

# VARIABLE-STEP UNCONDITIONALLY STABLE SECOND-ORDER APPROXIMATIONS

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From (implicit) Backward-Euler to Variable-Step Second-Order Conservative Unconditionally-Stable, by adding two lines of code

**1. One line of code to change a Backward Euler code into to a second-order, unconditionally stable, conservative method.** For the numerical approximation of a general evolution equation:

$$y'(t) = f(t, y(t)), \quad (1.1)$$

on the mesh points  $\{t_n\}_{n \geq 0}$ , and with the timestep  $\tau_n$ , such that:

$$t_{n+1} = t_n + \tau_n, \quad t_{n+1/2} = t_n + \frac{1}{2} \tau_n,$$

we recall the classical midpoint quadrature rule:

$$\frac{y_{n+1} - y_n}{\tau_n} = f(t_{n+1/2}, y_{n+1/2}), \quad (1.2)$$

where  $y_n \approx y(t_n)$ . The method (1.2) is ubiquitously presented and used [3, 7, 8, 13, 14, 16, 21, 22, 24–26] in the apparently different form:

$$\frac{y_{n+1} - y_n}{\tau_n} = f\left(t_{n+1/2}, \frac{y_{n+1} + y_n}{2}\right). \quad (1.3)$$

The reason for the wide use of (1.3) instead of (1.2) (see e.g. [22, page 133]) is due to the natural question: ‘*but which value should we take for  $y_{n+1/2}$ ?*’. The method (1.3) is an implicit second-order A-stable time-stepping method, and is the preferred method for solving evolutive conservative systems of partial differential equations (PDEs), along with the second order backward differentiation formula (BDF2) for dissipative PDEs.

From an algorithmic viewpoint, increasing the numerical accuracy of a complex legacy code, based on the first-order backward Euler (BE) method, to a second-order A-stable method, can be a difficult task. One straightforward solution would be to apply non-intrusive minimal modifications to the algorithm, i.e., by adding a few lines of code and post-processing the original BE solution into a ‘filtered’ higher-order solution. This is currently done in geophysical fluid dynamics, to improve the quality of the solution to the leap-frog method, by filtering it with Robert-Asselin or Robert-Asselin-Williams filters [1, 20, 28, 31–33, 35–37]. Recently, the BE solution was filtered into the solution to a second-order linear multistep method (LMM), similar to a BDF2 solution (see e.g., [19]), with a reduced discrete curvature and numerical dissipation. Most LMMs [11, 22], when considered with variable steps, do not preserve the zero-stability or unconditional A-stability properties of the constant step versions. For example, the variable step version of the trapezoidal method (Crank-Nicolson) is unstable [22], [34, pp. 181-182]; similarly, BDF2 loses zero-stability and A-stability with variable stepsize.

An alternative non-intrusive modification to the BE method, with the goal of defining a family of second-order, variable step, unconditionally stable one-step methods, relies on the successful resolution of the above question regarding (1.2). This alternative is based on the fact that both the midpoint (1.2) and the trapezoidal methods can be viewed as a sequence of backward-Euler then forward-Euler methods, respectively a forward-Euler then a backward-Euler method, where the first computation is performed at the time  $t_{n+1/2}$ , see e.g., [21, page 223] and [12, page 57].

Consequently, consider implementing the midpoint rule (1.2) by solving a backward-Euler step at the half-integer time step  $t_{n+1/2}$ , followed by a forward-Euler step to  $t_{n+1}$ :

$$\frac{y_{n+1/2} - y_n}{\tau_n/2} = f(t_{n+1/2}, y_{n+1/2}), \quad (\text{BE})$$

$$\frac{y_{n+1} - y_{n+1/2}}{\tau_n/2} = f(t_{n+1/2}, y_{n+1/2}). \quad (\text{FE})$$

