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A geometrically based grid refinement technique for multiphase flows

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ABSTRACT

An adaptive mesh refinement technique developed for the solution of scalar problems is extended to the simulation of two-phase flow problems, as a means of reducing the computational runtime associated with such problems. The methodology, involving the adaptive partition of the domain into uniformly discretised regions, is extended to systems of equations without increase in algorithmic complexity. By application first to the simpler case of the Euler equations of gas dynamics, the technique is shown to handle shocks without loss of accuracy and to result in significant CPU runtime reductions of over 90%. Application to more complex two-phase flow problems, including the flashing flow during the decompression of a pipeline, also show dramatic increase in computational performance.

1. Introduction

The prediction and simulation of problems involving compressible two-phase flows with phase transition is necessary in a number of industrial applications. Examples include study of cavitation in automotive fuel systems (Martynov et al., 2006), flash boiling of water during loss-of-coolant accidents in nuclear reactors (Nigmatulin and Soplenkov, 1994) and liquid boiling and expansion in refrigeration systems and heat pumps (Simões-Moreira and Bullard, 2003). In the particular context of Carbon Capture and Storage, the focus of such models has been on the flows resulting from pipeline decompression and failure (Brown et al., 2013b; Mahgerefteh et al., 2012; Munkejord et al., 2010).

For the simulation of such flows it is essential to incorporate a rigorous Equation of State (EoS) to accurately predict the thermodynamic properties and phase equilibria. However, the use of such an EoS in the context of a computational model necessarily incurs a significant computational overhead which, even when the simplifying assumption of one-dimensional flow is made, makes the simulation of large domains and long time scales impractical. Efforts to reduce the impact of this computational weight commonly focus on reducing the cost of evaluating the EoS itself, either by approximation of the thermodynamic model through interpolants (Swesty, 1996; Mahgerefteh and Abbasi, 2007) or more recently using Differential Algebra (Re et al., 2014). In cases where only a single component is of interest, as in the case of CO_2 (Wareing et al., 2012), simplified EoS have also been introduced.

As the number of evaluations of the EoS required is proportional to the discretisation used in a simulation, further reductions in runtime may be made by reducing the overall number of computational cells used while retaining accuracy where required. Hence, to complement the modelling strategies described above, the use of Adaptive Mesh Refinement (AMR) techniques represents another possible tool for further efficiency. The application of AMR for CFD is widespread (Pelanti and LeVeque, 2006; Gourma et al., 2013; Brown et al., 2014), with various methodologies applied ranging from the popular hierarchical box-structured techniques, first described by Berger and Oliger (1984), to moving grid methods (see for example Tang and Tang, 2003; Kelling et al., 2014). The former begin with an underlying coarse grid and proceed to identify and refine areas to a predefined level where required; though successful, the hierarchical approach requires the implementation of complex data structures (Berger, 1991) and a means for dealing with the artificial internal boundaries at the refined regions (Berger and Oliger, 1984; Berger and Le Veque, 1998). While not requiring such complex data structures, the moving grid technique has the drawback of requiring the solution of an additional equation.

As an alternative, a piecewise-uniform adaptive grid (PAG) method was developed by Fraga and Morris (1996). This technique, originally developed for the capture of soliton waves in dispersive equations, employs a single, piecewise uniform grid in which the spatial discretisation and time stepping algorithm are wholly decoupled. Importantly however, this method has only been applied to scalar problems without shocks.

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The aim of this paper is twofold: firstly, to extend the PAG method to systems of equations and to test the methodology in the presence of shock waves; secondly, to apply the technique to two-phase flows where a rigorous EoS is applied to quantify the increase in efficiency gained in problems of industrial interest.

The work proceeds as follows: Section 2 presents the PAG method and its adaptation to systems of equations. Section 3 presents the mathematical model for one-dimensional fluid flow, while Section 4 describes the numerical solution technique employed in this work, the AUSM+-up scheme (Liou et al., 2008).

Section 5 shows the verification of the PAG method in two shocktube test problems, the classical Sod's problem (1978) and a problem suggested by Toro (2009). Following this, the PAG method is applied to a transient two-phase problem to demonstrate its capability in capturing the pertinent flow phenomena including phase change and shock wave propagation. CO_2 is chosen as the working fluid given its extensive use as a refrigerant and its role in Carbon Capture and Sequestration (CCS). In each case, the impact of the use of the PAG method on the CPU runtime is reported. Conclusions are drawn in Section 6.

