Krylov subspace approximations for the exponential Euler method: error estimates and the harmonic Ritz approximant

E. J. Carr[1] I. W. Turner[2] M. Ilic[3]

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Abstract

We study Krylov subspace methods for approximating the matrix-function vector product $\varphi(tA)b$ where $\varphi(z) = (e^z - 1)/z$. This product arises in the numerical integration of large stiff systems of differential equations by the Exponential Euler Method (EEM), where the Jacobian matrix of the system defines the matrix A. Recently, this method has found application in the simulation of transport phenomena in porous media within mathematical models of wood drying and groundwater flow. In this work, we develop an *a posteriori* upper bound on the Krylov subspace approximation error and provide a new interpretation of a previously published error estimate. This leads to an alternative Krylov approximation to $\varphi(tA)b$, the so-called Harmonic Ritz approximant, which we find does not exhibit oscillatory behaviour of the residual error.

Contents

1 Introduction

Mathematical models for simulating transport phenomena in porous media take the form

$$\frac{\partial \psi_\ell}{\partial t} + \nabla \cdot q_\ell = 0 \quad \text{on } \Omega \,,$$

where ℓ denotes the conserved quantity, with appropriate conditions defined on the boundary $\partial\Omega$. For example, a three-equation model representing the conservation of water, energy and air is used for modelling the drying of wood [9]. For such problems, the Finite Volume Method (FVM) has been used with great success to solve the governing set of equations. In two dimensions, the domain Ω is tessellated with triangles and finite volumes are constructed around every node (vertex) in the mesh. For the three-equation wood-drying model and a mesh comprising of N_p nodes, the FVM leads to a system of differential equations of the form [2]

$$\frac{du}{dt} = g(u) \,, \quad u(0) = u_0 \,, \tag{1}$$

where $u \in \mathbb{R}^{3N_p}$ contains the unknown solution values, arranged in triplets, at each node in the mesh. Recently [2], it was found that the Exponential Euler Method (EEM) is effective for numerically integrating the resulting differential equation system (1). At each step of the integration process, EEM solves the linearised system

$$\frac{du}{dt} = g(u_n) + J(u_n)(u - u_n) \,, \quad u(t_n) = u_n \,,$$

exactly to obtain the approximate time-stepping formula

$$u_{n+1} = u_n + \tau_n \varphi\left(\tau_n J(u_n)\right) g(u_n) \,,$$

where $\varphi(z) = (e^z - 1)/z$, $\tau_n = t_{n+1} - t_n$ is the integration step and J is the Jacobian matrix of g [1, 2, 7, 8]. This integration strategy is by no means new but it was not until recently [1] that a stepsize control algorithm using local error estimation was provided for the problems of groundwater flow [1] and wood drying [2].

The focus of this paper concerns the computation of $\varphi(tA)b$ for the large sparse non-symmetric matrices A encountered in the aforementioned problems; the eigenvalues of these matrices typically have negative real components. Approximations to $\varphi(tA)b$ can be extracted from the m-dimensional

Krylov subspace

$$\mathcal{K}_m(A,b) = \text{span}\left\{b, Ab, \ldots, A^{m-1}b\right\} \subseteq \mathbb{R}^N, \quad A \in \mathbb{R}^{N\times N},$$

via Arnoldi's method, which produces the decomposition

$$AV_m = V_mH_m + \beta_m v_{m+1}e_m^T, \quad b = \beta_0 v_1, \tag{2}$$

where the columns $v_1, v_2, \ldots, v_m$ of $V_m \in \mathbb{R}^{N\times m}$ form an orthonormal basis for $\mathcal{K}_m(A,b)$, $H_m = V_m^TAV_m$ (since $V_m^Tv_{m+1} = 0$), $\beta_0 = \|b\|_2$, $\beta_m = \|(I - V_mV_m^T)Av_m\|_2$ and e_m is the mth column of the $m\times m$ identity matrix. The Krylov approximation reduces the evaluation of φ to the small $m\times m$ matrix H_m [1, 2, 7, 8]:

