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Convergence and component splitting for the Crank-Nicolson–Leap-Frog integration method

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ABSTRACT
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Convergence and Component Splitting for the Crank-Nicolson–Leap-Frog Integration Method

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Abstract

A new convergence condition is derived for the Crank-Nicolson–Leap-Frog integration scheme. The convergence condition guarantees second-order temporal convergence uniformly in the spatial grid size for a wide class of implicit-explicit splittings. This is illustrated by successfully applying component splitting to first-order wave equations resulting in such second-order temporal convergence. Component splitting achieves that only on part of the space domain Crank-Nicolson needs to be used. This reduces implicit solution costs when for Leap-Frog the step size is severely limited by stability only on part of the space domain, for example due to spatial coefficients of a strongly varying magnitude or locally refined space grids.

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Note: Work carried out within theme MAS1.

1 Introduction

CNLF (Crank-Nicolson–Leap-Frog) is a numerical integration method for systems of ordinary differential equations (ODEs)

$$w' = F(t,w)\,, \quad 0 < t \le T\,, \qquad w(0) = w_0\,, \tag{1.1}$$

where the vector function F allows a linear splitting

$$F(t,w) = F_0(t,w) + F_1(t,w)\,. \tag{1.2}$$

Typically F originates from spatial discretization of a Partial Differential Equation (PDE) and thus we think of systems (1.1) in the setting of the method of lines or semi-discretization [4]. Let w_n denote the CNLF approximation to $w(t_n)$ and $\tau = t_{n+1} - t_n$ the integration step size (taken constant here). Assuming that in addition to w_0 an approximation w_1 is available, the w_n are then defined by the two-step scheme

$$w_{n+1} - w_{n-1} = 2\tau F_0(t_n, w_n) + \tau F_1(t_{n+1}, w_{n+1}) + \tau F_1(t_{n-1}, w_{n-1})\,, \qquad n = 1, 2, \ldots\,. \tag{1.3}$$

For $F_0(t,w) = F(t,w)$ we recover the two-step, explicit midpoint rule which in the PDE literature is commonly called Leap-Frog. Likewise, if $F_1(t,w) = F(t,w)$, we recover the one-step, implicit

trapezoidal or Crank-Nicolson rule, here written down with a step size of length 2τ. CNLF is a classic two-step method within the class of so-called implicit-explicit linear multistep methods [1, 3, 4, 7] and is frequently used in Computational Fluid Dynamics (CFD) [8]. There the splitting (1.2) is used to treat convection terms (F_0) explicitly and viscous plus chemical reaction terms (F_1) implicitly [4].

The purpose of the current paper is to discuss (method of lines) convergence of CNLF governed by a special condition allowing a wider class of splittings than commonly used in CFD. Details are given in Section 2. As an application of this special convergence condition we will discuss component splitting for linear systems. Component splitting is akin to domain decomposition and to the approach of [6]. For CNLF it amounts to integrating on part of the space grid with LF (explicitly) and on the remaining part with CN (implicitly). This approach is useful in applications where for LF the step size τ is severely limited by stability on a small part of domain, for example due to spatial coefficients of a strongly varying magnitude or space grids with local refinements. Putting it differently, in such applications the aimed effect of component splitting is a significant reduction in implicit solution costs for CN. Details are given in Section 3. Section 4 is devoted to a one-space dimensional example emanating from the second-order wave equation. A similar two-space dimensional example is treated in Section 5. The paper finishes with concluding remarks in Section 6.

2 CNLF convergence

Over time intervals of finite length, CNLF is second-order consistent as an ODE integrator, that is, for a fixed dimension of (1.1). In a proper method of lines analysis, the dimension is not fixed as it depends on the underlying spatial grid size. Let the scalar h represent the spatial grid size. When we consider the dimension variable, in particular if we let $\tau, h \to 0$ simultaneously, temporal order constants that depend on h may grow unboundedly. This changes the consistency and convergence rate, with order reduction as a possible consequence [4]. In this section we discuss temporal convergence of CNLF in the method of lines setting, and thus all statements and results have to hold uniformly in the dimension of (1.1), that is, for the underlying spatial grid size $h \to 0$. Consequently, when we write $\mathcal{O}(\tau^p), p \geq 1$, we refer to asymptotics for simultaneously $\tau, h \to 0$ with the order constant involved independent of h. We also write $\mathcal{O}(1)$ and then we mean spatial boundedness for $h \to 0$. This will always be clear from the context.

Because we are interested in temporal convergence, we discuss convergence of w_n to $w(t_n)$, and thus neglect the spatial truncation error. This spatial error can be easily taken into account in our derivations when one would prefer to discuss temporal convergence towards the underlying PDE solution [4]. This, however, would be at the expense of more lengthy formulas without giving additional insight in temporal convergence.

