ON THE USE OF ADAPTIVE MOVING GRID METHODS IN COMBUSTION PROBLEMS °

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1. INTRODUCTION

The numerical solution of combustion problems arising from situations of industrial or theoretical interest has received an increasing attention in the past ten years. Accurately computing these combustion phenomena is an exciting challenge for numerical analysts because of the nonlinear coupling of various physical effects (a complex set of chemical reactions, heat and mass transfer, compressible turbulent flows, two-phase flows...) and also because of the stiffness of the corresponding mathematical models. Many of the numerical difficulties are due to the above physical effects acting on very disparate time and length scales.

This stiffness even exists in the simplest problem of combustion theory: the propagation of a premixed planar flame with a single one-step chemical reaction. Three different length scales are identified in this problem (see Fig. 5): the thickness of the reaction zone inside the flame, the thickness of the flame itself (i.e. of the region of sharp gradients), and the size of the domain in which the flame propagates. In addition to the presence of these disparate scales and sharp gradients concentrated in the thin flame region, the speed at which a flame front propagates and the overall burning rate of a gaseous mixture depend upon the inner structure of the thin flame and reaction regions. This is in contrast with a purely hydrodynamical shock wave, whose speed is solely influenced by the flow conditions outside the shock. It is therefore necessary, in a flame propagation problem, to *accurately solve the small length scales within the inner structure of the moving fronts*.

This can be accomplished by using computational grids whose nodes are highly *nonuniformly distributed in space*. A small mesh spacing is imposed inside the flame thickness and a coarse grid is used outside the flame, where the variables are almost constant. The irregular grid allows us to accurately resolve the sharp gradients in the problem while avoiding wasting computer time by overresolving the smooth solution regions. Comparisons between adaptive flame computations and similar simulations on uniform grids are very conclusive (see [29]), and the advantages of using adaptive mesh procedures for combustion problems are now widely recognized.

Many of the adaptive mesh procedures adjust or rezone the grid to improve the resolution of the solution and the approximation of the partial differential equations (PDEs) *at a fixed time*. This *static rezone* procedure is repeated during the calculation (sometimes as often as every time step) to insure an accurate resolution as the

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solution changes. But these adaptive static rezone methods may not be sufficient for the solution of unsteady combustion problems. In this paper we present the advantages resulting from *adaptively and continually moving the grid points* in time during the computation. These moving mesh or *dynamic rezone* methods can greatly improve the accuracy and efficiency of numerical simulations of combustion phenomena.

In Section 2 we present different reasons which lead to use an adaptive moving grid for the solution of systems of evolutionary PDEs developing sharp gradients. We then briefly describe in Section 3 several dynamic rezone methods, and illustrate the efficiency of some of these techniques for the solution of flame propagation problems in Section 4.

2. THE ADVANTAGES OF ADAPTIVELY MOVING THE NODES

2.1 The structure of a typical adaptive computer code for the solution of time-dependent PDEs is shown in Fig. 1 (see [14],[16],[19]): the semi-discrete PDE approximation is written in the form $U_t = F(U)$, where F is a nonlinear difference operator. The computational grid X is adapted to the variable profiles in two different ways:

- * a dynamic rezone is performed at every time step to define moving mesh equations for the node locations.
- * a static rezone procedure is used at some time levels during the computation, to redistribute the nodes and better resolve the solution. The total number of mesh points may change in this procedure.

2.2 Static rezone algorithms are often used without dynamically rezoning. For the solution of combustion problems, this can introduce stiffness and numerical instabilities. Consider the case of a moving front or discontinuity, and assume that the grid points locations are frozen between consecutive time levels (no dynamic rezone). If the front moves several mesh points per timestep, then the values of the variables at those points which are crossed by the front exhibit a very rapid variation in time (see Fig. 2). Since the time truncation error of the numerical method is proportional to $\Delta t^p \left| \frac{\partial^p U}{\partial t^p} \right|$ when a time integration scheme of order p is used, very rapid variations of the unknowns at some nodes result in large numerical errors. It is therefore necessary to use much smaller time steps, so that the front does not move more than one mesh point per time step. This need for small time steps is only related to accuracy considerations, and is true even for unconditionally stable implicit integration methods. Moreover, the problem is aggravated since the grid points are closer together near the front because of the local high spatial gradients.

This difficulty can be overcome by using local time steps (see [4],[5],[27]), or using a dynamic rezone algorithm to move the mesh points with the front so that their position remain near optimal. Then the front is less likely to cross the moving nodes and larger time steps can be taken (see Fig. 3). Thus static rezone methods may be inefficient when used alone. The dynamic rezone methods can overcome the inefficiencies by reducing the time variation of the solution at the moving mesh points to lower the numerical truncation errors.

