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A Half-Explicit, Non-Split Projection Method for Low Mach Number Flows

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Abstract

In the context of the direct numerical simulation of low MACH number reacting flows, the aim of this article is to propose a new approach based on the integration of the original differential algebraic (DAE) system of governing equations, without further differentiation. In order to do so, while preserving a possibility of easy parallelization, it is proposed to use a one-step index 2 DAE time-integrator, the Half Explicit Method (HEM). In this context, we recall why the low MACH number approximation belongs to the class of index 2 DAEs and discuss why the pressure can be associated with the constraint. We then focus on a fourth-order HEM scheme, and provide a formulation that makes its implementation more convenient. Practical details about the consistency of initial conditions are discussed, prior to focusing on the implicit solve involved in the method. The method is then evaluated using the Modified

KAPS Problem, since it has some of the features of the low MACH number approximation. Numerical results are presented, confirming the above expectations. A brief summary of ongoing efforts is finally provided.

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A Half-Explicit, Non-Split Projection Method for Low Mach Number Flows

1 Introduction

In the context of direct numerical simulation of reacting flow, the low MACH number approximation [25, 28, 20, 15, 16, 7, 26, 27] aims at projecting out acoustic phenomena when their effects are negligible. Analytically, the flow is modelled by a set of partial differential equations (PDEs) subject to an algebraic constraint. For the numerical solution of these, any space-discretization method leads to a set of differential-algebraic equations (DAEs) with differentiation index 2. Because of the inherent complexity of integrating directly such index 2 DAEs, numerous practical approaches have been proposed. Based on the differentiation of some equations of the initial system, they yield a weaker formulation. This results, in particular, in a possible drift-off from the proper index 2 submanifold [11].

Due to the present limits of computing resources, it has also been shown that adaptive mesh refinement (AMR) allows the level of resolution and problem complexity required for advances in combustion science. However, AMR involves several new difficulties such as hierarchical storage and handling and interpolation of time history. For this reason, one-step multi-stage time integrators appear to be the solution of choice in the context of AMR.

The goal of this work is therefore to propose a new solution strategy, aiming at integrating the original index 2 DAE by the means of a one-step scheme. An original approach for solving index 2 DAEs has been proposed by [10], consisting of adding an implicit solve of the algebraic constraint within each stage of an explicit RUNGE-KUTTA (ERK) scheme, and therefore called Half Explicit Methods (HEM). Although promising, especially because it allows the direct solution of the initial index 2 system, this method has not yet been demonstrated in the context of computational fluid dynamics. Several numerical difficulties have not been addressed, in particular concerning implicit solves and inconsistent initial physical conditions. Moreover, the question of whether it makes sense to consider the pressure as the degree of freedom of the constraint constituted by the equation of state has to be addressed.

In Section 2, we recall the mathematical formulation of the problem, then summarize

the classical approaches for its numerical solution. In Section 3, we formalize the problem as an index 2 DAE and briefly recall the mathematical basics of such systems. Then, we discuss the consistency between the pressure and the equation of state constraint. Finally, we introduce the Half Explicit Method and in particular its 5-stage, 4th order variant, HEM4. After recasting it in a more algorithmically suited formulation, we highlight a few implementation issues. Section 4 provides a numerical demonstration of the approach. In this goal, we make use of a test case, the Modified KAPS Problem, which is an index 2 DAE with two control parameters: one on the differential operator eigenvalues and the other on the algebraic constraint. Moreover, it has an analytical solution, allowing exact estimation of the accuracy of the method, the cost of its implicit part and its ability to recover from inconsistent initial conditions. We specialize HEM4 to this case, and compare it to both the analytical solution and an index-reduction projection method. This article concludes with a few remarks emphasizing the promising results and potential further improvements.

2 The Low MACH Number Approximation

First, this Section recalls the generally accepted mathematical formulation of the low MACH number approximation; then, classical solution methods are discussed; finally, we introduce a new approach, based on application of the HEM construction.

2.1 Statement of the Problem

The low MACH number approximation is strictly valid in the limit of zero MACH number M, however it is typically applied in practice for $M^2 < 0.1$. It neglects elastic compressibility of the fluid and the associated propagation of acoustic waves, such that the flow is effectively incompressible as regards flow dynamics; while it does allow for density variation in accordance with the state equation of the fluid at hand. The approximation procedure starts with the compressible flow equations, with suitable non-dimensionalization. It then involves expanding the flow variables in terms of a small parameter $\varepsilon = \gamma M^2$, where $\gamma = c_p/c_v$ is the ratio of constant pressure/volume specific heats of the gas. Thus, for $\phi \in \{u, p, \rho, T, Y_{i|i=1,\ldots,N}\}$,

$$\phi = \phi_0 + \varepsilon\phi_1 + \varepsilon^2\phi_2 + \cdots \tag{1}$$

where u is the velocity, p is pressure, ρ is density, T is temperature, and Y_i is the mass fraction of species i. One then finds the $\varepsilon \to 0$ limit of the governing equations by retaining

same order terms. As a result, the zeroth-order limit of the momentum equations leads to

$$\nabla p_0 = 0 \tag{2}$$

where p_0, the zeroth-order term in ε, is also known as the thermodynamic pressure. On the other hand, the pressure term remaining in the resulting low MACH number momentum equations involves the first-order pressure p_1, also known as the dynamic pressure. The thermodynamic pressure $p_0 = p_0(t)$ is constant in space and constrained by an integral mass conservation constraint on dp_0/dt over the domain of the problem. If the domain has open boundaries leading to the atmosphere, or any other "infinite" reservoir with constant p_0, then $dp_0/dt = 0$ and p_0 is constant in time. This will be the condition assumed in the present work. In the following, we drop the index on p_1, referring to it simply as p. All other field variables survive in the reduced equations in their zeroth-order terms only, where, again, we drop the subscript for convenience.

