THE UNSTABLE MODE IN THE CRANK-NICOLSON LEAP-FROG METHOD IS STABLE

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Abstract. This note proves that under the usual timestep condition $\Delta t |\Lambda| < 1$, derived from the scalar test problem $y' + ay + i\lambda y = 0$, all modes of the Crank-Nicolson Leap Frog (CNLF) approximate solution to the system

$$\frac{du}{dt} + Au + \Lambda u = 0$$
, for $t > 0$ and $u(0) = u_0$

where $A + A^T > 0$ and Λ is skew symmetric, are asymptotically stable. Thus, CNLF does indeed control the unstable mode.

 ${\bf Key}$ words. IMEX methods, Crank-Nicolson, Leap Frog, CNLF, unstable mode, computational mode

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1. Introduction. In this note we prove (asymptotic) stability of the so-called *unstable mode* (or *computational mode*) of the Crank-Nicolson Leap-Frog, CNLF, method for:

$$\frac{du}{dt} + Au + \Lambda u = 0, \text{ for } t > 0 \text{ and } u(0) = u_0$$

$$A: A + A^T > 0 \text{ and } \Lambda: \text{ skew symmetric.}$$
(1.1)

Here $u : [0, \infty) \to \mathbb{R}^d$ and the square, non-commutative, real matrices A, Λ have compatible dimensions. Under these conditions, the solution to (1.1) satisfies $u(t) \to 0$ as $t \to \infty$ so any growth in the approximate solution is a numerics induced instability. With superscript denoting the time step number, CNLF, the Implicit-Explicit (IMEX) combination of Crank-Nicolson and Leap Frog, is given by: given u^0, u^1 , for $n \ge 2$

$$\frac{u^{n+1} - u^{n-1}}{2\triangle t} + A \frac{u^{n+1} + u^{n-1}}{2} + \Lambda u^n = 0.$$
 (CNLF)

Root condition analysis for the scalar test problem $y' + ay + i\lambda y = 0$ leads to the timestep condition, necessary for stability, [JK63], and recently proven sufficient in [LT12],

$$\Delta t |\Lambda| < 1, \quad |\cdot| = \text{euclidean norm.} \tag{1.2}$$

However, in practical simulations, difficulties with CNLF's unstable mode occur. It is often reported that as $n\to\infty$

Stable Mode:
$$|u^{n+1} + u^{n-1}| \to 0$$
,
Unstable Mode: $|u^{n+1} - u^{n-1}| \to \infty$. (1.3)

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CNLF is used for many geophysical flow simulations from which experience with and fixes for the unstable mode are correspondingly large, e.g., [D10], [K03], [K12], [TL05], [A72], [R69], [W11], [JW11]. One mystery is that since CNLF is stable under (1.2), no growth is possible in theory and yet time filters to deal with (1.3) are nearly universal in practice, [JW11]. It is an open question to determine if this could be due to a gap for IMEX methods (e.g., [ARW95], [CM10], [FHV96], [HV03], [V80], [V09]) between necessary conditions from root condition analysis and sufficient ones for systems, to accumulation in the unstable mode of roundoff errors, to imperfect imposition of the timestep condition, to nonlinearities or other unknown causes. We prove that under (1.2) the CNLF unstable mode is (asymptotically) stable. This result, consistent with numerical tests in Section 3, supports the scenario that growth in the unstable mode is due to imperfect imposition of (1.2).

THEOREM 1.1. Suppose the timestep condition (1.2) holds. Then, all modes of CNLF are asymptotically stable:

$$u^n \to 0 \text{ as } n \to \infty \text{ and thus both}$$

 $u^{n+1} + u^{n-1} \to 0 \text{ and } u^{n+1} - u^{n-1} \to 0.$

2. Proof of asymptotic stability of the unstable mode. Denote the usual euclidean inner product and norm by $\langle w, v \rangle := w^T v$, $|v|^2 := \langle v, v \rangle$ and the A-norm (well defined since $A + A^T > 0$) by

$$|u|_A^2 := u^T A u.$$

Step 1: Energy Stability. In step 1 we follow [LT12]. Take the inner product of CNLF with $u^{n+1} + u^{n-1}$, add and subtract $|u^n|^2$ and multiply through by $2\triangle t$. This yields

$$\begin{bmatrix} |u^{n+1}|^2 + |u^n|^2 \end{bmatrix} - \begin{bmatrix} |u^n|^2 + |u^{n-1}|^2 \end{bmatrix}$$

$$\triangle t |u^{n+1} + u^{n-1}|_A^2 + 2\triangle t \langle \Lambda u^n, u^{n+1} + u^{n-1} \rangle = 0.$$
(2.1)

