Explicit Time-Scale Splitting Algorithm for Stiff ODE's

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Introduction

Much attention is recently devoted for the inclusion of detailed chemical kinetic mechanisms in the simulation of problems in the fields of combustion, hypersonic flows, and pollutant control. However, the largely separated time scales introduced by detailed chemistry make the set of governing equations stiff and their numerical solution prohibitively expensive.

The most successful attempts to cope with stiffness have been so far based on implicit schemes. Such a scheme is the family of multi-step, variable order, variable integration step implicit method due to Gear [1], which is among the most widely used technique to solve stiff ordinary differential equations (ODEs). Reacting flows in the hypersonic regime, reactive mixing layers, detonations and non equilibrium nozzle flows, are modeled by systems of partial differential equations (PDEs), and are frequently solved by a local implicit treatment of the stiff source terms according to the *method of lines* and the *time-step splitting* approach. Pre-conditioning techniques are also used to solve steady-state problems efficiently.

The implicit treatment of the stiff terms provides solutions which are accurate at the slow scales and stable at the fast scales. However, a significant fraction of the total computational time is devoted for the solution of the resulting non-linear systems of algebraic equations, the dimension of which is proportional to the number of chemical species in the detailed mechanism. This is the reason why the relatively limited effort required to deal with simple kinetic mechanisms, such as the one which describes air dissociation in the hypersonic regime, grows dramatically in the modeling of combustion of complex hydro-carbon mixtures.

In contrast, explicit schemes are simpler to implement, provide solutions of high- order accuracy at all scales and do not require the solution of algebraic systems at each time step. However, their stability requirements force the maximum integration step to be of the order of the fastest (smallest) time scale. When the problem is stiff, the ratio between the fastest scale and the scale by which the process evolves may grow very large (i.e., several orders of magnitude). In such a case, the calculations might progress uselessly at a very slow pace.

Here, a new explicit algorithm is presented which circumvents the stability limitations of the standard explicit schemes by resorting to the concepts embodied in the Computational Singular Perturbation (CSP) method. The original ideas and the mathematical background on which the CSP method is based are presented in [2, 3, 4, 5].

Given a stiff system of ODE's, the key to construct an efficient explicit scheme on the basis of CSP concepts is to split the contributions of the fast and slow time scales, account the effects of the fast scales at the start of each time step and proceed to the next point in time by taking into account the slow scales only. The development of the new explicit algorithm is done in view of future applications to systems of stiff PDE's, the stiffness of which is mainly related to the presence of a source term. The standard time-step splitting approach provides a consistent way of treating the non-linear coupling between the spatial operator and the source term, but it does not provide (and therefore cannot explicitly take advantage from) any information on how the spatial scales interact with the fast and slow time scales due to the

source term. When the fast time scales are related with the source term only, CSP allows the direct coupling of the spatial scales with the slow time scales due to the source term. Such a treatment of a stiff problem by an explicit algorithm eliminates the need for implicit or multi-step schemes. As a result, the solution of non-linear systems at each time step and the extra storage required is avoided. The CSP algorithm also provides an estimate of the order of magnitude of the dominant time scale, which can be used both to adjust (maximize) the integration step for time marching and to set the proper spatial discretization (grid resolution) in a PDE problem without resorting to an error control strategy.

Stiff problems handled by the CSP method

Consider the nonlinear initial value problem:

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{g}(y), \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \tag{1}$$

where $\boldsymbol{y}$ and $\boldsymbol{g}$ are N-dimensional (column) vectors. Suppose that, throughout the time domain of interest, the Jacobian matrix $J = grad(\boldsymbol{g})$ has M eigenvalues which have magnitudes much larger than the remaining $N - M$. If these M eigenvalues have negative real parts, are located away from the imaginary axis and if the time domain of interest is of the order of the reciprocal of the $(M + 1)$-th eigenvalue, then eq. (1) exhibits a boundary-layer type of stiffness.

The CSP method is based on the ability to split the N-dimensional domain of $\boldsymbol{y}$, in two subdomains each of which exhibits certain characteristics. One subdomain is M dimensional, contains the fast time-scales, and is responsible for the rapid changes the solution might exhibit. The other subdomain is $N - M$ dimensional, contains the slow time-scales, and is responsible for the smooth behavior of the solution. When $\boldsymbol{y}$ goes through a period of rapid changes (inner region or boundary layer), the component of the velocity vector $\boldsymbol{g}$ in the fast subdomain is significant. However, it becomes negligible when $\boldsymbol{y}$ exhibits a smooth behavior (outer region).