This model has been formalized by [15]. Ignoring body forces, radiant heat transfer and the SORET-DUFOUR effects [31], the governing equations for low MACH number non-reacting flow of a single species-fluid are given by the NAVIER-STOKES, energy, and mass conservation equations under the equation of state. Using the perfect gas law (*cf.* [19, 22]):

$$\begin{cases} \partial_t(\rho u) &= \operatorname{div}\tau - \operatorname{div}(\rho u \otimes u) - \operatorname{grad} p \\ \partial_t T &= -\langle u, \operatorname{grad} T\rangle + \dfrac{1}{\rho c_p}\operatorname{div}(\alpha \operatorname{grad} T) \\ \partial_t \rho &= -\langle u, \operatorname{grad}\rho\rangle - \rho \operatorname{div} u \\ \rho &= \dfrac{p_0}{RT} \end{cases} \tag{3}$$

where $\langle\cdot,\cdot\rangle$ and $\otimes$ are, respectively, the standard euclidean inner and tensorial products, τ is the viscous stress tensor, and R is the perfect gas constant. The above assumptions are for convenience, and in no way impact the generality of the present results. Using the material derivative, the system can be equivalently written as follows:

$$\begin{cases} \partial_t(\rho u) &= \operatorname{div}\tau - \operatorname{div}(\rho u \otimes u) - \operatorname{grad} p \\ D_t T &= \dfrac{1}{\rho c_p}\operatorname{div}(\alpha \operatorname{grad} T) \\ D_t \rho &= -\rho \operatorname{div} u \\ \rho &= \dfrac{p_0}{RT} \end{cases} \tag{4}$$

with $D_t \cdot = \partial_t \cdot + \langle u, \operatorname{grad} \cdot\rangle$.

2.2 Solution Strategies

The solution of the above system of equations is hampered by the absence of an equation for the pressure p. This is also the case for strictly incompressible flow with no density variation, however, the low MACH number equation system involves signifi cant additional complexity associated with the $D_t\rho$ term in the continuity equation and the equation of state algebraic constraint.

There is of course a vast literature on the solution of the incompressible and low MACH equations. Constraining the present discussion to the equations in terms of primitive variables in the eulerian context, solution strategies generally fall in two classes depending on whether the velocity and pressure fi elds are decoupled or not. Coupled constructions are generally of superior order of accuracy, are solved implicitly, and require signifi cant computational effort [30]. On the other hand, decoupled/operator-split constructions [8, 9, 21] are easier to implement in practice, and have been widely used, despite some accuracy consequences of the velocity-pressure decoupling. One of the most popular techniques in this class is the Projection method initially formulated by CHORIN [5, 6] and TEMAM [29] based on fractional-step methods. This method has been applied to both incompressible [14, 3, 12], and low MACH number [16, 26, 27, 17, 18] flows. The Projection scheme employs a fractional time integration procedure in each time step.

The general Projection scheme structure as applied to incompressible flow is as follows. In the fi rst fractional step, the momentum equations are integrated forward in time without the pressure gradient term. The provisional velocity fi eld computed in this step does not generally satisfy the divergence constraint provided by the continuity equation. The method then proceeds to fi nd the pressure fi eld by solving a pressure POISSON equation, derived by taking the divergence of the momentum equations and enforcing the continuity divergence constraint. This pressure fi eld is then used in a second fractional step to project the provisional velocity fi eld onto the submanifold determined by the divergence constraint, thereby arriving at the fi nal velocity fi eld for the time step.

The extension of this construction to low MACH number flow takes different forms, depending on whether a locally mass-conservative fractional-stepping procedure is used or not. Thus, when the momentum equations are written in a conservative form, in terms of ρu [16, 26, 27], Projection scheme implementations update the ρu fi eld in the fractional steps, such that the pressure POISSON equation derivation requires simply the application of the continuity equation, substituting $\partial\rho/\partial t$ for $\nabla\cdot(\rho u)$, where $\partial\rho/\partial t$ is found from the time integration of the density fi eld. In this construction, the energy equation is used for updating the temperature fi eld, and the density is retrieved from the state equation.

Alternative ρu Projection constructions [17, 18] follow similar lines, however they rely

on a derivation of the state equation constraint to arrive at an evolution equation for density. Another class of low MACH number Projection schemes [1, 23, 24, 22] is based on a non-conservative formulation of the momentum equations, and a Projection based on u rather than ρu. In these constructions, a divergence constraint on the velocity field is also formulated by differentiation of the state equation constraint using the material derivative operator, from whence a temperature derivative arises, and (3^4) is transformed by using (3^3):

$$\left\{\begin{array}{rcl} \partial_t(\rho u) &=& \mathrm{div}\tau - \mathrm{div}(\rho u \otimes u) - \mathrm{grad}p \\ \partial_t T &=& -\langle u, \mathrm{grad}T\rangle + \dfrac{1}{\rho c_p}\mathrm{div}(\alpha\,\mathrm{grad}T) \\ \partial_t \rho &=& -\langle u, \mathrm{grad}\rho\rangle - \rho\,\mathrm{div}u \\ \mathrm{div}u &=& \dfrac{1}{T\rho c_p}\mathrm{div}(\alpha\,\mathrm{grad}T). \end{array}\right. \tag{5}$$

It is important to acknowledge here the fact that, because of the differentiation of the original state-equation constraint on ρ, the resulting equations (5) with the divergence constraint are a weaker formulation than (3). Even though (5) has the same differential operator as (3), the constraint on div$u$ is intrisically weaker, *i.e.* results in a larger constraint submanifold, than that on ρ. However, the main advantage is that one now has an explicit expression for div$u$, which is needed in the requisite differentiation of the momentum equations necessary for formulating the pressure POISSON equation [1, 23, 24, 22]. Practically, the equations are decoupled and the methods aim at solving hydrodynamic and mass conservation equations for a given temperature while attempting to preserve the geometric invariant constituted by the constraint on div$u$. This implicitly assumes that the equation of state is automatically enforced. Nevertheless, it has been reported [22] that, in the regions where the velocity is supposed to be divergence-free, such schemes might fail at satisfying this property.

