UNCONDITIONAL STABILITY OF A CRANK-NICOLSON ADAMS-BASHFORTH 2 IMPLICIT-EXPLICIT NUMERICAL METHOD*

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Abstract. Systems of nonlinear partial differential equations modeling turbulent fluid flow and similar processes present special challanges in numerical analysis. Regions of stability of implicit-explicit methods are reviewed, and an energy norm based on Dahlquist's concept of G-stability is developed. Using this norm, a time-stepping Crank-Nicolson Adams-Bashforth 2 implicit-explicit method for solving spatially-discretized convection-diffusion equations of this type is analyzed and shown to be unconditionally stable.

Key words. convection-diffusion equations, unconditional stability, IMEX methods, Crank-Nicolson, Adams-Bashforth 2

AMS subject classifications. 76R50, 65L20, 65M12

1. Introduction.

The motivation of this work is to consider the stability of numerical methods when applied to ordinary differential equations (ODEs) of the form

$$u'(t) + Au(t) - Cu(t) + B(u)u(t) = f(t), \tag{1.1}$$

in which $A, B(u)$ and C are $d \times d$ matrices, $u(t)$ and $f(t)$ are d-vectors, and

$$A = A^T \succ 0, B(u) = -B(u)^T, C = C^T \succcurlyeq 0 \text{ and } \quad A - C \succ 0. \tag{1.2}$$

Here $\succ$ and $\succcurlyeq$ denote the positive definite and positive semidefinite ordering, respectively.

Models of the behavior of turbulent fluid flow using convection-diffusion partial differential equations discretized in the spatial variable give rise to a system of ODEs, such as

$$\dot{u}_{ij}(t) + b \cdot \nabla^h u_{ij} - (\epsilon_0(h) + \nu)\Delta^h u_{ij} + \epsilon_0(h) P_H(\Delta^h P_H(u_{ij})) = f_{ij}, \tag{1.3}$$

where Δ^h is the discrete Laplacian, ∇^h is the discrete gradient, $\epsilon(h)$ is the artificial viscosity parameters, and P_H denotes a projection onto a coarser mesh [2]. System (1.3) is of the form (1.1), (1.2) where

$$A = -(\epsilon_0(h) + \nu)\Delta^h, \quad C = \epsilon_0(h) P_h \Delta^h P_h, \quad B(u) = b \cdot \nabla^h.$$

In this case the matrix $B(\cdot)$ is constant, but in general it may depend on u, and thus the system is allowed to have a nonlinear part. A linear multistep method for the numerical integration a system $u'(t) = F(t, u)$, such as (1.1), is

$$\sum_{j=-1}^{k} \alpha_j u_{n-j} = \Delta t \sum_{j=-1}^{k} \beta_j F_{n-j}, \tag{1.4}$$

where t is defined on $\mathcal{I} = [t_0, t_0 + T] \subset \mathbb{R}$, $u_{n-j} \in \mathbb{R}^d$, $F_{n-j} = F(t_{n-j}, u_{n-j})$.

This work will discuss the regions of stability for IMEX methods applied to systems of the form (1.1), and prove that unconditional stability (the method's stability properties are independent of the choice of step-size Δt) holds for a proposed Crank-Nicolson Adams-Bashforth 2 (CNAB2) implicit-explicit (IMEX) numerical method,

$$\begin{aligned} &\frac{u_{n+1} - u_n}{\Delta t} + (A - C)^{\frac{1}{2}} \Big(A(A - C)^{-\frac{1}{2}} \tfrac{1}{2} u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A - C)^{-\frac{1}{2}} u_n + \tfrac{1}{2} C (A - C)^{-\frac{1}{2}} u_{n-1} \Big) \\ &\quad + B(\mathcal{E}_{n+\frac{1}{2}})(A - C)^{-\frac{1}{2}} \Big(\tfrac{1}{2} A (A - C)^{-\frac{1}{2}} u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A - C)^{-\frac{1}{2}} u_n + \tfrac{1}{2} C (A - C)^{-\frac{1}{2}} u_{n-1} \Big) \\ &\quad = f_{n+\frac{1}{2}}, \end{aligned} \tag{1.5}$$

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where $\mathcal{E}_{n+\frac{1}{2}} = \frac{3}{2}u_n + \frac{1}{2}u_{n-1}$, an explicit approximation of $u(t_{n+\frac{1}{2}})$. This method is a second-order convergent numerical scheme of the form (1.4). Section 2 discusses earlier related results for IMEX methods, Section 3 motivates the unconditional stability analysis of (1.5) by deriving illustrative stability results for related scalar IMEX methods. With these results in mind, unconditional stability of method (1.5) is proven in Section 4, and demonstrated by numerical tests in Section 5. Section 6 briefly discusses an obvious draw-back to method (1.5) and concludes.

2. Previous IMEX Stability Results. In [5], Frank *et al.* consider applying IMEX methods to a system of ODEs of the form

$$u'(t) = F(t, u(t)) + G(t, u(t)),$$

where F is the stiff, and G the non-stiff parts of the system. Considering the scalar test equation

$$u'(t) = \lambda u(t) + \gamma u(t),$$

they find that under these conditions, $\lambda\Delta t$ and $\gamma\Delta t$ lying in the regions of stability of their respective methods are sufficient conditions for the IMEX method to be assymptotically stable. As is demonstrated in Section 3, these are not necessary conditions when the system is under assymptions (1.2), which is due to the additional requirement that $A - C$ be positive-definite.

Akrivis *et al.* study a system of the same form as (1.1) except that B is not assumed to be self-adjoint instead of skew-symmetric. They analyze a general class of methods that are implicit in all linear terms, and explicit in all nonlinear terms, and show these methods to be absolutely stable [1].

Finally, Anitescu *et al.* [2] show that the first-order IMEX method

$$\frac{u_{n+1} - u_n}{\Delta t} + Au_{n+1} - Cu_n + B(u)u_{n+1} = f_{n+1} \tag{2.1}$$

is unconditionally stable. Unlike [1] there are two linear terms, one of which will be approximated explicitly, while the solution vector in the nonlinear term $B(u)u(t)$ is computed using an implicit scheme.

3. Stability for Scalar IMEX Methods. Consider the Cauchy problem

$$y'(t) = (\epsilon + \nu)\lambda y(t) - \epsilon\lambda y(t), \tag{3.1}$$

$$y : \mathbb{R} \to \mathbb{R}, \quad y(0) = 1, \quad \lambda < 0, \quad 0 < \nu, \quad 0 < \epsilon. \tag{3.2}$$

Note that this is the Dahlquist test-problem $y'(t) = \nu\lambda y(t)$, with exact solution $y(t) = e^{\nu\lambda t}$, broken into two parts.

DEFINITION 3.1. *A-stability (Dahlquist 1963). The multistep method (1.4) applied to the Cauchy test problem (3.1) is A-stable if $A \supseteq \mathbb{C}^-$ (where A is entire region of stability for the method). This is equivalent to requiring the numerical solutions $|u_n| \to 0$ as $t_n \to +\infty$ [6].*

A method's A-stability region can be illustrated by plotting its root locus curve, that is, the values of $\Delta t\lambda\nu$ corresponding to the stability boundary roots $|\zeta(\Delta t\lambda\nu)| = 1$ of its generating polynomials. Recall that for stability the roots of these polynomials must be lie within the unit circle ($\zeta_j(\Delta t\lambda\nu) \le 1$ in modulus) [6].