2.1 Consistency

To begin with we substitute the exact solution $w(t)$ of (1.1) into (1.3) by which we introduce the local truncation error $\delta_n, n \geq 1$, for the integration step from t_n to t_{n+1}, that is,

$$w(t_{n+1}) - w(t_{n-1}) = 2\tau F_0(t_n, w(t_n)) + \tau F_1\left(t_{n+1}, w(t_{n+1})\right) + \tau F_1(t_{n-1}, w(t_{n-1})) + \delta_n\,. \quad (2.1)$$

Now denote, as in Section IV.4.2 of [4],

$$\varphi(t) = F_0(t, w(t))\,. \quad (2.2)$$

Eliminating the F_1-terms through (1.1) and (1.2), and expanding only w and w', then gives after a short calculation the expansion

$$\delta_n = \sum_{j=3,5,\,\ldots} 2\left(\frac{1}{j!} - \frac{1}{(j-1)!}\right)\tau^j w^{(j)}(t) + \tau\left(\varphi(t-\tau) - 2\varphi(t) + \varphi(t+\tau)\right)\,, \quad t = t_n\,. \quad (2.3)$$

We here tacitly assume temporal smoothness, that is, sufficient differentiability of $w(t)$ such that $w^{(j)}(t) = \mathcal{O}(1)$ for any j-th derivative of $w(t)$ encountered in the analysis.[1)] The sum starts of with τ^3 and contains only solution derivatives. This means that asymptotically the sum is only determined by temporal smoothness of the exact ODE solution. So this part of the local error is $\mathcal{O}(\tau^3)$, that is, retains the second-order ODE consistency when we simultaneously let $\tau, h \to 0$.

Next consider the remaining term $\tau\left(\varphi(t-\tau) - 2\varphi(t) + \varphi(t+\tau)\right)$ of (2.3). If [4]

$$\varphi(t) = \mathcal{O}(1) \text{ and three times differentiable,} \tag{2.4}$$

this term is also $\mathcal{O}(\tau^3)$, meaning that $\delta_n = \mathcal{O}(\tau^3)$. So if (2.4) applies, the ODE consistency of order two is retained for simultaneously $\tau, h \to 0$. The condition $\varphi(t) = \mathcal{O}(1)$ is the crucial one. It requires that components of $F_0(t, w(t))$ do not grow in size for decreasing spatial grid size. This holds for common splittings (1.2) used in CFD, because there the semi-discrete vector function $F_0(t, w)$ typically does incorporate boundary values. We refer to [4] for illustrative examples. Further, differentiability of $\varphi(t) = F_0(t, w(t))$ is a natural smoothness requirement. Altogether this explains that for CFD applications, CNLF often works very satisfactorily from the accuracy point of view, because the temporal accuracy it delivers only depends on the smoothness of the sought solution and order reduction does not occur.

However, there do exist splittings (1.2) for which the condition $\varphi(t) = \mathcal{O}(1)$ is violated, whereas CNLF still retains its temporal second order for simultaneously $\tau, h \to 0$ (an example is component splitting which is proposed in Section 3). This means that a special convergence condition exists which is more general than (2.4) in the sense that it covers a wider class of splittings. The next subsection is devoted to this special condition.

2.2 A special convergence condition

The results presented here are inspired by Lemma II.2.3 from [4] which has been introduced to examine related convergence issues for one-step methods. That lemma assumes linearity. We will here consider the nonlinear problem (1.1) (although in Section 3 and in the remainder linear problems will be used). Throughout we assume stability and existence of CNLF approximations uniformly in the dimension of (1.1). So our analysis focuses on consistency and we take any requirement associated to stability and existence of CNLF approximations for granted.

Let $e_n = w(t_n) - w_n$ denote the global error with $e_0 = 0$ and e_1 to be defined later (see Section 2.3). Introduce the integrated Jacobian

$$F'_{k,m} = \int_0^1 \frac{\partial F_k}{\partial w}(t_m, \sigma w(t_m) + (1-\sigma)w_m)d\sigma. \tag{2.5}$$

Subtracting (1.3) from (2.1) and applying the mean value theorem for vector functions, then yields the global error recursion

$$e_{n+1} - e_{n-1} = 2\tau F'_{0,n}e_n + \tau F'_{1,n+1}e_{n+1} + \tau F'_{1,n-1}e_{n-1} + \delta_n\,, \qquad n = 1, 2, \ldots\,, \tag{2.6}$$

or, equivalently,

$$e_{n+1} = 2\tau R_1 F'_{0,n}e_n + Re_{n-1} + R_1\delta_n\,, \qquad n = 1, 2, \ldots\,, \tag{2.7}$$

where

$$R_1 = (I - \tau F'_{1,n+1})^{-1} \quad \text{and} \quad R = R_1(I + \tau F'_{1,n-1})\,. \tag{2.8}$$

Observe that R is the global error amplification operator of CN for the problem $w' = F_1(t, w)$ when applied with step size 2τ. So, in view of our stability and existence assumption, we may assume that both R and R_1 exist and are bounded for $h \to 0$ and any $\tau > 0$. This means that we can interpret $R_1\delta_n$ as local error and if $\delta_n = \mathcal{O}(\tau^p)$ for simultaneously $\tau, h \to 0$, then this also holds for $R_1\delta_n$.

[1)] Spatial convergence assures that for $h \to 0$, the j-th temporal derivative $w^{(j)}(t)$ converges to the corresponding derivative of the underlying PDE solution, allowing us to write $w^{(j)}(t) = \mathcal{O}(1)$.

