A Non-Split Projection Strategy 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 semi-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 solver involved in the method. The method is then evaluated using the Modified KAP5 Problem, since it has some of the features of the low Mach number approximation. Numerical results are presented, confirming the validity of the strategy. A brief summary of ongoing efforts is finally provided.

KEY WORDS

Low Mach number flow, projection schemes, differential algebraic equations, DAE, half explicit method, HEM, modified KAP5 problem.
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 1 manifold [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 solvers 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 a 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 $\epsilon = \gamma M^2$, where $\gamma = c_p/c_v$ is the ratio of constant pressure/volume specific heats of the gas. Thus, for $\phi \in \{u, \rho, T, Y_i \mid i = 1, \ldots, N \}$,

$$\phi = \phi_0 + \epsilon \phi_1 + \epsilon^2 \phi_2 + \cdots \quad (2.1)$$

where $u$ is the velocity, $p$ is pressure, $\rho$ is density, $T$ is temperature, and $Y_i$ is the mass fraction of species $i$. One then finds the $\epsilon \to 0$ limit of the governing equations by retaining same order terms. As a result,
the zeroth-order limit of the momentum equations leads to
\[ \nabla p_0 = 0 \]  
(2.2)
where \( p_0 \), the zeroth-order term in \( \epsilon \), 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 in [15]. Ignoring body forces, radiant heat transfer and the Soret-Dufour effects [11], 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 with the equation of state. Using the perfect gas law (cf [19, 22]):

\[
\begin{align*}
\partial_t (\rho u) &= \text{div} \tau - \text{div} (\rho u \otimes u) - \text{grad} p \\
\partial_t T &= - \langle u, \text{grad} T \rangle + \frac{1}{\rho c_p} \text{div} (\alpha \text{grad} T) \\
\partial_t \rho &= - \langle u, \text{grad} \rho \rangle - \rho \text{div} u \\
\rho &= \frac{p_0}{RT}
\end{align*}
\]  
(2.3)

where \( \langle \cdot, \cdot \rangle \) and \( \otimes \) are, respectively, the standard euclidean inner and tensorial products, \( \tau \) 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:

\[
\begin{align*}
\partial_t (\rho u) &= \text{div} \tau - \text{div} (\rho u \otimes u) - \text{grad} p \\
D_t T &= \frac{1}{\rho c_p} \text{div} (\alpha \text{grad} T) \\
D_t \rho &= - \rho \text{div} u \\
\rho &= \frac{p_0}{RT}
\end{align*}
\]  
(2.4)

with \( D_t = \partial_t \cdot + \langle u, \text{grad} \cdot \rangle \).

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 significant 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 fields are decoupled or not. Coupled constructions are generally of superior order of accuracy, are solved implicitly, and require significant 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 first fractional step, the momentum equations are integrated forward in time without the pressure gradient term. The provisional velocity field computed in this step does not generally satisfy the divergence constraint provided by the continuity equation. The method then proceeds to find the pressure field by solving a pressure Poisson equation, derived by taking the divergence of the momentum equations and enforcing the continuity divergence constraint. This pressure field is then used in a second fractional step to project the provisional velocity field onto the submanifold determined by the divergence constraint, thereby arriving at the final velocity field 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 \( \rho u \) [16, 26, 27], Projection scheme
implementations update the \( \rho u \) field in the fractional steps, such that the pressure POISSON equation derivation requires simply the application of the continuity equation, substituting \( \partial p / \partial t \) for \( \nabla \cdot (\rho u) \), where \( \partial p / \partial t \) is found from the time integration of the density field. In this construction, the energy equation is used for updating the temperature field, and the density is retrieved from the state equation.

Alternative \( \rho u \) 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 \( \rho u \). 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 (2.3) is transformed by using (2.3):

\[
\begin{align*}
\partial_t (\rho u) & = \text{div} \tau - \text{div} (\rho u \otimes u) - \text{grad} p \\
\partial_t T & = -\langle u, \text{grad} T \rangle + \frac{1}{\rho c_p} \text{div}(\alpha \text{grad} T) \\
\partial_t \rho & = -\langle u, \text{grad} \rho \rangle - \rho \text{div} u \\
\text{div} u & = \frac{1}{T \rho c_p} \text{div}(\alpha \text{grad} T).
\end{align*}
\]

(2.5)