The aim here is to explore IMEX methods which, when applied to the Cauchy test problem (3.1) as stated, display stable behavior. Let us consider methods which apply an implicit scheme to the first part, and an explicit scheme to the second part. A-priori it is not obvious which mixed methods will exhibit stable behavior (if at all), and if so, whether the stability properties of the implicit or explicit part will dominate.

3.1. Backward Euler Forward Euler IMEX. Let us first investigate an IMEX method which is Backward Euler for the implicit part and Forward Euler for the explicit part (BEFE):

$$\frac{u_{n+1} - u_n}{\Delta t} = (\epsilon + \nu)\lambda u_{n+1} - \epsilon\lambda u_n. \tag{3.3}$$

This method can be solved for u_n in terms of λ, ϵ, ν, and an initial condition u_0. Iterating backward n times gives the sequence of numerical solutions

$$u_n = u_0\Big(\frac{1 - \epsilon\lambda\Delta t}{1 - (\epsilon + \nu)\lambda\Delta t}\Big)^n.$$

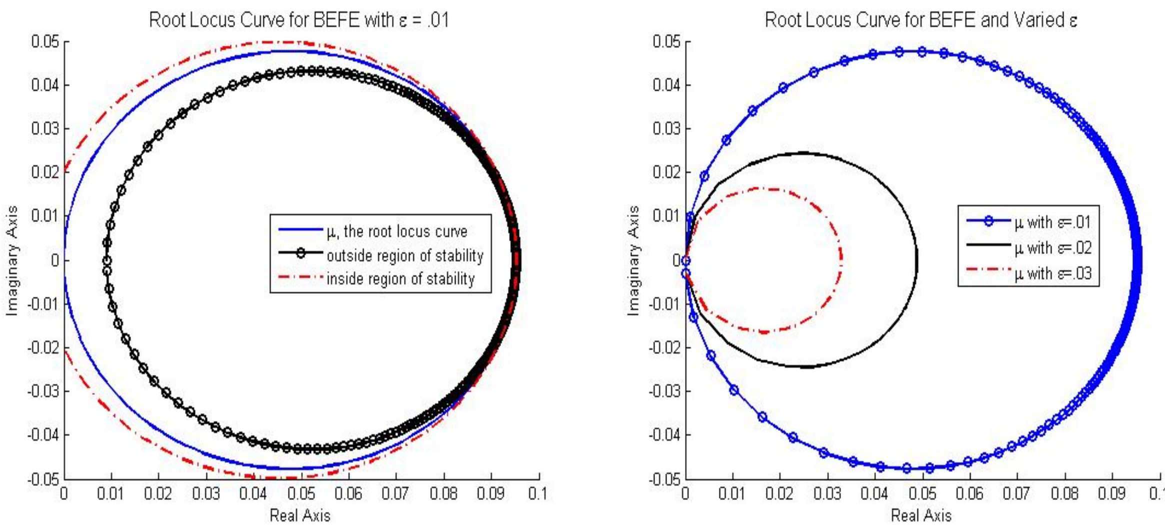

Fig. 3.1: Root Locus Curves for BEFE

As $n \to +\infty$, $|u_n| \to 0$ if $\left|\frac{1-\epsilon\lambda\Delta t}{1-(\epsilon+\nu)\lambda\Delta t}\right| < 1$. The assumptions in (3.2) are sufficient for this to hold. None of these conditions is dependent on the choice of step-size Δt, so we can immediately conclude that this method is unconditionally stable.

Note that if ϵ is allowed to be zero, we recover the Backward Euler method, which has the solution

$$u_n = u_0\Big(\frac{1}{1-\nu\lambda\Delta t}\Big)^n.$$

Figure 3.4 shows the convergence of the energy of the solutions of BE and BEFE for initial condition $u_0 = 1$, $\lambda = -10000$, $\nu = .001$, $\Delta t = .01$, $\epsilon = .01$ (for the BEFE scheme). Notice that BE converges faster than BEFE mixed method. This illustrates that the advantages of using an IMEX method come at the cost of decreased speed of convergence of the method's solutions.

To see the stability region of the BEFE method in terms of step-size and eigenvalues, take $\zeta^n = u_n$, $\mu = \Delta t\lambda\nu$, and solving the method (3.3) for μ gives the root locus curve

$$\mu = \nu\frac{\rho(\zeta)}{\sigma(\zeta)} = \nu\frac{\zeta - 1}{(\alpha+\nu)\zeta - \epsilon}. \tag{3.4}$$

Since $|e^{i\theta}| = 1$ for all θ, taking $\zeta = e^{i\theta}$ in (3.4) and letting θ vary in $[0, 2\pi]$ produces the desired stability region (with ν=.001).

The first plot in Figure 3.2 illustrates that the BEFE IMEX method is stable for any choice of μ outside the solid blue line, which is to say the method (3.3) is A-stable since any choice of $\Delta t\lambda\nu$ in $\mathbb{C}^-$ will be stable and the solution u_n will converge to zero as n gets large. The second plot in Firgure 3.2 shows, somewhat counterintuitively, that the stability region of BEFE is growing with ϵ; that is, the region of absolute stability grows as the scaling of the explicit part of the method approaches that of the implicit.

3.2. Crank-Nicolson Adams-Bashforth 2 IMEX. We are interested in finding a second-order convergent IMEX method that is also A-stable. Consider

$$\frac{u_{n+1} - u_n}{\Delta t} = (\epsilon+\nu)\lambda\Big(\frac{u_{n+1}+u_n}{2}\Big) - \epsilon\lambda\big(\tfrac{3}{2}u_n - \tfrac{1}{2}u_{n-1}\big), \tag{3.5}$$

which is a Crank-Nicolson second-order (implicit) method for the first part of the Cauchy problem (3.1), and Adams-Bashforth 2 second-order (explicit) for the second part. If ϵ is allowed to be zero we recover Crank-Nicolson:

$$u_n = \Big[\frac{1+\frac{1}{2}\Delta t\nu\lambda}{1-\frac{1}{2}\Delta t\nu\lambda}\Big]^n.$$