Furthermore adaptively moving the nodes can also reduce the number of static rezones: since the grid is continually adapted to the solution, the mesh points need to be redistributed less often. This may also reduce numerical errors since each static rezone introduces an interpolation error when the solution is interpolated from the old mesh to the new one, and these errors are often greater than the integration errors between two static rezones. Moreover these interpolations can be costly if done accurately and conservatively (see [15]).

2.3 The dynamic rezone methods have specific advantages when implicit time integration schemes are used. Implicit methods are often used in numerical combustion, both because of the disparity of the time scales involved in complex chemical mechanisms (see [18]), and because of the very subsonic velocity of the gas flows in flame propagation problems (see [11],[24]).

At each time step when using an implicit method we must solve a non linear algebraic system. This is usually done with an iterative method relying on the Jacobian J of the discrete PDEs system (e.g. Newton's method). The reduced time variation of the solution, resulting from adaptively moving the nodes, makes this discrete system easier to solve. In particular, if the solution slowly varies with time, it is easy to find a good starting guess for the iterative method.

A more interesting potential of dynamic rezoning for implicit methods is related to the computation of the Jacobian matrix J . In combustion problems, this Jacobian can be written as the sum of two terms: $J = J_c + J_t$, where J_c represents the Jacobian of the chemical source terms, and J_t denotes the Jacobian of the diffusive and convective transport terms. The matrix J_c depends non linearly on the mass fraction variables and on the temperature at the mesh points. Since it is expensive to compute, J_c is used for many time steps once evaluated, and is recomputed only when the solution has changed so much that the iterative method converges unbearably slowly. A moving mesh method which reduces the variation of the solution values will also reduce the variation of the Jacobian J_c , and require us to reevaluate it much less often while preserving an acceptable convergence of the Newton's method, thus saving computer time.

The other part J_t of the Jacobian depends on the mesh spacings, which are modified by the dynamic rezoning; but this matrix is cheaper to compute than J_c and can be updated more often. When using dynamic rezone algorithms in which the nodes velocities smoothly vary in space, as the ones presented in [16] or in Section 3.4, the Jacobian J_t also slowly varies.

3. A BRIEF OVERVIEW OF SOME MOVING MESH METHODS

The literature on dynamic rezone methods is filled with approaches based on different view points. At every time step, the nodes velocities can be defined

- * to reduce the global truncation error (in time and in space) of the discrete approximation (see [9],[16],[22],[23]),
- * or to lower only one of these errors, the time truncation error (or the time variation of the solution; see [14],[16]) or the spatial error (see [16]),

* or in some specific cases (such as for hyperbolic systems of conservation laws or unsteady flame propagation problems; see [12],[17],[20]) the mesh points velocities are determined so that the mesh follows some identified structure of the solution (for instance shock waves or flame fronts).

In this section we give a brief overview of several of these methods which can be of interest for combustion problems. We refer the reader to the bibliography for more details.

3.1. The moving finite element method

The moving finite element method (see [9],[22],[23]) is among the most popular of the available dynamic rezone methods, because of its well-established mathematical basis: the derivation of the nodes velocities relies on the variational formulation used in the finite-element method and introduces the mesh velocities in order to globally minimize some norm of the error. This method has proved to be efficient for several stiff one-dimensional and some two-dimensional problems (including a flame propagation problem; see [9]). Nevertheless this method tightly couples the mesh equations to the solution equations, increasing the size of the algebraic system to be solved implicitly at every time step (the time integration is necessarily implicit since one has to use the constant non diagonal mass matrix of the finite-element approximation). Moreover, some "ad hoc" terms or penalty functions must be added to the nodes velocities based on the variational arguments, in order to avoid the distortion of the grid.

3.2. The time-variation method

This method is based on the arguments presented in Section 2.2. When a moving mesh is used, the semi-discrete system of differential equations to be integrated in time becomes:

$$\frac{dU}{dt} = F(U) + U_x X_t, \quad \frac{dX}{dt} = X_t,$$

instead of $U_t = F(U)$ alone. In these equations, $U(t)$ is the vector whose components $U_i(t)$ are the values of the numerical solution at the moving nodes $X_i(t)$, and X_t is the vector of the nodes velocities, determined by the dynamic rezone algorithm (the notation $\dot{X}$ will also be used). For sake of simplicity, we restrict ourselves to the case of a single PDE in a one-dimensional geometry; the method can be easily extended to the case of systems in higher spatial dimensions (see [14],[16]).