It is important to acknowledge here the fact that, because of the differentiation of the original state-equation constraint on \( \rho \), the resulting equations (2.5) with the divergence constraint are a weaker formulation than (2.3). Even though (2.5) has the same differential operator as (2.3), the constraint on \( \text{div} u \) is intrinsically weaker, i.e. results in a larger constraint submanifold, than that on \( \rho \). However, the main advantage is that one now has an explicit expression for \( \text{div} u \), 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 \( \text{div} u \). 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 (2.3). 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 (2.3) 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 \( \Omega \) and \([0, t_f] \) respectively denote the geometric domain of interest and the relevant time interval, the functions:

\[
\begin{align*}
\rho u : \Omega \times [0, t_f] & \rightarrow \mathbb{R}^{\dim \Omega} \\
T : \Omega \times [0, t_f] & \rightarrow \mathbb{R} \\
\rho : \Omega \times [0, t_f] & \rightarrow \mathbb{R} \\
p : \Omega \times [0, t_f] & \rightarrow \mathbb{R}
\end{align*}
\]

(3.1)

are substituted by the following:

\[
\begin{align*}
\tilde{\rho u} : [0, t_f] & \rightarrow \mathbb{R}^{N \dim \Omega} \\
\tilde{T} : [0, t_f] & \rightarrow \mathbb{R}^N \\
\tilde{\rho} : [0, t_f] & \rightarrow \mathbb{R}^N \\
\tilde{p} : [0, t_f] & \rightarrow \mathbb{R}^N
\end{align*}
\]

(3.2)

where \( N \) is the number of nodes of the grid. In this context, (2.3) implies that

\[
(\forall k \in \{1, \ldots, N\}) \quad \begin{cases}
\partial_t \tilde{\rho u}_k = A(\tilde{\rho}, \tilde{\rho u}) - B(\tilde{p}) \\
\partial_t \tilde{T}_k = C(\tilde{\rho}, \tilde{\rho u}, \tilde{T}) \\
\partial_t \tilde{\rho}_k = D(\tilde{\rho}, \tilde{\rho u}) \\
0 = R\tilde{\rho}_k \tilde{T}_k - \tilde{p}_0
\end{cases}
\]

(3.3)
where $A$, $B$, $C$ and $D$ are time-dependent functions of the vectorial unknowns depending on the space-discretization scheme. These functions can be assumed to have sufficient regularity (e.g., polynomial interpolants). Finally, defining $y$ as $(\rho, \rho \bar{u}, T)$, this yields:

$$
\begin{align*}
\forall k \in \{1, \ldots, N\} \quad \begin{cases} 
\partial_t y_k &= f_k(y, \rho) \\
0 &= g_k(y_k)
\end{cases} \\
(\forall k \in \{1, \ldots, N\} \quad \begin{cases} 
\partial_t y &= f(y, z) \\
0 &= g(y)
\end{cases}
\end{align*} \tag{3.4}
$$

or, with $z = \rho$,

$$
\begin{align*}
\begin{cases} 
\partial_t y &= f(y, z) \\
0 &= g(y)
\end{cases}
\end{align*} \tag{3.5}
$$

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. $C^0(\mathbb{R}^n, \mathbb{R}^m)$), the following system of equations with unknowns $y$ in $C^0(\mathbb{R}_+, \mathbb{R}^n)$ and $z$ in $C^0(\mathbb{R}_+, \mathbb{R}^m)$:

$$
\begin{align*}
\begin{cases} 
y' &= f(y, z) \\
0 &= g(y, z)
\end{cases} \\
(y_0, z_0) &= (y(0), z(0))
\end{align*} \tag{3.6}
$$

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

$$
\frac{dy}{dt}(y) \cdot f(y, z) = g(y) \cdot f(y, z) = 0, \tag{3.7}
$$

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 $\text{Ker}g$, the kernel of $g$ (cf. [11]).

Indeed, (3.5) 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:

$$
\begin{align*}
\begin{cases} 
\varphi_1'(t) &= f_1(t) + p(t) \\
\varphi_2(t) &= f_2(t, \varphi_2(t)) + \varphi_1(t) \\
0 &= \varphi_2(t) - 1
\end{cases} \\
(\varphi_{i0}, 1) &= (\varphi_1(0), \varphi_2(0))
\end{align*} \tag{3.8}
$$

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 (3.8) has a solution $(\varphi_1, \varphi_2, p) \in C^1 \times C^1 \times C^0$ given by

$$
\begin{align*}
\forall t \in \mathbb{R} \\
\varphi_1(t) &= \varphi_{i0} + \int_0^t f_1(s) + p(s) \, ds \\
\varphi_2(t) &= 1
\end{align*} \tag{3.9}
$$