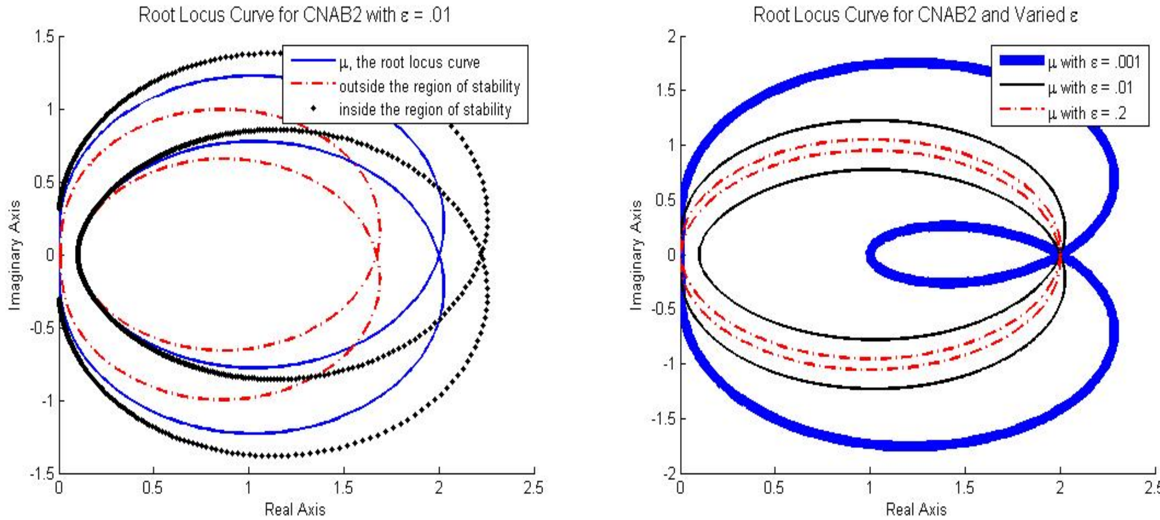

Fig. 3.2: Root Locus Curves for CNAB2

The characteristic polynomial of method (3.5) is

$$\Pi(r) = (1 - \tfrac{1}{2}\Delta t(\epsilon + \nu)\lambda)r^2 - (1 + \tfrac{1}{2}\Delta t(\epsilon+\nu)\lambda - \tfrac{3}{2}\Delta t\epsilon\lambda)r - \tfrac{1}{2}\epsilon\lambda\Delta t r^0 = 0.$$

This second-degree polynomial has two roots,

$$r_{1,2} = \frac{\left(1 - \Delta t\epsilon\lambda - \frac{1}{2}\Delta t\nu\right) \pm \frac{1}{2}\sqrt{4 + 4\Delta t\lambda\nu + \Delta t^2\nu\lambda^2(\nu - 8\epsilon)}}{2 - \Delta t\lambda\epsilon - \Delta t\lambda\nu}.$$

Drawing on results from the theory of difference equations, the analytical solutions of the CNAB2 scalar method (3.5) can be written as

$$u_n = \gamma_1 r_1^n + \gamma_2 r_2^n.$$

Using initial conditions u_0, u_1 to solve for γ_1, γ_2 gives

$$u_n = +\frac{u_1 + r_2 u_0}{r_1 + r_2} r_1^n + \frac{u_1 + r_1 u_0}{r_1 + r_2} r_2^n.$$

The second plot in Figure 3.4 shows the convergence of the energy of the solutions of Crank-Nicolson and Crank-Nicolson Adams Bashforth 2 for initial conditions $u_0 = 1$, $u_1 = .8$, $\lambda = -10000$, $\nu = .001$, $\Delta t = .5$, $\epsilon = .01$. As with BE and BEFE, pure Crank-Nicolson converges faster than the mixed method.

For method (3.5) the root locus curve is

$$\Delta t\lambda\nu = \nu\frac{\rho(\zeta)}{\sigma(\zeta)} = \nu\frac{\zeta^2 - \zeta}{(\epsilon+\nu)(\frac{\zeta^2+\zeta}{2}) - \epsilon(\frac{3}{2}\zeta - \frac{1}{2})}. \tag{3.6}$$

The first plot in Figure 3.2 shows the region of stability for CNAB2 IMEX is similar to that of BEFE IMEX, and this method is also A-stable. The second plot shows the root locus curves corresponding to different values of ϵ. As with BEFE, the region of stability is growing with ϵ. This plot is similar, except for the size of the stability region, for any choice of $\epsilon \neq 0$.

Figure 3.3 shows that for for $\epsilon = .001$ and $\epsilon = .01$ the region of stability for BEFE is relatively larger than that of CNAB2. This reflects the fact that using a higher order method comes at the cost of a decreased region of stability.

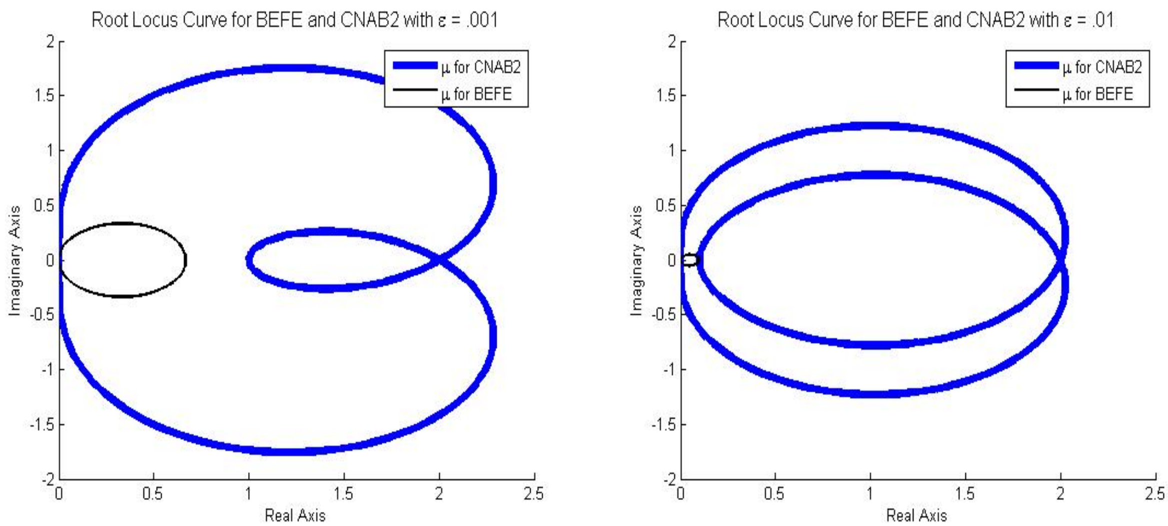

Fig. 3.3: Root Locus Curves of BEFE compared to CNAB2

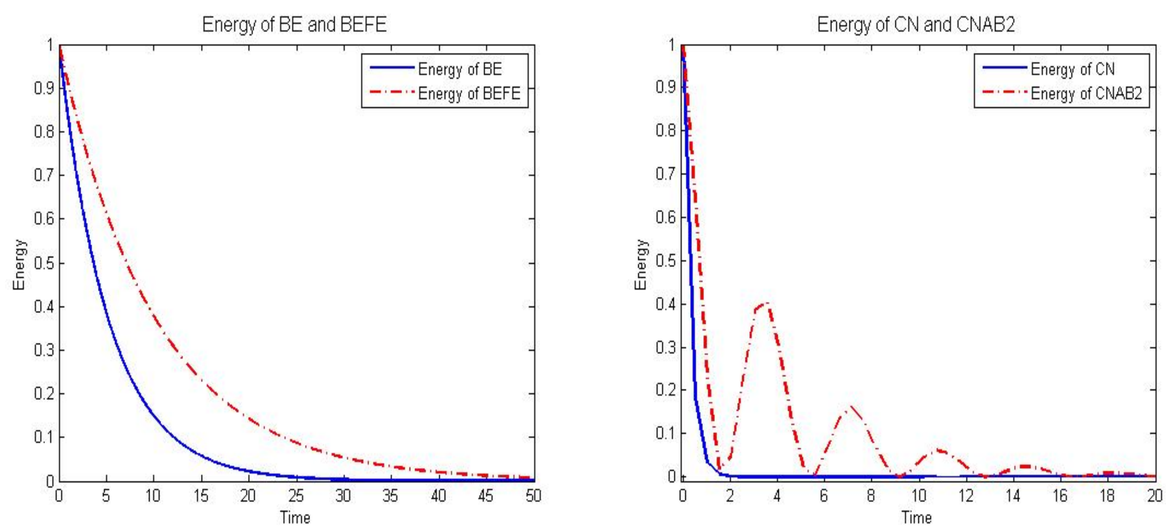

Fig. 3.4: Energy comparisons for BE to BEFE, CN to CNAB2

3.3. G-stability. Now let us study the stability of the two aforementioned methods under the lens of a stability definition that is both more complex and in some cases more useful. Consider the Lipschitz condition

$$\mathrm{Re}\langle F(t,u) - F(t,\hat{u}), u - \hat{u}\rangle \leq L\|u - \hat{u}\|^2. \tag{3.7}$$

If the system $u'(t) = F(t,u)$ satisfies (3.7) with $L = 0$, then its solutions are contractive. In this case we wish to know which linear multistep methods also have contractive solutions, and are thus G-stable as defined in Definition 3.2 stated below. Let

$$U_n = (u_{n+k-1}, u_{n+k-2}, ..., u_n)^T$$

be a sequence of numerical solutions to (1.4), and define the G-norm of U_n to be $\|U_n\|_G^2 = U_n^T G U_n$.

