

REFACTORIZATION OF A VARIABLE STEP, UNCONDITIONALLY STABLE METHOD OF DAHLQUIST, LINIGER AND NEVANLINNA

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Abstract. The one-leg, two-step time-stepping scheme proposed by Dahlquist, Liniger and Nevanlinna has clear advantages in complex, stiff numerical simulations: unconditional G -stability for variable time-steps and second-order accuracy. Yet it has been underutilized due, partially, to its complexity of direct implementation. We prove herein that this method is equivalent to the backward Euler method with pre- and post arithmetic steps added. This refactorization eases implementation in complex, possibly legacy codes. The realization we develop reduces complexity, including cognitive complexity and increases accuracy over both first order methods and constant time steps second order methods.

1. Introduction. Numerical methods for evolution equations are designed based on accuracy and stability. The theory of both is highly developed for constant time step and linear problems. Less is known for variable time steps and nonlinear problems. These cases are subtle. For example, for increasing time steps, the BDF2 method loses A -stability and suffers non-physical energy growth in the approximate solution [1]. Even the trapezoidal method is unstable when used with variable time steps, see e.g. [2], [3, pp. 181-182]. Dahlquist, Liniger and Nevanlinna in [2] proposed a one parameter δ -family of variable-step, one-leg, two-step methods (DLN), which are second-order accurate, and variable-step, nonlinearly, long-time stable. Its detailed specification (given in Section 2), is sufficiently Gordian to deter its use in complex applications, in which a method with DLN's excellent properties should be valued. Our preliminary work on adaptive time-stepping for flow problems [4, 5] shows that (DLN) has promise, motivating the work herein.

Refactorization generally means restructuring of an existing algorithm without changing its behaviour. The goal of refactorization is to reduce complexity by creating a simple and clean logical structure, improving implementation, code readability, source maintainability and extensibility. Herein we show how (DLN) can be refactorized to be easily implemented in an intricate, possibly legacy/black-box code, without modifying the 'assemble and solve' portion. While our refactorization can work for other base methods, to fix ideas for $y' = f(t, y)$, we consider a method based on the fully implicit Euler method

$$\frac{y^{\text{new}} - y^{\text{old}}}{t^{\text{new}} - t^{\text{old}}} = f(t^{\text{new}}, y^{\text{new}}). \quad (\text{BE})$$

Figure 2.1 illustrates the implementation of the (DLN) method in Algorithm 1, by adding a pre-filter step to the data ahead of the nonlinear solver (BE), and a poster-filter step after the solver (BE). This algorithmic idea is our first contribution. In Section 3 we prove a new expression for the local truncation error, which simplifies the time-adaptive implementation of (DLN), and also recall its variable step G -stability property.

2. The DLN method and its refactorization. We consider a numerical approximation of the initial value problem

$$y'(t) = f(t, y(t)), \quad y(0) = y_0. \quad (2.1)$$

at times $\{t_n\}_{n \geq 0}$, with the time step $k_n = t_{n+1} - t_n$. To present the method of [2], let $\varepsilon_n = (k_n - k_{n-1}) / (k_n + k_{n-1})$ denote the step size variability and $\delta \in [0, 1]$ be an arbitrary parameter. The (DLN) method is a 2-step method with coefficients:

$$\begin{bmatrix} \alpha_2 \\ \alpha_1 \\ \alpha_0 \end{bmatrix} = \begin{bmatrix} \frac{1}{2}(\delta + 1) \\ -\delta \\ \frac{1}{2}(\delta - 1) \end{bmatrix}, \quad \begin{bmatrix} \beta_2^{(n)} \\ \beta_1^{(n)} \\ \beta_0^{(n)} \end{bmatrix} = \begin{bmatrix} \frac{1}{4} \left(1 + \frac{1-\delta^2}{(1+\varepsilon_n\delta)^2} + \varepsilon_n^2 \frac{\delta(1-\delta^2)}{(1+\varepsilon_n\delta)^2} + \delta \right) \\ \frac{1}{2} \left(1 - \frac{1-\delta^2}{(1+\varepsilon_n\delta)^2} \right) \\ \frac{1}{4} \left(1 + \frac{1-\delta^2}{(1+\varepsilon_n\delta)^2} - \varepsilon_n^2 \frac{\delta(1-\delta^2)}{(1+\varepsilon_n\delta)^2} - \delta \right) \end{bmatrix}. \quad (2.2)$$

