Refactorization of the midpoint rule

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Abstract

An alternative formulation of the midpoint method is employed to analyze its advantages as an implicit second-order absolutely stable timestepping method. Legacy codes originally using the backward Euler method can be upgraded to this method by inserting a single line of new code. We show that the midpoint method, and a theta-like generalization, are B-stable. We outline three estimates of local truncation error that allow adaptive time-stepping.

Keywords: backward Euler, midpoint rule, second-order, symplectic, Hamiltonian, energy conservation, A-stable and B-stable, blackbox / legacy code, partitioning algorithms, time adaptivity

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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:

$$y'(t) = f(t, y(t)), \tag{1.1}$$

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

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

we recall the classical midpoint quadrature rule:

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

where $y_n \approx y(t_n)$. The method (1.2) is ubiquitously presented and used [8, 11, 12, 19, 31, 30, 29, 27, 26, 21, 18] in the apparently different form:

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

The reason for the wide use of (1.3) instead of (1.2) (see e.g. [27, page 133]) is due to the natural question: '*but which value should we take for $y_{n+1/2}$?*'. The method (1.3) is

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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 stability and accuracy of the solution to the leap-frog (explicit midpoint) method, by filtering it with Robert-Asselin or Robert-Asselin-Williams filters [38, 3, 40, 42, 41, 25, 33, 37, 36]. 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., [24]), with a reduced discrete curvature and numerical dissipation.

Most LMMs [27, 16], 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 [16],[39, pp. 181-182]; similarly, BDF2 loses zero-stability and A-stability when used with a variable stepsize. The trapezoidal method, even in the constant step case, is *A*-stable but not *B*-stable [1]. Also, "it is not known which of the LMMs preserve quadratic invariants" [5].

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., [26, page 223] and [17, 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}:

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

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

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):

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

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. The second formulation (BEFE), while equivalent, makes it obvious how to bootstrap an existing Euler code to a second-order accurate, unconditionally energy stable, conservative, symplectic code. An important characteristic of (1.2) is the fact that it is a one-leg two-step method, which 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 τ_n (see e.g., [23, 22]), 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 accurate, energy conservative, stable method. (We recall that Dahlquist's barrier limits the accuracy of A-stable linear multistep methods to second-order.) Moreover, the midpoint rule is a symplectic method for general Hamiltonian systems, conserving all quadratic Hamiltonians [2, 5], unconditionally stable (A-stable and B-stable [7, 1]). Another important remark 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, time-adaptivity can also be implemented with non-intrusive minimal algorithmic changes, mitigating the fact that the midpoint rule is not a Poisson map [26].

For coupled complex systems, like ocean-atmosphere, groundwater-surface water, fluid-structure interactions, or magnetohydrodynamics, 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 routinely 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 [6], 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 [34, 35].

2. Generalization to a θ-like method

We remark also that (BEFE) is a particular instance of the one-leg 'θ-like' method:

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

implemented as:

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

which can be rewritten as:

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

Notice that (2.1) is not the classical linear multistep θ method [20, page 182], but Cauchy's one-leg version (see e.g. [9, pp. 40], also [13, 14, 15]):

$$\frac{y_{n+1} - y_n}{\tau_n} = f\big(t_{n+\theta}, \theta_n y_{n+1} + (1-\theta_n) y_n\big), \tag{2.4}$$

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

Remark 2.1. *It was recently proved in [4], for the Navier-Stokes equations, that the solutions constructed using the one-leg method* (2.4) *(with* $\theta_n = \frac{1}{2} + \tau_n^{1-\varepsilon}$*) for the finite-difference time-discretization and the finite element method for the spatial-discretization, give rise to suitable weak solutions in the sense of Scheffer and Caffarelli-Kohn-Nirenberg.*

In the following we mean stability in the sense of B-stability [7], which implies A-stability [13]. We say a method is B-stable if $\forall f$ satisfying $\langle f(u) - f(v), u - v\rangle \leq 0$ $\forall u, v$ in a Hilbert or a Banach space, it holds that $\|y_{n+1} - z_{n+1}\| \leq \|y_n - z_n\|$, where $\{y_n\}_{n\geq 0}, \{z_n\}_{n\geq 0}$ are two sequences of approximations computed with the method. (Here $\langle \cdot, \cdot \rangle$ denotes the inner product / duality mapping of the Hilbert / Banach space, and $\| \cdot \|$ denotes its norm.) Dahlquist introduced a similar criterion for certain types of multistep methods, G-stability (Dahlquist 1975, see e.g., [12] or [28, p.308]), which is equivalent to A-stability for constant step linear multistep methods.