Definition 3.2. *G-stability (Dahlquist 1976)[3]. A multistep numerical method is G-stable if the system of ODEs $u' = F(t,u)$ satisfies (3.7) with $L = 0$, and if there exists a symmetric positive-definite matrix (SPD)*

G, such that

$$\|U_{n+1} - \hat{U}_{n+1}\|_G \leq \|U_n - \hat{U}_n\|_G, \tag{3.8}$$

for all steps n and step-sizes $\Delta t > 0$, where $\hat{U}_n$ is a sequence of solutions for (1.4) that correspond to different initial conditions than U_n.

Thus, we can use G-stability to test the behavior of a method where the underlying ODE is linear or nonlinear, providing that it satisfies the Lipschitz condition with $L = 0$. In the nonlinear case, we have G-stability when the difference of the solutions $U_n - \hat{U}_n$ are not growing in the G-norm.

3.4. G-stability of Scalar Crank-Nicolson Adams-Bashforth 2. Showing that the method in question is G-stable involves checking that the conditions of the G-stability definition hold. Since our underlying ODE (3.1) is linear, we can consider the Lipschitz and G-norm conditions

$$\mathrm{Re}\langle F(t,u), u)\rangle \leq 0, \qquad \|U_{n+1}\|_G \leq \|U_n\|_G, \tag{3.9}$$

respectively. It is easy to see that if $\lambda < 0$ and $\nu > 0$ then $\langle \nu\lambda u, u\rangle = \nu\lambda u^2 \leq 0$, and the Lipschitz condition is satisfied. Thus, the task is to see if we can construct a G that satisfies the G-stability definition.

The G-matrix corresponding to this method can be generated directly or indirectly using the proof Dahlquist's equivalence theorem as is done in Subsection 3.4.2 [4].

3.4.1. Direct Computation of G. First, consider the inner-product

$$\Big\langle (\epsilon+\nu)\lambda(\frac{u_{n+1}+u_n}{2}) - \epsilon\lambda(\tfrac{3}{2}u_n - \tfrac{1}{2}u_{n-1}), \frac{u_{n+1}-u_n}{\Delta t})\Big\rangle \geq 0, \tag{3.10}$$

which holds because they are the RHS and LHS of method (3.5) under consideration. Multiplying by $-\frac{1}{\Delta t}$ and expanding gives

$$E = -c_1 u_{n+1}^2 - (c_2 - c_1)u_{n+1}u_n + c_2 u_n^2 - c_3 u_{n+1}u_{n-1} + c_3 u_n u_{n-1} \leq 0 \tag{3.11}$$

where

$$c_1 = \tfrac{1}{2}(\epsilon+\nu)\lambda, \qquad c_2 = \tfrac{1}{2}(\epsilon+\nu)\lambda - \tfrac{3}{2}\epsilon\lambda, \qquad c_3 = \tfrac{1}{2}\epsilon\lambda.$$

Now consider the equation

$$E = \|U_{n+1}\|_G^2 - \|U_n\|_G^2 + \|a_2 u_{n+1} + a_1 u_{n+1} + a_0 u_n\|^2, \qquad a_0, a_1, a_2 \in \mathbb{R}. \tag{3.12}$$

Imposing $E \leq 0$ implies $\|U_{n+1}\|_G^2 \leq \|U_n\|_G^2$, since $\|a_2 u_{n+1} + a_1 u_{n+1} + a_0 u_n\|^2 \geq 0$. Let

$$G = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}. \tag{3.13}$$

Thus, if the matrix G produced by matching the coefficients of (3.11) to those of (3.12) is SPD, method (3.5) is G-stable by Definition 3.2.

Following this approach and letting $g_{12} = g_{21}$ produces the following nonlinear system of six equations in six unknowns:

$$\begin{array}{llll} u_{n+1}^2: & -c_1 = g_{11} + a_2^2, & u_{n+1}u_n: & c_1 - c_2 = 2g_{12} + 2a_2 a_1 \\ u_n^2: & c_2 = g_{22} - g_{11} + a_1^2 & u_{n+1}u_n: & -c_3 = 2a_2 a_0 \\ u_{n-1}^2: & 0 = -g_{22} + a_0^2 & u_n u_{n-1}: & c_3 = -2g_{12} + 2a_1 a_0. \end{array} \tag{3.14}$$

Solving this system produces the G-matrix

$$G = \frac{\lambda}{4}\begin{pmatrix} -\epsilon - 2\nu & \epsilon \\ \epsilon & -\epsilon \end{pmatrix}. \tag{3.15}$$

This matrix is symmetric by construction, and it is easy to see that if $\lambda < 0$ all its principle minors have a positive determinant, and therefore this G is positive-definite by Sylvester's Criterion. Thus, by Definition 3.2 this IMEX method is G-stable (as well as A-stable, as demonstrated in the previous section). This, as Dahlquist was finally able to prove in 1978, is not a coincidence.

THEOREM 3.3. *(Dahlquist 1978)[4]: If a method's generating polynomials ρ, σ, have no common divisor, then the method is G-stable if and only it is A-stable.*

Figure 3.5 shows the convergence of the energy and G-norm of the solutions of the Crank-Nicolson Adams-Bashforth 2 schemes for initial conditions $u_0 = 1$, $u_1 = .8$, $\epsilon = .01$, $\lambda = -10000$, $\nu = .001$, and $\Delta t = .5$,). Notice that the G-norm is monotonically decreasing, as the G-stability definition requires.

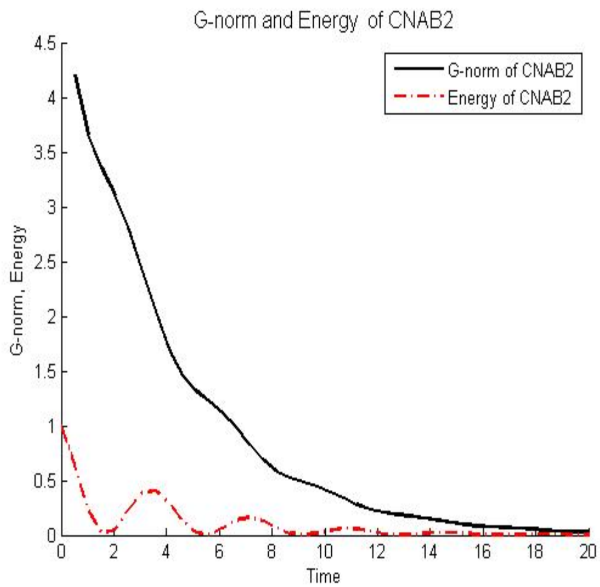

Fig. 3.5: G-norm and Energy decay of CNAB2 method

3.4.2. Constructing G Using Generating Polynomials. By following the proof of Theorem 3.3 (see [4], [6]) one can derive a procedure for computing the G matrix that relies on algebraic manipulation of the the method's generating polynomials rather than solving a nonlinear system as is required for computing G directly.