Next, using skew symmetry rearrange

+

$$2 \triangle t \langle \Lambda u^n, u^{n+1} + u^{n-1} \rangle = 2 \triangle t \langle \Lambda u^n, u^{n+1} \rangle - 2 \triangle t \left\langle \Lambda u^{n-1}, u^n \right\rangle.$$

Define the first energy (which is positive if $\Delta t |\Lambda| < 1$, [LT12])

$$E^{n+1/2} := |u^{n+1}|^2 + |u^n|^2 + 2\Delta t \langle \Lambda u^n, u^{n+1} \rangle.$$

Collecting terms we obtain

$$E^{n+1/2} - E^{n+1/2} + \Delta t |u^{n+1} + u^{n-1}|_A^2 = 0.$$
(2.2)

This implies that the stable mode $u^{n+1} + u^{n-1} \to 0$ as $n \to \infty$. Indeed, summing for $n = 1, \dots, N$ and then letting $N \to \infty$, we see that

$$\sum_{n=1}^{\infty} |u^{n+1} + u^{n-1}|_A^2 < \infty$$

and thus the n^{th} term $|u^{n+1} + u^{n-1}|_A^2 \to 0$.

Step 2: A second estimate. Take the inner product of CNLF with $u^{n+1}-u^{n-1}$ and multiply through by $2\triangle t\delta$ where $\delta > 0$ will be determined later. This gives

$$\Delta t \delta \left\langle A(u^{n+1} + u^{n-1}), u^{n+1} - u^{n-1} \right\rangle$$

+ $\delta |u^{n+1} - u^{n-1}|^2 + 2\delta \Delta t \left\langle \Lambda u^n, u^{n+1} - u^{n-1} \right\rangle = 0.$ (2.3)

Split the operator A into two parts, $A := A_s + A_{ss}$ where A_s is symmetric and A_{ss} is skew-symmetric. The first term of (2.3) becomes

$$\langle A(u^{n+1}+u^{n-1}), u^{n+1}-u^{n-1} \rangle$$

= $\langle A_s(u^{n+1}+u^{n-1}), u^{n+1}-u^{n-1} \rangle + \langle A_{ss}(u^{n+1}+u^{n-1}), u^{n+1}-u^{n-1} \rangle$
= $\langle A_s u^{n+1}, u^{n+1} \rangle - \langle A_s u^{n-1}, u^{n-1} \rangle + \langle A_{ss}(u^{n+1}+u^{n-1}), u^{n+1}-u^{n-1} \rangle$
= $|u^{n+1}|_A^2 - |u^{n-1}|_A^2 + \langle A_{ss}(u^{n+1}+u^{n-1}), u^{n+1}-u^{n-1} \rangle$

since the A-norm holds the property $|v|_A^2 = \langle A_s v, v \rangle$. Use the above equality for the first term in (2.3) and add and subtract $\Delta t \delta |u^n|_A^2$ to gain

$$\begin{split} \left[\delta \triangle t | u^{n+1} |_A^2 + \delta \triangle t | u^n |_A^2 \right] &- \left[\delta \triangle t | u^n |_A^2 + \delta \triangle t | u^{n-1} |_A^2 \right] \\ &+ \delta \triangle t \left\langle A_{ss} (u^{n+1} + u^{n-1}), u^{n+1} - u^{n-1} \right\rangle \\ &+ \delta | u^{n+1} - u^{n-1} |^2 + 2\delta \triangle t \left\langle \Lambda u^n, u^{n+1} - u^{n-1} \right\rangle = 0. \end{split}$$
(2.4)

Define the second energy

$$\mathcal{E}^{n+1/2} := E^{n+1/2} + \delta \triangle t |u^{n+1}|_A^2 + \delta \triangle t |u^n|_A^2$$