Assuming stability, the standard approach of global error analysis is to transfer all preceding local errors to the global error by means of the recursion (2.7). This will yield a bound for e_n of the size of $\tau^{-1}R_1\delta_n$. Thus, if $e_1 = \mathcal{O}(\tau^2)$ and (2.4) holds, we have $e_n = \mathcal{O}(\tau^2), n \geq 1$, that is, second-order convergence for simultaneously $\tau, h \to 0$. However, if the condition $\varphi = \mathcal{O}(1)$ is violated, so that we do not know whether $R_1\delta_n = \mathcal{O}(\tau^3)$, the standard approach of estimating the global errors will also transfer to e_n any possible order reduction in the local error resulting from this violation. Fortunately, this conclusion is too pessimistic in the sense that if $\varphi = \mathcal{O}(1)$ is violated, we can still have second-order convergence for simultaneously $\tau, h \to 0$. To show this, we adopt the approach of Lemma II.2.3 from [4]. That lemma amounts to finding a suitable expression for $R_1\delta_n$ such that we can modify the recursion (2.7) into a new one from which second-order convergence can be concluded. In so doing, we introduce the new condition which replaces $\varphi = \mathcal{O}(1)$.

A suitable expression for $R_1\delta_n, n \geq 1$, that works, is

$$R_1\delta_n = (I - 2\tau R_1 F'_{0,n} - R)\xi_n + \eta_n \qquad \text{such that} \qquad \xi_n = \mathcal{O}(\tau^2)\,, \quad \eta_n = \mathcal{O}(\tau^3)\,. \tag{2.9}$$

Thus we have to establish the existence of the errors vectors $\xi_n = \mathcal{O}(\tau^2)$ and $\eta_n = \mathcal{O}(\tau^3)$ for $n \geq 1$. We postpone this for a while and introduce the modified global errors

$$\hat{e}_n = e_n - \xi_n\,, \quad n \geq 0\,. \tag{2.10}$$

Inserting expression (2.9) into (2.7) yields

$$\hat{e}_{n+1} = 2\tau R_1 F'_{0,n}\hat{e}_n + R\hat{e}_{n-1} + \hat{\delta}_n\,, \qquad n = 1, 2, \dots\,, \tag{2.11}$$

where

$$\hat{\delta}_n = \xi_n - \xi_{n+1} + R(\xi_{n-1} - \xi_n) + \eta_n\,, \qquad n = 1, 2, \dots\,. \tag{2.12}$$

Consequently, if $\xi_n = \mathcal{O}(\tau^2), n \geq 0$, and $\eta_n = \mathcal{O}(\tau^3), n \geq 1$, the new local error $\hat{\delta}_n = \mathcal{O}(\tau^3)$ for all $n \geq 1$. Hence, instead of (2.7), recursion (2.11) can be used to establish second-order convergence for simultaneously $\tau, h \to 0$, since $\hat{e}_n = \mathcal{O}(\tau^2)$ implies $e_n = \mathcal{O}(\tau^2)$. What remains to be done is to verify (2.9) and to incorporate the starting error associated with the computation of w_1 into this analysis.

First we verify (2.9). Consider the local error expression (2.3) to which ξ_n and η_n are to be adapted. We choose η_n equal to the sum in (2.3) multiplied by R_1. The assumption $\eta_n = \mathcal{O}(\tau^3), n \geq 1$, is hereby satisfied because R_1 is bounded. There remains to define $\xi_n, n \geq 1$, through the relation

$$(I - 2\tau R_1 F'_{0,n} - R)\,\xi_n = \tau R_1\,(\varphi(t_{n-1}) - 2\varphi(t_n) + \varphi(t_{n+1}))\,. \tag{2.13}$$

Multiplying from left by $I - \tau F'_{1,n+1}$ then yields

$$A_n\,\xi_n = -\frac{1}{2}(\varphi(t_{n-1}) - 2\varphi(t_n) + \varphi(t_{n+1}))\,, \tag{2.14}$$

with A_n defined as

$$A_n = \frac{1}{2}F'_{1,n-1} + F'_{0,n} + \frac{1}{2}F'_{1,n+1}\,. \tag{2.15}$$

The new condition that replaces (2.4) and verifies condition $\xi_n = \mathcal{O}(\tau^2)$ from (2.9) now follows as

$$\varphi(t) \text{ is three times differentiable and solutions } \xi_n \text{ of (2.14) are bounded for } h \to 0\,. \tag{2.16}$$

This new condition does not require $\varphi(t) = \mathcal{O}(1)$ and therefore covers a wider class of splittings than (2.4) (an example is component splitting which we discuss in Section 3). If $\varphi(t) = \mathcal{O}(1)$ is violated, we can still have $\xi_n = \mathcal{O}(\tau^2)$ from (2.14), because for $h \to 0$ the grid function $A_n\xi_n$ can be unbounded for bounded ξ_n. In other words, the mapping from $-\frac{1}{2}(\varphi(t_{n-1}) - 2\varphi(t_n) + \varphi(t_{n+1}))$ to ξ_n through (2.14) is a discrete spatial integration which can turn an unbounded function into a bounded one.