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

**Proof.** Since $f_1$ and $f_2$ are $C^1$ functions, $p$ is $C^0$, then $\varphi_1$ is also $C^1$ and is given by:

$$
\begin{align*}
\forall t \in \mathbb{R} \\
\varphi_1(t) &= \varphi_{i0} + \int_0^t (f_1(s) + p(s)) \, ds
\end{align*} \tag{3.10}
$$

Now, the second differential equation implies that $\varphi_2$ is also $C^1$ and

$$
\forall t \in \mathbb{R} \\
\varphi_2(t) = \varphi_2(0) + \int_0^t (f_2(s, \varphi_2(s)) + \varphi_1(s)) \, ds
$$

(3.11)
Enforcing the constraint and the consistency of the initial conditions, it follows that

$$
(\forall t \in \mathbb{R}) \quad \int_0^t (f_2(s, 1) + \varphi_1(s)) \, ds = 0 \quad (3.12)
$$
whence

$$
(\forall t \in \mathbb{R}) \quad f_2(t, 1) + \varphi_1(t) = 0. \quad (3.13)
$$

Finally, combining (3.13) with the first equation of (3.8) yields

$$
(\forall t \in \mathbb{R}) \quad p(t) = -\partial_t f_2(t, 1) - f_1(t). \quad (3.14)
$$

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 scheme we intend to use to solve (2.3) is the Half-Explicit s-stage Method (HEM), introduced by [10] in order to integrate DAE2 systems. It can be stated as follows:

$$
(\forall i \in \{1, \ldots, s\}) \quad \begin{cases}
Y_i = y_0 + h \sum_{j=1}^{i-1} a_{ij} f(Y_j, Z_j) \\
0 = g(Y_i) \\
y_1 = y_0 + h \sum_{j=1}^s b_j f(Y_j, Z_j) \\
0 = g(y_1)
\end{cases} \quad (3.15)
$$

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 coefficients in order to get order 4 time-accuracy for $y$ with a $s = 5$ steps scheme:

$$(a_{ij}) = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
\frac{3}{10} & 0 & 0 & 0 & 0 \\
\frac{1+4\sqrt{3}}{30} & \frac{11-4\sqrt{3}}{30} & 0 & 0 & 0 \\
\frac{-79+11\sqrt{3}}{180} & \frac{24+11\sqrt{3}}{90} & \frac{-9+7\sqrt{3}}{4} & 0 & 0 \\
\frac{150+5\sqrt{3}}{180} & \frac{8+7\sqrt{3}}{6} & \frac{-9-7\sqrt{3}}{4} & \frac{9-\sqrt{3}}{4} & 0
\end{pmatrix}
$$

and

$$(b_i) = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & \frac{16}{36} & \frac{16}{36} & \frac{1}{9} & 0 \\
0 & \frac{1}{10} & \frac{4+\sqrt{3}}{10} & \frac{4+\sqrt{3}}{10} & \frac{1}{9} & 0 \\
0 & \frac{1}{10} & \frac{4-\sqrt{3}}{10} & \frac{4-\sqrt{3}}{10} & \frac{1}{9} & 0 \\
0 & \frac{1}{10} & \frac{4+\sqrt{3}}{10} & \frac{4-\sqrt{3}}{10} & \frac{1}{9} & 0
\end{pmatrix}
$$

thus

$$(c_i) = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
\frac{3}{10} & \frac{4-\sqrt{3}}{10} & \frac{4+\sqrt{3}}{10} & \frac{1}{9} & 0 \\
0 & \frac{1}{10} & \frac{4+\sqrt{3}}{10} & \frac{4-\sqrt{3}}{10} & \frac{1}{9} & 0 \\
0 & \frac{1}{10} & \frac{4+\sqrt{3}}{10} & \frac{4-\sqrt{3}}{10} & \frac{1}{9} & 0 \\
0 & \frac{1}{10} & \frac{4+\sqrt{3}}{10} & \frac{4-\sqrt{3}}{10} & \frac{1}{9} & 0
\end{pmatrix}
$$

Remark 3.2. The $(c_i)$ coefficients do not appear explicitly in the scheme as stated in 3.15, they indicate the time increments corresponding to each stage. For example, $Y_2$ is an approximation of $y(t_0 + \frac{3}{10}h)$. These coefficients will in fact be used later, when extrapolating the initial guesses for the $Z_i$.