The key step is adding (2.2) and (2.4) which gives

$$\mathcal{E}^{n+1/2} - \mathcal{E}^{n-1/2} + \Delta t |u^{n+1} + u^{n-1}|_A^2 + \delta |u^{n+1} - u^{n-1}|^2 + \delta \Delta t \left\langle A_{ss}(u^{n+1} + u^{n-1}), u^{n+1} - u^{n-1} \right\rangle + 2\delta \Delta t \left\langle \Lambda u^n, u^{n+1} - u^{n-1} \right\rangle = 0.$$

Summing this from n = 1 to N gives

$$\mathcal{E}^{N+1/2} + \sum_{n=1}^{N} \left[\Delta t | u^{n+1} + u^{n-1} |_{A}^{2} + \delta | u^{n+1} - u^{n-1} |^{2} \right] + Q_{1} + Q_{2} = \mathcal{E}^{1/2}, \quad (2.5)$$
$$Q_{1} := \sum_{n=1}^{N} \delta \Delta t \left\langle A_{ss}(u^{n+1} + u^{n-1}), u^{n+1} - u^{n-1} \right\rangle,$$
$$Q_{2} := \sum_{n=1}^{N} 2\delta \Delta t \left\langle \Lambda u^{n}, u^{n+1} - u^{n-1} \right\rangle.$$

Step 3: Bounding $|Q_1|$ & $|Q_2|$. For Q_1 note that

$$\begin{split} \left\langle A_{ss}(u^{n+1}+u^{n-1}), u^{n+1}-u^{n-1} \right\rangle \\ &\leq |A_{ss}||u^{n+1}+u^{n-1}||u^{n+1}-u^{n-1}| \\ &\leq \frac{1}{2\epsilon} |A_{ss}||u^{n+1}+u^{n-1}|^2 + \frac{\epsilon}{2} |A_{ss}||u^{n+1}-u^{n-1}|^2 \end{split}$$

where $\epsilon > 0$. Hence

$$|Q_1| \le \sum_{n=1}^N \frac{\delta \triangle t}{2\epsilon} |A_{ss}| |u^{n+1} + u^{n-1}|^2 + \sum_{n=1}^N \frac{\delta \triangle t\epsilon}{2} |A_{ss}| |u^{n+1} - u^{n-1}|^2$$
3

For Q_2 note that

$$\begin{split} \langle \Lambda u^n, u^{n+1} - u^{n-1} \rangle \\ &= \frac{1}{2} \langle \Lambda (u^n - u^{n-2}), u^{n+1} - u^{n-1} \rangle + \frac{1}{2} \langle \Lambda (u^n + u^{n-2}), u^{n+1} - u^{n-1} \rangle \\ &\leq \frac{1}{2} |\Lambda| |u^n - u^{n-2}| |u^{n+1} - u^{n-1}| + \frac{1}{2} |\Lambda| |u^n + u^{n-2}| |u^{n+1} - u^{n-1}| \\ &\leq \frac{1}{2} |\Lambda| \left(\frac{1}{2} |u^n - u^{n-2}|^2 + \frac{1}{2} |u^{n+1} - u^{n-1}|^2 \right) + \\ &\quad + \frac{1}{2} |\Lambda| \left(\frac{1}{2\epsilon} |u^n + u^{n-2}|^2 + \frac{\epsilon}{2} |u^{n+1} - u^{n-1}|^2 \right). \end{split}$$

Then

$$2\delta\Delta t \sum_{n=1}^{N} \frac{1}{2} |\Lambda| \left(\frac{1}{2} |u^n - u^{n-2}|^2 + \frac{1}{2} |u^{n+1} - u^{n-1}|^2 \right) = \frac{\delta}{2} \Delta t |\Lambda| |u^{N+1} - u^{N-1}|^2 + \delta \Delta t |\Lambda| \left(|u^N - u^{N-2}|^2 + \dots + |u^3 - u^1|^2 \right) + \frac{\delta}{2} \Delta t |\Lambda| |u^2 - u^0|^2 \leq \delta \Delta t |\Lambda| \sum_{n=1}^{N} |u^{n+1} - u^{n-1}|^2,$$