As the system evolves in time, the two subdomains "rotate". CSP follows the movement of the two subdomains and inspects the projection of $\boldsymbol{g}$ into the fast subdomain. When the trajectory leaves the inner region, this projection becomes exponentially small. CSP then provides a simplified system of equations which produces an approximation of the "exact" solution but contains no fast time-scales. This way, the fast time-scales, which cause the numerical difficulties, are retained only when needed and are discarded when they have no effect on the evolution of the system. This process is done in such a way that the computed solution stays within the desired accuracy.

In order to split the source term $\boldsymbol{g}$ into a fast and a slow component, the $\boldsymbol{y}$-domain must be resolved in an appropriate manner. Let R^N be the domain of $\boldsymbol{y}$ and $[\boldsymbol{a}_1(t), ..., \boldsymbol{a}_N(t)]$ be a set of column basis vectors which span R^N at time t. The corresponding set of orthogonal row vectors is denoted as $[\boldsymbol{b}^1(t), ..., \boldsymbol{b}^N(t)]$. The vector $\boldsymbol{g}$ can now be expanded in terms of these sets of basis vectors as follows:

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{a}_1 f^1 + ... + \boldsymbol{a}_N f^N = \boldsymbol{a}_r f^r + \boldsymbol{a}_s f^s \qquad \text{where} \qquad f^i = \boldsymbol{b}^i \odot \boldsymbol{g} \qquad i = 1, N \tag{2}$$

is the "amplitude" of $\boldsymbol{g}$ in the "direction" of $\boldsymbol{a}_i$, and the indices r and s denote summation ($r = 1, M$ and $s = M + 1, N$). The projection of $\boldsymbol{g}$ being small over the fast subdomain can be expressed by the M equations (of partial equilibrium state):

$$f^r \approx 0 \qquad r = 1, M \tag{3}$$

The M equations (3) describe the manifold in the space of $\boldsymbol{y}$ on which the trajectory in the outer region moves according to the ODE equation:

$$\frac{d\boldsymbol{y}}{dt} \approx \boldsymbol{a}_s f^s \qquad s = M + 1, N \tag{4}$$

The explicit algorithm based on the CSP method

Three are the basic steps to build the new explicit algorithm: (i) identification of the number of exhausted modes M at a given time, (ii) construction of the CSP basis vectors and (iii) integration of the stiff ODE system according to a time-scale explicit algorithm.

Detection of the exhausted fast modes

The criterion is the following. Let us first introduce a "small" vector $\boldsymbol{\epsilon}$ built on the basis of the solution vector $\boldsymbol{y}$, as follows:

$$\epsilon^i = \epsilon^i_{rel} \, |y^i| + \epsilon^i_{abs} \tag{5}$$

where ϵ^i_{rel} and ϵ^i_{abs} are the maximum relative and absolute errors on the i-th variable respectively. The algorithm to find the number of exhausted modes M is based on the inequality:

$$\tau(L+1)|\sum_{j=1,L} a^i_j f^j| < \epsilon^i \tag{6}$$

where L is a running counter of the modes ranging from 1 to N. The first time the inequality above is satisfied allows, the number of exhausted modes, M, is set equal to $L-1$. The condition (6) guarantees that the trajectory remains close to the manifold within specified bounds and is not diverted far from it by marching in time according to the simplified non-stiff eq. (4).