$$\varphi(tA)b \approx \beta_0V_m\varphi(tH_m)e_1\,. \tag{3}$$

In practice, beginning at $m = 1$, the dimension of the Krylov subspace is increased and the procedure terminated when the approximation (3) is deemed sufficiently accurate. In the literature, criteria for terminating this approximation procedure are based on the true error [7]:

$$\varepsilon_m = \varphi(tA)b - \beta_0V_m\varphi(tH_m)e_1\,. \tag{4}$$

Since $\varphi(tA)b$ is unknown, this true error (4) must be estimated or bounded. One error estimate due to Hochbruck, Lubich and Selhofer [7] performs reasonably well in simulation codes [1, 2]. In Section 2.1, we attempt to improve upon this error estimate by developing an upper bound on the 2-norm of the true error (4) for those matrices encountered in wood drying and groundwater flow applications.

In Section 2.2, we provide a new interpretation of the error estimate of Hochbruck et al. [7] by introducing the concept of a "differential equation residual". This concept relies on the fact that the matrix function $t\varphi(tA)b$ exactly satisfies a suitably-defined differential equation. This notion of a residual leads to an alternative Krylov approximation to $\varphi(tA)b$, which we derive by extending methods developed for linear systems that enforce orthogonality of the residual vector and a specified m-dimensional subspace of constraints (see Section 2.3).

2 Krylov approximation to $\varphi(tA)b$

2.1 An a posteriori error bound

Using the Cauchy integral formula, the error of the mth Krylov approximation (4) is represented as [7]

$$\varepsilon_m = \frac{1}{2\pi i}\oint_\Gamma \varphi(z)(zI - tA)^{-1}r_m(z)\,dz\,, \tag{5}$$

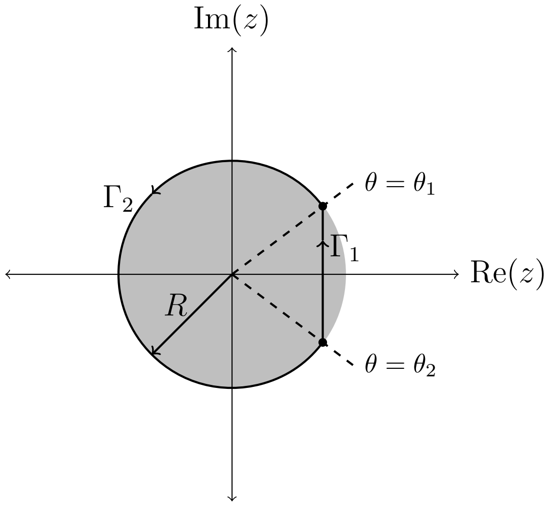

Figure 1: Contour of integration $\Gamma = \Gamma_1 \cup \Gamma_2$ used in error bound derivation. We take $\Gamma_1 : z = \alpha + iy$, $R\sin(\theta_2) \leq y \leq R\sin(\theta_1)$ and $\Gamma_2 : z = Re^{i\theta}$, $\theta_1 \leq \theta \leq \theta_2$ where $\theta_1 = \arccos(\alpha/R)$ and $\theta_2 = 2\pi - \arccos(\alpha/R)$.

where the contour of integration Γ encloses the eigenvalues of both tA and tH_m, and where

$$r_m(z) = b - (zI - tA)x_m = t\beta_0\beta_m e_m^T(zI - tH_m)^{-1}e_1 v_{m+1} \tag{6}$$

is the residual error associated with the Full Orthogonalisation Method (FOM) approximation $x_m = \beta_0 V_m(zI - tH_m)^{-1}e_1$ to the solution of the z-shifted linear system $(zI - tA)x = b$ [7].

