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Efficient time integrators in the numerical method of lines

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Abstract

The numerical method of lines has long been acknowledged as a very powerful approach to the numerical solution of time dependent partial differential equations. This method, in its original form, involved making a simple approximation to the space derivatives, and by so doing reducing the problem to that of solving a system of initial value ordinary differential equations, and then using a “black box” package as the time integrator. However in the past twenty years or so, moving mesh algorithms in space have been developed and this allows much more challenging problems (for example those with moving fronts) to be solved efficiently and reliably. Regridding of the space variables poses special problems for the time integrator since sufficient back information to allow multistep formulae to run at high order is not available immediately after the regridding has been performed . In this paper we survey some of the options available for the time integration when using a moving grid method of lines code. In particular we derive ‘Runge–Kutta starters’ for use after grid adaptation has been carried out and we show how a considerable saving in computational effort can be made if just a few spatial points are moved during each regridding.

MSC: 65L05; 65N06; 65N12; 65N22

Keywords: Time dependent PDEs; Method of lines; Runge–Kutta formulae; Static and dynamic regridding; Moving mesh algorithms

1. Introduction

The method of lines (MOL) is a well known technique for the numerical solution of time dependent partial differential equations. A typical MOL approach can be regarded as consisting of two distinct parts.

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Given a partial differential equation of the form

$$\partial u/\partial t = f(u), \tag{1.1}$$

where u is a vector of dependent variables, f is a spatial differential operator and t is time, the first step of the MOL approach is to approximate the spatial derivatives e.g. terms such as $\partial u/\partial x$ and $\partial^2 u/\partial x^2$ typically using either finite differences or finite elements. This produces a system of ordinary differential equations of the general form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = g(u, t) \tag{1.2}$$

and this time dependent initial value problem can be solved using a standard integrator. Indeed one of the main reasons for the popularity of the MOL approach is the availability of powerful 'off the shelf' integrators for solving (1.2).

In its original form, the MOL approach typically involved first fixing the grid in the spatial variable, then approximating the spatial derivatives, and finally solving the resulting system of time dependent ODEs. In this approach, the mesh on which the spatial derivatives are approximated is never changed. However for very difficult problems, such as those with steep moving fronts for example, many grid points in space will be required to properly resolve the complex spatial behaviour. If, as a typical example, we consider a shock wave arising in incompressible flow then, if a fixed mesh spacing is used, a very fine spatial grid is required over the whole spatial domain in order to capture and resolve the high spatial gradient. Outside of the regions of high spatial activity a large number of nodes will be wasted since a fine mesh is not required in regions where the solution is relatively smooth. In many ways this problem is reminiscent of early attempts to solve stiff systems of initial value problems using a non-stiff integrator. Clearly what we would ideally want to do in our MOL algorithm is to use a fine spatial mesh in regions where there is a large spatial gradient and to use a coarse mesh elsewhere.

The development of algorithms which employ spatial regridding and the consequent emergence of MOL codes which use a non-uniform grid in space, has presented some serious additional problems to the codes which perform the time integration. Typically a user may wish to use a multistep method for the time integration since these are amongst the most efficient algorithms currently available. However after a space regridding has been performed, there is the difficulty that there may not be enough past solution values available to run the code at high order using a multistep method. One option is to re-start the time integrator at order one so that no past values are required. However we reject this approach since in general it has proved to be very inefficient. It is this restarting problem for the time integrator after a mesh spacing has been performed which will mainly concern us in this paper. In Hyman et al. [17] this procedure of restarting with a multistep formula is termed a warm restart. They achieve this by interpolating the history array of the code DASSL to get the past values that are needed by the multistep code. They also show by means of examples that a warm restart can give great efficiency. In this paper we consider the problem of obtaining a warm restart by using classes of integration formula which require no additional back values of the solution so that no interpolation is needed. The possible disadvantages of performing frequent interpolation are discussed in [17]. We will not be concerned at all with algorithms for the spatial grid adaptation (the reader is referred to [20] and the many references contained in this book for a description of this). Instead we will analyse classes of methods already available for the efficient integration of general stiff initial value problems and see which of these can be suitably modified so that