The generating polynomials for scalar CNAB2 IMEX are

$$\rho(\zeta) = \zeta^2 - \zeta, \qquad \sigma(\zeta) = (\epsilon + \nu)(\tfrac{\zeta^2+\zeta}{2}) - \epsilon(\tfrac{3}{2}\zeta - \tfrac{1}{2}).$$

Define the function

$$E(\zeta) = \tfrac{1}{2}(\rho(\zeta)\sigma(\tfrac{1}{\zeta}) + \rho(\tfrac{1}{\zeta})\sigma(\zeta)),$$

which for CNAB2 is

$$\begin{aligned} E(\zeta) &= \tfrac{1}{2}((\zeta^2 - \zeta)((\alpha + \nu)(\tfrac{\frac{1}{\zeta^2}+\frac{1}{\zeta}}{2}) - \epsilon(\tfrac{3}{2}\zeta - \tfrac{1}{2}))(\tfrac{1}{\zeta}) + (\tfrac{1}{\zeta^2} - \tfrac{1}{\zeta})((\epsilon + \nu)(\tfrac{\zeta^2+\zeta}{2}) - \epsilon(\tfrac{3}{2}\zeta - \tfrac{1}{2}))) \\ &= \frac{\epsilon(\zeta - 1)^2}{4\zeta^2} \\ &= \Big[\frac{\sqrt{\epsilon}}{2}[(\zeta - 1)^2]\Big]\Big[\frac{\sqrt{\epsilon}}{2}][(\tfrac{1}{\zeta} - 1)^2]\Big] \\ &= a(\zeta)a(\tfrac{1}{\zeta}). \end{aligned}$$

Define the function $P(\zeta,\omega) = \frac{1}{2}(\rho(\zeta)\sigma(\omega)+\rho(\omega)\sigma(\zeta))-a(\zeta)a(\omega)$, which with some simplification and factoring becomes

$$\begin{aligned}P(\zeta,\omega) &= \tfrac{1}{4}[-\epsilon(\zeta-1)^2(\omega-1)^2 + \epsilon(\omega-1)\omega - \zeta(\alpha(2\nu-4\epsilon)\omega + 3\alpha\omega^2) + \zeta^2(\epsilon - 3\epsilon\omega + 2(\epsilon+\nu)\omega^2))]\\ &= (\zeta\omega - 1)\Big(\frac{(\epsilon+2\nu)}{4}\zeta\omega - \frac{\epsilon}{4}\zeta - \frac{\epsilon}{4}\omega + \frac{\epsilon}{4}\Big)\\ &= (\zeta\omega-1)(g_{11}\zeta\omega - g_{12}\zeta - g_{21}\omega + g_{22}).\end{aligned}$$

This yields the matrix

$$G = \frac{1}{4}\begin{pmatrix}\epsilon+2\nu & -\epsilon\\ -\epsilon & \epsilon\end{pmatrix}, \tag{3.16}$$

which is SPD. Multiplying (3.16) by the positive constant $-\lambda$ gives the same result as computing G directly as in the previous section.

Somewhat surprisingly, under assumptions (3.2) the method's stability properties are driven by its implicit part, and this is the motivation that leads to the separation of linear parts A and C as done in (1.1).

4. Unconditional Stability of the Crank-Nicolson Adams Bashforth 2 IMEX Method (1.5). Let us now return to considering a system of ODEs (1.1) under assumptions (1.2).

The CNAB2 method proposed in Section 1 is a member of a broader family of three level, second order time-stepping schemes [8]:

$$\begin{aligned}&\frac{(\theta+\frac{1}{2})u_{n+1} - 2\theta u_n + (\theta-\frac{1}{2})u_{n-1}}{\Delta t}\\ &+ (A-C)^{\frac{1}{2}}\Big(A(A-C)^{-\frac{1}{2}}\theta u_{n+1} + \big((1-\theta)A - (\theta+1)C\big)(A-C)^{-\frac{1}{2}}u_n + C(A-C)^{-\frac{1}{2}}\theta u_{n-1})\Big)\\ &\quad + B(\mathcal{E}_{n+\theta})(A-C)^{-\frac{1}{2}}\Big(A(A-C)^{-\frac{1}{2}}\theta u_{n+1} + \big((1-\theta)A - (\theta+1)C\big)(A-C)^{-\frac{1}{2}}u_n + C(A-C)^{-\frac{1}{2}}\theta u_{n-1})\Big)\\ &= f_{n+\theta},\end{aligned} \tag{4.1}$$

where $\mathcal{E}_{n+\theta}$ is an implicit or explicit second order approximation of u_{n+1} and $\theta \in [\frac{1}{2}, 1]$. Taking $\theta = \frac{1}{2}$, and $\mathcal{E}_{n+\theta} = \frac{3}{2}u_n - \frac{1}{2}u_{n-1}$, gives method (1.5), as introduced in Section 1.

Here we will consider the stability properties of the method (1.5). However, unlike the examples in the previous chapter, the system under consideration will be d-dimensional and be in terms of non-commmuting coefficient matrices A, B, C, where B is allowed to be nonlinear. This added complexity is worthwhile since many processes have highly nonlinear behavior, but it comes at the cost of greatly complicating stability analysis.

4.1. Well-Posedness of the Problem. Nonlinearity of problem (1.1) will prohibit the Lipschitz condition (3.7) from holding globally. This is not trivial, since it means none of the well-known global stability results for the underlying problem will necessarily hold (for a discussion of the well-posedness of globally Lipschitz continuous Cauchy problems see [7], Chapter 10). The system is, however, locally stable.

THEOREM 4.1. *Local Stability of Nonlinear System (1.1). Under assumptions (1.2), the solution of ODE* (1.1) *is bounded as*

$$\|u(t)\|_2^2 \leq \|u(0)\|_2^2 e^t + F_T^2(e^t - 1), \quad \textit{where} \;\; F_T^2 = \max_{t\in[0,T]} \|f(t)\|_2^2,$$

is therefore stable for all $t \in \mathcal{I} = [0, T]$, for all finite T.

For the proof of Theorem 4.1 see [2]. This result ensures that problem (1.1) is well-behaved locally, which is to say that its exact solutions $u(t)$ do not blow up on $\mathcal{I}$. This allows us to conclude that the problem is sufficiently well-posed in at least a local sense, and we can discuss stability of a numerical method for approximation of its solution on $\mathcal{I}$.

4.2. Transformation of the Method. In [2] the numerical solution u_n provided by the BEFE IMEX method (2.1) is shown to be nonincreasing,

$$\|u_{n+1}\|_E \le \|u_n\|_E, \qquad E = I + \Delta t C,$$

in the energy norm E, and this condition is sufficient to conclude the method is unconditionally stable. The aim of this section will be analogous in nature. Borrowing heavily from the G-stability concepts developed in Section 3.3, given an appropriately chosen transformation of the method, it can be proved that the numerical solutions are decreasing at each time step in the G-norm, and the method is unconditionally stable on the interval of interest $\mathcal{I}$.