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Note that $\{\alpha_\ell\}_{\ell=0}^2$ are step size independent, while $\{\beta_\ell^{(n)}\}_{\ell=0}^2$ are step size dependent. Define the average step size \widehat{k}_n as follows:

$$\widehat{k}_n = \alpha_2 k_n - \alpha_0 k_{n-1} = \delta \frac{k_n - k_{n-1}}{2} + \frac{k_n + k_{n-1}}{2}. \quad (2.3)$$

The variable step DLN method of [2] as a one-leg¹ method is

$$\frac{\alpha_2 y_{n+1} + \alpha_1 y_n + \alpha_0 y_{n-1}}{\widehat{k}_n} = f\left(\beta_2^{(n)} t_{n+1} + \beta_1^{(n)} t_n + \beta_0^{(n)} t_{n-1}, \beta_2^{(n)} y_{n+1} + \beta_1^{(n)} y_n + \beta_0^{(n)} y_{n-1}\right). \quad (\text{DLN})$$

REMARK 1. The (DLN) methods are indexed by the free parameter $\delta \in [0, 1]$.

When $\delta = 1$, the (DLN) method becomes the (implicit) midpoint rule [7, 8]

$$\frac{y_{n+1} - y_n}{k_n} = f\left(\frac{1}{2}(t_{n+1} + t_n), \frac{1}{2}(y_{n+1} + y_n)\right), \quad (\text{one-step midpoint})$$

while for $\delta = 0$, the (DLN) method is the (implicit) midpoint rule with double time step

$$\frac{y_{n+1} - y_{n-1}}{k_n + k_{n-1}} = f\left(\frac{1}{2}(t_{n+1} + t_{n-1}), \frac{1}{2}(y_{n+1} + y_{n-1})\right). \quad (\text{two-step midpoint})$$

The value $\delta = \frac{2}{3}$ was chosen by Dahlquist, Liniger and Nevanlinna in [2], in order to minimize the error constant in the local truncation error (LTE) and to preserve good stability properties.

The value $\delta = \frac{2}{\sqrt{5}}$ was suggested by Kulikov and Shindin in [9] to provide the best stability at infinity, a property close to the L-stability of Ehle [10, 11], and computed by minimizing the spectral radius of the companion matrix [12].

To reduce the complexity of implementing (DLN), we consider its implementation through pre- and post-processes of an implicit (backward) Euler method, described in Algorithm 1, and illustrated in Figure 2.1.

Input: y_n, y_{n-1} and t_{n-1}, t_n, t_{n+1} ;

// Pre-process : **interpolation**

// Evaluate quantities in (2.2) and (2.3)

$$\begin{aligned} \alpha_2 &= \frac{1}{2}(\delta + 1), & \alpha_1 &= -\delta, & \alpha_0 &= \frac{1}{2}(\delta - 1), \\ \beta_2^{(n)} &= \frac{1}{4} \left(1 + \frac{1 - \delta^2}{(1 + \varepsilon_n \delta)^2} + \varepsilon_n^2 \frac{\delta(1 - \delta^2)}{(1 + \varepsilon_n \delta)^2} + \delta \right), \\ \beta_1^{(n)} &= \frac{1}{2} \left(1 - \frac{1 - \delta^2}{(1 + \varepsilon_n \delta)^2} \right), & \beta_0^{(n)} &= 1 - \beta_2^{(n)} - \beta_1^{(n)}, & \widehat{k}_n &= \alpha_2 k_n - \alpha_0 k_{n-1}. \end{aligned}$$