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We point out that solving the equations (BE)-(FE) is equivalent to, and reduces to only solving (BE), and then applying a time-filter, as the (FE) step is equivalent to a linear extrapolation. Hence we evaluate  $y_{n+1} = 2y_{n+1/2} - y_n$ , and the equation (BE)-(FE) can be thought of as a single process designated as (BEFE):

$$\begin{cases} \frac{y_{n+1/2} - y_n}{\tau_n/2} = f(t_{n+1/2}, y_{n+1/2}), \\ y_{n+1} = 2y_{n+1/2} - y_n. \end{cases} \quad (\text{BEFE})$$

Notice that the second step can also be written as:

$$y_{n+1/2} = \frac{y_{n+1} + y_n}{2},$$

and therefore both (1.2) and (1.3) yield exactly the same numerical approximations, i.e., (1.2) is a second-order accurate, unconditionally A-stable method. An important characteristic of (1.2) is the fact that it is a one-leg two-step method, which, as in the case of the trapezoidal rule, makes it easy to view it as a variable-step method, without losing the stability property. There are several options as to how to adapt the time-step  $\tau_n$  (see e.g., [17, 18]), namely how to estimate the local truncation error.

This implementation (BEFE) of the midpoint method is consequential from the viewpoint of its potential applications for time-stepping methods of complex partial differential equations. The first advantage is the ease of non-intrusive implementation: it takes one line of code to transform a first-order dissipative method to a second-order conservative stable method. (We recall that Dahlquist's barrier limits the accuracy of A-stable linear multistep methods to second-order.) A second advantage is that the constant in the local truncation error of (1.3), when seen in the implementation (BEFE) is  $\frac{1}{24}$ , instead of the usual  $-\frac{1}{12}$ . Thirdly, since midpoint is a one step method, time-adaptivity can be implemented with non-intrusive minimal algorithmic changes.

For coupled complex systems, like magnetohydrodynamics, ocean-atmosphere, groundwater-surface water, or fluid-structure interactions, the current trend is to employ partitioning methods of implicit-explicit type, which solve each equation separately by a legacy code, and transfer information between the subdomains and algorithms. This breaking of the monolithic approach ubiquitously comes at the cost of stability. Most existing partitioned stable methods are only first-order accurate in time. The (BEFE) implementation opens the path of extending the current partitioning first-order stable methods to second-order accurate variable-step unconditionally stable methods, by manipulating the computed solution at  $t_{n+1/2}$  in a stable manner. Recently, this approach has been applied to problems in fluid-structure interaction [2], magnetohydrodynamics and ocean-atmosphere modeling. Note also that the computed solution at  $t_{n+1/2}$  allows further manipulation, such as modular spatial filtering, in order to improve the qualitative properties of the numerical simulations [29, 30].

**2. Generalization to a  $\theta$ -like method.** We remark also that (BEFE) is a particular instance of the one-leg ' $\theta$ -like' method:

$$\frac{y_{n+1} - y_n}{\tau_n} = f(t_{n+\theta}, y_{n+\theta_n}), \quad (2.1)$$

implemented as:

$$\begin{cases} \frac{y_{n+\theta_n} - y_n}{\theta_n \tau_n} = f(t_{n+\theta_n}, y_{n+\theta_n}), \\ \frac{y_{n+1} - y_{n+\theta_n}}{(1 - \theta_n) \tau_n} = f(t_{n+\theta_n}, y_{n+\theta_n}). \end{cases} \quad (2.2)$$

which can be rewritten as:

$$\begin{cases} \frac{y_{n+\theta_n} - y_n}{\theta_n \tau_n} = f(t_{n+\theta_n}, y_{n+\theta_n}), \\ y_{n+1} = \frac{1}{\theta_n} y_{n+\theta_n} - \left(\frac{1}{\theta_n} - 1\right) y_n. \end{cases} \quad (2.3)$$

Notice that (2.1) is not the classical linear multistep  $\theta$  method [15, page 182], but Cauchy’s one-leg version (see e.g. [4, pp. 40], also [6, 9, 10]):

$$\frac{y_{n+1} - y_n}{\tau_n} = f(t_{n+\theta}, \theta y_{n+1} + (1 - \theta)y_n),$$

since, as above, we have from the second part of (2.3) that  $y_{n+\theta} = \theta y_{n+1} + (1 - \theta)y_n$ .