Proposition 2.1. *The midpoint method* (BE)-(FE)*, and the* θ*-method* (2.2) *for* $\frac{1}{2} \leq \theta_n \leq 1$*, 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 $\theta_n = 1/2$. First, for B-stability, we consider the equation (2.4) for $\{y_{n+1}\}$ and respectively $\{z_{n+1}\}$. Then subtract, take the inner product with $\tau_n(y_{n+\theta_n} - z_{n+\theta_n})$, use the Cauchy-Schwarz inequality and the definition to obtain

$$\begin{aligned} 0 &\geq \tau_n \langle f(\theta_n, y_{n+\theta_n}) - f(\theta_n, z_{n+\theta_n}), y_{n+\theta_n} - z_{n+\theta_n}\rangle \\ &= \langle y_{n+1} - z_{n+1}, \theta_n(y_{n+1} - z_{n+1}) + (1-\theta_n)(y_n - z_n)\rangle \\ &= \theta_n \|y_{n+1} - z_{n+1}\|^2 + (\theta_n - 1)\|y_n - z_n\|^2 - (2\theta_n - 1)\langle y_{n+1} - z_{n+1}, y_n - z_n\rangle \\ &\geq \big(\theta_n \|y_{n+1} - z_{n+1}\| + (1-\theta_n)\|y_n - z_n\|\big)\big(\|y_{n+1} - z_{n+1}\| - \|y_n - z_n\|\big), \end{aligned}$$

which yields $\|y_{n+1}-z_{n+1}\| \leq \|y_n - z_n\|$.
For the energy equality we proceed in a similar manner. Multiplying both equations in (2.2) by $2\theta_n\tau_n y_{n+\theta_n}$ and $2(1-\theta_n)\tau_n y_{n+\theta_n}$ respectively, and applying the polarization identity we obtain:

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

Summation and the use of (2.2)

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

completes the argument. $\square$

3. Time-step adaptivity

We begin this section by a small observation: the local truncation error[1] of the midpoint method (BEFE) is:

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

The same formula holds for the 'θ–like' method (2.1), provided $\theta_n = \frac{1}{2} + \frac{1}{2}\tau_n^2$.

Therefore, we can adaptively adjust the time step τ_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 $\|\widehat{T}_{n+1}\| \approx \texttt{tol}$ (see e.g. [23]). The time-step τ_n^{new} which imposes that $\widehat{T}_{n+1}$ is sufficiently small is given by:

$$\tau_n^{new} = \kappa\tau_n \left|\texttt{tol}/\|\widehat{T}_{n+1}\|\right|^{\frac{1}{3}}, \tag{3.2}$$

where $\kappa = 1$. We found that more conservative coefficient values of the (safety coefficient [27, p.168], [26, p.255]) $\kappa = 0.90 \div 0.95$ minimize the number of time step rejections in the adaptive algorithm, while increasing the number of time intervals[2].

There are numerous ways in which the time-step adaptivity can be implemented (see e.g. [23]), out of which we briefly[3] present two methods. The first choice estimates the local truncation error by the difference between the numerical midpoint solution and a second-order approximation, given by a formula similar to the explicit Adams-Bashforth 2 (AB2) method. This method is related to the classical AB2 (see e.g., [27, p. 398]), the difference being that it uses the function values evaluated at

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[1] The local truncation error holds provided the solution is smooth enough.