// Define the refactorization coefficients

$$\begin{cases} a_1^{(n)} = \beta_1^{(n)} - \frac{\alpha_1 \beta_2^{(n)}}{\alpha_2}, & a_0^{(n)} = 1 - a_1^{(n)}, & b^{(n)} = \frac{\beta_2^{(n)}}{\alpha_2}, \\ c_2^{(n)} = \frac{1}{\beta_2^{(n)}}, & c_1^{(n)} = -\frac{\beta_1^{(n)}}{\beta_2^{(n)}}, & c_0^{(n)} = -\frac{\beta_0^{(n)}}{\beta_2^{(n)}}. \end{cases} \quad (2.4)$$

// Evaluate the time-step for BE

$$(\Delta t)_n^{\text{BE}} \leftarrow b^{(n)} \widehat{k}_n$$

// Set the BE time interval: $[t^{\text{new}} - (\Delta t)_n^{\text{BE}}, t^{\text{new}}]$, and y_n^{old}

$$t^{\text{new}} \leftarrow \beta_2^{(n)} t_{n+1} + \beta_1^{(n)} t_n + \beta_0^{(n)} t_{n-1}; \quad y^{\text{old}} \leftarrow a_1^{(n)} y_n + a_0^{(n)} y_{n-1};$$

// **backward Euler**

Solve for y^{new} : $\frac{y^{\text{new}} - y^{\text{old}}}{(\Delta t)_n^{\text{BE}}} = f(t^{\text{new}}, y^{\text{new}})$

// Post-process : **extrapolation**

$$y_{n+1} \leftarrow c_2^{(n)} y^{\text{new}} + c_1^{(n)} y_n + c_0^{(n)} y_{n-1};$$

// the DLN solution

Output: y_{n+1} , If desired: Estimate Error and adapt k_n

Algorithm 1: Refactorization of the (DLN) method

¹The ‘one-leg’ term was coined by Dahlquist in 1975 [6] to name the multistep methods which involve only one value of f in each step. In particular, the leapfrog and BDF methods are one-leg multistep methods.

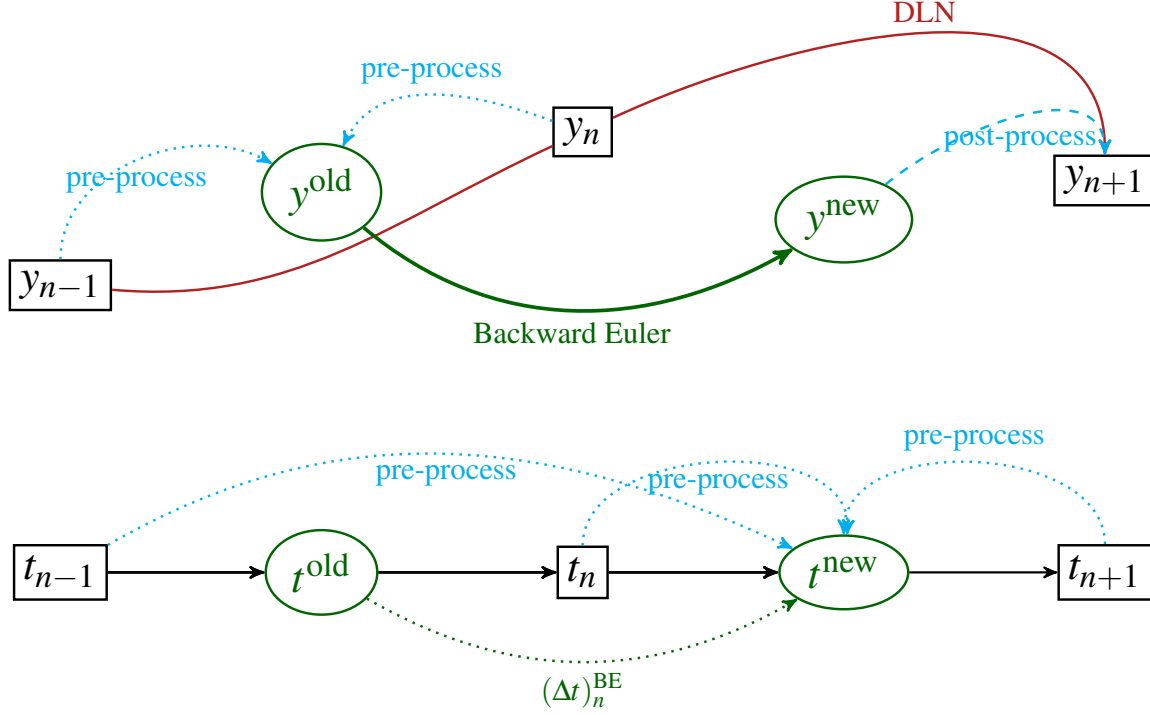


FIG. 2.1. Refactorization of the (DLN) method as a pre- and post-processed (BE) method