3.4. An Equivalent Formulation of the Scheme

Contrary to appearances, the implicitness of (3.15) 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 (3.15), 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 (3.15) is equivalent to:

$$
(\forall i \in \{1, \ldots, s-1\}) \quad \begin{cases}
X_i = y_0 + h \sum_{j=1}^{i-1} a_{i+1,j} f(Y_j, Z_j) \\
0 = g(X_i + h a_{i+1,1} f(Y_1, Z_1)) \\
Y_{i+1} = X_i + h a_{i+1,i} f(Y_i, Z_i) \\
X_s = y_0 + h \sum_{j=1}^s b_j f(Y_j, Z_j) \\
0 = g(X_s + h b_s f(Y_s, Z_s)) \\
y_1 = X_s + h b_s f(Y_s, Z_s)
\end{cases} \quad (3.19)
$$

Proof. It follows directly from (3.15) that, at each stage $i \in \{1, \ldots, s-1\}$, $Z_i$ must be a solution of the following non-linear equation in the unknown $z$:

$$
g \left( y_0 + h \sum_{j=1}^{i-1} a_{i+1,j} f(Y_j, Z_j) + h a_{i+1,i} f(Y_i, z) \right) = 0 \quad (3.20)
$$

and that $Z_s$ must be a solution of

$$
g \left( y_0 + h \sum_{j=1}^{s-1} b_j f(Y_j, Z_j) + h b_s f(Y_s, z) \right) = 0. \quad (3.21)
$$
thus, (3.20) and (3.21) imply that

\[(\forall i \in \{1, \ldots, s-1\}) \quad g(X_i + k_i f(Y_i, Z_i)) = 0,\]

which proves the sufficient condition.

Conversely, if (3.19) is satisfied, then so are (3.20) and (3.21), except for the case \(i = 1\), corresponding to the initial consistency condition \(g(y_0) = 0\) which is true by hypothesis.

\[\square\]

**Remark 3.3.** This new formulation of the HEM scheme explicitly requires the consistency of \(y_0\), but this condition is also present, albeit implicitly, in (3.15).

### 3.5. Practical Implementation Issues

Clearly, (3.19) 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 (3.19) at any stage \(i\) using an exact Newton algorithm would evaluate the derivative of \(\phi_i(z) = g(X_i + h \theta + f(Y_i, z))\), given by:

\[
\frac{\partial \phi_i}{\partial z}(z) = h \theta + f(Y_i, z) \cdot \frac{\partial f}{\partial z}(Y_i, z).
\]

Evaluating \(\frac{\partial \phi_i}{\partial z}(z)\) 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: \(\frac{\partial \phi_i}{\partial z}(z)\) 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 (3.7). Nevertheless, according to (3.19), \(g(y_0 + h \theta + f(y_0, Z_1)) = 0\), 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 automatically 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 \(\text{Ker}g\): either arbitrarily, in which case there is an infinite number of ways to proceed, or with respect to some direction, e.g., one which makes sense physically.

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### 4. NUMERICAL TEST: THE MODIFIED KAPS PROBLEM

The Modified 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.

#### 4.1. Statement of the Problem

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

\[
\begin{cases}
  y'_1 &= -(2 + \varepsilon^{-1})y_1 + \varepsilon^{-1}y_2^2 \\
  y'_2 &= -\exp(1 - z^2) \\
  y_2^2 &= y_1 \exp(\alpha(1 - \cos(y_1 - y_2^2))) \\
  y_1(0) &= 1 \\
  y_2(0) &= 1 \\
  z(0) &= 1.
\end{cases}
\]

(\(\forall t \in \mathbb{R}_+\))

(4.1)

The eigenvalues of \(\frac{\partial f}{\partial y_1}\) are 0 and \(-(2 + \varepsilon^{-1})\), thus can be made as distant from each other as desired. In addition, \(\alpha\) allows modification of the submanifold geometry. Moreover, MK has the following analytical solution:

\[
\begin{cases}
  y_1(t) &= e^{-2t} \\
  y_2(t) &= e^{-t} \\
  y_3(t) &= \sqrt{1 + t}
\end{cases}
\]

(4.2)

which is independent of both \(\alpha\) and \(\varepsilon\). These features make MK an excellent test case for DAE2 schemes.

#### 4.2. The Constraints

By definition, the index 2 submanifold \(\text{Ker}g\) depends solely on the parameter \(\alpha \in \mathbb{R}\). For all \(\alpha\), \(y_1 = y_2^2\) implies \(g(y_1, y_2) = 0\) thus the parabola \(P: y_1 = y_2^2\) is a submanifold of \(\text{Ker}g\); moreover, the analytical solution of MK belongs to \(P\) by inspection. In fact, the geometry of \(\text{Ker}g\) becomes increasingly complicated as \(|\alpha|\) grows, but \(P\) 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,