Straightforwardly applying the ideas of Section 2.2, we may think of defining the nodes velocities by minimizing the time variation of the solution U . The problem $\text{Min}_{X_t} |F(U) + U_x X_t|^2$ is easily solved to give $X_t = -\frac{F(U)}{U_x}$ and $U_t = 0$. Even if $U_x \neq 0$, we are left with a difficulty similar to the initial one: instead of solving the solution equations on a fixed mesh, we are solving the mesh equations at constant solution. We have traded one set of problems (integrating the solution) for an equally difficult set (integrating the mesh).

The errors in the solution and mesh equations can be balanced by minimizing

the time variations of both variables U and X . To be more specific, we define the grid points velocities as the solution of $\text{Min}_{X_i} |F(U) + U_x X_i|^2 + \gamma |X_i|^2$ where γ is a positive scaling parameter. This minimization problem is again quadratic in X_i and yields:

$$\frac{dU_i}{dt} = -\frac{\gamma F_i(U)}{\gamma + U_x(X_i)^2}, \quad \frac{dX_i}{dt} = -\frac{F_i(U) U_x(X_i)}{\gamma + U_x(X_i)^2}.$$

This method has been successfully used for solving systems of PDEs developing sharp gradients (see [14],[16] for more details). It has the advantages that the solution and the mesh equations are not necessarily coupled (also see [26]). A penalty function may also need to be added to reduce the grid distortion.

3.3. The "equidistributing mesh approach"

In this third algorithm, the grid points will be moved in order to *improve their spatial distribution* and therefore reduce the spatial truncation errors.

This approach relies on the concept of "mesh function": a mesh function m is a performance index which locally measures how well the solution is represented and also how well the spatial differential operators in the PDEs are approximated on a given grid. Such mesh functions are usually used in static rezoning methods for defining a new adapted grid. They can be based for example on local truncation errors (see [20],[23],[28]) or on the arc length or curvature of the solution (see [7],[8],[18],[21],[29]).

Once a mesh function m is defined, an optimal grid is a grid which minimizes $|m|$ for a given norm $|| \cdot ||$. This often amounts to equidistributing the mesh function, i.e. to seek for a mesh which satisfies $m_{i+1/2} = \text{Constant}$ for all node index i . With this in mind, we derive mesh points velocities which guide the grid towards an equidistributing mesh, by requiring at each time step:

$$\frac{d}{dt} m_{i+1/2} = -\frac{1}{\tau} (m_{i+1/2} - \bar{m}). \quad (1)$$

In this equation, $\bar{m}$ is an average value of the mesh function, and τ is the time scale over which the mesh relaxes towards an equidistributing mesh (this time scale is to be defined from the physical time scales involved in the system of PDEs; see [1],[16] for more details about the choice of the grid relaxation time τ). Several ways of deriving from (1) an explicit expression of the nodes velocities $\dot{X}$ are presented in [16]; for instance, one can evaluate the mesh points velocities from the following positive definite symmetric tridiagonal linear system:

$$m_{i+1/2} \frac{\Delta \dot{X}_{i+1/2}}{\Delta X_{i+1/2}} - m_{i-1/2} \frac{\Delta \dot{X}_{i-1/2}}{\Delta X_{i-1/2}} = -\frac{1}{\tau} (m_{i+1/2} - m_{i-1/2}), \quad (2)$$

(the velocities of the first and last nodes being prescribed a priori).

This equidistributing mesh approach has been an efficient method on our one-dimensional test problems (see [16]). Some care of the mesh distortion must also be taken. The method can be generalized to two-dimensional problems using the ideas in [13].

REMARK: The time variation and the equidistributing mesh approaches can be combined in order to define nodes velocities which take care of both time and space errors (see [16]).

3.4. A method for free flame propagation problems

We end this section by presenting a dynamic rezone method which is particularly appropriate for simulating the free propagation of a flame in an "infinite" duct - a basic problem of combustion theory.

Consider the simple test problem of a planar flame freely propagating in a channel. Assuming (to simplify the presentation of the method) a single one-step chemical reaction and a Lewis number equal to unity, we can describe the phenomenon with the following reaction-diffusion equation (in normalized form; see [20],[25]):

$$T_t - T_{xx} = \Omega(T) = \frac{\beta^2}{2} (1-T) \exp\left(-\frac{\beta(1-T)}{1-\alpha(1-T)}\right), \quad (3)$$

with the boundary conditions:

$$T(-\infty) = 0, \quad T(+\infty) = 1. \quad (4)$$

In these equations, T is a reduced temperature variable and Ω is the normalized chemical reaction rate (β and α are nondimensionalized parameters). It is well known that the solution of (3)-(4) develops sharp gradients and converges to a traveling wave moving with a constant speed towards the cold mixture (towards negative x). If this problem is solved in a fixed computational domain $[X_1, X_N]$, the region of sharp gradients continually moves towards the left boundary X_1 of the domain, which makes necessary either to use a very efficient dynamic rezoning algorithm, or to continually perform static rezones. Moreover, one runs the risk that the flame leaves the computational domain before the end of the calculation. This can be avoided by taking advantage of the fact that the problem (3)-(4) is posed in an infinite domain and moving all the nodes with the same speed towards the left at each time. Equation (3) then becomes:

$$T_t - T_{xx} = \Omega(T) + V(t)T_x, \quad (5)$$

where $V(t)$ is the time-dependent velocity of all the nodes at time t . The best choice for $V(t)$ is given by (see [20]):

$$V(t) = - \int_{X_1}^{X_N} \Omega(x,t) dx. \quad (6)$$

which is the average physical instantaneous flame speed at time t . The effect of the additional convective term $V(t)T_x$ in (5) is to keep the flame inside the domain and to allow the convergence of the solution to a steady state. During the simulation, the flame will be deformed but will stay at the same place in the computational domain.

This moving node technique is very appropriate for flame propagation problems and has been successfully used for many one- or two-dimensional combustion problems, including flame extinction and instabilities (see [2],[3],[10]). It is inexpensive

and easy to use since only one velocity is to be evaluated at each time step, and dynamic grid distortion is not a concern. Of course, since all the nodes move with the same speed, this method should be combined with static rezone or other dynamic rezone algorithms.

4. NUMERICAL EXAMPLE

In this section, we solve the test problem (3)-(4) for $\beta = 10$ and $\alpha = 0.8$. We use a dynamic rezone algorithm combining the methods presented in Sections 3.3 and 3.4 above. More precisely, the nodes velocities take the form:

$$\frac{dX_i}{dt} = V(t) + V_i(t) \text{ for } i = 1, 2, \dots, N ;$$

in this expression, $V(t)$ is the average flame speed given by (6), and $V_i(\cdot)$ is the i^{th} node velocity evaluated from the linear system (2), with $V_1(t) = V_N(t) = 0$. The grid relaxation time τ is simply equal to the time scale used to nondimensionalize the governing equation (3) (the flame transit time), i.e. $\tau = 1$, and the mesh function m is identical to the one used in [19],[20].

We use the classical initial temperature profile (see [20],[25]):

$$T(x,0) = \begin{cases} e^x & \text{if } x \leq 0 , \\ 1 & \text{if } x \geq 0 . \end{cases}$$

The calculation is performed with 30 moving mesh points. In order to show the efficiency of the dynamic rezone algorithm, the 30 nodes are initially equally spaced in the interval $[-10,10]$, and no static rezone is used. An explicit time integration scheme is used (see [19],[20] for more details).

The initial temperature and reaction rate profiles are presented in Fig. 4. Figure 5 shows the steady temperature and reaction rate profiles, at time $t = 4.5$, in the computational domain $[-4.22,15.78]$. The stars on the solution plots indicate the 30 mesh points used in the calculation. It clearly appears that the thin flame and reaction zones are finely resolved, and the relative error on the steady flame propagation speed $V(+\infty)$ is less than 3.10^{-3} . The trajectories of the 30 moving nodes are presented in Fig. 6, while Fig. 7 shows the trajectories of the mesh points in the moving reference frame [i.e. the curves $\frac{dX_i}{dt} = V_i(t)$]. It can be observed that the moving mesh tends to a steady state in the moving reference frame ($V_i(+\infty) \rightarrow 0$ for all i), and the steady grid is an equidistributing mesh for the steady solution.

5. CONCLUSION

We have presented the reasons and advantages of adaptively moving the mesh points for the solution of time-dependent PDEs systems developing sharp gradients, and more specifically for combustion problems. Several available adaptive dynamic rezone methods have been briefly reviewed, and the effectiveness of these algorithms for combustion problems has been illustrated by the numerical solution of a simple flame propagation problem.

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Figure 1: Structure of an adaptive computer code for solving systems of PDEs.

Figure 2: The front will cross several mesh points per time step on a fixed grid unless small time steps are taken. This introduces large errors into the solution.

Figure 3: Larger time steps can be taken if the mesh moves with the front. The time variation of U and X is small compared with that of Fig. 2.

Figure 4: Temperature and reaction rate profiles at time $t = 0$.

Figure 5: Steady-state temperature and reaction rate profiles.

Figure 6: Trajectories of the moving mesh points for $t \leq 4.5$.

Figure 7: Trajectories of the moving mesh points in the moving reference frame for $t \leq 4.5$.