In general, it is well established that the splitting inherent in traditional Projection scheme approaches has consequences on the accuracy of computations [3] even in incompressible flow. These are typically remedied by clever choices of boundary conditions [13] or by algebraic splitting [12]. The additional differentiation of the equation of state algebraic constraints can potentially compound these difficulties by projecting on constraint submanifolds larger than the submanifold corresponding to the state equation constraint induced by the initial governing equations (3). The present work pursues remedies for both of these difficulties by focusing on the original coupled constrained PDE system, and pursuing Half Explicit time integration strategies (HEM), rather than traditional fully-implicit constructions, for the resulting semidiscretized equations.

3 A Non-Split Projection Strategy

We propose an approach for solving the initial system (3) without prior differentiation and without operator splitting.

3.1 Index 2 Differential Algebraic Equations

Formally, a space-discretization leads to the substitution of functions depending on space and time variables by time only depending vector functions. More precisely, if Ω and $[0,t_f]$ respectively denote the geometric domain of interest and the relevant time interval, the functions:

$$\begin{array}{rrcl} \rho u: & \Omega\times[0,t_f] & \longrightarrow & \mathbb{R}^{\dim\Omega} \\ T: & \Omega\times[0,t_f] & \longrightarrow & \mathbb{R} \\ \rho: & \Omega\times[0,t_f] & \longrightarrow & \mathbb{R} \\ p: & \Omega\times[0,t_f] & \longrightarrow & \mathbb{R} \end{array} \tag{6}$$

are substituted by the following:

$$\begin{array}{rrcl} \widetilde{\rho u}: & [0,t_f] & \longrightarrow & \mathbb{R}^{N\dim\Omega} \\ \widetilde{T}: & [0,t_f] & \longrightarrow & \mathbb{R}^{N} \\ \widetilde{\rho}: & [0,t_f] & \longrightarrow & \mathbb{R}^{N} \\ \widetilde{p}: & [0,t_f] & \longrightarrow & \mathbb{R}^{N} \end{array} \tag{7}$$

where N is the number of nodes of the grid. In this context, (3) implies that

$$(\forall k\in\{1,\ldots,N\}) \quad \left\{ \begin{array}{rcl} \partial_t\widetilde{\rho u}_k &=& A(\widetilde{\rho},\widetilde{\rho u})-B(\widetilde{p}) \\ \partial_t\widetilde{T}_k &=& C(\widetilde{\rho},\widetilde{\rho u},\widetilde{T}) \\ \partial_t\widetilde{\rho}_k &=& D(\widetilde{\rho},\widetilde{\rho u}) \\ 0 &=& R\widetilde{\rho}_k\widetilde{T}_k-p_0 \end{array} \right. \tag{8}$$

where A, B, C and D are time-dependent polynomial functions of the vectorial unknowns depending on the space-discretization scheme. Finally, defining y as $(\widetilde{\rho},\widetilde{\rho u},\widetilde{T})$, this yields:

$$(\forall k\in\{1,\ldots,N\}) \quad \left\{ \begin{array}{rcl} \partial_t y_k &=& f_k(y,\widetilde{p}) \\ 0 &=& g_k(y_k) \end{array} \right. \tag{9}$$

or, with $z=\widetilde{p}$,

$$\left\{ \begin{array}{rcl} \partial_t y &=& f(y,z) \\ 0 &=& g(y) \end{array} \right. \tag{10}$$

which is a set of differential-algebraic equations. For the sake of clarity, we recall here a few essential definitions; see for example [11] for a comprehensive discussion.

Definition 3.1. Given n and m in $\mathbb{N}^*$, f in $C^0(\mathbb{R}^{n+m},\mathbb{R}^n)$ and g in $C^0(\mathbb{R}^{n+m},\mathbb{R}^m)$ (resp. $C^1(\mathbb{R}^n,\mathbb{R}^m)$), the following system of equations with unknows y in $C^1(\mathbb{R}_+,\mathbb{R}^n)$ and z in $C^0(\mathbb{R}_+,\mathbb{R}^m)$:

$$\left\{\begin{array}{rcll} y' & = & f(y,z) & \\ 0 & = & g(y,z) & \text{(resp.}g(y)\text{)} \\ (y_0,z_0) & = & (y(0),z(0)) & \end{array}\right. \tag{11}$$

is a differential-algebraic equation with differentiation index 1 (resp. 2) or DAE1 (resp. DAE2). Given such a DAE2, the equation which arises when combining the differential equation with the derivative of the algebraic constraint is called the hidden constraint of the DAE2.

Remark 3.1. Gathering the differential equation of a DAE2 along with its hidden constraint

$$\frac{\mathrm{d}g}{\mathrm{d}y}(y)\cdot f(y,z) = g_y(y)\cdot f(y,z) = 0, \tag{12}$$

constitutes a DAE1. Integrating the latter instead of the former (index-reduction) is much easier. Although benevolent in some particular cases (*e.g.* incompressible fluids), this can lead to a drift-off from the proper submanifold Ker$g$, the kernel of g (*cf.* [11]).

Indeed, (10) is an index 2 DAE, with $n = N(\dim\Omega+2)$ and $m = N$. Our aim is to solve it using a time integrator designed for DAE2 systems.

3.2 Can the Pressure Be Associated with the Constraint?

Since the pressure is usually associated with the divergence constraint, we now discuss the relevance of using the pressure as the algebraic variable along with the equation of state as the constraint. We illustrate this with a simpler model system that has an analytical solution and can be solved without differentiating the index 2 algebraic constraint while, nevertheless, retrieving an equation for the pressure. In this simplified case, we show that the pressure can be tied to the index 2 constraint which motivates a similar approach for the full low MACH number flow problem. Consider the following system:

$$\left\{\begin{array}{rcl} \varphi_1'(t) & = & f_1(t)+p(t) \\ \varphi_2'(t) & = & f_2(t,\varphi_2(t))+\varphi_1(t) \\ 0 & = & \varphi_2(t)-1 \\ (\varphi_{1_0},1) & = & (\varphi_1(0),\varphi_2(0)). \end{array}\right. \tag{13}$$

For the sake of brevity, and since this is not the main goal of this article, we only provide an existence result with a suboptimal hypothesis regarding the regularity of the right-hand side functions. The result could be made more general at the expense of a more detailed discussion.