We recall that in the following we mean stability in the sense of  $G$ -stability (Dahlquist 1975, see e.g., [8] or [23, p.308]), which is equivalent to  $A$ -stability for constant step linear multistep methods.

PROPOSITION 2.1. *The midpoint method (BE)-(FE), and the  $\theta$ -method (2.2) for  $\theta_n \geq \frac{1}{2}$ , are unconditionally-stable, and the following equality holds:*

$$\frac{1}{2}\|y_{n+1}\|^2 - \frac{1}{2}\|y_n\|^2 + \frac{2\theta_n - 1}{2}\|y_{n+1} - y_n\|^2 = \tau_n \langle f(t_{n+\theta_n}, y_{n+\theta_n}), y_{n+\theta_n} \rangle.$$

*Proof.* We prove the result only for (2.2), since the midpoint method is obtained by taking  $\theta_n = 1/2$ . Multiplying both equations in (2.2) by  $\theta_n \tau_n y_{n+\theta_n}$  and  $(1 - \theta_n) \tau_n y_{n+\theta_n}$  respectively, and applying the polarization identity we obtain:

$$\begin{aligned} \frac{1}{2}\|y_{n+\theta_n}\|^2 - \frac{1}{2}\|y_n\|^2 + \frac{1}{2}\|y_{n+\theta_n} - y_n\|^2 &= \theta_n \tau_n f(t_{n+\theta_n}, y_{n+\theta_n}) y_{n+\theta_n}, \\ \frac{1}{2}\|y_{n+1}\|^2 - \frac{1}{2}\|y_{n+\theta_n}\|^2 - \frac{1}{2}\|y_{n+1} - y_{n+\theta_n}\|^2 &= (1 - \theta_n) \tau_n f(t_{n+\theta_n}, y_{n+\theta_n}) y_{n+\theta_n}. \end{aligned}$$

Summation and the use of (2.2) completes the argument.  $\square$

**3. Time-step adaptivity.** We begin this section by a small observation: the local truncation error of the midpoint method (BEFE) is:

$$T_{n+1} = \frac{1}{24} \tau_n^3 y'''(t_{n+1/2}) + \mathcal{O}(\tau_n^5). \quad (3.1)$$

The same formula holds for the ‘ $\theta$ -like’ method (2.1), provided  $\theta_n = \frac{1}{2} + \frac{1}{2} \tau_n^2$ .

Therefore, we can adaptively adjust the time step  $\tau_n$  by enforcing an estimate of the local truncation error (1.2), denoted  $\widehat{T}_{n+1}$ , to equal a tolerance, i.e., such that the  $\|\widehat{T}_{n+1}\| \approx \text{tol}$  (see e.g. [18]). The time-step  $\tau_n^{new}$  which imposes that  $\widehat{T}_{n+1}$  is sufficiently small is given by:

$$\tau_n^{new} = \tau_n \left| \frac{\text{tol}}{\|\widehat{T}_{n+1}\|} \right|^{\frac{1}{3}}. \quad (3.2)$$

There are numerous ways in which the time-step adaptivity can be implemented (see e.g. [18]), out of which we present three methods. The first choice is based on the estimation of the LTE using Taylor expansions. The other two options estimate the local truncation error by the difference between the numerical midpoint solution and a second-order, and respectively a third-order approximation, given by formulae similar to the explicit Adams-Bashforth 2 (AB2) and Adams-Bashforth 3 (AB3) methods. These two methods are related to the classical AB2 and AB3 (see e.g., [22, p. 398]), the difference being that they use the function values evaluated at half-times

$f_{n+1/2}, f_{n-1/2}, f_{n-3/2}, f_{n-5/2}$ .

