Accepted Manuscript

Operator splitting for chemical reaction systems with fast chemistry

Axel Ariaan Lukassen, Martin Kiehl

PII: S0377-0427(18)30349-2
DOI: https://doi.org/10.1016/j.cam.2018.06.001
Reference: CAM 11731

To appear in: *Journal of Computational and Applied Mathematics*

Received date : 13 October 2017
Revised date : 1 June 2018

Please cite this article as: A.A. Lukassen, M. Kiehl, Operator splitting for chemical reaction systems with fast chemistry, *Journal of Computational and Applied Mathematics* (2018), https://doi.org/10.1016/j.cam.2018.06.001

Operator splitting for chemical reaction systems with fast chemistry

Axel Ariaan Lukassen and Martin Kiehl

Department of Mathematics, TU Darmstadt, Germany
lukassen@mathematik.tu-darmstadt.de, kiehl@mathematik.tu-darmstadt.de

Abstract

Splitting methods are frequently used for large scale chemical reaction systems. The main reason is the reduced computational cost for solving the subproblems in comparison to the time integration of the full problem. However, a splitting error is introduced. The most popular splitting schemes are the first order Lie-Trotter splitting and the second order Strang splitting. However, in case of stiff differential equations the Strang splitting suffers from order reduction and both schemes have order one for stiff differential equations. Therefore, the step size restrictions due to the low order can result in a prohibitive small step size. Hence, splitting schemes with order larger than one are necessary for stiff differential equations. The Richardson extrapolation of the Lie-Trotter splitting is a second order scheme. In this paper we examine differential equations with a fast chemical source term and a slow transport term. Thus, all stiffness of the system is related to the chemical source term. We show that the Richardson extrapolation does not suffer from order reduction in this case. Furthermore, we perform a stability analysis of the extrapolated splitting scheme for a linear test problem. Thereby the operators of the test problem do not commute.

Keywords: Chemical Reaction System, Order Reduction, Richardson extrapolation, Splitting Methods, Stiffness

1. Introduction

Operator splitting is frequently used in large scale engineering problems like chemical reaction systems with transport. The most common splitting schemes are the Lie-Trotter splitting of order one and the Strang splitting [1, 2] of order two. However, in [3, 4, 5] it is shown that the Strang splitting suffers from order reduction in the stiff case. Therefore, practical estimation of the splitting error might fail, and the possible step size of the splitting method is prohibitive for the numerical computation of many problems. The Richardson extrapolation (in general [6, 7, 8], for splitting methods [9, 10, 11]) of the Lie-Trotter splitting is a second order scheme. In this paper we show that the Richardson extrapolation does not suffer from order reduction if all stiffness is related to the chemical source term. Furthermore, we examine stability of the extrapolated splitting scheme.

In the following we consider the application of the splitting schemes to chemical reaction systems with transport, which results in nonlinear differential equations. The corresponding differential equation is a partial differential equation, but after discretization in space we obtain an ordinary differential equation

$$\frac{\mathrm{d}z}{\mathrm{d}t} = f(z) + g(z), \qquad z(t_0) \text{ is given}. \tag{1.1}$$