2. The piecewise-uniform adaptive grid (PAG) method

The PAG method (Fraga and Morris, 1992, 1996) is based on identifying regions of the spatial domain that require refinement through the analysis of the geometry of the solution profile. The original application domain was the solution of *soliton*-generating (Zabusky and Kruskal, 1965) nonlinear dispersive wave equations. The geometric analysis was used to identify the locations of solitons, based on the assumption that the critical regions of the spatial domain were those where the solitons were present. No other criteria, such as *a posteriori* error estimation, were used in defining the adapted grid.

An important property of the grid generated by this method is that the points are distributed in a *piecewise-uniform* fashion. This was motivated by the observation that many numerical methods, both for discretisation in the spatial dimension and for time-stepping, have been developed with an implicit assumption of uniformity in the grid spacing. When non-uniformity is present, these methods often suffer losses in accuracy, typically losing one order of accuracy, and become more susceptible to stability issues (Russell and Christiansen, 1978). It was found that if non-uniformity in the adapted grid were present in regions that were not critical, i.e. those where a coarser grid was appropriate, problems with accuracy and stability were minimised. Hence, the PAG method was constructed to generate a nonuniform grid which consists of a set of contiguous non-overlapping uniform sub-meshes, without the use of artificial internal boundary conditions.

The basic approach of the PAG method can be summarised as follows: locate each soliton in the solution, place a fine mesh, with uniform spacing h_{goal}, so as to cover the support for each soliton and fill in the gaps between each fine mesh with more coarsely spaced points. Each sub-interval, be it the support for a soliton or a gap between two solitons, is discretised uniformly. However, any numerical method used will work on the whole mesh at once, considering it to be a nonuniform mesh overall.

In the original implementation (Fraga and Morris, 1996), it was noted that it was not necessary to use the solution values alone to identify regions of uniformity. Instead, an approximation to the first derivative of the solution profile, using a simple first-order finite difference approximation, could be used to locate regions of large change in the spatial dimension, such as shocks. The PAG construction could be applied to the first derivative of the solution with no change in the underlying algorithm. This suggested improvement was considered in the simulation of a fixed bed system (Fraga, 1998) and is used as the basis for application below.

Algorithm 1. Extension of PAG algorithm (Fraga and Morris, 1996) for adaptive grid generation with multiple dependent variables

Given: Profile for each of m indicator variables $\mathbf{I}_i$ at positions x_i, $i = 1, \ldots, n$
Returns: Adapted grid suitable for all dependent variables.

for $j \leftarrow 1$ to m **do**
  $I_{\min} \leftarrow \min_i(I_i^j)$
  $I_{\max} \leftarrow \max_i(I_i^j)$
  $\text{cutoff}_j \leftarrow I_{\min} + \frac{I_{\max} - I_{\min}}{S_{\min}}$
end for
$S = \emptyset$ {Initially empty combined interval list}
for $i \leftarrow 1$ to n **do**
  if not *in_soliton* **then**
    if $\text{any}_j(I_i^j > \text{cutoff}_j)$ **then**
      in_soliton $\leftarrow$ *true*
      start_of_interval $\leftarrow x_i$
    end if
  else
    if $\text{all}_j(I_i^j < \text{cutoff}_j)$ **then**
      in_soliton $\leftarrow$ *false*
      end_of_interval $\leftarrow x_i$
      $S \leftarrow$ *insert*([*start_of_interval*, *end_of_interval*])
    end if
  end if
end for
generate new grid based on intervals of refinement S

The PAG method has only ever been used for single equations. Application to problems with multiple dependent variables, such as the problems described below, requires extending the PAG algorithm to base the adaptive grid generation on multiple solution profiles simultaneously. The extended algorithm is described in Algorithm 1. The solution profile for each indicator variable is analysed simultaneously using the base PAG procedure for identifying regions of refinement. The resulting grid will possibly have more points than required at any given spatial location for a given dependent variable but there will be at least one variable that requires that level of refinement. Having a single adapted grid for all dependent variables makes the implementation of a numerical procedure easier.

3. Model formulation

3.1. Fluid dynamics

The governing equations for one-dimensional single-fluid flow are based on the Euler equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} = 0, \tag{1}$$

where

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix}, \quad \mathbf{F}(\mathbf{U}) = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u H \end{pmatrix}.$$

and where u and ρ are the velocity and density respectively. P is the system pressure, E and H represent the specific total mixture energy and total enthalpy respectively, defined as:

$$E = e + \frac{1}{2}u^2 \tag{2}$$

$$H = E + \frac{P}{\rho}, \tag{3}$$

where e is the specific internal energy.