**Result:** Adaptive midpoint rule

**initialization:** set  $\text{tol}$ , compute  $y_1$  and  $\tau_0$  with a one step second-order accurate method, such that  $\tau_0$  is in the convergence range (see e.g., [5, page 367]);

compute  $y_2$  and  $\tau_1$  with a second order accurate method,  $t_2 = t_1 + \tau_1$ ;

$t^{\text{new}} = t_2, \tau^{\text{new}} = \tau_1$ ;

for  $n \geq 2$  (i.e.,  $t^{\text{new}}, \tau^{\text{new}}, y_n, y_{n-1}, y_{n-2}$  are given);

**while**  $t^{\text{new}} \leq T$  **do**

$\tau_n \leftarrow \tau^{\text{new}}$  ;

    evaluate  $y_{n+1}$  with the midpoint rule (1.2);

    evaluate  $\widehat{T}_{n+1}$  with (LTE-Taylor), (LTE-AB2) or (LTE-AB3);

$\tau^{\text{new}} \leftarrow \tau_n \|\text{tol} / \|\widehat{T}_{n+1}\|\|^{1/3}$ ;

**if**  $\|\widehat{T}_{n+1}\| \leq \text{tol}$  **then**

$t_{n+1} \leftarrow t_n + \tau^{\text{new}}, t^{\text{new}} \leftarrow t_{n+1}, n+1 \leftarrow n$

**end**

**end**

**3.1. Estimation of the local truncation error using Taylor expansions.** In order to estimate the numerical value of  $\widehat{T}_{n+1}$ , we need to evaluate  $y'''(t_n)$ . We proceed by using Taylor expansions:

$$y'(t_{n+1/2}) = y'(t_n) + \frac{\tau_n}{2} y''(t_n) + \frac{\tau_n^2}{8} y'''(t_n) + \mathcal{O}(\tau_n^3),$$

$$y'(t_{n-1/2}) = y'(t_n) - \frac{\tau_{n-1}}{2} y''(t_n) + \frac{\tau_{n-1}^2}{8} y'''(t_n) + \mathcal{O}(\tau_{n-1}^3),$$

$$y'(t_{n-3/2}) = y'(t_n) - \frac{2\tau_{n-1} + \tau_{n-2}}{2} y''(t_n) + \frac{(2\tau_{n-1} + \tau_{n-2})^2}{8} y'''(t_n) + \mathcal{O}(\tau_{n-1}^3 + \tau_{n-2}^3),$$

which, eliminating  $y'(t_n)$  and  $y''(t_n)$ , gives:

$$\frac{y'(t_{n+1/2}) - y'(t_{n-1/2})}{\tau_n + \tau_{n-1}} - \frac{y'(t_{n-1/2}) - y'(t_{n-3/2})}{\tau_{n-1} + \tau_{n-2}} = \frac{1}{8} (\tau_n + 2\tau_{n-1} + \tau_{n-2}) y'''(t_n) + \mathcal{O}(\tau_n^2 + \tau_{n-1}^2 + \tau_{n-2}^2).$$

Using the numerical method (1.2), the LTE (3.1) can finally be estimated in terms of the computed solutions:

$$\begin{aligned} \widehat{T}_{n+1} &= \frac{\tau_n^3}{3(\tau_n + 2\tau_{n-1} + \tau_{n-2})} \left( \frac{f_{n+1/2} - f_{n-1/2}}{\tau_n + \tau_{n-1}} - \frac{f_{n-1/2} - f_{n-3/2}}{\tau_{n-1} + \tau_{n-2}} \right) \quad (\text{LTE-Taylor}) \\ &= \frac{\tau_n^3}{3(\tau_n + 2\tau_{n-1} + \tau_{n-2})} \left( \frac{\frac{y_{n+1} - y_n}{\tau_n} - \frac{y_n - y_{n-1}}{\tau_{n-1}}}{\tau_n + \tau_{n-1}} - \frac{\frac{y_n - y_{n-1}}{\tau_{n-1}} - \frac{y_{n-1} - y_{n-2}}{\tau_{n-2}}}{\tau_{n-1} + \tau_{n-2}} \right) \\ &= \frac{\tau_n^3}{3(\tau_n + 2\tau_{n-1} + \tau_{n-2})} \left( y_{n+1} \frac{1}{\tau_n(\tau_n + \tau_{n-1})} - y_n \frac{\tau_n + \tau_{n-1} + \tau_{n-2}}{\tau_n \tau_{n-1} (\tau_{n-1} + \tau_{n-2})} \right. \\ &\quad \left. + y_{n-1} \frac{\tau_n + \tau_{n-1} + \tau_{n-2}}{\tau_{n-1} \tau_{n-2} (\tau_n + \tau_{n-1})} - y_{n-2} \frac{1}{\tau_{n-2} (\tau_{n-1} + \tau_{n-2})} \right). \end{aligned}$$