Proposition 3.1. *If f_1, f_2 are C^1 functions, then* (13) *has a C^1 solution $(\varphi_1, \varphi_2, p)$ given by:*

$$(\forall t \in \mathbb{R}) \quad \left\{ \begin{array}{rcl} p(t) & = & -\partial_t f_2(t,1) - f_1(t) \\ \varphi_1(t) & = & \varphi_{1_0} + \displaystyle\int_0^t \big(f_1(s) + p(s)\big)\,\mathrm{d}s \\ \varphi_2(t) & = & 1. \end{array} \right. \tag{14}$$

In addition, this solution can be obtained without differentiating the constraint.

Proof. Assuming that p is a C^1 function, then φ_1 is also C^1 and is given by:

$$(\forall t \in \mathbb{R}) \quad \varphi_1(t) = \varphi_{1_0} + \int_0^t \big(f_1(s) + p(s)\big)\,\mathrm{d}s. \tag{15}$$

Now, the second differential equation implies that φ_2 is also C^1 and

$$(\forall t \in \mathbb{R}) \quad \varphi_2(t) = \varphi_2(0) + \int_0^t \big(f_2(s, \varphi_2(s)) + \varphi_1(s)\big)\,\mathrm{d}s. \tag{16}$$

Enforcing the constraint and the consistency of the initial conditions, it follows that

$$(\forall t \in \mathbb{R}) \quad \int_0^t \big(f_2(s,1) + \varphi_1(s)\big)\,\mathrm{d}s = 0 \tag{17}$$

whence

$$(\forall t \in \mathbb{R}) \quad f_2(t,1) + \varphi_1(t) = 0. \tag{18}$$

Finally, combining (18) with the first equation of (13) yields

$$(\forall t \in \mathbb{R}) \quad p(t) = -\partial_t f_2(t,1) - f_1(t). \tag{19}$$

□

In other words, Proposition 3.1 illustrates that the pressure can be viewed as a generalized scalar LAGRANGE multiplier associated with the equation of state constraint.

3.3 The Half-Explicit RUNGE-KUTTA Method

The Half-Explicit s-stage Method (HEM), introduced by [10] in order to integrate DAE2 systems, can be stated as follows:

$$\begin{cases} Y_i &= y_0 + h\sum_{j=1}^{i-1} a_{ij} f(Y_j, Z_j) & (\forall i \in \{1,...,s\}) \\ 0 &= g(Y_i) & (\forall i \in \{1,...,s\}) \\ y_1 &= y_0 + h\sum_{j=1}^{s} b_j f(Y_j, Z_j) & \\ 0 &= g(y_1) & \end{cases} \tag{20}$$

where $h \in \mathbb{R}_+^*$, y_0 and y_1 respectively denote the time-step and the two values of y at the beginning and the end of a step.

According to [2], we will use the following coeffi cients in order to get order 4 time-accuracy for y with a $s = 5$ steps scheme:

$$(a_{ij}) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \frac{3}{10} & 0 & 0 & 0 & 0 \\ \frac{1+\sqrt{6}}{30} & \frac{11-4\sqrt{6}}{30} & 0 & 0 & 0 \\ \frac{-79-31\sqrt{6}}{150} & \frac{-1-4\sqrt{6}}{30} & \frac{24+11\sqrt{6}}{25} & 0 & 0 \\ \frac{14+5\sqrt{6}}{6} & \frac{-8+7\sqrt{6}}{6} & \frac{-9-7\sqrt{6}}{4} & \frac{9-\sqrt{6}}{4} & 0 \end{pmatrix} \tag{21}$$

and

$$(b_i) = \begin{pmatrix} 0 & 0 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \end{pmatrix} \tag{22}$$

thus

$$(c_i) = \begin{pmatrix} 0 & \frac{3}{10} & \frac{4-\sqrt{6}}{10} & \frac{4+\sqrt{6}}{10} & 1 \end{pmatrix} \tag{23}$$

3.4 An Equivalent Formulation of the Scheme

Contrary to appearences, the implicitness of (20) does not involve the differential but the algebraic variable. In fact, a closer look at the scheme shows that, for $i \neq 1$, knowledge of Z_{i-1} is required in order to compute Y_i. Now, each Y_i must satisfy the algebraic equation; thus there should be, at each stage, at least a degree of freedom allowing the enforcement of this constraint. In fact, precisely because nothing is imposed on Z_1, there is at each stage $i \neq 1$ one, and only one, such degree of freedom: the previous stage algebraic value, Z_{i-1}. For the same reason, the only free parameter allowing compliance with the step algebraic constraint is not y_1, but Z_s. In fact, the implicitness is transfered from the differential to the

algebraic stage values. This is why we propose to re-formulate (20), in such a way as to make it more convenient for implementation purposes.

Proposition 3.2. *Assuming* $g(y_0) = 0$ *and* $Y_1 = y_0$, *then* (20) *is equivalent to:*

$$\left\{\begin{array}{rcll} X_i & = & y_0 + h\sum_{j=1}^{i-1} a_{i+1,j} f(Y_j, Z_j) & (\forall i \in \{1,..,s-1\}) \\ 0 & = & g(X_i + h a_{i+1,i} f(Y_i, Z_i)) & (\forall i \in \{1,..,s-1\}) \\ Y_{i+1} & = & X_i + h a_{i+1,i} f(Y_i, Z_i) & (\forall i \in \{1,..,s-1\}) \\ X_s & = & y_0 + h\sum_{j=1}^{s-1} b_j f(Y_j, Z_j) & \\ 0 & = & g(X_s + h b_s f(Y_s, Z_s)) & \\ y_1 & = & X_s + h b_s f(Y_s, Z_s) & \end{array}\right. \tag{24}$$

Proof. It follows directly from (20) that, at each stage $i \in \{1,..,s-1\}$, Z_i must be a solution of the following non-linear equation in the unknown z:

$$g\left(y_0 + h\sum_{j=1}^{i-1} a_{i+1,j} f(Y_j, Z_j) + h a_{i+1,i} f(Y_i, z)\right) = 0 \tag{25}$$

and that Z_s must be a solution of:

$$g\left(y_0 + h\sum_{j=1}^{s-1} b_j f(Y_j, Z_j) + h b_s f(Y_s, z)\right) = 0. \tag{26}$$

thus, (25) and (26) imply that

$$(\forall i \in \{1,..,s-1\}) \quad g(X_i + k_i f(Y_i, Z_i)) = 0, \tag{27}$$

which proves the suffi cient condition.
Conversely, if (24) is satisfi ed, then so are (25) and (26), except for the case $i = 1$, corresponding to the initial consistency condition $g(y_0) = 0$ which is true by hypothesis. □

Remark 3.2. This new formulation of the HEM scheme explicitly requires the consistency of y_0, but this condition is also present, albeit implicitly, in (20).