[2] From (3.2) we see that if $\widehat{T}_{n+1} > \texttt{tol}$, then τ_n is decreased, and the algorithm repeats the midpoint rule step with a reduced time-step. Respectively, if $\widehat{T}_{n+1} \leq \texttt{tol}$, then τ_n is increased, and the computation moves to the next time interval, with the increased time step. The safety factor $\kappa < 1$ reduces the probability of the new time-steps being rejected in the [**if** $\|\widehat{T}_{n+1}\| \leq \texttt{tol}$] test in the Algorithm 1.

[3] An expanded version of this report is available at www.mathematics.pitt.edu/research/technical-reports

half-times $f_{n+1/2}, f_{n-1/2}, f_{n-3/2}$. The other option is based on the estimation of the LTE using Taylor expansions.

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Result: Adaptive midpoint rule
initialization: set 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., [10, 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-AB2) or (LTE-Taylor);
    $\tau^{\text{new}} \leftarrow \kappa\tau_n \left|\mathtt{tol}/\|\widehat{T}_{n+1}\|\right|^{\frac{1}{3}}$;
    if $\|\widehat{T}_{n+1}\| \leq \mathtt{tol}$ then
        $t_{n+1} \leftarrow t_n + \tau^{\text{new}}$, $t^{\text{new}} \leftarrow t_{n+1}$, $n \leftarrow n+1$
    end
end
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3.1. *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 $\mathscr{O}(\Delta t^2)$ midpoint-solution y_{n+1} and another second-order approximation, $y_{n+1}^{\widetilde{AB2}}$, obtained by a variable-step Adams-Bashforth 2-like method

$$y_{n+1}^{\widetilde{AB2}} = y_n \frac{(\tau_n + \tau_{n-1})(\tau_n + \tau_{n-1} + \tau_{n-2})}{\tau_{n-1}(\tau_{n-1} + \tau_{n-2})} - y_{n-1} \frac{\tau_n(\tau_n + \tau_{n-1} + \tau_{n-2})}{\tau_{n-1}\tau_{n-2}} + y_{n-2} \frac{\tau_n(\tau_n + \tau_{n-1})}{\tau_{n-2}(\tau_{n-1} + \tau_{n-2})},$$

and its local truncation error (under the ‘localization assumption’, i.e. back values are exact, see e.g. [23, p.70], [32, p.56]) can be written:

$$\widetilde{T_{n+1}^{AB2}} = \tau_n^3 y'''(t_{n+1/2})\mathscr{R}_n, \quad \text{where} \quad \mathscr{R}_n = \frac{1}{24} + \frac{1}{8}\left(1 + \frac{\tau_{n-1}}{\tau_n}\right)\left(1 + 2\frac{\tau_{n-1}}{\tau_n} + \frac{\tau_{n-2}}{\tau_n}\right).$$

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

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

where $y_{n+1}^{\text{midpoint}}$ denotes the midpoint solution from (BEFE).

3.2. *Estimation of the local truncation error using Taylor expansions*

In order to estimate the numerical value of $\widehat{T}_{n+1}$, we evaluate $y'''(t_n)$, in a manner similar to [23], manipulating Taylor expansions. Using the numerical method (1.2), the LTE (3.1) can be estimated in terms of the computed solutions as follows:

$$\begin{aligned}\widehat{T}_{n+1} = \frac{\tau_n^3}{3(\tau_n + 2\tau_{n-1} + \tau_{n-2})}\Bigg(& y_{n+1}\frac{1}{\tau_n(\tau_n + \tau_{n-1})} - y_n \frac{\tau_n + \tau_{n-1} + \tau_{n-2}}{\tau_n\tau_{n-1}(\tau_{n-1} + \tau_{n-2})}\\ &+ y_{n-1}\frac{\tau_n + \tau_{n-1} + \tau_{n-2}}{\tau_{n-1}\tau_{n-2}(\tau_n + \tau_{n-1})} - y_{n-2}\frac{1}{\tau_{n-2}(\tau_{n-1} + \tau_{n-2})}\Bigg).\end{aligned} \tag{LTE-Taylor}$$

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