**3.2. Estimation of the local truncation error using a variable step AB-2 solution.** Here we estimate the local truncation error at  $t_{n+1}$  by evaluating the difference between the  $\mathcal{O}(\Delta t^2)$  midpoint-solution  $y_{n+1}$  and another second-order approximation,  $\widetilde{y}_{n+1}^{\text{AB2}}$ , obtained by a variable-step Adams-Bashforth 2-like method. Let  $\Pi_1(t)$  be the polynomial interpolating  $f(y(t))$  at nodes  $\{t_{n-1/2}, t_{n-3/2}\}$  and values  $\{f_{n-1/2}, f_{n-3/2}\}$ , which by (BEFE) denote:

$$f_{n-1/2} = \frac{y_n - y_{n-1}}{\tau_{n-1}}, \quad f_{n-3/2} = \frac{y_{n-1} - y_{n-2}}{\tau_{n-2}}.$$

Then the solution to the AB2-like with variable step is:

$$\widetilde{y}_{n+1}^{\text{AB2}} = y_n + \int_{t_n}^{t_{n+1}} \Pi_1(t) dt = y_n + f_{n-1/2} \frac{\tau_n(\tau_n + 2\tau_{n-1} + \tau_{n-2})}{\tau_{n-1} + \tau_{n-2}} - f_{n-3/2} \frac{\tau_n(\tau_n + \tau_{n-1})}{\tau_{n-1} + \tau_{n-2}}$$

$$= y_n \frac{(\tau_n + \tau_{n-1})(\tau_n + \tau_{n-1} + \tau_{n-2})}{\tau_{n-1}(\tau_{n-1} + \tau_{n-2})} - y_{n-1} \frac{\tau_n(\tau_n + \tau_{n-1} + \tau_{n-2})}{\tau_{n-1}\tau_{n-2}} + y_{n-2} \frac{\tau_n(\tau_n + \tau_{n-1})}{\tau_{n-2}(\tau_{n-1} + \tau_{n-2})}, \quad (\text{AB2-like})$$

and its local truncation error (under the ‘localization assumption’, i.e. back values are exact, see e.g. [18, p.70], [27, p.56]) can be written:

$$\widetilde{T}_{n+1}^{AB2} = \tau_n^3 y'''(t_{n+1/2}) \left( \frac{1}{24} + \frac{1}{8} \left( 1 + \frac{\tau_{n-1}}{\tau_n} \right) \left( 1 + 2 \frac{\tau_{n-1}}{\tau_n} + \frac{\tau_{n-2}}{\tau_n} \right) \right).$$

For brevity, we denote the error coefficient in the right hand side, which depends on timestep ratios, by:

$$\mathcal{R}_n = \frac{1}{24} + \frac{1}{8} \left( 1 + \frac{\tau_{n-1}}{\tau_n} \right) \left( 1 + 2 \frac{\tau_{n-1}}{\tau_n} + \frac{\tau_{n-2}}{\tau_n} \right).$$

Then, from (3.1) and the expression above, we obtain the following approximation of the local truncation error of the midpoint rule (BEFE):

$$\widehat{T}_{n+1} = (y_{n+1}^{\text{midpoint}} - y_{n+1}^{\widetilde{AB2}}) \frac{1}{1 - 1/(24\mathcal{R}_n)}, \quad (\text{LTE-AB2})$$

where  $y_{n+1}^{\text{midpoint}}$  denotes the midpoint solution from (BEFE), and  $y_{n+1}^{\widetilde{AB2}}$  is given in (AB2-like).