Since $B(u)$ is assumed to be skew-symmetric, multiplying method (1.5) from the left by the vector

$$\Big[(A-C)^{-\frac{1}{2}}\Big(\tfrac{1}{2}A(A-C)^{-\frac{1}{2}}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big)\Big]^T \tag{4.2}$$

will cause the nonlinear term

$$B(\mathcal{E}_{n+\frac{1}{2}})(A-C)^{-\frac{1}{2}}\Big(\tfrac{1}{2}A(A-C)^{-\frac{1}{2}}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big)$$

to disappear, leaving

$$\begin{aligned}
&\Big\langle (A-C)^{-\frac{1}{2}}\Big(\tfrac{1}{2}A(A-C)^{-\frac{1}{2}}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big),\\
&\frac{u_{n+1}-u_n}{\Delta t} + (A-C)^{\frac{1}{2}}\Big(A(A-C)^{-\frac{1}{2}}\tfrac{1}{2}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big)\Big\rangle\\
&= \Big\langle (A-C)^{-\frac{1}{2}}\Big(\tfrac{1}{2}A(A-C)^{-\frac{1}{2}}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big), f_{n+\frac{1}{2}}\Big\rangle.
\end{aligned}$$

By the properties of the inner-product and Euclidian norm, this can be rearranged as

$$\begin{aligned}
&\frac{1}{\Delta t}\Big\langle u_{n+1}-u_n\,,\,(A-C)^{-\frac{1}{2}}\Big(A(A-C)^{-\frac{1}{2}}\tfrac{1}{2}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big)\Big\rangle\\
&+ \Big\|\Big(A(A-C)^{-\frac{1}{2}}\tfrac{1}{2}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big)\Big\|_2^2\\
&= \Big\langle f_{n+\frac{1}{2}}\,,\,(A-C)^{-\frac{1}{2}}\Big(A(A-C)^{-\frac{1}{2}}\tfrac{1}{2}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big)\Big\rangle.
\end{aligned} \tag{4.3}$$

Focusing on the first line of (4.3), the goal will be to simplify the transformed method into positive pieces using the G-norm to group and compare terms, as was done in the G-stability examples in Section 3.4. The G-stability matrix is calculated using the proceedure derived from the proof of Theorem 3.3, as demonstrated in Subsection 3.4.2. Method (1.5) and its corresponding characteristic polynomials yield matrix

$$G = \begin{pmatrix} (A-C)^{-\frac{1}{2}}(\frac{1}{2}A - \frac{1}{4}C)(A-C)^{-\frac{1}{2}} & -(A-C)^{-\frac{1}{2}}(\frac{1}{4}C)(A-C)^{-\frac{1}{2}} \\ -(A-C)^{-\frac{1}{2}}(\frac{1}{4}C)(A-C)^{-\frac{1}{2}} & (A-C)^{-\frac{1}{2}}(\frac{1}{4}C)(A-C)^{-\frac{1}{2}} \end{pmatrix}. \tag{4.4}$$

Referring to the G-stability examples in Section 3.4, taking $A = -(\alpha+\nu)\lambda$, $C = -\alpha\lambda$, and ignoring $(A-C)^{-\frac{1}{2}}$ terms, G matches matrix (3.15).

4.3. G-norm. We now wish to check that G is a symmetric positive-definite matrix so it can be used to finish putting the transformed method (4.3) into norms and positive terms.

4.3.1. Symmetry of G. The G matrix defined in (4.4) is a 2×2 block-partitioned matrix with submatrices of size $d \times d$. Since the off-diagonal blocks are the same, symmetry of the four blocks is sufficient to conclude G is symmetric also.

Since A and C are both symmetric by assumptions (1.2), adding or subtracting positive-definite multiples of them also results in symmetric matrices. By properties of diagonalizable matrices, $(A-C)^{-\frac{1}{2}}$ is symmetric. This is sufficient to conclude that each block of G is symmetric, and therefore G is also.

4.3.2. Positive-Definiteness of G. If G is PD the following will be strictly positive for any choice of d-dimensional vectors u, v not equal to zero:

$$\left\| \begin{bmatrix} u \\ v \end{bmatrix} \right\|_G^2 = \left\langle \begin{bmatrix} u \\ v \end{bmatrix}, G \begin{bmatrix} u \\ v \end{bmatrix} \right\rangle. \tag{4.5}$$

LEMMA 4.2. *G is a positive-definite matrix.*

Proof. Expanding equation (4.5) gives

$$\begin{aligned} \left\langle \begin{bmatrix} u \\ v \end{bmatrix}, G \begin{bmatrix} u \\ v \end{bmatrix} \right\rangle = \tfrac{1}{4} \Big[& u^T [(A-C)^{-\frac{1}{2}} (2A - C)(A-C)^{-\frac{1}{2}}] u - u^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] v \\ & - v^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] u + v^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] v \Big]. \end{aligned} \tag{4.6}$$

Subtracting and adding $\frac{1}{4}\big[u^T[(A-C)^{-\frac{1}{2}}C(A-C)^{-\frac{1}{2}}]u\big]$ to (4.6) and using the fact that

$$u^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] v = \big[u^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] v \big]^T = v^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] u$$

gives

$$\begin{aligned} & \left\langle \begin{bmatrix} u \\ v \end{bmatrix}, G \begin{bmatrix} u \\ v \end{bmatrix} \right\rangle = \tfrac{1}{4} \Big[u^T [(A-C)^{-\frac{1}{2}} (2A - C)(A-C)^{-\frac{1}{2}}] u - u^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] u \\ & + u^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] u - 2u^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] v + v^T [(A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}] v \Big]. \end{aligned}$$

The first two terms can be combined and simplified to be

$$\tfrac{1}{4} u^T [(A-C)^{-\frac{1}{2}} (2A - 2C)(A-C)^{-\frac{1}{2}}] u = \tfrac{1}{2} u^T u,$$

which we will call the energy of the method's solutions. Take $F = (A-C)^{-\frac{1}{2}} C (A-C)^{-\frac{1}{2}}$. Since $F = F^T$, the remaining terms can be factored as

$$\begin{aligned} & \tfrac{1}{4} [u^T (F^{\frac{1}{2}})^T F^{\frac{1}{2}} u - 2u^T (F^{\frac{1}{2}})^T F^{\frac{1}{2}} v + v^T (F^{\frac{1}{2}})^T F^{\frac{1}{2}} v] \\ & = \tfrac{1}{4} \langle F^{\frac{1}{2}} u - F^{\frac{1}{2}} v, F^{\frac{1}{2}} u - F^{\frac{1}{2}} v \rangle \\ & = \tfrac{1}{4} \| F^{\frac{1}{2}} u - F^{\frac{1}{2}} v \|_2^2 \geq 0, \end{aligned}$$

and the result immediately follows. ◻

4.4. Unconditional Stability Result. As proved above, the matrix G is symmetric and positive-definite, and therefore the expression defined in (4.5) is a G-norm.