$$(2.6)$$

and

$$2\delta\Delta t \sum_{n=1}^{N} \frac{1}{2} |\Lambda| \left(\frac{1}{2\epsilon} |u^{n} + u^{n-2}|^{2} + \frac{\epsilon}{2} |u^{n+1} - u^{n-1}|^{2} \right)$$

$$= \frac{\delta\Delta t |\Lambda|}{2\epsilon} \sum_{n=1}^{N-1} |u^{n+1} + u^{n-1}|^{2} + \frac{\epsilon\delta\Delta t |\Lambda|}{2} \sum_{n=1}^{N} |u^{n+1} - u^{n-1}|^{2}$$

$$\leq \frac{\delta\Delta t |\Lambda|}{2\epsilon} \sum_{n=1}^{N} |u^{n+1} + u^{n-1}|^{2} + \frac{\epsilon\delta\Delta t |\Lambda|}{2} \sum_{n=1}^{N} |u^{n+1} - u^{n-1}|^{2}.$$
(2.7)

Thus, $|Q_2|$ is now bounded by combining (2.6) and (2.7) as follows

$$|Q_2| \le \delta \Delta t |\Lambda| (1 + \frac{\epsilon}{2}) \sum_{n=1}^N |u^{n+1} - u^{n-1}|^2 + \frac{\delta \Delta t |\Lambda|}{2\epsilon} \sum_{n=1}^N |u^{n+1} + u^{n-1}|^2.$$

Hence

$$\begin{split} |Q_1| + |Q_2| &\leq \delta \Delta t \Big(|\Lambda| (1 + \frac{\epsilon}{2}) + \frac{\epsilon}{2} |A_{ss}| \Big) \sum_{n=1}^N |u^{n+1} - u^{n-1}|^2 \\ &+ \frac{\delta \Delta t}{2\epsilon} \Big(|\Lambda| + |A_{ss}| \Big) \sum_{n=1}^N |u^{n+1} + u^{n-1}|^2. \end{split}$$

Step 4: Using the $Q_1 \& Q_2$ estimates in the energy inequality. Inserting

this estimate for Q_1 and Q_2 into the energy inequality and collecting terms gives

$$\mathcal{E}^{N+1/2} + \delta \left(1 - (1 + \frac{\epsilon}{2}) \Delta t |\Lambda| - \frac{\epsilon}{2} \Delta t |A_{ss}| \right) \sum_{n=1}^{N} |u^{n+1} - u^{n-1}|^2 + \Delta t \sum_{n=1}^{N} \left(|u^{n+1} + u^{n-1}|_A^2 - \frac{\delta}{2\epsilon} \left(|\Lambda| + |A_{ss}| \right) |u^{n+1} + u^{n-1}|^2 \right) \le C(u^0, u^1).$$
(2.8)

Step 5: Estimating the unstable mode. Since the RHS, $C(u^0, u^1)$, is independent of N, we can let $N \to \infty$ and conclude that

$$\delta\left(1 - (1 + \frac{\epsilon}{2})\Delta t |\Lambda| - \frac{\epsilon}{2}\Delta t |A_{ss}|\right) \sum_{n=1}^{\infty} |u^{n+1} - u^{n-1}|^2 + \Delta t \sum_{n=1}^{\infty} \left(|u^{n+1} + u^{n-1}|_A^2 - \frac{\delta}{2\epsilon} \left(|\Lambda| + |A_{ss}|\right)|u^{n+1} + u^{n-1}|^2\right) < \infty.$$

From this we shall deduce that $\sum_{n=1}^{\infty} |u^{n+1}-u^{n-1}|^2 < \infty$ and thus $|u^{n+1}-u^{n-1}|^2 \to 0$ as $n \to \infty$. To make this step, two conditions are required: the second sum must be non-negative and the coefficient of the first sum positive. That coefficient is positive if

$$\epsilon < 2 \frac{1 - \Delta t |\Lambda|}{\Delta t |\Lambda| + \Delta t |A_{ss}|}$$

Since $\epsilon > 0$ is arbitrary, this condition can be satisfied if the stability condition $\Delta t |\Lambda| < 1$ holds. For the second sum to be non-negative, it suffices that

$$|u^{n+1} + u^{n-1}|_A^2 - \frac{\delta(|\Lambda| + |A_{ss}|)}{2\epsilon}|u^{n+1} + u^{n-1}|^2 \ge 0$$

