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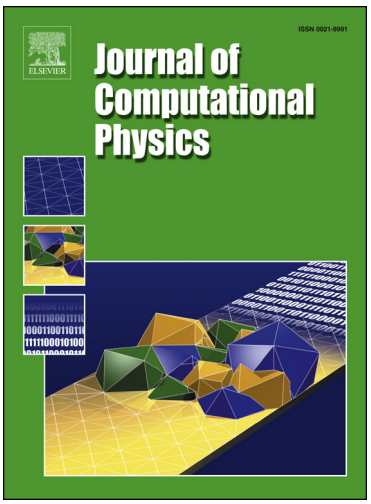

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High Order Methods for the Integration of the Bateman Equations and Other Problems of the Form of $y' = F(y,t)y$

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Abstract

This paper introduces two families of A-stable algorithms for the integration of $y' = F(y,t)y$: the extended predictor-corrector (EPC) and the exponential-linear (EL) methods. The structure of the algorithm families are described, and the method of derivation of the coefficients presented. The new algorithms are then tested on a simple deterministic problem and a Monte Carlo isotopic evolution problem.

The EPC family is shown to be only second order for systems of ODEs. However, the EPC-RK45 algorithm had the highest accuracy on the Monte Carlo test, requiring at least a factor of 2 fewer function evaluations to achieve a given accuracy than a second order predictor-corrector method (center extrapolation / center midpoint method) with regards to Gd-157 concentration.

Members of the EL family can be derived to at least fourth order. The EL3 and the EL4 algorithms presented are shown to be third and fourth order respectively on the systems of ODE test. In the Monte Carlo test, these methods did not overtake the accuracy of EPC methods before statistical uncertainty dominated the error.

The statistical properties of the algorithms were also analyzed during the Monte Carlo problem. The new methods are shown to yield smaller standard deviations on final quantities as compared to the reference predictor-corrector method, by up to a factor of 1.4.

Keywords: Depletion, Bateman equations, Burnup calculations, Predictor-corrector, Exponential-linear

1. Introduction

In the study of nuclear reactors, it is often useful to know how the composition of fuel develops throughout the life of the reactor. This process as a whole is known as depletion. This evolution with time is governed by the Bateman equations [1]. In its most simple form, the Bateman equations can be written as $y' = F(y,t)y$, where y is a vector of nuclide quantities, and F is a matrix representing decay and reaction rates.

The function F can be calculated in a few ways, but the two main categories of interest are deterministic and stochastic methods. Deterministic solutions can be extremely quick, depending on how one approximates the physics. Conversely, a typical Monte Carlo function evaluation makes no approximations, but can take many hundreds of thousands of CPU hours to evaluate. Thus, when F is evaluated with Monte Carlo, the cost to integrate y in time is almost entirely due to the number of function evaluations.

This conflicts with the main difficulty in solving the Bateman equations. The equations are incredibly stiff. While the average engineering problem considers time scales of months, the eigenvalues of F can have values on the order of -10^{21} s^{-1} [2]. Section 2 of this paper focuses on how current methods solve this problem. The predictor and predictor-corrector family of methods are introduced, as well as the matrix exponent these algorithms rely on.

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