Since $\alpha_0 + \alpha_1 + \alpha_2 = 0$, $\beta_0^{(n)} + \beta_1^{(n)} + \beta_2^{(n)} = 1$, the coefficients $a_i^{(n)}, b^{(n)}, c_i^{(n)}$ satisfy $a_0^{(n)} + a_1^{(n)} = 1, c_2^{(n)} + c_1^{(n)} + c_0^{(n)} = 1$.

THEOREM 2.1. Algorithm (1) is equivalent to the (DLN) method.

Proof. First using the notations (2.4), the post-processing step writes

$$y^{\text{new}} = \frac{1}{c_2^{(n)}} y_{n+1} - \frac{c_1^{(n)}}{c_2^{(n)}} y_n - \frac{c_0^{(n)}}{c_2^{(n)}} y_{n-1} = \beta_2^{(n)} y_{n+1} + \beta_1^{(n)} y_n + \beta_0^{(n)} y_{n-1}.$$

Using also the pre-processing relations, the backward Euler step in Algorithm 1

$$\frac{y^{\text{new}} - y^{\text{old}}}{(\Delta t)_n^{\text{BE}}} = f(t^{\text{new}}, y^{\text{new}}) \quad (\text{DLN2BE})$$

translates to

$$\begin{aligned} & \frac{1}{\widehat{k}_n} \left(\frac{1}{b^{(n)} c_2^{(n)}} y_{n+1} - \frac{1}{b^{(n)}} \left(\frac{c_1^{(n)}}{c_2^{(n)}} + a_1^{(n)} \right) y_n - \frac{1}{b^{(n)}} \left(\frac{c_0^{(n)}}{c_2^{(n)}} + a_0^{(n)} \right) y_{n-1} \right) \\ & = f \left(\beta_2^{(n)} t_{n+1} + \beta_1^{(n)} t_n + \beta_0^{(n)} t_{n-1}, \beta_2^{(n)} y_{n+1} + \beta_1^{(n)} y_n + \beta_0^{(n)} y_{n-1} \right). \end{aligned}$$

Finally, by (2.4), this shows that the backward-Euler based Algorithm 1 yields the solution of the (DLN) method. \square

2.1. Related Work. The (DLN) method is variable-step G -stable outgrowth of a method of Liniger [13], which is non-autonomous A -stable (i.e. for $y' = \lambda(t)y$). The pre- and post-process steps in the Algorithm 1 are akin to time filters, highly developed as numerical methods in atmospheric science [14–18]. Recently it was noticed in [19] that this technique for adding stability can also increase accuracy. The idea of prefilter \rightarrow simple method \rightarrow postfilter was developed in a different direction for constant time steps in [20].

The refactorization of an algorithm to reduce its cognitive complexity has been used in [7] to rearrange a family of one-leg one-step methods into a backward Euler code followed by post-processing, and further applied for partitioning multi-physics problems [8, 21–23]. In [24], the authors describe the implementation of the (DLN) formulas in a Nordsieck formulation [25, 26] essentially identical to that of the backward differentiation formulas, facilitating to adapt Nordsieck formulation codes like DIFSUB [27, 28] to the (DLN) formulas.

3. Convergence analysis of (DLN). While stability and consistency were already addressed in [2], we present complementary details on both which are useful for developing an adaptive (DLN) method.

