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Journal of Computational and Applied Mathematics 183 (2005) 245–258

JOURNAL OF
COMPUTATIONAL AND
APPLIED MATHEMATICS

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A MATLAB implementation of upwind finite differences and adaptive grids in the method of lines

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Received 20 May 2004; received in revised form 6 September 2004

Abstract

In this paper, we report on the development of a MATLAB library for the solution of partial differential equation systems following the method of lines. In particular, we focus attention on upwind finite difference schemes and grid adaptivity, i.e., grid movement or grid refinement. Several algorithms are presented and their performance is demonstrated with illustrative examples including a fixed-bed reactor with periodic flow reversal, a model of flame propagation, and the Korteweg–de Vries equation.

MSC: 65M20; 65M06; 65M50

Keywords: Partial differential equations; Grid refinement; Moving grid; Catalytic combustion; Flame propagation; Korteweg–de Vries equation

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1. Introduction

Computational modeling is now routinely applied in various disciplines of science and engineering. As the systems under consideration are often characterized by several independent variables, e.g., space and time, they are described by sets of, generally nonlinear, partial differential equations (PDEs). One

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doi:10.1016/j.cam.2004.12.030

of the most popular approaches to the numerical solution of PDE models is the method of lines (MOL), which proceeds in two separate steps:

- approximation of the spatial derivatives using finite difference, finite element or finite volume techniques;
- time integration of the resulting semi-discrete (discrete in space, but continuous in time) equations using an appropriate solver.

The success of the MOL stems from its simplicity of implementation and the availability of high-quality time integrators for solving a wide range of problems, including ordinary differential equations (ODEs), and mixed systems of algebraic and ordinary differential equations (AEs and ODEs forming a system of differential-algebraic equations (DAEs)).

Several general-purpose FORTRAN libraries, e.g., NAG [1,8] or DSS/2 [12], can be used to develop codes following the MOL approach. Recently, several MATLAB-based libraries have also been proposed for the solution of ODE/DAE systems [13] and for the solution of PDE systems using spectral methods [18,14]. MATLAB is now widely available in industry and academia and provides a very convenient basis for the development of MOL tools, allowing compact vector/matrix operations, and requiring minimum programming expertise.

In a recent paper [16], the authors report on the development of a collection of MATLAB routines (called MATMOL) implementing various finite difference schemes (FDs) and flux limiters, as well as a discussion of some preliminary results concerning the implementation of a grid refinement strategy. The present paper elaborates on these preliminary results and focuses attention on the following techniques applied to PDE problems with solutions displaying moving fronts (e.g., moving fronts of temperature and concentration, water waves):

- upwind finite difference schemes for the solution of convection–diffusion–reaction problems, with application to a catalytic fixed-bed reactor operated with periodic flow reversal;
- a dynamic grid adaptation strategy based on the equidistribution principle and ideas borrowed from [17,2], with application to a flame propagation problem and Korteweg–de Vries equation;
- a more elaborate version of our static grid refinement strategy, with application to the same two standard problems.

This paper is organized as follows. The next section briefly introduces the MOL strategy and the development of MATLAB routines for spatial discretization. Section 3 presents upwind finite difference schemes and their application to a catalytic combustion problem [4]. In Section 4, the MATLAB implementation of a moving grid algorithm, similar in spirit to the FORTRAN code MOVGRD [17,2], is discussed. The algorithm is then applied to two standard PDE problems, i.e., Dwyer and Sanders' flame propagation problem [3], and the classical Korteweg–de Vries equation [7]. Section 5 presents the MATLAB implementation of a static grid refinement algorithm, based on the FORTRAN code AGEREG [10], and its application to the two standard PDE problems considered in the previous section. Finally, Section 6 draws some conclusions.

2. A MATLAB-based method of lines library

Consider the PDE problem

$$x_t = f(z, t, x, x_z, x_{zz}, x_{zzz}, \ldots), \quad z \in \Omega, \quad t \geqslant 0, \tag{1}$$