + 2B_{aq} \leftrightarrow C_{aq} \qquad 0.1 x_{Caq} = x_A x_B^2$$
$$3A_{org} + 2B_{org} \leftrightarrow C_{org} \qquad 0.1 y_C^2 = y_A^3 y_B^2$$
$$A_{aq} \leftrightarrow A_{org} \qquad y_A = 2 x_A$$
$$B_{aq} \leftrightarrow B_{org} \qquad y_B = 2 x_B$$
$$B_{aq} + D_{aq} \leftrightarrow D_{org} \qquad y_D = 100 x_B x_B$$

Density laws : ρ_{aq}, ρ_{org}

Variable fluxes with phase swelling

4 Pulsed Colums, 5 more fictitious species, 1 more kinetics and 3 more equilibria



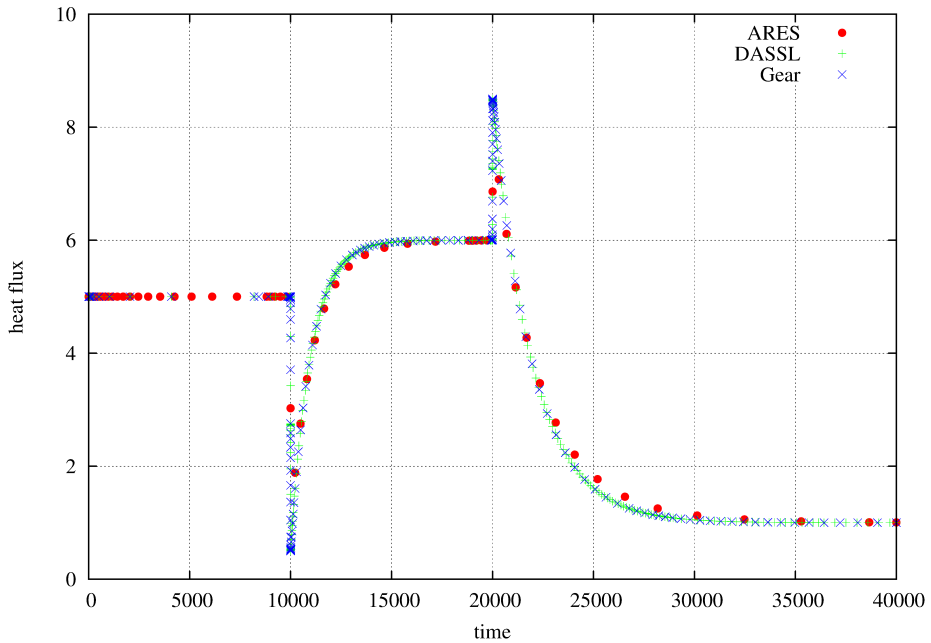
$$A_{aq} + D_{aq} \rightarrow 2E_{aq} + 3F_{aq} \quad \lambda = 12 x_C x_D$$

$$E_{aq} + 3F_{aq} \leftrightarrow G_{aq} \quad 10^{-15} x_G = x_E x_F^3$$
$$F_{aq} \leftrightarrow F_{org} \quad y_F = 2 x_F^{1.5}$$
$$G_{aq} \leftrightarrow G_{org} \quad \frac{1}{2} y_G^2 = x_G$$

Analytical case study : 2 fast reactions, with a threshold temperature.

$$A \to B \quad \lambda(\theta \geq 1100) = 0.001a \quad \mathcal{H} = 45000$$
$$B \to C \quad \lambda(\theta \geq 2100) = 0.005b \quad \mathcal{H} = -25000$$

Heating device : $\theta(t) = 100 + 0.1t$. We monitor the needed heat flux Φ :



$\longrightarrow$ Steady plateaux $\Phi = 5$, $\Phi = 6$ and $\Phi = 1$ accurately given by ARES, with much less simulation times.

$\longrightarrow$ As expected : Gear or DASSL more accurate on transient regimes.

method	Gear	DASSL	ARES	ARES delayed
case study 1	114	172	78	81
case study 2	294	492	295	189
case study 3	3.6	6	0.8	0.8

How to choose an ideal number of iterations I_u ?

A DAE system contains both algebraic and differential equations :

- For differential equations, decreasing the timestep hopefully means that the overall function giving y^{k+1} in relation to y^k may become **contractive**.
- However, the presence of purely algebraic equations, independent from time derivatives, invalidates or at least challenges this strategy.

