

Numerical Methods of Rational Form for Reaction Diffusion Equations

Said Algarni*

*Department of Mathematics and Statistics
King Fahd University of Petroleum and Minerals

Resumo

The purpose of this study was to investigate select numerical methods that demonstrate good performance in solving PDEs that couple diffusion and reaction terms.

The simple form of a reaction diffusion equation is the following

$$u_t(x, t) = \alpha u_{xx} + f(u),$$

where u is an order-parameter field, e.g., population density, chemical concentration, magnetization, which depends on space x and time t . The order-parameter may be either scalar or vector, depending on the number of variables that describe the physical system. The order-parameter evolves in time due to a local reaction, described by the nonlinear term $f(u)$, in conjunction with spatial diffusion. The coefficient α can be a diagonal matrix or in some cases a full matrix to account for so-called cross-diffusion terms. In most cases, however, α can be a scalar where the amount of diffusion is the same in all coordinate directions, or it could be dependent on time and space $\alpha(x, t)$. These types of equations have numerous fields of application such as environmental studies, biology, chemistry, medicine, and ecology.

Our aim was to investigate and develop accurate and efficient approaches which compare favourably to other applicable methods. In particular, we investigated and adapted a relatively new class of methods based on rational polynomials. Namely, Padé time stepping (PTS), which is highly stable for the purposes of the present application and is associated with lower computational costs. Furthermore, PTS was optimized for our study to focus on reaction diffusion equations. Due to the rational form of PTS method, a local error control threshold (LECT) was proposed. Numerical runs were conducted to obtain the optimal LECT. In addition, new schemes based on both PTS and splitting methods were established.

Based on the results, we found PTS alone and combined via splitting with other approaches provided favourable performance in certain and wide ranging parameter regimes.

Referências

- [1] Amundsen, D., Bruno, O., *Time stepping via one-dimensional Padé approximation*, J. of Sci. Comp., 2007, 30, pp. 83-115.
- [2] Baker, G. A., Graves-Morris, P., *Padé Approximants Part 1: Basic Theory*, Encyclopedia of Mathematics and Its Applications, Vol. 13, Addison-Wesley, 1981.