LEMMA 4.3. *Let u_n satisfy (1.5) for all $n \in \{2, \dots, \frac{T}{\Delta t}\}$. Then*

$$\begin{aligned} & \frac{1}{\Delta t} \Big\langle u_{n+1} - u_n \,,\, (A-C)^{-\frac{1}{2}} \Big(\tfrac{1}{2} A (A-C)^{-\frac{1}{2}} u_{n+1} + \big(\tfrac{1}{2} A - \tfrac{3}{2} C\big)(A-C)^{-\frac{1}{2}} u_n + \tfrac{1}{2} C (A-C)^{-\frac{1}{2}} u_{n-1} \Big) \Big\rangle \\ & = \frac{1}{\Delta t} \left\| \begin{bmatrix} u_{n+1} \\ u_n \end{bmatrix} \right\|_G^2 - \frac{1}{\Delta t} \left\| \begin{bmatrix} u_n \\ u_{n-1} \end{bmatrix} \right\|_G^2 + \frac{1}{4 \Delta t} \| \big(u_{n+1} - 2u_n + u_{n-1} \big) \|_F^2. \end{aligned} \tag{4.7}$$

4.4.1. Energy Bound. The proof of Lemma 4.2 allows us to conclude that

$$\left\| \begin{bmatrix} u \\ v \end{bmatrix} \right\|_G^2 \geq \frac{1}{2} u^T u > 0, \tag{4.8}$$

that is, the energy of the solutions is bounded from above by their G-norm, and this is independent of Δt. From (4.8) we have convergence of the solutions in the G-norm implies convergence of their energy.

4.4.2. Energy Equality. To see that the method is unconditionally stable consider the following energy equality, which holds for u_0, u_1 given inital conditions at all time steps $n = 1$ through $N-1$:

$$\begin{aligned}
&\frac{1}{\Delta t}\left\| \begin{bmatrix} u_N \\ u_{N-1} \end{bmatrix} \right\|_G^2 + \frac{1}{4\Delta t}\sum_{n=1}^{N-1} \|u_{n+1} - 2u_n + u_{n-1}\|_F^2 \\
&\quad + \sum_{n=1}^{N-1} \left\| \tfrac{1}{2}A(A-C)^{-\frac{1}{2}}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1}) \right\|^2 \\
&= \frac{1}{\Delta t}\left\| \begin{bmatrix} u_1 \\ u_0 \end{bmatrix} \right\|_G^2 \\
&\quad + \sum_{n=1}^{N-1} \Big\langle f_{n+\frac{1}{2}}, (A-C)^{-\frac{1}{2}}\Big(\tfrac{1}{2}A(A-C)^{-\frac{1}{2}}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1})\Big)\Big\rangle.
\end{aligned} \tag{4.9}$$

Notice Lemma 4.3 and the Energy Equality (4.9) immediately imply G-stability in the case of $f(t) = 0$. That is, if the the energy source (forcing function) is removed, stability of the method requires that the G-norm of the solutions decays weakly at each time step n. To see that this note that

$$\begin{aligned}
&\frac{1}{\Delta t}\left\| \begin{bmatrix} u_{n+1} \\ u_n \end{bmatrix} \right\|_G^2 - \frac{1}{\Delta t}\left\| \begin{bmatrix} u_n \\ u_{n-1} \end{bmatrix} \right\|_G^2 + \frac{1}{4\Delta t}\big\|(u_{n+1} - 2u_n + u_{n-1})\big\|_F^2 \\
&+ \left\| \tfrac{1}{2}A(A-C)^{-\frac{1}{2}}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1}) \right\|^2 = 0
\end{aligned}$$

holds for all $n \in \{1, N-1\}$. Further,

$$\frac{1}{4\Delta t}\big\|(u_{n+1} - 2u_n + u_{n-1})\big\|_F^2 \geq 0,$$

since F is a positive-definite matrix. Thus we have

$$\left\| \begin{bmatrix} u_{n+1} \\ u_n \end{bmatrix} \right\|_G^2 \leq \left\| \begin{bmatrix} u_n \\ u_{n-1} \end{bmatrix} \right\|_G^2.$$

Since this result is independent of the the size of time-step Δt, we have unconditional stablility when $f(t) = 0$.

4.4.3. Energy Estimate. When $f(t) \neq 0$ for some $t \in \mathcal{I}$, the effect of $f_{n+\frac{1}{2}}$ on the Energy Equality (4.9) is ambiguous. By applying Cauchy-Schwarz and Young's Inequalities, the Energy Bound (4.8), and combining like-terms, we can use (4.9) to derive the following energy estimate to bound the effect of f on the energy in the system:

$$\begin{aligned}
&\|u_N\|^2 + \tfrac{1}{2}\sum_{n=1}^{N-1} \big\|u_{n+1} - 2u_n + u_{n-1}\big\|_F^2 \\
&\qquad + \Delta t\sum_{n=1}^{N-1} \big\|\tfrac{1}{2}A(A-C)^{-\frac{1}{2}}u_{n+1} + \big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}u_n + \tfrac{1}{2}C(A-C)^{-\frac{1}{2}}u_{n-1}\big\|^2 \\
&\leq 2\left\| \begin{bmatrix} u_1 \\ u_0 \end{bmatrix} \right\|_G^2 + \Delta t\sum_{n=1}^{N-1} \big\|(A-C)^{-\frac{1}{2}}f_{n+\frac{1}{2}}\big\|^2.
\end{aligned} \tag{4.10}$$

Inequality (4.10) gives that solutions u_N are bounded from above by the G-norm of initial conditions and a positive term depending on f, so although monotonicity is no longer required, boundedness is retained.

5. Numerical Experiments. Consider the general form of the linear multistep numerical method (1.4). Method (1.5) is of this form, where $k = 2$ and

$$\begin{aligned}
&\alpha_{-1} = I, \qquad \alpha_0 = -I, \qquad \alpha_1 = 0\\
&\beta_{-1} = -(A-C)^{\frac{1}{2}}\tfrac{1}{2}A(A-C)^{-\frac{1}{2}} - B(\mathcal{E}_{n+\frac{1}{2}})(A-C)^{-\frac{1}{2}}\tfrac{1}{2}A(A-C)^{-\frac{1}{2}}\\
&\beta_0 = -(A-C)^{\frac{1}{2}}\big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}} - B(\mathcal{E}_{n+\frac{1}{2}})(A-C)^{-\frac{1}{2}}\big(\tfrac{1}{2}A - \tfrac{3}{2}C\big)(A-C)^{-\frac{1}{2}}\\
&\beta_1 = -(A-C)^{\frac{1}{2}}\tfrac{1}{2}C(A-C)^{-\frac{1}{2}} - B(\mathcal{E}_{n+\frac{1}{2}})(A-C)^{-\frac{1}{2}}\tfrac{1}{2}C(A-C)^{-\frac{1}{2}}.
\end{aligned}$$

Applying this method for solving the system (1.1) will require solving for the vector u_{n+1} in terms of u_n, u_{n-1} (given two initial condition vectors u_0, u_1), that is

$$u_{n+1} = \big[I - h\beta_{-1}\big]^{-1}\Big[\big[I + h\beta_0\big]u_n + h\beta_1 u_{n-1}\Big]. \tag{5.1}$$

The method requires the inversion

$$\big[I - h\beta_{-1}\big]^{-1} = \big[I + h(A-C)^{\frac{1}{2}}\tfrac{1}{2}A(A-C)^{-\frac{1}{2}} + hB(\mathcal{E}_{n+\frac{1}{2}})(A-C)^{-\frac{1}{2}}\tfrac{1}{2}A(A-C)^{-\frac{1}{2}}\big]^{-1}.$$

In practice (5.1) will not be solved by computing the inverse since this would be overly costly and introduce large round-off error. Also of note is that in general, A, B, and C do not commute, and thus the calculation in (5.1) appears to be somewhat more costly than method (2.1) due to the additional $(A-C)^{-\frac{1}{2}}$ and $(A-C)^{\frac{1}{2}}$ terms. As seen in the previous section, the fact that these matrices do not commute plays a critical role in the stability analysis developed in Section 4.