**3.3. Estimation of the local truncation error using a variable step AB-3 solution.** We choose to estimate the local truncation error at  $t_{n+1}$  by evaluating the difference between the  $\mathcal{O}(\Delta t^2)$  midpoint-solution  $y_{n+1}$  and a third-order approximation,  $u_{n+1}$ , obtained by the variable-step Adams-Bashforth 3 method (see e.g., [22, p. 398]). We denote:

$$f_{n-1/2} = \frac{y_n - y_{n-1}}{\tau_{n-1}}, \quad f_{n-3/2} = \frac{y_{n-1} - y_{n-2}}{\tau_{n-2}}, \quad f_{n-5/2} = \frac{y_{n-2} - y_{n-3}}{\tau_{n-3}},$$

and let  $\Pi_2(t)$  be the polynomial interpolating  $f(y(t))$  at nodes  $\{t_{n-1/2}, t_{n-3/2}, t_{n-5/2}\}$  and values  $\{f_{n-1/2}, f_{n-3/2}, f_{n-5/2}\}$ :

$$\Pi_2(t) = f_{n-1/2} + \frac{f_{n-1/2} - f_{n-3/2}}{t_{n-1/2} - t_{n-3/2}} (t - t_{n-1/2}) + \frac{\frac{f_{n-1/2} - f_{n-3/2}}{t_{n-1/2} - t_{n-3/2}} - \frac{f_{n-3/2} - f_{n-5/2}}{t_{n-3/2} - t_{n-5/2}}}{t_{n-1/2} - t_{n-5/2}} (t - t_{n-1/2})(t - t_{n-3/2}).$$

Hence:

$$u_{n+1} \approx y_n + \int_{t_n}^{t_{n+1}} \Pi_2(t) dt = y_n + \tau_n \left[ f_{n-1/2} + \frac{f_{n-1/2} - f_{n-3/2}}{t_{n-1/2} - t_{n-3/2}} \frac{\tau_n + \tau_{n-1}}{2} + \frac{\frac{f_{n-1/2} - f_{n-3/2}}{t_{n-1/2} - t_{n-3/2}} - \frac{f_{n-3/2} - f_{n-5/2}}{t_{n-3/2} - t_{n-5/2}}}{t_{n-1/2} - t_{n-5/2}} \cdot \left( \frac{1}{3} \tau_n^2 + \frac{1}{2} \tau_{n-1}^2 + \frac{3}{4} \tau_n \tau_{n-1} + \frac{1}{4} \tau_n \tau_{n-2} + \frac{1}{4} \tau_{n-1} \tau_{n-2} \right) \right],$$

and therefore the local truncation error can be approximated by:

$$\widehat{T}_{n+1} = \tau_n \left[ f_{n-1/2} + \frac{f_{n-1/2} - f_{n-3/2}}{t_{n-1/2} - t_{n-3/2}} \frac{\tau_n + \tau_{n-1}}{2} + \frac{\frac{f_{n-1/2} - f_{n-3/2}}{t_{n-1/2} - t_{n-3/2}} - \frac{f_{n-3/2} - f_{n-5/2}}{t_{n-3/2} - t_{n-5/2}}}{t_{n-1/2} - t_{n-5/2}} \cdot \left( \frac{1}{3} \tau_n^2 + \frac{1}{2} \tau_{n-1}^2 + \frac{3}{4} \tau_n \tau_{n-1} + \frac{1}{4} \tau_n \tau_{n-2} + \frac{1}{4} \tau_{n-1} \tau_{n-2} \right) \right]. \quad (\text{LTE-AB3})$$

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