3.1. Consistency error. In [9, 29], the variable time-step (DLN) method was implemented in an adaptive manner, using a local and global error estimator. Similar to [2], the authors of [6, 9, 24, 29] use the classical definition of the local truncation error

$$\mathcal{L}_1(y(t), t_{n+1}, k_n) = \frac{1}{\widehat{k}_n} \sum_{\ell=0}^2 \alpha_\ell y(t_{n-1+\ell}) - f\left(t_{n,\beta}, \beta_2^{(n)} y(t_{n+1}) + \beta_1^{(n)} y(t_n) + \beta_0^{(n)} y(t_{n-1})\right),$$

where $t_{n,\beta} = \beta_2^{(n)} t_{n+1} + \beta_1^{(n)} t_n + \beta_0^{(n)} t_{n-1}$. The above definition follows the approach taken in the analysis of linear multistep methods (see e.g. [30, page 27]), and involves both the differentiation defect $\mathcal{L}_d = \frac{1}{\widehat{k}_n} \sum_{\ell=0}^2 \alpha_\ell y(t_{n-1+\ell}) - f(t_{n,\beta}, y(t_{n,\beta}))$, and the interpolation defect $\mathcal{L}_i = f(t_{n,\beta}, y(t_{n,\beta})) - f(t_{n,\beta}, \sum_{\ell=0}^2 \beta_\ell^{(n)} y(t_{n-1+\ell}))$. Dahlquist raised in [31] the question of the appropriateness of this viewpoint: “We accept this definition, but *we do not accept \mathcal{L}_1 as the adequate local truncation error!*”

Using the refactorized form (DLN2BE) and Theorem 2.1, we now prove that the local truncation error of the one-leg (DLN) method can be evaluated only by the differentiation defect (LTE), similarly to the midpoint rule [7] and the Runge-Kutta methods. The new expression (LTE) simplifies greatly the error estimation.

PROPOSITION 3.1. *The local truncation error of (DLN) is the differentiation error and*

$$\mathcal{L}_d(y(t), t_{n+1}, k_n) \approx \frac{y'''(t_n)}{2} \left[\frac{1}{\widehat{3k}_n} (k_n^3 - \frac{\alpha_0}{\alpha_2} k_{n-1}^3) - \frac{1}{\alpha_2} (\beta_2^{(n)} k_n - \beta_0^{(n)} k_{n-1})^2 \right]. \quad (\text{LTE})$$

Proof. The consistency order and the coefficient of the leading term in (LTE) follow by Taylor expansions. On one hand, since (DLN) can be refactorized as the one-step method (DLN2BE), we further write the (DLN) method as follows

$$\frac{\alpha_2 y_{n+1} + \alpha_1 y_n + \alpha_0 y_{n-1}}{\widehat{k}_n} = f(t^{\text{new}}, y^{\text{new}}). \quad (3.1)$$

On the other hand, when we integrate (2.1) on $[t_{n-1}, t_n]$ and on $[t_n, t_{n+1}]$, multiply the results by $\frac{1-\delta}{2}$ and $\frac{1+\delta}{2}$, respectively, and add, we obtain

$$\frac{1+\delta}{2} y(t_{n+1}) - \delta y(t_n) - \frac{1-\delta}{2} y(t_{n-1}) = \frac{1-\delta}{2} \int_{t_{n-1}}^{t_n} f(t, y(t)) dt + \frac{1+\delta}{2} \int_{t_n}^{t_{n+1}} f(t, y(t)) dt.$$

Finally, approximating both integrals in the right hand-side with the chord quadrature rule, with t^{new} as the point of evaluation on both intervals, gives

$$\frac{1+\delta}{2} y(t_{n+1}) - \delta y(t_n) - \frac{1-\delta}{2} y(t_{n-1}) \approx \left(\frac{1+\delta}{2} (t_{n+1} - t_n) - \frac{\delta-1}{2} (t_n - t_{n-1}) \right) f(t^{\text{new}}, y(t^{\text{new}})).$$

which by (2.2)-(2.3) yields the (3.1) method. \square

REMARK 2. *In particular, for $\delta = 1$ and $\delta = 0$, from (LTE) we have that*

$$\mathcal{L}^{\text{(one-step midpoint)}} \approx \frac{1}{24} k_n^3 y'''(t_n), \quad \mathcal{L}^{\text{(two-step midpoint)}} \approx \frac{1}{24} (k_n + k_{n-1})^3 y'''(t_n).$$