3.5 Practical Implementation Issues

Clearly, (24) involves the solution of s non-linear equations, one at each stage. These equations are not, in general, algebraically solvable and, therefore, iterative methods must

be considered. In addition, solving (24) at any stage i using an exact[1] NEWTON algorithm would require an evaluation of the derivative of $\phi_i(z) = g(X_i + ha_{i+1,i} f(Y_i, z))$, given by:

$$\frac{\mathrm{d}}{\mathrm{d}z}\phi_i(z) = ha_{i+1,i} g_y(X_i + ha_{i+1,i} f(Y_i, z)) \cdot \frac{\partial}{\partial z} f(Y_i, z). \tag{28}$$

Evaluating $\frac{\mathrm{d}}{\mathrm{d}z}\phi_i(z)$ at each stage can be computationally prohibitive. This is in particular the case with the numerical example proposed in this article and is likely to be the same for low MACH number flows. We therefore chose here to solve each of these non-linear equations using an approximate NEWTON method: $\frac{\mathrm{d}}{\mathrm{d}z}\phi_i(z)$ is approximated *via* a difference formula.

Another practical issue is that of inconsistent initial conditions that can result in an ill-posed problem. Moreover, this can be numerically hidden, since the scheme might converge but produce meaningless results. Although only the differential variable of a DAE2 seems to be initially constrained, this is also the case for the algebraic variable, because of the hidden constraint (12). Nevertheless, according to (24), $g(y_0 + ha_{21} f(y_0, Z_1)) = 0$, thus z_0 is actually not used. Consequently, it is not necessary to provide a consistent z_0 prior to each step. In a sense, the consistency is automaticaly enforced by setting $z_0 = Z_1$. In the case of an inconsistent y_0, the only solution is to replace it by a projection on Kerg: either arbitrarily, in which case there is an infi nite number of ways to proceed, or with respect to some direction, *e.g.* one which makes sense physically.

4 Numerical Test: the Modifi ed KAPS Problem

The Modifi ed KAPS Problem is a differential-algebraic system, with differentiation index 2, introduced in [4]. We briefly recall here the properties which make it a good test case for low MACH number reacting flow time-integrators. As it seems that no literature is available concerning the qualitative properties of its algebraic submanifold, we will also briefly discuss them.

[1] at least theoretically, but not numerically.

4.1 Statement of the Problem

The Modified KAPS Problem (MK) is a DAE2 introduced in [4] as follows: given $(\alpha,\varepsilon) \in \mathbb{R} \times \mathbb{R}_+^*$, solve the following system for y_1, y_2 and z:

$$(\forall t \in \mathbb{R}_+) \quad \begin{cases} y_1' &= -(2+\varepsilon^{-1})y_1 + \varepsilon^{-1}y_2^2 \\ y_2' &= -\exp(1-z^2) \\ 0 &= y_2^2 - y_1 \exp[\alpha(1-\cos(y_1-y_2^2))] \\ (y_1(0),y_2(0)) &= (1,1) \\ z(0) &= 1. \end{cases} \tag{29}$$

The eigenvalues of $\frac{\partial f}{\partial y}$ are 0 and $-(2+\varepsilon^{-1})$, thus can be made as distant from each other as desired. In addition, α allows modification of the submanifold geometry. Moreover, MK has the following analytical solution:

$$(\forall t \in \mathbb{R}_+) \quad (y_1(t),y_2(t),z(t)) = \left(e^{-2t}, e^{-t}, \sqrt{1+t}\right), \tag{30}$$

which is independent of both α and ε. These features make MK an excellent test case for DAE2 schemes.

4.2 The Constraints

By definition, the index 2 submanifold Kerg depends solely on the parameter $\alpha \in \mathbb{R}$. For all α, $y_1 = y_2^2$ implies $g(y_1,y_2) = 0$ thus the parabola $\mathcal{P} : y_1 = y_2^2$ is a submanifold of Kerg; moreover, the analytical solution of MK belongs to $\mathcal{P}$ by inspection. In fact, the geometry of Kerg becomes increasingly complicated as $|\alpha|$ grows, but $\mathcal{P}$ is invariant: the numerical scheme must be capable of staying on it. Now, in order to compare our HEM implementation with an index-reduction approach, let us examine the hidden constraint, and define $d_{12} = y_1 - y_2^2$ for convenience. Then,

Proposition 4.1. *The hidden constraint of MK is*

$$(1+\alpha y_1 \sin d_{12})(2y_1+\varepsilon^{-1}d_{12})e^{\alpha(1-\cos d_{12})} - 2y_2(\alpha y_1 e^{\alpha(1-\cos d_{12})}\sin d_{12}+1)e^{1-z^2} = 0 \tag{31}$$

Proof. By applying (12) to the particular f and g induced by (29). □

Remark 4.1. In addition, given y, the analytical solution of the hidden constraint, when it exists, is given by:

$$z = \pm\sqrt{\ln\left(\frac{2\left(\exp\left(\alpha(\cos(y_1 - y_2^2) - 1)\right) + \alpha y_1 \sin(y_1 - y_2^2)\right) y_2}{(1 + \alpha y_1 \sin(y_1 - y_2^2))(2y_1 + \varepsilon^{-1}(y_1 - y_2^2))}\right) + 1}\,. \tag{32}$$

Alternatively, it is also convenient to see the algebraic constraint as a two-dimensional submanifold $\mathcal{H}$ of $\mathbb{R}^3$, where the third coordinate is given by α, as illustrated in Figure 1.