Our interest concerns matrices tA whose eigenvalues have real components less than some positive value α. Consequently, the contour of integration Γ is chosen as the boundary of the region formed by the intersection of the disk $|z| \leq R$ with the half-plane $\mathrm{Re}(z) \leq \alpha$. Taking the limit as R tends to infinity (to enclose all eigenvalues with real components less than α), produces the following Cauchy-integral representation

$$\varphi(\lambda) = \lim_{R\to\infty} (I_1 + I_2) \ , \quad I_j = \frac{1}{2\pi i}\int_{\Gamma_j} \frac{\varphi(z)}{z - \lambda}\, dz \ , \ j = 1, 2$$

for $\mathrm{Re}(\lambda) < \alpha$. The second integral in this representation is bounded above as follows

$$|I_2| = \left| \frac{1}{2\pi}\int_{\theta_1}^{\theta_2} \frac{\varphi(Re^{i\theta})}{Re^{i\theta} - \lambda} Re^{i\theta} d\theta \right| \leq \frac{1}{2\pi}\int_{\theta_1}^{\theta_2} \frac{e^{R\cos\theta} + 1}{R - |\lambda|}\, d\theta \,,$$

$$\leq \frac{e^\alpha + 1}{2\pi(R - |\lambda|)}(\theta_2 - \theta_1)\,,$$

where we have used $R\cos\theta \leq \alpha$ for $\theta_1 \leq \theta \leq \theta_2$. Taking the limit as R approaches infinity we obtain

$$\left|\lim_{R\to\infty} I_2\right| = \lim_{R\to\infty} |I_2| = 0\,.$$

The significance of this result is that the error representation (5) can be expressed as

$$\varepsilon_m = \frac{1}{2\pi}\int_{-\infty}^{\infty} \varphi(\alpha + iy)\,((\alpha + iy)I - tA)^{-1}\, r_m(\alpha + iy)\, dy\,. \qquad (7)$$

In the following proposition, we provide an upper bound on the 2-norm of ε_m by considering this integral representation.

Proposition 1 *Suppose $A = PDP^{-1}$ and $H_m = Y_m\Lambda_m Y_m^{-1}$ are diagonalisable with eigenvalues λ_j, $j = 1,\ldots,N$ and μ_k, $k = 1,\ldots,m$. Furthermore, take $\lambda_{\max}$ to be the maximum real component of the eigenvalues of A. Then for α positive and $\alpha > t\lambda_{\max}$, the 2-norm of the Krylov approximation error $\varepsilon_m = \varphi(tA)b - \beta_0 V_m \varphi(tH_m)e_1$ satisfies*

$$\|\varepsilon_m\|_2 \leq \mathcal{C}_m(\alpha)\, \|r_m(\alpha)\|_2\,, \qquad (8)$$

where

$$\mathcal{C}_m(\alpha) = \frac{\kappa_2(P)(e^\alpha + 1)}{2\alpha^{1/2}(\alpha - t\lambda_{\max})^{1/2}} \prod_{k=1}^{m}\left[1 + \left(\frac{t\,\mathrm{Im}(\mu_k)}{\alpha - t\,\mathrm{Re}(\mu_k)}\right)^2\right]^{1/2}\,, \qquad (9)$$

$\kappa_2(P)$ is the 2-norm condition number of P, and $r_m(\alpha)$ is the residual error associated with the FOM *approximation to $(\alpha I - tA)^{-1}b$.*

Proof: Taking norms of (7) gives

$$\|\varepsilon_m\|_2 \leq \frac{1}{2\pi}\int_{-\infty}^{\infty} |\varphi(\alpha + iy)|\, \left\|((\alpha + iy)I - tA)^{-1}\right\|_2 \|r_m(\alpha + iy)\|_2\, dy\,.$$