To demonstrate that the proposed CNAB2 method (1.5) is unconditionally stable consider the following numerical experiments.

5.1. Experiment 1. Take

$$A = (\epsilon+\nu)\begin{pmatrix}100 & 0\\ 0 & 1\end{pmatrix}, \qquad C = \epsilon\begin{pmatrix}100 & 0\\ 0 & 1\end{pmatrix}, \qquad B(\mathcal{E}_{n+\frac{1}{2}}) = \sqrt{u_1^2+u_2^2}\begin{pmatrix}0 & 100\\ -100 & 0\end{pmatrix}, \qquad f(t) = 0,$$

where u_1 and u_2 denote the first and second elements of the vector $\frac{3}{2}u_n - \frac{1}{2}u_{n-1}$ (not the time step). Let $\nu = .001$, and initial conditions be $u_1 = u_2 = [1,1]^T$.

The first plot in Figure 5.1 shows the convergence of the energy and G-norms for CNAB2 (1.5) with $d = 2$, and $\epsilon = .01$. Notice that as in the scalar example in Section 3 (see Figure 3.5), the G-norm decreases monotonically, even though the energy of the solution does not. The second plot shows the convergence of the G-norm for CNAB2 (1.5) with $d = 2$ and $f(t) = 0$ for various Δt.

5.2. Experiment 2. Now we relax the restrictions on C and $f(t)$ to study the case where C is not diagonal, and $f(t) \neq 0$ for some t. Taking

$$C = \epsilon\begin{pmatrix}100 & -1\\ -1 & 1\end{pmatrix}, \qquad f(t) = e^{-t},$$

implies that

$$A - C = \begin{pmatrix}100\nu & \epsilon\\ \epsilon & \nu\end{pmatrix}.$$

Recalling that $A-C$ is required to be positive-definite, by Sylvester's Criterion we see that $A-C$ is positive-definite when $100\nu^2 - \epsilon^2 > 0$, which is satisfied by all ν and ϵ such that $10\nu > \epsilon$. $\epsilon = .009$, satisfies the inequality for $\nu = .001$.

Figure 5.2 shows the energy and G-norms for various Δt under the new conditions on C and $f(t)$. Notice that when $\Delta t = 0.25$ the G-norm is not monotically decreasing until $t \simeq 1$. This is due to the forcing function $f(t) = e^{-t}$, and is an illustration of the Energy Estimate (4.10), which says that the solutions in the G-norm are bounded by solutions at previous steps *and* a norm depending on the forcing function $f(t)$. The Energy Bound (4.8) holds in both experiments, as the theory requires.

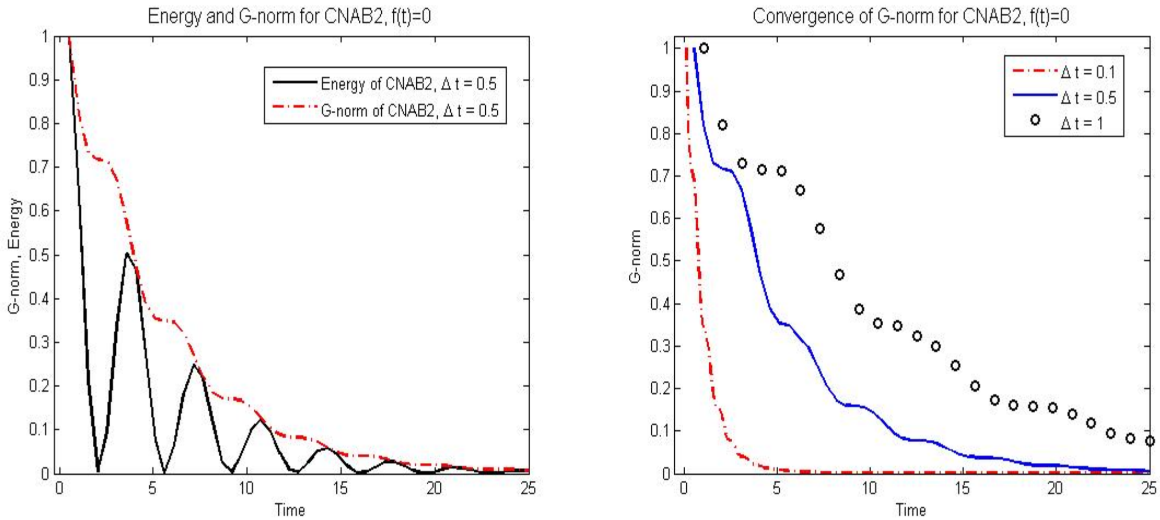

Fig. 5.1: Convergence CNAB2 with $f(t) = 0$

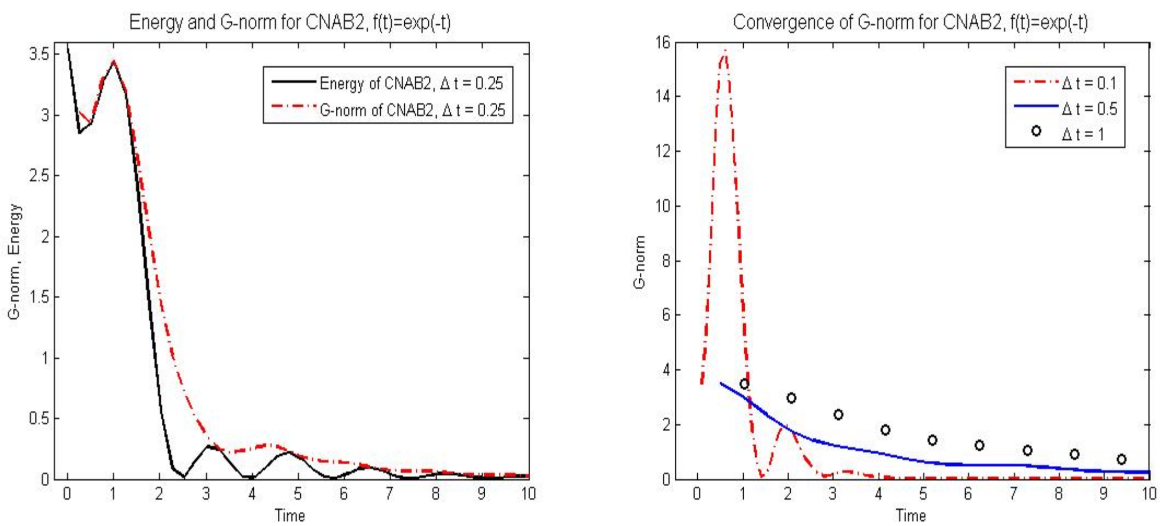

Fig. 5.2: Convergence CNAB2 with $f(t) = e^{-t}$

6. Conclusion. The Crank-Nicolson Adams-Bashforth 2 second-order method analyzed herein offers an improvement over the first-order method proposed in [2] in terms of accuracy, though it does so at the expense of being considerably more computationally expensive. Nonetheless, the fact that it is unconditionally stable, and thus accomodates any choice of Δt makes it an attractive method in terms of its stability properties.

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