Construction of the basis vectors

The algorithm for the construction of the basis vector sets $\boldsymbol{a}_i$ and $\boldsymbol{b}^i$ is based on the recursive CSP formulas for the basis vectors [2, 3, 4, 5]. By neglecting the time derivative terms (which account for non-linear effects), these formulas are:

$$A(s_1+1) \;=\; JA(s_1)\left[BJA(s_1)\right]^{-1} \qquad B, J = const \tag{7}$$

$$B(s_2+1) \;=\; \left[B(s_2)JA\right]^{-1} B(s_2)J \qquad A, J = const \tag{8}$$

where the matrixes A and B collect the right and left M fast eigenvectors respectively:

$$A = (\, \boldsymbol{a}_1 \quad \ldots \quad \boldsymbol{a}_M \,) \qquad ; \qquad B = (\, \boldsymbol{b}^1 \quad \ldots \quad \boldsymbol{b}^M \,)^T$$

and the initial guesses $A(0)$ and $B(0)$ are arbitrary matrixes. The refinements (7) and (8) are not coupled to each other; i.e., the number of s_1-refinements might not be equal to the number of s_2-refinements. Independent of the number of s_1- and s_2-refinements, the resulting vectors produce an orthonormal basis.

If the problem is fully non-linear, the vectors produced with one refinement provide leading order accuracy. Since the time derivative terms were neglected in the recursive formulas (7) and (8), more refinements do not provide higher accuracy. In general, eq. (1) is considered to be non-linear. Therefore, only one refinement is, in principle, necessary. When the problem is linear, the accuracy increases with the number of s_1/s_2-refinements. Therefore, the degree of quasi-linearity of eq. (1) is exploited by letting s_1 and s_2 obtain values higher than zero.

When the s_1/s_2-refinements do have an effect, each s_1-refinement (eq. 7) improves the stability of the scheme while each s_2-refinement (eq. 8) improves the accuracy.

Integration of the stiff ODE system

Let us assume that, at a certain stage of the process evolution, the trajectory has exited the inner region and the first M column vector $\boldsymbol{a}_r$ span the fast subdomain of $\boldsymbol{y}$, while the remaining $N-M$ column vectors $\boldsymbol{a}_s$ span the slow subdomain of $\boldsymbol{y}$. With these definitions, the original ODE system (2) can also be written as:

$$\frac{d\boldsymbol{y}}{dt} \;=\; \boldsymbol{a}_r f^r \;+\; \mathrm{P}\boldsymbol{g} \tag{9}$$

where, the projection matrix P defined as:

$$\mathrm{P} \;=\; \mathrm{I} \;-\; \boldsymbol{a}_r \boldsymbol{b}^r \tag{10}$$

maps $\boldsymbol{g}$ onto the slow subdomain of $\boldsymbol{y}$. The time change of $\boldsymbol{y}$ is obtained by integrating system (9) over an interval of time Δt, according to the expression:

$$\boldsymbol{y}(T+\Delta t) \;-\; \boldsymbol{y}(T) \;=\; \int_T^{T+\Delta t} \boldsymbol{a}_r f^r dt \;+\; \int_T^{T+\Delta t} \mathrm{P}\boldsymbol{g} dt \tag{11}$$

As demonstrated in [2, 3, 4, 5], the amplitudes of the fast modes f^r evolve in time according to the equations:

$$\frac{df^r}{dt} \;=\; \lambda^r_{r'}[f^{r'} \;-\; f^{r'}_\infty] \qquad \text{where} \qquad \lambda^r_{r'} = \left(\frac{d\boldsymbol{b}^r}{dt} + \boldsymbol{b}^r J\right)\boldsymbol{a}_{r'} \tag{12}$$

Given that the trajectory is in the outer (slow) region, f^r reaches the asymptotically small value f^r_∞ which expresses the contribution of the slow scales to the amplitude of the fast modes and is defined as:

$$f^r_\infty = -\tau^r_{r'}\lambda^{r'}_s f^s \qquad \text{where} \qquad \lambda^{r'}_s = \left(\frac{d\boldsymbol{b}^{r'}}{dt} + \boldsymbol{b}^{r'} J\right)\boldsymbol{a}_s \tag{13}$$

and the matrix $\tau^r_{r'}$ is defined as the inverse of $\lambda^r_{r'}$.