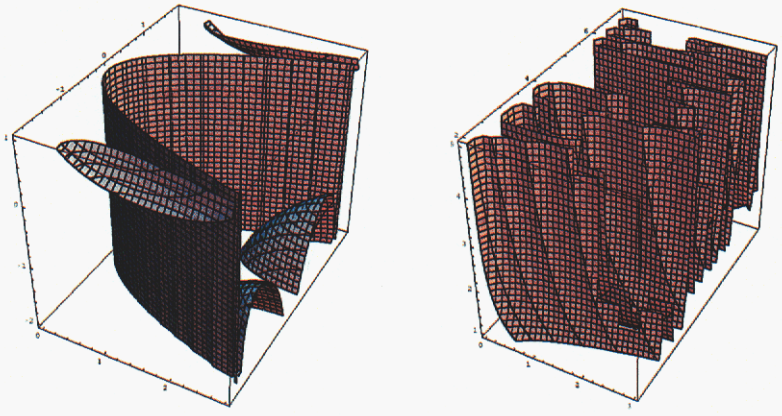

Figure 1. Sections of the constraint submanifold $\mathcal{H} \subset \mathbb{R}^3$.

4.3 Numerical Results

Our HEM4 implementation for MK is now compared to both the analytical solution (30) and to an index-reduction with a local state space form ERK4 (irERK4), *cf.* [11], based on inserting the index 1 constraint at each stage and at the end of each step of an ERK4 scheme. Practically, our irERK4 does not solve the equations (31) but directly uses (32), in order to estimate the drift-off *per se* by avoiding implicit solve failures. It should be noted that this advantage is artifi cal and would not be possible in the general case, since an explicit solution of the index 1 constraint would not be available. In contrast, the HEM4 scheme must solve the 5 non-linear equations of (24), by the means of a perturbed, or approximated, NEWTON solve. This requires in particular the provision of the initial guesses for the

Z_i. Considering the fact that HEM's stage order is only unity (*cf.* [10]), we decided to extrapolate these guesses linearly from previous stage values, when available, as follows:

Z_1^*	z_0
Z_2^*	Z_1
Z_3^*	$\frac{-1+\sqrt{6}}{3}Z_1 + \frac{4-\sqrt{6}}{3}Z_2$
Z_4^*	$\frac{12+2\sqrt{6}}{5}Z_2 - \frac{7+2\sqrt{6}}{5}Z_3$
Z_5^*	$\frac{1-\sqrt{6}}{2}Z_3 + \frac{1+\sqrt{6}}{2}Z_4$

Remark 4.2. Although Z_1 (previous implicit solution) and z_0 (previous step value) are known when Z_2^* is needed, they are both approximations of $z(t_0)$; therefore, one cannot extrapolate in time from them. We simply set $Z_2^* = Z_1$, since z_0 is not necessarily consistent.

Starting with the consistent $y_0 = (1, 1)$ and $z_0 = 1$, we highlight the most signifi cant results. Figure 2 illustrates how, even with small time-steps and the simplest possible Kerg,

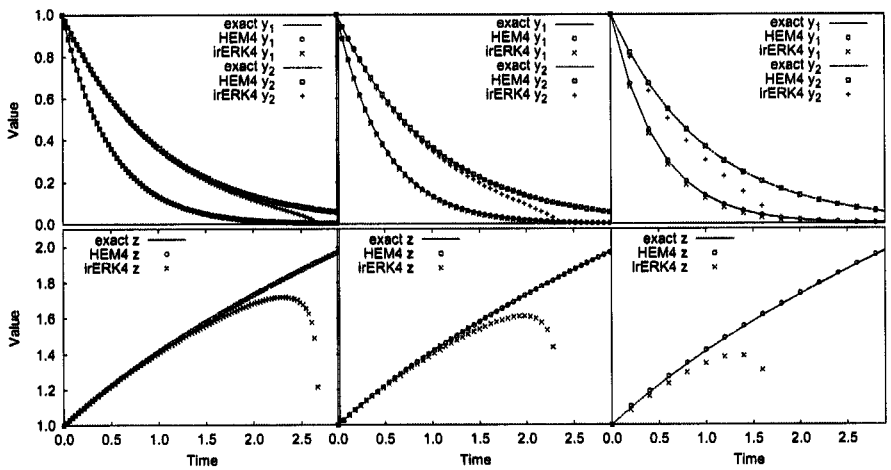

Figure 2. HEM4, irERK4 and exact solutions with $\alpha = 0$, $\varepsilon = 1$ and, from left to right, $h = 0.03$, 0.06 and 0.15.

irERK4 drifts away from Kerg while HEM4 remains stable. Figure 3 shows that, as the geometry of Kerg is made more complex, irERK4 diverges sooner; this is not related to the search for the submanifold, since irERK4 uses (32). On the other hand, HEM4 remains

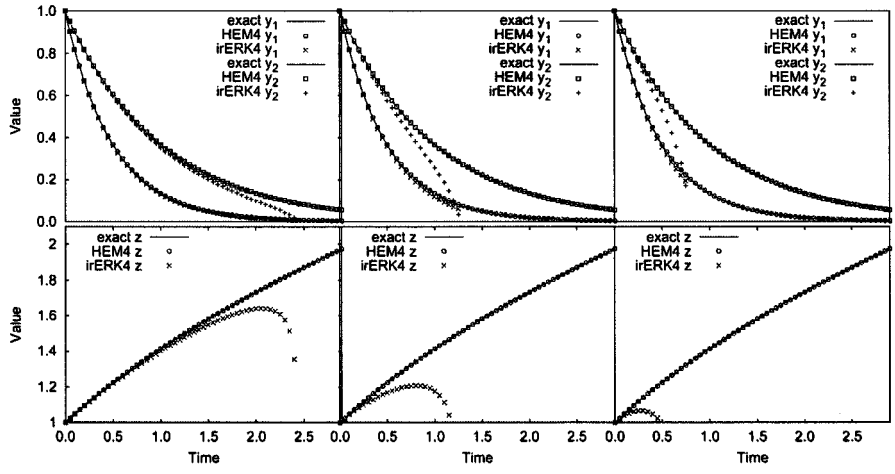

Figure 3. HEM4, irERK4 and exact solutions with $h = 0.05$, $\varepsilon = 1$ and, from left to right, $\alpha = 0$, 4 and 9.

on Kerg, as expected; moreover, it is largely insensitive to α (except for very large time-steps, where the index 2 projection fails). One could expect the differential operator to become stiffer as $\varepsilon \to 0$, thus making any explicit scheme unstable; this is what happens with irERK4 (Fig. 4). On the contrary, HEM4 remains stable[2] even though its "differential part" is explicit. Contrary to what was expected, and for any ε, MK is not stiff along $\mathcal{P}$; but, because of the drift-off, irERK4 does not benefi t from this.