We make use of the results

$$|\varphi(\alpha + iy)| \leq \frac{e^\alpha + 1}{|\alpha + iy|}\,,$$

$$\left\|((\alpha + iy)I - tA)^{-1}\right\|_2 \leq \kappa_2(P) \max_{j=1,\ldots,N} \frac{1}{|(\alpha + iy) - t\lambda_j|}\,,$$

and

$$\|r_m(\alpha+iy)\|_2 = \prod_{k=1}^{m} \frac{|\alpha - t\mu_k|}{|\alpha+iy-t\mu_k|}\, \|r_m(\alpha)\|_2\,, \\ \le \prod_{k=1}^{m}\left[1+\left(\frac{t\,\mathrm{Im}(\mu_k)}{\alpha - t\,\mathrm{Re}(\mu_k)}\right)^2\right]^{1/2} \|r_m(\alpha)\|_2\,.$$

The third result follows from expressing $e_m^T(zI - tH_m)^{-1}e_1$ in the definition of the residual vector (6) in adjoint–determinant form for both $z=\alpha+iy$ and $z=\alpha$ and then taking norms. Using these results one obtains

$$\|\varepsilon_m\|_2 \le \kappa_2(P)\,(e^{\alpha}+1)\prod_{k=1}^{m}\left[1+\left(\frac{t\,\mathrm{Im}(\mu_k)}{\alpha - t\,\mathrm{Re}(\mu_k)}\right)^2\right]^{1/2} \\ \times \max_{j=1,\ldots,N}\int_{-\infty}^{\infty}\frac{1}{|\alpha+iy|}\frac{1}{|(\alpha+iy)-t\lambda_j|}\,dy\,\|r_m(\alpha)\|_2\,.$$

The integral can then be bounded above using the Cauchy–Schwarz Inequality,

$$I = \max_{j=1,\ldots,N}\int_{-\infty}^{\infty}\frac{1}{|\alpha+iy|}\frac{1}{|(\alpha+iy)-t\lambda_j|}\,dy \\ \le \max_{j=1,\ldots,N}\left(\int_{-\infty}^{\infty}\frac{1}{|\alpha+iy|^2}\,dy\right)^{1/2}\left(\int_{-\infty}^{\infty}\frac{1}{|\alpha+iy-t\lambda_j|^2}\,dy\right)^{1/2} \\ = \max_{j=1,\ldots,N}\left(\frac{\pi}{\alpha}\right)^{1/2}\left(\frac{\pi}{\alpha - t\,\mathrm{Re}(\lambda_j)}\right)^{1/2}\,.$$

♠

Remark 2 In the case when the matrix is not diagonalisable, one must use the Jordan canonical form [5]. This will be the subject of future research.

Proposition 1 provides an upper bound that can be used to terminate the approximation procedure. However, it requires knowledge of the values of $\kappa_2(P)$ and $\lambda_{\max}$. A practical error estimate based on this bound is obtained by estimating these values using the projected matrix H_m, via the approximations $\kappa_2(P)\approx\kappa_2(Y_m)$ and $\lambda_{\max}\approx\mu_{\max}=\max_{k=1,\ldots,m}\mathrm{Re}(\mu_k)$. This produces the estimate $\mathcal{C}_m(\alpha)\approx\tilde{\mathcal{C}}_m(\alpha)$ for use in (8) where

$$\tilde{\mathcal{C}}_m(\alpha) = \frac{\kappa_2(Y_m)(e^{\alpha}+1)}{2\alpha^{1/2}(\alpha - t\mu_{\max})^{1/2}}\prod_{k=1}^{m}\left[1+\left(\frac{t\,\mathrm{Im}(\mu_k)}{\alpha - t\,\mathrm{Re}(\mu_k)}\right)^2\right]^{1/2}\,. \qquad (10)$$