2.3 Starting error

A natural scheme to provide w_1 is the related first-order implicit-explicit Euler scheme

$$w_1 - w_0 = \tau F_0(t_0, w_0) + \tau F_1(t_1, w_1)\,. \tag{2.17}$$

Its error $e_1 = w(t_1) - w_1$ satisfies

$$e_1 = R_1\,(I + \tau F'_{0,0})\,e_0 + R_1\delta_0\,, \qquad R_1 = (I - \tau F'_{1,1})^{-1}\,, \tag{2.18}$$

with as local error $\delta_0 = w(t_1) - w(t_0) - \tau F_0(t_0, w(t_0)) - \tau F_1(t_1, w(t_1))$. Eliminating F_1 reveals

$$\delta_0 = \mathcal{O}(\tau^2) + \tau(\varphi(t_1) - \varphi(t_0))\,. \tag{2.19}$$

Therefore, if (2.4) applies, $e_1 = R_1\delta_0 = \mathcal{O}(\tau^2)$ and (2.17) can be used to start up CNLF to achieve $\mathcal{O}(\tau^2)$ global errors for simultaneously $\tau, h \to 0$ for all $n \geq 1$.

Surprisingly, if (2.4) is violated, the combination implicit-explicit Euler–CNLF may suffer from order reduction which is solely due to the implicit-explicit Euler computation during the first step. We will illustrate this numerically in Section 4 and explain it here through the modified error analysis based on Lemma II.2.3 from [4]. This analysis assumes that $R_1\delta_0$ can be written as

$$R_1\delta_0 = (I - R_1(I + \tau F'_{0,0}))\xi_0 + \eta_0 \quad \text{such that} \quad \xi_0 = \mathcal{O}(\tau) \quad \text{and} \quad \eta_0 = \mathcal{O}(\tau^2)\,, \tag{2.20}$$

and involves the modified global errors $\hat{e}_0 = e_0 - \xi_0$ and $\hat{e}_1 = e_1 - \xi_1$ through the relation.

$$\hat{e}_1 = R_1\,(I + \tau F'_{0,0})\,\hat{e}_0 + \hat{\delta}_0\,, \qquad \hat{\delta}_0 = \xi_0 - \xi_1 + \eta_0\,. \tag{2.21}$$

Herein ξ_0 and η_0 are still to be defined whereas ξ_1 is a CNLF quantity given by (2.14). It is natural to choose for η_0 the $\mathcal{O}(\tau^2)$ term from (2.19) multiplied with R_1, retaining $\mathcal{O}(\tau^2)$. The remaining term $(I - R_1(I + \tau F'_{0,0}))\xi_0$ featuring in (2.20) then fits if

$$(I - R_1(I + \tau F'_{0,0}))\xi_0 = \tau R_1(\varphi(t_1) - \varphi(t_0))\,, \tag{2.22}$$

that is, if

$$B\,\xi_0 = \varphi(t_0) - \varphi(t_1)\,, \qquad B = F'_{0,0} + F'_{1,1}\,. \tag{2.23}$$

This condition is similar to (2.14) and may verify the condition $\xi_0 = \mathcal{O}(\tau)$ from (2.20). However, this gives $\hat{e}_0 = -\xi_0 = \mathcal{O}(\tau)$ rather than $\mathcal{O}(\tau^2)$. Also, ξ_0 is contained in the new local error $\hat{\delta}_1$ defined by (2.12), where ξ_0 also must be $\mathcal{O}(\tau^2)$ to take effect. More precisely, the modified error analysis succeeds for CNLF alone due to cancelation from the ξ-differences in (2.12). Apparently, this cancelation does not take place if we compute w_1 by means of the implicit-explicit Euler scheme.

In conclusion, if $\varphi(t) = \mathcal{O}(1)$ does not hold, while the aim is second-order CNLF convergence for simultaneously $\tau, h \to 0$, one should refrain from using implicit-explicit Euler as starting scheme. An alternative is to use the full Crank-Nicolson scheme CN at the start. CN does not suffer from order reduction and when CNLF is combined with CN, it is immediately seen that we will have second-order convergence for simultaneously $\tau, h \to 0$ under constraint (2.16) for all succeeding steps. The price to pay is that for computing w_1 we do not exploit splitting, but this is the case for a single step only.

3 Component splitting

We now proceed with linear systems

$$w' = Aw + f(t)\,, \tag{3.1}$$

accompanied with the split operators

$$F_0(t, w) = A_0 w + f_0(t)\,, \qquad F_1(t, w) = A_1 w + f_1(t)\,, \tag{3.2}$$

for which CNLF becomes

$$\begin{aligned} w_{n+1} - w_{n-1} &= 2\tau\left[(A_0 w_n + f_0(t_n)\right] + \\ &\quad \tau\left[A_1(w_n + w_{n+1}) + f_1(t_n) + f_1(t_{n+1})\right], \qquad n = 1, 2, \ldots . \end{aligned} \tag{3.3}$$

Our purpose here is to introduce what we call component splitting, which is an example of a splitting which violates the condition $\varphi(t) = \mathcal{O}(1)$ while CNLF retains its second-order temporal convergence for simultaneously $\tau, h \to 0$. We owe this to the new condition (2.16) derived from equation (2.14), which in the current linear case reads

$$A\,\xi_n = -\frac{1}{2}(\varphi(t_{n-1}) - 2\varphi(t_n) + \varphi(t_{n+1}))\,. \tag{3.4}$$

For a three times differentiable $\varphi(t)$, sufficient for (2.16) to hold is that a grid function $\nu = \mathcal{O}(1)$ exists such that $A\nu = \varphi(t)$.