Let us consider a DAE system containing only one algebraic equation :

$$\begin{bmatrix} y_A - y_A^{n-1} - h_n f_1(y) \\ \dots \\ y_{p-1} - y_{p-1}^{n-1} - h_n f_{p-1}(y) \\ f_p(y) \end{bmatrix} = 0 \tag{6}$$

If we decompose the jacobian $J = J_1 + h_n J_2$, where J_1 gathers all terms independant of h_n, the Newton step writes :

$$\begin{bmatrix} y_A^k - y_A^{n-1} - h_n f_1(y^k) \\ \dots \\ y_{p-1}^k - y_{p-1}^{n-1} - h_n f_{p-1}(y^k) \\ f_p(y^k) \end{bmatrix} = \begin{bmatrix} (1 + \frac{\partial f_p}{\partial y_A}(y^k))(y_A^k - y_A^{k+1}) \\ \dots \\ (1 + \frac{\partial f_p}{\partial y_{p-1}}(y^k))(y_{p-1}^k - y_{p-1}^{k+1}) \\ \sum_{j=1}^{p} \frac{\partial f_p}{\partial y_j}(y^k)(y_j^k - y_j^{k+1}) \end{bmatrix} + h_n J_2[y^k - y^{k+1}] \quad (7)$$

This simplifies as :

$$\begin{bmatrix} -y_A^{n-1} - h_n f_1(y^k) \\ \dots \\ -y_{p-1}^{n-1} - h_n f_{p-1}(y^k) \\ f_p(y^k) \end{bmatrix} = -y^{k+1} + \begin{bmatrix} \frac{\partial f_p}{\partial y_A}(y^k)(y_A^k - y_A^{k+1}) \\ \dots \\ \frac{\partial f_p}{\partial y_{p-1}}(y^k)(y_{p-1}^k - y_{p-1}^{k+1}) \\ y_p^{k+1} + \sum_{j=1}^{p} \frac{\partial f_p}{\partial y_j}(y^k)(y_j^k - y_j^{k+1}) \end{bmatrix} + h_n J_2[y^k - y^{k+1}] \quad (8)$$

Convergence leading to y^n can be interpeted here as the fixed point of that function :

$$y^{k+1} = M^{-1}\left(\begin{bmatrix} y_A^{n-1} + h_n f_1(y^k) \\ \dots \\ y_{p-1}^{n-1} + h_n f_{p-1}(y^k) \\ f_p(y^k) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_p}{\partial y_A}(y^k) y_A^k \\ \dots \\ \frac{\partial f_p}{\partial y_{p-1}}(y^k) y_{p-1}^k \\ \sum_{j=1}^{p} \frac{\partial f_p}{\partial y_j}(y^k) y_j^k \end{bmatrix} + h_n J_2 y^k\right) \tag{9}$$

$\longrightarrow$ Strong assumptions on f_p and its derivatives to ensure contraction ! Whereas, in the purely differential case (f_p and the p^{th} line disappear) :

$$y^{k+1} = (Id_p + h_n J_2)^{-1}\left(\begin{bmatrix} y_A^{n-1} + h_n f_1(y^k) \\ \dots \\ y_{p-1}^{n-1} + h_n f_{p-1}(y^k) \end{bmatrix} + h_n J_2 y^k\right) \tag{10}$$

$\longrightarrow M = Id_p + h_n J_2$ can be made contractive for a certain h_n, in the vicinity of the Newton search

In the general context of real chemical equilibria, the algebraic equations will come in many unpleasant shapes and impose (at best !) a **lower bound to the number of Newton iterations needed, independently of the value of** h_n.

$\longrightarrow$ A good rule of thumb is to give I_u a value close to that of the lower bound, which depends on the system.

$\longrightarrow$ A guess can be made from the behaviour of the system in the first timesteps : $I_u = I_1$ and $I_{max} = 3I_u$ ($\gamma_a = 1.2$ and $\gamma_d = 0.5$ for ARES and $\gamma_a = 1.5$ and $\gamma_d = 0.8$ for ARES delayed).

- ARES aims at solving a paradox : due to Stiff Nonlinear DAE, reactive transport simulations are usually very costly but it is common to have to run a transient calculation in order obtain a steady state in a robust way, although this costly transient calculation itself is not necessarily of interest.
- By allowing a relative loss of accuracy on a transient calculation, ARES may help in providing the desired result at a reduced cost, by proposing an intermediate approach between overly simple methods such as the constant timestep Euler scheme and complex high-order approaches.
- ARES is very easy to implement and to use, since it uses very few parameters.