2.2 New interpretation of error estimate

Firstly, we briefly outline the estimate of the true error (4) given by Hochbruck et al. [7]. Consider the Cauchy-integral representation (5), which can be expressed as

$$\varepsilon_m = \frac{1}{2\pi i}\int_\Gamma \varphi(z)\epsilon_m(z)\,dz\,,$$

where $\epsilon_m(z) = x - x_m$ is the true error associated with the FOM approximation $x_m = \beta_0 V_m(zI - tH_m)^{-1}e_1$ to the solution of the z-shifted linear system $(zI - tA)x = b$. Hochbruck et al. [7] argue that since the termination of FOM for this linear system is typically based on the residual error $r_m(z)$ rather than the true error $\epsilon_m(z)$, one can substitute for $\epsilon_m(z)$ the error indicator $r_m(z)$ (6) giving

$$\varepsilon_m \approx \frac{1}{2\pi i}\int_\Gamma \varphi(z)r_m(z)\,dz \;= t\beta_0\beta_m e_m^T\varphi(tH_m)e_1 v_{m+1}\,.$$

We now provide a new interpretation of the resulting error estimate by introducing the concept of a differential equation residual. This relies on the fact that the function $x(t) = t\varphi(tA)b = A^{-1}(e^{tA} - I)b$ satisfies

$$\frac{dx}{dt} = Ax + b\,, \quad x(0) = 0. \tag{11}$$

We replace $\varphi(tA)b$ by its Krylov approximation (3) and hence define the approximation $x_m(t) = t\beta_0 V_m\varphi(tH_m)e_1 = \beta_0 V_m H_m^{-1}(e^{tH_m} - I)e_1$. One way to measure how well x_m approximates x (and hence determine the accuracy of the Krylov approximation (3)) is to measure how well x_m satisfies the differential equation (11). We propose to measure this through the "differential equation residual", defined as

$$\rho_m = b + Ax_m - \frac{dx_m}{dt}\,, \tag{12}$$

where $\rho_m = 0$ when $x_m = x$ and one assumes a small value of $\|\rho_m\|$ means x_m is a good approximation to x. We note that a similiar error interpretation has been given for the matrix exponential by Celledoni and Moret [4]. Making use of the Arnoldi decomposition (2) and noting that $b = \beta_0 V_m e_1$, one obtains

$$\begin{aligned}\rho_m &= b + t\beta_0 AV_m\varphi(tH_m)e_1 - \beta_0 V_m e^{tH_m}e_1\,,\\ &= b + t\beta_0 AV_m\varphi(tH_m)e_1 - \beta_0 V_m(tH_m\varphi(tH_m) + I_m)e_1\,,\\ &= t\beta_0\left(AV_m - V_mH_m\right)\varphi(tH_m)e_1\,,\\ &= t\beta_0\beta_m e_m^T\varphi(tH_m)e_1 v_{m+1}\,,\end{aligned} \tag{13}$$

as a measure of the accuracy of the approximation (3), which is identical to the error estimate proposed by Hochbruck et al. [7]. As we see in the next section, this error interpretation can be used to construct an alternative Krylov approximant to $\varphi(tA)b$.

2.3 Harmonic Ritz approximation

For linear systems, Krylov projection methods extract an approximate solution from $\mathcal{K}_m$ by forcing the residual vector to be orthogonal to an m-dimensional subspace of constraints $\mathcal{W}_m \subseteq \mathbb{R}^N$. We extend this idea to the "differential equation residual" introduced in Section 2.2 to produce an alternative Krylov approximation to $\varphi(tA)b$.

First, we note that each vector $x_m \in \mathcal{K}_m$ is expressible in the form $x_m = V_m y_m$ where $y_m \in \mathbb{R}^m$. This produces the general form of the residual vector (12)

$$\rho_m = b + AV_m y_m - V_m \frac{dy_m}{dt},$$

where we have assumed y_m is a function of t.