3.2. G-stability. Let $\langle \cdot, \cdot \rangle$ and $\|\cdot\|$ denote the inner product and ℓ^2 -norm in Euclidean space \mathbb{C}^d . For any pair of solutions $u(t), v(t)$ of (2.1), a necessary and sufficient condition [32, page 384] for $\|u(t) - v(t)\|$ to be a non-increasing function of t is the *contractivity* (one-sided Lipschitz) condition on f :

$$\operatorname{Re}\langle f(t, u) - f(t, v), u - v \rangle \leq 0, \quad \forall t \geq 0, \quad \forall u, v \in \mathbb{C}^d. \quad (\text{contractivity})$$

The system (2.1) for which f satisfies the (contractivity) condition is called *dissipative*, see e.g. the Definition in [33, page 268]. We recall that a Runge-Kutta method is *B-stable*, if the (contractivity) condition implies $\|y_{n+1} - z_{n+1}\| \leq \|y_n - z_n\|$ for any $\{y_n\}, \{z_n\}$ numerical solutions, see e.g. [34, page 359], or Definition 12.2 in [12]. Similarly, a 2-step linear multistep method is called *G-stable* [12, 32, 35, 36] if there exists a real positive definite matrix G such that its one-leg version is contractive, namely $\|Y_{n+1} - Z_{n+1}\|_G \leq \|Y_n - Z_n\|_G$, where $Y_n = [y_n^r, y_{n-1}^r]^r$. In the case of the (DLN) method, there exists such a positive definite matrix (independent of the step size)

$$G(\delta) := \begin{bmatrix} \frac{1}{4}(1 + \delta)\mathbb{I}_d & 0 \\ 0 & \frac{1}{4}(1 - \delta)\mathbb{I}_d \end{bmatrix}, \quad \forall \delta \in [0, 1].$$

As pointed out by Dahlquist in [37], both *B-stability* and *G-stability* imply *A-stability*, and *A-stability* implies *G-stability* for constant time steps.

PROPOSITION 3.2. *The (DLN) method is unconditionally G-stable, and*

$$\left\langle \sum_{\ell=0}^2 \alpha_\ell y_{n-1+\ell}, \sum_{\ell=0}^2 \beta_\ell^{(n)} y_{n-1+\ell} \right\rangle_{\mathbb{R}^d} = \left\| \begin{bmatrix} y_{n+1} \\ y_n \end{bmatrix} \right\|_{G(\delta)}^2 - \left\| \begin{bmatrix} y_n \\ y_{n-1} \end{bmatrix} \right\|_{G(\delta)}^2 + \left\| \sum_{\ell=0}^2 \gamma_\ell^{(n)} y_{n-1+\ell} \right\|^2, \quad (3.2)$$

where the γ -coefficients are $\gamma_1^{(n)} = -\frac{\sqrt{\delta(1-\delta^2)}}{\sqrt{2(1+\varepsilon_n\delta)}}$, $\gamma_2^{(n)} = -\frac{1-\varepsilon_n}{2}\gamma_1^{(n)}$, $\gamma_0^{(n)} = -\frac{1+\varepsilon_n}{2}\gamma_1^{(n)}$. The ‘energy’ identity (3.2), implicit in [2], follows from algebraic manipulations, see e.g. [4]. The *G-stability* of (DLN), i.e. $\|Y_{n+1} - Z_{n+1}\|_{G(\delta)} \leq \|Y_n - Z_n\|_{G(\delta)}$, follows from (3.2) and the (contractivity) assumption. The only (DLN) methods which yield the ℓ^2 invariance of the solution are the symplectic (one-step midpoint) and (two-step midpoint) rules: the numerical dissipation $\left\| \sum_{\ell=0}^2 \gamma_\ell^{(n)} y_{n-1+\ell} \right\|^2$ vanishes if and only if $\delta \in \{0, 1\}$.

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