In what follows we take A skew-symmetric with non-zero entries proportional to h^{-1} assuming that A originates from spatial discretization of a first-order wave equation. For skew-symmetric problems, component splitting is then defined by

$$\begin{aligned} A_0 &= A - SAS\,, \quad & f_0(t) &= (I - S)f(t)\,, \\ A_1 &= SAS\,, & f_1(t) &= Sf(t)\,, \end{aligned} \tag{3.5}$$

where S is a diagonal matrix with its entries S_{jj} obeying the rule

$$S_{jj} = \begin{cases} 0 & j\text{-th component of } w \text{ to be treated with LF,} \\ 1 & j\text{-th component of } w \text{ to be treated with CN.} \end{cases} \tag{3.6}$$

The definition of S is rather general so that we have some freedom in choosing S in an actual application. An important practical consideration is of course stability of CNLF. In this connection it is noteworthy that by left and right multiplying by S, A_0 and A_1 are skew-symmetric if A is skew-symmetric. Skew-symmetry of A_1 guarantees that the CN-matrix $I - \tau A_1$ is inversely bounded for any $\tau > 0$ and $h \to 0$. Also, the stability interval of LF is purely imaginary. So skew-symmetry of A_0 makes sense either.

Remark 3.1 For skew-symmetric problems $w' = Aw$, the stability properties of LF and CN are known and well understood [4]. The CN scheme $w_{n+1} = w_n + \frac{\tau}{2}A(w_{n+1} + w_n)$ can be proven to be stable for all $\tau > 0$ and the LF scheme $w_{n+1} = w_{n-1} + 2\tau A w_n$ if τ is smaller than one over the spectral radius of A. Likewise, for the linear CNLF scheme (3.3) stability can be proven if τ is smaller than one over the spectral radius of A_0, but under the restriction that A_0 and A_1 do commute [3]. However, as defined in (3.5), A_0 and A_1 cannot commute. We don't know of proven stability results for CNLF for non-commuting split matrices. Numerical experiments indicate that τ smaller than one over the spectral radius of A_0 is sufficient for stability, which we believe we owe to the skew-symmetry of A_0. In the numerical tests presented later on we will use values for τ practically equal to the spectral radius of A_0. $\diamond$

Let us examine condition (2.4) and equation (3.4) which is connected with condition (2.16). The requirement $\varphi(t) = \mathcal{O}(1)$ from (2.4) reads

$$\varphi(t) = (A - SAS)w(t) + (I - S)f(t) = w'(t) - S(ASw(t) - f(t)) = \mathcal{O}(1)\,. \tag{3.7}$$

The derivative $w'(t) = \mathcal{O}(1)$. So for (3.7) to hold it is necessary that $ASw(t) - f(t) = \mathcal{O}(1)$. This, however, cannot be true, since there will exist components which are proportional to h^{-1} (assuming a spatial discretization of a first-order wave equation). Specifically, (3.7) is violated at components for which the corresponding row remains unchanged ($S_{jj} = 1$), while one or more non-zero entries in this row have been put to zero due to the right-multiplication of A with S (in columns for which the associated entry $S_{kk} = 0$). Right-multiplication by S breaks up the divided

difference formula in parts leading to divided differences of solution values that no longer combine into a consistent derivative approximation. This suggests to avoid right-multiplication, and thus to define $A_0 = A - SA, A_1 = SA$. However, then we loose the skew-symmetry of A_0 and A_1 with loss of accuracy and even numerical instability as a possible consequence (confirmed by tests with the application of Section 4.1).

Next consider equation (3.4). We have to prove that a grid function $\nu = \mathcal{O}(1)$ exists such that $A\nu = \varphi(t)$. From the discussion above follows that $\varphi(t)$ has $\mathcal{O}(1)$ components and components proportional to h^{-1}. The mapping $\varphi \to \nu$ through $A\nu = \varphi(t)$ is a discrete spatial integration that will remove the h^{-1}-factor of $\varphi(t)$, implying that $\nu = \mathcal{O}(1)$. For the examples of Sections 4 and 5, we have verified the condition $\nu = \mathcal{O}(1)$ by solving $A\nu = \varphi(0)$ numerically for the grids Ω_h and matrices S specified in these examples.

4 Component splitting: a 1D illustration

In this section we numerically illustrate the component splitting introduced in Section 3 for the wave equation $U_{tt} = U_{xx}$ written in the first-order form

$$\begin{pmatrix} U_t \\ V_t \end{pmatrix} = \begin{pmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}, \qquad 0 < x < 1\,, \quad 0 < t \le T\,. \tag{4.1}$$

The solution reads $U(x,t) = \frac{1}{2}(g(x+t) + g(x-t))$, $V(x,t) = \frac{1}{2}(g(x+t) - g(x-t))$ for any differentiable given function g. We choose $g(x) = (\sin(\pi x))^{100}$ and for discretization we prescribe U and V at the two boundary points $x = 0, 1$ and the initial time $t = 0$. We emphasize that our sole purpose with this example is to numerically illustrate the second-order CNLF convergence and the order reduction when the implicit-explicit Euler scheme is used to start up, rather than solving a practical problem. For this purpose the current one-dimensional wave equation problem will do.