To produce the FOM approximate solution of a linear system, one chooses $\mathcal{W}_m = \mathcal{K}_m$. Interestingly, forcing ρ_m to be orthogonal to $\mathcal{K}_m$, that is $V_m^T \rho_m = 0$, we obtain

$$\begin{aligned} V_m^T b + (V_m^T A V_m) y_m - (V_m^T V_m) \frac{dy_m}{dt} &= 0, \\ \beta_0 e_1 + H_m y_m - \frac{dy_m}{dt} &= 0, \end{aligned}$$

due to the columns of V_m forming an orthonormal basis. The solution of this differential equation is $y_m = t\beta_0 \varphi(tH_m)e_1$ and hence $x_m = t\beta_0 V_m \varphi(tH_m)e_1$, which reproduces the Krylov approximation defined by (3).

Another Krylov projection method for linear systems, the Generalised Minimal Residual Method (GMRES), is often preferred over FOM since the resulting approximate solution minimises the 2-norm of the residual vector over $\mathcal{K}_m$. For linear systems, this choice of the constraint space $\mathcal{W}_m$ is well known, however, the choice that minimises the 2-norm of ρ_m is not as straight forward.

As a result, we take $\mathcal{W}_m = A\mathcal{K}_m$, which produces the GMRES approximate solution to the linear system $Ax = b$. Forcing ρ_m to be orthogonal to $A\mathcal{K}_m$ requires

$$(AV_m)^T \left(b + AV_m y_m - V_m \frac{dy_m}{dt} \right) = 0.$$

Using the Arnoldi decomposition (2),

$$(V_m H_m + \beta_m v_{m+1} e_m^T)^T \left(\beta_0 V_m e_1 + \left(V_m H_m + \beta_m v_{m+1} e_m^T \right) y_m - V_m \frac{dy_m}{dt} \right) = 0\,,$$

and given that v_{m+1} is orthogonal to each column of V_m, we obtain

$$\beta_0 H_m^T e_1 + \left(H_m^T H_m + \beta_m^2 e_m e_m^T \right) y_m - H_m^T \frac{dy_m}{dt} = 0\,.$$

Assuming H_m^T is invertible and denoting $H_m^{-T} = (H_m^T)^{-1}$ one obtains

$$\beta_0 e_1 + \left(H_m + \beta_m^2 H_m^{-T} e_m e_m^T \right) y_m - \frac{dy_m}{dt} = 0\,.$$

The solution of this differential equation is $y_m = t\beta_0 \varphi(t\mathcal{H}_m) e_1$ where $\mathcal{H}_m = H_m + \beta_m^2 H_m^{-T} e_m e_m^T$ and hence $x_m = t\beta_0 V_m \varphi(t\mathcal{H}_m) e_1$. This defines the alternative Krylov approximation

$$\varphi(tA)b \approx \beta_0 V_m \varphi(t\mathcal{H}_m) e_1\,, \quad \mathcal{H}_m = H_m + \beta_m^2 f_m e_m^T\,, \tag{14}$$

where the evaluation of φ occurs at a matrix given by a rank-one update on H_m and $f_m = H_m^{-T} e_m$. We refer to the case $f_m = H_m^{-T} e_m$ as the harmonic Ritz approximant since the eigenvalues of $\mathcal{H}_m$ are the harmonic Ritz values of A with respect to the subspace $\mathcal{K}_m$. We note that a generalised version of (14) was derived by Hochbruck and Hochstenbach [6] using a different strategy. For (14), the "differential equation residual" is defined as

$$\begin{aligned}
\rho_m &= b + t\beta_0 A V_m \varphi(t\mathcal{H}_m) e_1 - \beta_0 V_m e^{t\mathcal{H}_m} e_1\,,\\
&= b + t\beta_0 A V_m \varphi(t\mathcal{H}_m) e_1 - \beta_0 V_m (t\mathcal{H}_m \varphi(t\mathcal{H}_m) + I_m) e_1\,,\\
&= t\beta_0 \left(A V_m - V_m \mathcal{H}_m \right) \varphi(t\mathcal{H}_m) e_1\,,\\
&= t\beta_0 \beta_m e_m^T \varphi(t\mathcal{H}_m) e_1 \left[v_{m+1} - \beta_m V_m f_m \right]\,.
\end{aligned} \tag{15}$$

One notes that setting $f_m = 0$ in Equations (14) and (15) produces the standard Krylov approximation, which we refer to in the next section as the Ritz approximant.