Remark 4.3. The numerical tests also show that the number of NEWTON iterations needed to converge within the prescribed tolerance is generally less than 7, which indicates that the loss of second order convergence of the NEWTON iterations, because the $\frac{\mathrm{d}}{\mathrm{d}z}\phi_i(z)$ are approximate, is not an issue.

5 Conclusions and Perspectives

In this article, we have presented a new non-split projection strategy for low MACH number flows that takes into account the intrisic index 2 differential algebraic formulation that results from semi-discretization of the governing equations. In addition, being one-step, this scheme can be easily combined to adaptive mesh refi nement. We have used a reduced model that has some of the characteristics of the semi-discretized low MACH number flow

[2]until ε reaches machine precision.

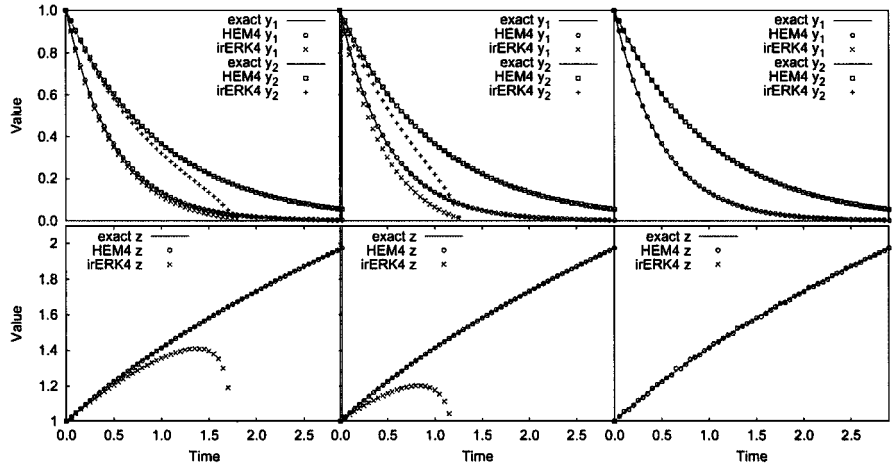

Figure 4. HEM4, irERK4 and exact solutions with $\alpha = 1$, $h = 0.05$ and, from left to right, $\varepsilon = \frac{1}{3}$, 0.1 and 10^{-14}.

governing equations in order to illustrate analytically that the pressure can be viewed as a generalized LAGRANGE multiplier associated with the index 2 constraint constituted by the equation of state. We have therefore proposed to use in this context a one-step, multi-stage index 2 DAE scheme, HEM, for the numerical solution of low MACH number flow equations. Finally, we have numerically illustrated the approach and compared it to an index-reduction projection strategy with a test case allowing in particular for variable manifold complexity. Moreover, because of its inherent simplicity, porting it to more complex DAE2 systems such as[3] low MACH number reacting flow can be confi dently considered. For these reasons, we have decided to proceed accordingly, while exploring in parallel several related issues:

5.1 Stiffness

As indicated in Section 4.3, the Modifi ed KAPS Problem does not permit an assessment of HEM stability when the differential operator becomes stiff. Therefore, we propose to examine the behavior of the HEM scheme on a slightly modifi ed version of the system by

[3]but not restricted to.

keeping the same g and z, but taking y in $C^1(\mathbb{R}^4, \mathbb{R}^3)$ along with the following system:

$$(\forall t \in \mathbb{R}_+) \begin{cases} y_1' & = & -\varepsilon^{-1}(y_1 - e^{-2y_3}) - 2y_2^2 \\ y_2' & = & -\exp(1-z^2) \\ y_3' & = & 1 \\ 0 & = & y_2^2 - y_1 \exp[\alpha(1-\cos(y_1 - y_2^2))] \\ (y_1(0), y_2(0), y_3(0)) & = & (1,1,1) \\ z(0) & = & 1. \end{cases} \tag{33}$$

so that (30) remains valid and $y_3(t) = t$ for all t in $\mathbb{R}_+$. This new problem is also a DAE2.

5.2 Order in z

In the case where Z_s is used as an approximation of $z_1 = z(t_0 + h)$, then z is only first-order accurate. Solving for z_1 the hidden (index 1) constraint:

$$g_y(y_1) f(y_1, z_1) = 0 \tag{34}$$

would provide a better approximation. Unfortunately, this approach seems unrealistic in our case, in particular with the "real" low MACH number approximation problem. An alternate approach is to approximate, for $i \in \{1, \ldots, s-1\}$, the derivatives $y'(x_0 + c_i h)$ with a forward EULER method:

$$\tilde{y}(x_0 + c_i h)' = \frac{Y_{i+1} - Y_i}{(c_{i+1} - c_i)h} \tag{35}$$

then to use a polynomial extrapolation, through these $s-1$ points, in order to obtain an approximation $\tilde{y}_1'$ of $y(x_0 + h)' = y_1'$. Finally, solve

$$\tilde{y}_1' = f(y_1, z_1) \tag{36}$$

for z_1, *e.g.*, with an approximate NEWTON method.

References

[1] A.S. Almgren, J.B. Bell, P. Colella, L.H. Howell, and M. Welcome. A Conservative Adaptive Projection Method for the Variable Density Incompressible Navier-Stokes Equations. *J. Comput. Phys.*, 142:1–46, 1998.