We semi-discretize (4.1) on a non-uniform grid $\Omega_h = (x_j)$ covering $[0, 1]$ by means of the difference method

$$U_j' = \frac{V_{j+1} - V_{j-1}}{x_{j+1} - x_{j-1}}\,, \quad V_j' = \frac{U_{j+1} - U_{j-1}}{x_{j+1} - x_{j-1}}\,, \quad U_j(t) \approx U(x_j, t)\,, \quad V_j(t) \approx V(x_j, t)\,. \tag{4.2}$$

This vertex-centered method yields 2nd-order convergence for all practical non-uniform grids [4], Section III.4.1. Next we assemble components U_j, V_j in a vector w so that we can write (4.2) in the linear system form (3.1). Using the natural ordering of components, this gives

$$A = \begin{pmatrix} 0 & D \\ D & 0 \end{pmatrix}, \qquad f(t) = \begin{pmatrix} f^U(t) \\ f^V(t) \end{pmatrix}, \tag{4.3}$$

where D is the associated finite-difference matrix and the source functions f^U, f^V contain the prescribed boundary values. Because D is skew-symmetric (in an appropriate inner product norm [4]), matrix A is also skew-symmetric. The CNLF scheme (3.3) is now defined by choosing S as

$$S = \begin{pmatrix} S_D & 0 \\ 0 & S_D \end{pmatrix}, \tag{4.4}$$

with S_D being the actual diagonal component-splitting matrix. Below we will make two different choices for Ω_h and accompanying S_D.

4.1 Non-uniform grid test

First we let Ω_h be composed of a uniform coarse grid and a uniform fine grid, with the aim of applying LF on the coarse grid and CN on the fine grid by means of CNLF, with a step size τ dictated for LF on the coarse grid.

The coarse grid covers $[0, 0.45] \cup [0.55, 1]$ with grid size h_1 and $2m_1$ points such that $m_1 h_1 = 0.45$. The fine grid covers $(0.45, 0.55)$ with grid size $h_2 \ll h_1$ and m_2 points such that $(m_2+1)h_2 = 0.1$. So the total number of grid points covering $[0, 1]$ is $2m_1+m_2$. We order the components U_j, V_j into w (from left to right, first the U_j, then the V_j, natural ordering) and give S_D zero entries $(S_D)_{jj}$ for $1 \le j \le m_1 - 2$ and $m_1 + m_2 + 3 \le j \le 2m_1 + m_2$ and ones elsewhere. This means that we apply CN on the fine grid covering $[0.45, 0.55]$, including one grid point left of $x = 0.45$ and one right of $x = 0.55$. With this definition of S_D, we achieve that all entries of the LF-matrix A_0 are proportional to h_1^{-1} and do not depend on the fine grid size h_2. Obviously, this is needed since we wish to integrate with a step size τ dictated for LF by the coarse grid.

CNLF has been applied six times over the time interval $[0, T]$ with $T = 0.25$, using $h_1 = 2^{-j}/40\,, h_2 = h_1/10$, $j = 1(1)6$ (slightly adjusted to get integer values for m_1, m_2). Hence the grid size at the refined patch is ten times smaller. The temporal step size is chosen near the maximal stable step size for LF would LF be applied alone on the uniform grid of (the coarse grid) size h_1 on the whole space interval, that is, $\tau = T/N$, $N = \lceil T/h_1 \rceil + 1$. Lest we miss the obvious, we let $\tau, h \to 0$ simultaneously since our aim is to test convergence uniformly in h.

The results for CNLF (with CN as starting scheme) are in full agreement with the above analysis confirming second-order convergence, see left plot of Figure 4.1 which shows infinity-norm accuracy for solution U versus the number of time steps at time T (o - marks). The dashed line represents exact order two convergence. We have also run CNLF with BE as starting scheme using the same grids and step sizes. The results confirm the anticipated order reduction from two to one ($*$-marks). For a further comparison CN alone has been applied (+-marks). We see that the accuracy for second-order CNLF is even slightly better meaning that the error constants have even become slightly smaller. This, of course, is problem and solution dependent while also the definition of the component splitting-matrix S_D plays a role. Overall the current test fully supports component splitting for CNLF.

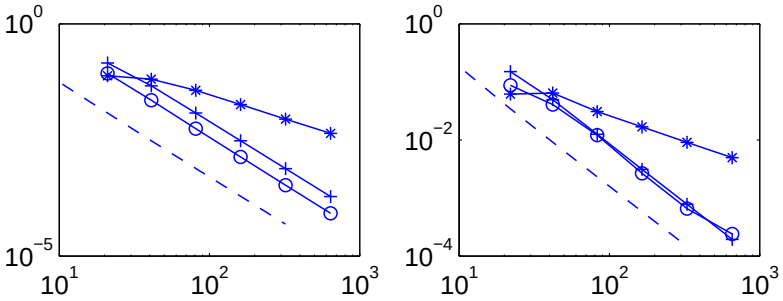

Figure 4.1: Results for the wave equation (4.1).

4.2 Uniform grid test with random splitting

Our second choice for Ω_h is a uniform grid with grid size $h = 1/(m+1)$ accompanied with a matrix S_D defined randomly. Let $y = \text{rand}(m, 1) \in R^m$ be a vector of random numbers between 0 and 1 generated by the Matlab command rand. We then define $(S_D)_{jj} = 0$ if $y_j \le \frac{1}{2}$ and $(S_D)_{jj} = 1$ if $y_j > \frac{1}{2}$. The random definition of S_D is of course only of theoretical interest. However, regarding convergence it yields an interesting test.