3 Numerical experiments

All numerical experiments are conducted in Matlab Version 7.1 based on a single representative matrix $A = J(u_n)$ of size 1899×1899 and vector $b = g(u_n)$ extracted from a low temperature wood-drying simulation [2, 3].

The real and imaginary eigenvalue components of A range from -1.0000×10^2 to -7.4344×10^{-5} and -5.0217×10^{-4} to 5.0217×10^{-4}, respectively.

First, we assess the performance of the error bound derived in (8) and (9) of Section 2.1 and the error estimate defined by (10) for a time step of $t = 200$ (see Figure 2). Recall that the error estimate is obtained by using the approximations $\kappa_2(P) \approx \kappa_2(Y_m)$ and $\lambda_{\max} = \mu_{\max} \approx \max_{k=1,\ldots,m} \mathrm{Re}(\mu_k)$ in the bound. In these results, $\alpha > 0$ can be freely chosen. We find increasing the value of α provides a sharper bound for large m but a poorer bound for small m. This trade-off occurs due to two reasons: the appearance of the term $\exp(\alpha)$ in the constants $\mathcal{C}_m(\alpha)$ and $\tilde{\mathcal{C}}_m(\alpha)$ and the faster convergence of the linear system residual $r_m(\alpha)$ for larger α. Note, however, that for both the error bound and error estimate, a value of α could not be found that improved upon the "differential equation residual" error (estimate of Hochbruck et al. [7]).

We now assess the performance of both the Ritz and harmonic Ritz approximants to $\varphi(tA)b$, defined in (14) with $f_m = 0$ and $f_m = H_m^{-T}e_m$ respectively (see Figure 3). Eigenvalue decompositions are used to compute both $\varphi(tH_m)$ and $\varphi(t\mathcal{H}_m)$. Our initial experiments discovered that for some values of m, a single positive harmonic Ritz value was produced that eroded the accuracy of the given harmonic Ritz approximant. We found it necessary to discard these eigenvalues by approximating $\varphi(t\mathcal{H}_m)$ by

$$\varphi(t\mathcal{H}_m) \approx \sum_{\mathrm{Re}(\theta_j)<0} \varphi(t\theta_j) y_j z_j^T \,, \quad \mathcal{H}_m Y_m = \Theta_m Y_m \,,$$

where y_j is the jth column of Y_m such that (θ_j, y_j) is an eigenpair of $\mathcal{H}_m$ and z_j^T is the jth row of Y_m^{-1}. Time steps of $t = 50$ and $t = 200$ (slower convergence) are both tested. From the plot, it is clear that the behaviour of the "differential equation residual" error for the harmonic Ritz approximant is more favourable than the standard Ritz approximant. The former eliminates the oscillation, providing a smooth monotone decreasing residual error.

4 Conclusions

In this paper, we have derived an *a posteriori* upper bound on the Krylov subspace approximation error for the matrix-function vector product $\varphi(tA)b$. This error bound provides a mechanism through which the quality of the Krylov approximant can be assessed as the dimension of the subspace is increased. We have also introduced the concept of a "differential equation residual" and used this definition to explain why a previously defined error estimate performs adequately in predicting when to terminate the Krylov