This can be attained by picking $\delta = \epsilon \lambda_{\min}(A_s) / (|\Lambda| + |A_{ss}|)$, where $\lambda_{\min}(A_s)$ denotes the minimum eigenvalue of A_s . With this condition on Δt and choice of δ , we conclude that the sum below converges

$$\sum_{n=1}^{\infty} |u^{n+1} - u^{n-1}|^2 \le C < \infty.$$
(2.9)

Thus the n^{th} term $|u^{n+1} - u^{n-1}|^2 \to 0$ and $|u^{n+1} + u^{n-1}|^2_A \to 0$ from Step 1. Hence, $u^n \to 0$ and all modes, including the unstable mode, are controlled.

3. Numerical Exploration of the Unstable Mode. There are (at least) three natural conjectures about the growth of the unstable mode¹. The first is that practical simulations often occur with many accompanying perturbations. Thus the matrix Λ will only be skew symmetric to $O(\varepsilon)$, where ε is the magnitude of the errors in numerical integration, computer arithmetic, function evaluation, previous calculations and so on used to generate Λ and form the product Λu . These perturb the eigenvalues of Λ to be outside the stability interval of leap-frog, $\{z : \operatorname{Re}(z) = 0, -1 < \operatorname{Im}(z) < +1\}$. CN contributes damping of the stable mode sufficient to control its growth, leaving the

¹These scenarios owe much to many lively discussions with Catalin Trenchea, for which we are appreciative.

unstable mode's growth to accumulate. The **second** is that practical simulations often occur for implicitly defined operators Λ . The singular values of Λ are not available and guesses of $|\Lambda|$ based on physical reasoning or preliminary calculations are used instead. As a result, the timestep condition $\Delta t |\Lambda| < 1$ may be slightly violated. This results in an instability that begins small, is damped in the stable mode by CN and accumulates in the unstable mode. The **third** is that the unstable mode occurs only in cases not covered by the theorem such as with A = A(u). Practical simulations often occur with Λ a linear operator (as covered) but A = A(u) a nonlinear operator with $\langle A(u), u \rangle \geq 0$ for which step 2 in the proof fails.

We give three tests to check these scenarios.

Test 1:A has large skew symmetric part. Let

$$A = \begin{bmatrix} 10^4 & 10^3 \\ -10^3 & 10^{-4} \end{bmatrix}$$

which has symmetric part $A_s = diag\{10^4, 10^{-4}\}$ and skew symmetric part $A_{ss} = antidiag\{-10^3, 10^3\}$ and consider the 2 × 2 system

$$\frac{du}{dt} + (10^4u + 10^3v) - v = 0, \ \frac{dv}{dt} + (10^{-4}v - 10^3u) + u = 0.$$

The matrix Λ is

$$\Lambda = \begin{bmatrix} 0 & -1 \\ +1 & 0 \end{bmatrix}$$

We apply CNLF over a long time interval:

$$\frac{u^{n+1} - u^{n-1}}{2\triangle t} + 10^4 \frac{u^{n+1} + u^{n-1}}{2} + 10^3 \frac{v^{n+1} + v^{n-1}}{2} - v^n = 0,$$

$$\frac{v^{n+1} - v^{n-1}}{2\triangle t} + 10^{-4} \frac{v^{n+1} + v^{n-1}}{2} - 10^3 \frac{u^{n+1} + u^{n-1}}{2} + u^n = 0,$$

with starting conditions $u^0 = v^0 = u^1 = +1, v^1 = -1$. We calculate $|\Lambda| = 1$ so the time step condition is $\Delta t < 1$. We test:

- For $\Delta t = 1.01(> 1)$ CNLF is unstable. Figure 3.1 verifies that the instability occurs in only the unstable mode (a scenario suggested by root condition analysis [D10]).
- For $\Delta t = 0.99 < 1$, CNLF is energy stable. All modes are observed to be stable in figure 3.4 over a very long time interval.