We again used the three schemes applied on the non-uniform grids in Section 4.1, here for $h = 2^{-j}/40$, $j = 1(1)6$ (slightly adjusted to get integer values for m) and $\tau = T/N$, $N = \lceil T/h \rceil + 1$. Although somewhat less regular due to the random nature of matrix S_D, the results are again fully in line with the consistency and convergence analysis and very satisfactory for second-order CNLF, see right plot of Figure 4.1 which shows the results in the same manner as in the left plot.

5 Component splitting: a 2D illustration

For a further numerical illustration we consider the linear, two-space dimensional PDE system

$$\begin{pmatrix} U_t \\ V_t \\ W_t \end{pmatrix} = \begin{pmatrix} 0 & \frac{\partial}{\partial y} & -\frac{\partial}{\partial x} \\ d\frac{\partial}{\partial y} & 0 & 0 \\ -d\frac{\partial}{\partial x} & 0 & 0 \end{pmatrix} \begin{pmatrix} U \\ V \\ W \end{pmatrix}, \tag{5.1}$$

where $U = U(x, y, t)$, etc., $0 < x, y < 1$ and $0 < t \le T$. The components U, V, W are prescribed at $t = 0$ and U is prescribed zero on the boundary for $t \ge 0$. The coefficient d is positive and space-dependent. The initial functions and coefficient d will be specified below. Note that U satisfies the 2nd-order wave equation $U_{tt} = (dU_x)_x + (dU_y)_y$ and that (5.1) is akin to the TE-form and TM-form of Maxwell's equations, see e.g. [2, 5].

For first-order systems of this type a staggered space grid is attractive. We semi-discretize by means of second-order, central differences on the uniform, staggered grid with grid size $h = 1/m$, such that U is approximated at (x_i, y_j) for $i, j = 1\,(1)\,m-1$, V at $(x_i, y_{j+1/2})$ for $i = 1\,(1)\,m-1$ and $j = 0\,(1)\,m-1$, and W at $(x_{i+1/2}, y_j)$ for $i = 0\,(1)\,m-1$ and $j = 1\,(1)\,m-1$. With this staggering we only need U from the boundary, and since U vanishes there, we end up with a linear, homogeneous system of ODEs which we denote by

$$w' = Aw\,, \qquad A = \begin{pmatrix} 0 & V_{[y]} & -W_{[x]} \\ U_{[y]} & 0 & 0 \\ -U_{[x]} & 0 & 0 \end{pmatrix}, \tag{5.2}$$

where $W_{[x]}$ is the difference matrix for $\partial/\partial x$ acting on component W, etc. The ordering for w is supposed to be based on the natural ordering along horizontal grid lines, while first collecting all U-components, etc. This ordering defines the central difference matrices contained in A. For convenience of presentation, the encountered d-values on the grid are contained in $U_{[x]}$ and $U_{[y]}$. In conclusion, A is a sparse difference matrix of dimension $(m-1)^2 + 2m(m-1)$ and A is diagonally similar to the skew-symmetric matrix obtained for $d(x, y) = 1$. CNLF applied to (5.2) is given by the integration formula (3.3) with zero source functions.

Similar to (4.4), we choose S in the diagonal form

$$S = \begin{pmatrix} S_U & 0 & 0 \\ 0 & S_V & 0 \\ 0 & 0 & S_W \end{pmatrix}, \tag{5.3}$$

where the diagonal matrix S_U, etc., needs to be specified for the actual PDE problem (5.1) in accordance with (3.6). For (5.1) we choose as initial functions $U(x, y, 0) = \sin(2\pi x)\sin(2\pi y), V(x, y, 0) = 0, W(x, y, 0) = 0$ and d is chosen as the strongly peaked function

$$d(x, y) = 0.95 + 9.05\, e^{-(2000\,((x-\frac{1}{2})^2 + (y-\frac{1}{2})^2))}\,, \tag{5.4}$$

with values between 0.95 and 10.0. This means that would LF be applied alone, for time stepping stability the step size τ would be restricted to approximately $\tau_F/10$, where $\tau_F = h/2\sqrt{2}$ is the step size limit for LF for constant $d = 1$. This situation calls for CNLF applied with $\tau = \tau_F$ and component splitting, such that near the center point of the space domain CN is applied and elsewhere LF. We then integrate with a tenfold larger step size while only on a small part of the domain implicit calculations are needed. This is achieved by a proper definition of S_U, S_V and S_W. For the results given below we have applied the rule: $d(x_i, y_j) \ge 1.0$ implies $(S_U)_{kk} = 1$ for entries associated with $(x_i, y_j), (x_i, y_{j\pm1}), (x_{i\pm1}, y_j)$, $(S_V)_{kk} = 1$ for entries associated with $(x_i, y_{j\pm1/2})$, and $(S_W)_{kk} = 1$ for entries associated with $(x_{i\pm1/2}, y_j)$. Entries not assigned to one are zero.