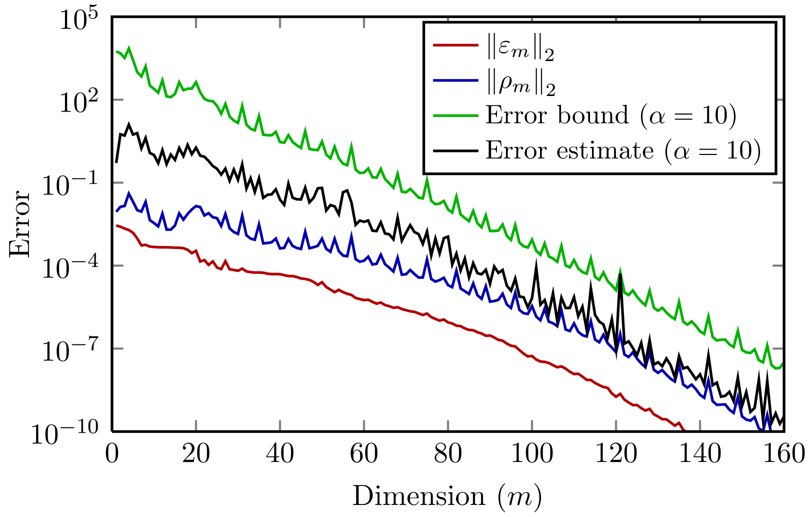

Figure 2: Accuracy of error estimates and error bounds to $\varepsilon_m = \varphi(tA)b - \beta_0 V_m \varphi(tH_m)e_1$ for a time step of $t = 200$. Comparison of the "differential equation residual" (13), error bound (given in Equations 8 and 9) and error estimate defined by (10).

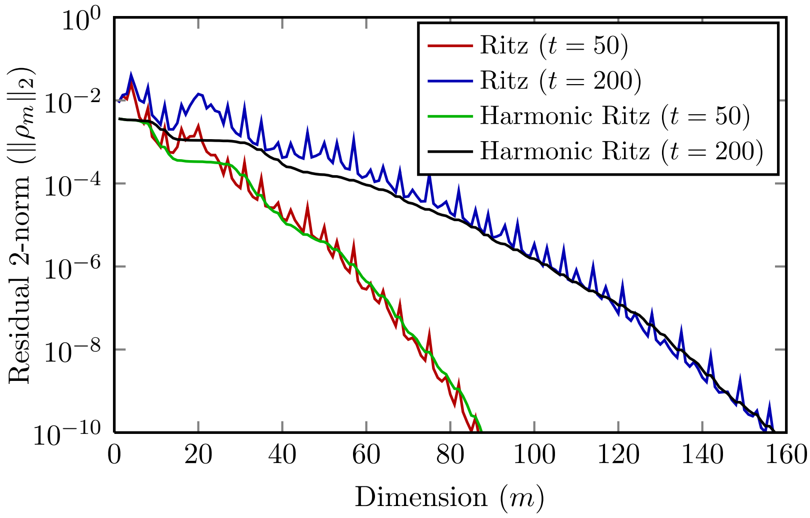

Figure 3: Accuracy of Krylov approximants to $\varphi(tA)b$. Comparison of the "differential equation residual" error (15) for the Ritz ($f_m = 0$) and Harmonic Ritz ($f_m = H_m^{-T} e_m$) approximants for two values of the time step t.

subspace approximation procedure. This finding identified an alternative Krylov subspace approximation to $\varphi(tA)b$ that provided "smoother" residual errors than the standard approximation featured in the literature. We believe this alternative approximation has potential and our intention will be to utilise this result in future versions of our Exponential Euler Method (EEM) simulation code for further case studies in modelling transport processes in porous media.

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Author addresses

1. **E. J. Carr**, Mathematical Sciences, Queensland University of Technology, Brisbane, Australia.
mailto:elliot.carr@qut.edu.au

2. **I. W. Turner**, Mathematical Sciences, Queensland University of Technology, Brisbane, Australia.
mailto:i.turner@qut.edu.au

3. **M. Ilic**, Mathematical Sciences, Queensland University of Technology, Brisbane, Australia.
mailto:m.ilic@qut.edu.au