Test 2: Small perturbations of Λ . Let $A = diag\{10^4, 10^{-4}\}$ and consider the 2×2 system

$$\frac{du}{dt} + 10^4 u + \varepsilon_1 u - v = 0, \ \frac{dv}{dt} + 10^{-4} v + \varepsilon_2 v + u = 0.$$

The matrix Λ is thus

$$\Lambda_{\varepsilon_1,\varepsilon_2} = \begin{bmatrix} \varepsilon_1 & -1 \\ +1 & \varepsilon_2 \end{bmatrix}$$

in which skew symmetry is broken by the small, random coefficients ε_1 and ε_2 . We apply CNLF over a long time interval:

$$\frac{u^{n+1} - u^{n-1}}{2\triangle t} + 10^4 \frac{u^{n+1} + u^{n-1}}{2} + \varepsilon_1 u^n - v^n = 0,$$

$$\frac{v^{n+1} - v^{n-1}}{2\triangle t} + 10^{-4} \frac{v^{n+1} + v^{n-1}}{2} + \varepsilon_2 v^n + u^n = 0,$$



Fig. 3.1. For $\triangle t = 1.01$ the unstable mode grows and the stable mode decays



FIG. 3.2. For $\triangle t = .99$ the both unstable and stable modes decay

with starting conditions $u^0 = v^0 = u^1 = +1, v^1 = -1$. We calculate $|\Lambda_{0,0}| = 1$ so the time step condition is $\Delta t < 1$. We test:

- For $\Delta t = 1.01(> 1)$ and $\varepsilon_1 = \varepsilon_2 = 0$ CNLF is unstable. Figure 3.3 verifies that the instability once again occurs in only the unstable mode.
- For $\Delta t = 0.99 < 1$, CNLF is energy stable if $\varepsilon_1 = \varepsilon_2 = 0$; we pick $\varepsilon_1 = \varepsilon_2 = 10^{-4}$ and check for growth in the unstable mode in figure 3.4. All modes are observed to be stable over a very long time interval.



Fig. 3.3. For $\bigtriangleup t=1.01$ the unstable mode grows and the stable mode decays



FIG. 3.4. For $\bigtriangleup t = .99$ the both unstable and stable modes decay

Test 3: Nonlinear version of Test 2. Consider the 2×2 nonlinear system

$$\frac{du}{dt} + a_1(u) + \varepsilon_1 u - v = 0, \quad \frac{dv}{dt} + a_2(v)10^{-4}v + \varepsilon_2 v + u = 0,$$

where $a_1(u) = 10^4 |u|u$, and $a_2(v) = 10^{-4} |v|v$.

The matrix Λ is thus

$$\Lambda_{\varepsilon_1,\varepsilon_2} = \begin{bmatrix} \varepsilon_1 & -1 \\ +1 & \varepsilon_2 \end{bmatrix}$$

in which skew symmetry is broken by the small coefficients ε_1 and ε_2 . We apply



FIG. 3.5. For $\Delta t = 1.01$ the unstable mode grows and the stable mode decays

CNLF over a long time interval:

$$\frac{u^{n+1} - u^{n-1}}{2\Delta t} + a_1 \left(\frac{u^{n+1} + u^{n-1}}{2}\right) + \varepsilon_1 u^n - v^n = 0,$$

$$\frac{v^{n+1} - v^{n-1}}{2\Delta t} + a_2 \left(\frac{v^{n+1} + v^{n-1}}{2}\right) + \varepsilon_2 v^n + u^n = 0,$$

with starting conditions $u^0 = v^0 = u^1 = +1, v^1 = -1$. We calculate $|\Lambda_{0,0}| = 1$ so the two time step condition is $\Delta t < 1$. We observe that:

- For $\Delta t = 1.01(> 1)$ and $\varepsilon_1 = \varepsilon_2 = 0$ CNLF is unstable; The instability again occurs in only the unstable mode, figure 3.5.
- For $\Delta t = 0.99 < 1$, CNLF is energy stable (as Step 1 of the proof extends to this nonlinear case) if $\varepsilon = 0$. Pick $\varepsilon_1 = \varepsilon_2 = 10^{-4}$ in this test and find all modes go to zero (figure 3.6); there is no growth in the unstable mode.

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FIG. 3.6. For $\triangle t = 1.01$ both the unstable and the stable mode decay

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