Regarding implementation, at each CNLF step we have to solve the linear system of algebraic equations $(I - \tau A_1)w_{n+1} = r$ with r the current right-hand side vector. Let r_u, r_v, r_w denote the

sub-vectors of r belonging to U, V, W. Let u_{n+1}, etc., denote the sub-vectors of w_{n+1}. The linear system then takes the form

$$\begin{pmatrix} I & -\tau S_U V_{[y]} S_V & \tau S_U W_{[x]} S_W \\ -\tau S_V U_{[y]} S_U & I & 0 \\ \tau S_W U_{[x]} S_U & 0 & I \end{pmatrix} \begin{pmatrix} u_{n+1} \\ v_{n+1} \\ w_{n+1} \end{pmatrix} = \begin{pmatrix} r_u \\ r_v \\ r_w \end{pmatrix}, \tag{5.5}$$

which is solved by

$$\begin{aligned} (I - \tau^2 \mathcal{M})\, u_{n+1} &= r_u + \tau S_U V_{[y]} S_V r_v - \tau S_U W_{[x]} S_W r_w\,, \\ v_{n+1} &= r_v + \tau S_V U_{[y]} S_U u_{n+1}\,, \\ w_{n+1} &= r_w - \tau S_W U_{[x]} S_U u_{n+1}\,, \end{aligned} \tag{5.6}$$

where $\mathcal{M}$ is the $(m-1)^2 \times (m-1)^2$ sparse matrix

$$\mathcal{M} = S_U V_{[y]} S_V U_{[y]} S_U + S_U W_{[x]} S_W U_{[x]} S_U\,. \tag{5.7}$$

Since $\mathcal{M}$ is symmetric non-positive definite (being the related 2nd-order central difference operator for the 2nd-order wave equation for U), this is an attractive form for numerical implementation (we used sparse LU).

Using this implementation, we have applied CNLF (with CN as starting scheme) four times, namely, for $m = h^{-1} = 10 \cdot 2^{j-1}, j = 1(1)4$ with $\tau = T/N, N = \lceil T/\tau_F \rceil + 1$ (so again τ and h decrease simultaneously). Since we have no exact solution available, the same runs have been carried out with CN alone. Adopting these CN-approximations as reference approximations, Table 5.1 gives for component U at time $T = 1.0$ the L_2-norm of the CN-approximations and the relative differences in the L_2-norm. Figure 5.1 plots U at the initial time on the 160×160 grid (left plot) and the CN approximation on this grid at $T = 1$ (right plot).

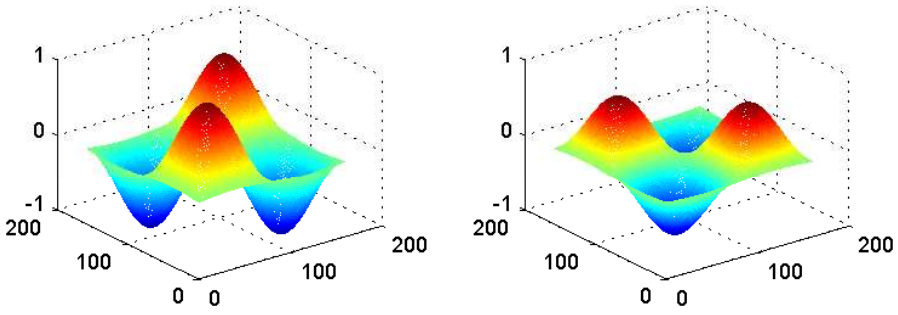

Figure 5.1: Component U of the two-dimensional test problem .

The relative differences are small and fully in line with our positive findings for the one-dimensional problem of Section 4. Clearly, also for the current two-dimensional problem CNLF is stable using the maximal stable step size for LF alone with $d(x, y) = 1.0$. As a further check on accuracy of CNLF, we have also computed the relative differences between CN alone and LF alone, the latter applied with a tenfold smaller step size τ, see fourth column of Table 5.1. The latter differences are only about two to three times smaller, which confirms the good performance of CNLF applied with component splitting. Finally, regarding efficiency, in the table we also give the numbers of nonzero entries of $\mathcal{M}$ with and without splitting. These numbers reveal the gain in sparsity for $\mathcal{M}$ due to component splitting and hence the reduction in implicit solution costs for CN alone.

m	L_2-norm	rel.diff. CN-CNLF	rel.diff. CN-LF	nnz without split	nnz with split
20	0.3609	$0.487\,10^{-1}$	$0.170\,10^{-1}$	1729	45
40	0.3662	$0.135\,10^{-1}$	$0.452\,10^{-2}$	7449	97
80	0.3650	$0.354\,10^{-2}$	$0.173\,10^{-2}$	30889	305
160	0.3635	$0.147\,10^{-2}$	$0.830\,10^{-3}$	125769	1181

Table 5.1: Results for the test problem from Section 5.

6 Concluding remarks

The contribution of this paper is twofold, (i) a new convergence condition for the Crank-Nicolson–Leap-Frog integration method guaranteeing second-order temporal convergence uniformly in the spatial grid size for a wide class of implicit-explicit splittings, (ii) component splitting which we have introduced and illustrated for first-order wave equations. The new convergence condition explains why for component splitting the second-order is maintained for simultaneously $\tau, h \to 0$. In addition to such second-order convergence, in our numerical tests Crank-Nicolson–Leap-Frog turned out to be comparably accurate as full Crank-Nicolson, which is a clear asset for component splitting. The approach is definitely also of interest for the three-dimensional Maxwell equations discretized on a staggered space grid as in the popular Yee scheme [9], since all derivations given in Section 5 on the two-dimensional problem carry over to the three-dimensional Maxwell equations.

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