[2] V. Brasey. *Half explicit methods for semi-explicit differential-algebraic equations of index* 2. Phd thesis 2664, Universit'e de Genève, CH, 1994.

[3] D.L. Brown, R. Cortez, and M.L. Minion. Accurate projection methods for the incompressible navier-stokes equations. *J. Comput. Phys.*, 168:464–499, 2001.

[4] J.C. Butcher and P. Chartier. Parallel general linear methods for stiff ordinary differential and differential-algebraic equations. *Appl. Numer. Math.*, 17(3):213–222, 1995.

[5] A.J. Chorin. Numerical Solution of the Navier-Stokes Equations. *Math. Comput.*, 22:745–762, 1968.

[6] A.J. Chorin. On the Convergence of Discrete Approximations to the Navier-Stokes Equations. *Math. Comput.*, 23:341–353, 1969.

[7] A.F. Ghoniem. Computational methods in turbulent reacting flow. *Lectures in Applied Math.*, 24:199–265, 1986.

[8] P.M. Gresho. On the theory of semi-implicit projection methods for viscous incompressible flow and its implementation via a fi nite element method that also introduces a nearly consistent mass matrix, part 1: Theory. *Int. J. Numer. Meth. Fluids*, 11:587–620, 1990.

[9] P.M. Gresho. On the theory of semi-implicit projection methods for viscous incompressible flow and its implementation via a fi nite element method that also introduces a nearly consistent mass matrix, part 2: Implementation. *Int. J. Numer. Meth. Fluids*, 11:621–659, 1990.

[10] E. Hairer, C. Lubich, and M. Roche. *The Numerical Solution of Differential-Algebraic Systems by* RUNGE-KUTTA *Methods*, volume 1409 of *Lecture Notes in Mathematics*. Springer-Verlag, 1989.

[11] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations II, Stiff and Differential-Algebraic Problems*, volume 14 of *Springer Series in Computational Mathematics*. Springer-Verlag, 1996.

[12] M.O. Henriksen and J. Holmen. Algebraic splitting for incompressible navier-stokes equations. *J. Comput. Phys.*, 175:438–453, 2002.

[13] G.E. Karniadakis, M. Israeli, and S.A. Orzag. High-order splitting methods for the incompressible navier-stokes equations. *J. Comput. Phys.*, 97:414, 1991.

[14] J. Kim and P. Moin. Application of a fractional-step method to incompressible navier-stokes equations. *J. Comput. Phys.*, 59:308–323, 1985.

[15] A. Majda and J. Sethian. The derivation and numerical solution of the equations for zero mach number combustion. *Comb. Sci. and Technology*, 42:185–205, 1985.

[16] P.A. McMurtry, W.-H. Jou, J.J. Riley, and R.W. Metcalfe. Direct numerical simulations of a reacting mixing layer with chemical heat release. *AIAA J.*, 24(6):962–970, June 1986.

[17] H.N. Najm. A Conservative Low Mach Number Projection Method for Reacting Flow Modeling. In S.H. Chan, editor, *Transport Phenomena in Combustion*, volume 2, pages 921–932. Taylor and Francis, Wash. DC, 1996.

[18] H.N. Najm and P.S. Wyckoff. Premixed Flame Response to Unsteady Strain-Rate and Curvature. *Combustion and Flame*, 110(1-2):92–112, 1997.

[19] H.N. Najm, P.S. Wyckoff, and O.M. Knio. A Semi-Implicit Numerical Scheme for Reacting Flow. I. Stiff Chemistry. *J. Comp. Phys.*, 143(2):381–402, July 1998.

[20] S. Paolucci. On the fi ltering of sound from the navier-stokes equations. SAND Report SAND82-8257, Sandia National Laboratories, Livermore, California, December 1982.

[21] S.V. Patankar. *Numerical Heat Transfer and Fluid Flow*, chapter 6. Hemisphere Pub. Corp., McGraw-Hill Co., New York, 1980.

[22] R. Pember. An adaptive projection method for unsteady, low-mach number combustion. *Combust. Sci. and Tech.*, 140:123–168, 1998.

[23] R.B. Pember, A.S. Almgren, J.B. Bell, P. Colella, L.H. Howell, and M.Lai. A higher-order projection method for the simulation of unsteady turbulent nonpremixed combustion in an industrial burner. Preprint UCRL-JC-118634, Lawrence Livermore National Laboratory, Livermore, CA, December 1994.

[24] R.B. Pember, L.H. Howell, J.B. Bell, P. Colella, W.Y. Crutchfi eld, W.A. Fiveland, and J.P. Jesse. An Adaptive Projection Method for the Modeling of Unsteady Low-Mach Number Combustion. Technical Report LBL-38551, Lawrence Berkeley National Laboratory, Berkeley, CA, October 1997.

[25] R.G. Rehm and H.R. Baum. The equations of motion for thermally driven, buoyant flows. *J. of Research of the National Bureau of Standards*, 83(3):297–308, May-June 1978.

[26] C. Rutland, J.H. Ferziger, and B.J. Cantwell. Effects of strain, vorticity, and turbulence on premixed flames. Report TF-44, Thermosciences Div., Mech. Eng., Stanford Univ., Stanford, CA, October 1989.

[27] C.J. Rutland and J.H. Ferziger. Simulations of flame-vortex interactions. *Combustion and Flame*, 84:343–360, 1991.

[28] G.I. Sivashinsky. Hydrodynamic theory of flame propagation in an enclosed volume. *Acta Astronautica*, 6:631–645, 1979.

[29] R. Temam. Sur l'approximation de la solution des ´equations de navier-stokes par la m´ethode des pas fractionnaires II. *Arch. Rat. Mech. Anal.*, 33:377–385, 1969.

[30] S. Turek. On discrete projection methods for the incompressible navier-stokes equations: An algorithmic approach. *Comput. Methods Appl. Mech. Eng.*, 143:271–288, 1997.

[31] F.A. Williams. *Combustion Theory*. Addison-Wesley, New York, 2nd edition, 1985.

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