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EVALUATING MATRIX FUNCTIONS FOR EXPONENTIAL INTEGRATORS VIA CARATHÉODORY-FEJÉR APPROXIMATION AND CONTOUR INTEGRALS*

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Abstract. Among the fastest methods for solving stiff PDE are exponential integrators, which require the evaluation of $f(A)$, where A is a negative semidefinite matrix and f is the exponential function or one of the related "φ functions" such as $\varphi_1(z) = (e^z - 1)/z$. Building on previous work by Trefethen and Gutknecht, Minchev, and Lu, we propose two methods for the fast evaluation of $f(A)$ that are especially useful when shifted systems $(A + zI)x = b$ can be solved efficiently, e.g. by a sparse direct solver. The first method is based on best rational approximations to f on the negative real axis computed via the Carathéodory-Fejér procedure. Rather than using optimal poles we approximate the functions in a set of common poles, which speeds up typical computations by a factor of 2 to 3.5. The second method is an application of the trapezoid rule on a Talbot-type contour.

Key words. matrix exponential, exponential integrators, stiff semilinear parabolic PDEs, rational uniform approximation, Hankel contour, numerical quadrature

AMS subject classification. 65L05, 41A20, 30E20

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