Solving eq. (12) for f^r, substituting it into the integral (11), integrating by parts and using eq. (13) yields:

$$\boldsymbol{y}(T+\Delta t) \;=\; \boldsymbol{y}(T) \;+\; (\boldsymbol{a}_r\tau^r_{r'}f^{r'})_{t=T+\Delta t} \;-\; (\boldsymbol{a}_r\tau^r_{r'}f^{r'})_{t=T} \;-\; \int_T^{T+\Delta t} \frac{d}{dt}[\boldsymbol{a}_r\tau^r_{r'}]f^{r'}dt$$

$$+\; \int_T^{T+\Delta t} \boldsymbol{a}_r f^r_\infty dt \;+\; \int_T^{T+\Delta t} \mathrm{P}\boldsymbol{g} dt \tag{14}$$

Over the time scale $\Delta t \approx O(\tau(M+1))$, the basis vectors vary very slowly. Thus: $d[\boldsymbol{a}_r\tau^r_{r'}]/dt \approx 0$, which allows to drop the integral and to factorize out the term $(\boldsymbol{a}_r\tau^r_{r'})_{t=T}$. Moreover, the term $f^{r'}(T+\Delta t)$ can be replaced by its asymptotic value f^r_∞. Therefore, eq. (14) can be written as:

$$\boldsymbol{y}(T+\Delta t) \;=\; \boldsymbol{y}(T) \;-\; (\boldsymbol{a}_r\tau^r_{r'})_{t=T}f^{r'}(T) \;+\; \int_T^{T+\Delta t} \mathrm{P}\boldsymbol{g} dt \;+\; SMALL \tag{15}$$

where

$$SMALL \;=\; +\; (\boldsymbol{a}_r\tau^r_{r'})_{t=T}f^{r'}_\infty \;+\; \int_T^{T+\Delta t} \boldsymbol{a}_r f^r_\infty dt \;-\; \int_T^{T+\Delta t} \frac{d}{dt}[\boldsymbol{a}_r\tau^r_{r'}]f^{r'}dt \tag{16}$$

collects all small contributions. Eq. (15), with the SMALL terms neglected, is in a form suited to write a class of time-scale splitting explicit schemes of integration. The contribution of the fast modes to the time change of $\boldsymbol{y}$ is given by the relation:

$$\tilde{\boldsymbol{y}}(T) \;=\; \boldsymbol{y}(T) \;-\; (\boldsymbol{a}_r\tau^r_{r'})_{t=T}f^{r'}(T+\Delta t) \tag{17}$$

where the amplitude of the fast modes f^r is evaluated at the next time level $T+\Delta t$ to make the algorithm stable, and the slow mode contribution is accounted for by the equation:

$$\boldsymbol{y}(T+\Delta t) \;=\; \tilde{\boldsymbol{y}}(T) \;+\; \int_T^{T+\Delta t} \mathrm{P}\boldsymbol{g} dt \tag{18}$$

It is easy to show that eq. (17) provides a leading order solution to eqs. (3), describing the manifold on which the trajectory moves. In essence, eq. (17) corrects the error introduced by the omission of the fast modes in eq. (18), by bringing the trajectory back on the manifold.

The time-scale splitting, represented by eqs. (17-18) becomes more and more accurate as the separation between the smallest eigenvalue $\lambda(M)$ related to the fast modes and the largest eigenvalue of the slow modes $\lambda(M+1)$ increases. A measure of this separation is provided by the ratio $\varepsilon = |\lambda(M+1)/\lambda(M)|$. The correct order of magnitude of the time scale Δt over which the slow contribution evolves is provided by $\tau(M+1)$ defined as the inverse of $|\lambda(M+1)|$. This value provides a measure of the time step Δt for the numerical integration of eq. (18).

Validation of the New Algorithm

The validation of the explicit algorithm will be done on the basis of the auto-ignition of a combustible mixture behind a steady, normal shock wave. This problem displays the main features related to the subject under study, but it remains simple enough to allow a thorough analysis of the performance of the schemes.

The flow is assumed to be inviscid and non-conducting. Detailed finite rate chemical kinetics is included, making the governing equations stiff. With these assumptions, the relevant flow model equations are the reactive Euler equations. To illustrate and evaluate the properties of the new algorithm, a one-dimensional approximation is employed.

The performance analysis is carried out for the auto-ignition process initiated by a normal shock of combustible mixtures of hydrogen/air and methane/air. The kinetics of the hydrogen/air mixture is described by a mechanism which involves 33 reactions, 13 species, and 3 elements; the kinetics of the methane/air mixture is governed by a mechanism which involves 260 reactions, 49 species and 4 elements.

A parametric investigation will been carried out to asses the performance of the new algorithm. Its performance will be compared against the results delivered by LSODE.

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