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A PRESSURE CORRECTION LOCAL DEFECT CORRECTION ALGORITHM FOR LAMINAR FLAME SIMULATION

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Abstract. We present a numerical algorithm to solve the zero-Mach number approximation of the governing equations for laminar flames. The ingredients of the algorithm are a Pressure Correction (PC) method to decouple the computation of velocity and pressure, and a multi-level Local Defect Correction (LDC) method to solve the resulting set of (non)linear boundary value problems. The PC method is based on a constraint equation, rather than the continuity equation, describing expansion of the gas mixture due to combustion. Moreover, we combine the PC method with implicit Euler time integration to compute steady flames. Boundary value problems for laminar flames are characterised by a high activity region, the so-called flame front, where the solution varies rapidly. The basic idea of the LDC method is to compute a global coarse grid solution, that is accurate enough to represent the solution outside the flame front, and a sequence of local fine grid solutions to capture all the details in the flame front. Moreover, these fine grid solutions are subsequently used to improve the coarse grid solution by a defect correction technique. We have applied our PC LDC algorithm to simulate a two-dimensional methane/air flame.

1 INTRODUCTION

Numerical simulation codes for laminar flames are a useful tool to study flames and/or design burning devices. With the ever increasing power of modern computers, it is nowadays possible to simulate realistic combustion phenomena; see e.g. [6]. However, numerical flame simulation is still a demanding task, for several reasons. First, in a flame many reactions take place involving many different species, and conservation laws for each of these have to be solved. Consequently, the mathematical model consists of a large set of partial differential equations in two- or even three-dimensional space. Second, the governing equations are extremely stiff, meaning that they allow for solutions with largely varying
time and space scales. More specifically, very rapid variations occur in the flame front, which is a very thin zone between the unburnt and burnt gases where all the reactions and heat production takes place, whereas outside the flame front the solution is almost constant. A third difficulty is that the chemical source terms are extremely nonlinear in the temperature. Finally, transport models, e.g., for heat flux or mass diffusion, are often very complicated and result in many coupling terms in the set of governing equations.

A numerical method for laminar flame simulation should at least satisfy the following requirements. First, a nonuniform grid is absolutely mandatory in order to capture the detailed structure of the flame front. Second, space discretisation methods should be accurate in all regimes of the flow. Third, time integration methods should be efficient and be able to handle stiff equations. Recently, time splitting methods have been applied in flame simulations; see e.g. [25]. The basic idea is to split the set of governing equations in several subsystems, for the sake of time integration, such that the different subsystems can be solved efficiently; see e.g. [19] for a detailed account. Fourth, iterative solution methods for (nonlinear) algebraic systems should be fast, and in particular, robust. Finally, a projection method to decouple the pressure and velocity computation is highly desirable. Projection methods were initially introduced for incompressible flow, but are nowadays also widely used in the numerical simulation of low-Mach number compressible flow and flames; see e.g. [1].

A lot of research on all these numerical techniques needed for flame simulation is going on, although not always in the context of flame simulation. In this paper we focus on one aspect of flame simulation, i.e., local grid refinement methods for boundary value problems (BVPs) characterised by a high activity region. There are basically two options, i.e., unstructured versus structured grids. Unstructured grids are often used in combination with the FEM and applied to myriad problems. FEM simulations of laminar flames on unstructured grids are presented in e.g. [9, 11]. A finite difference method leading to unstructured grids is the Local Rectangular Refinement (LRR) method [7, 8]. This method uses a rectangular grid with ending grid lines, that require special discretisation stencils. On the other hand, the so-called Adaptive Mesh Refinement (AMR) methods [1] are based on structured, rectangular grids, possibly even uniform. AMR in combination with time splitting and a projection method is applied to laminar flames in [12]. The references cited above are a short list of recent publications, that is certainly not exhaustive.

Local uniform grids have several advantages over nonuniform grids: they can be represented by simple data structures, allow accurate discretisation methods and there exist efficient iterative solution methods for the resulting algebraic systems. For these reasons, we restrict ourselves to uniform grids, and the solution method we employ is the Local Defect Correction (LDC) method. The basic idea of the method is as follows. First, we compute the solution on a global coarse grid, that is fine enough to represent the solution outside the flame front. However, this coarse grid is certainly not fine enough to capture the detailed structure of the flame inside the flame front. Therefore, we cover the flame front with a sequence of local fine grids, and recompute the solution there using Dirichlet
boundary data from the next coarser grid solution. Finally, we use the fine grid solutions to improve the coarse grid solution by a defect correction technique. The LDC method is developed and analysed for elliptic boundary value problems in, e.g., [13, 2, 3, 15], and further extended to parabolic initial boundary value problems in [23, 24]. Applications to flame simulation are presented in, e.g., [16], where the method is used to solve the thermodiffusive model, and in [4], to solve the streamfunction-vorticity formulation of a diffusion flame.

We have organized the remainder of our paper as follows. In section 2 we briefly summarize the governing equations. We describe the pressure correction algorithm for these equations in Section 3. Next, in Section 4 we give an outline of the multi-level LDC method, and subsequently in Section 5, we apply it to the BVPs derived in Section 3. Application of our method to a two-dimensional steady methane/air flame is given in Section 6. Conclusions are formulated in Section 7.

2 GOVERNING EQUATIONS

In this section we present a mathematical model for laminar, premixed flames under atmospheric conditions. Typically, we consider the combustion of hydrocarbons in air. The species in the flame are numbered 1 through $N_s$. Species $N_s$ is nitrogen and is present in abundance, while the other species are considered trace species. The governing equations for such flames are the conservation equations of mass, momentum and energy of the gas mixture and the balance equations of mass for the trace species. These equations can be written in the following form [26, 28]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

(1a)

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \mathbf{T} + \rho \mathbf{g},$$

(1b)

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{v} h) - \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h \right) = \nabla \cdot \mathbf{J}_h,$$

(1c)

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) - \frac{1}{Le_i} \nabla \cdot \left( \frac{\lambda}{c_p} \nabla Y_i \right) = \omega_i, \quad (i = 1, 2, \ldots, N_s - 1).$$

(1d)

The independent variables in (1) are the density $\rho$, the flow velocity $\mathbf{v}$, the hydrostatic pressure $p$, the specific enthalpy $h$ and the species mass fractions $Y_i$. Other variables/constants in (1) are the (Newtonian) stress tensor $\mathbf{T}$, the gravitational acceleration $\mathbf{g}$, the thermal conductivity $\lambda$, the specific heat at constant pressure $c_p$, the enthalpy diffusion flux $\mathbf{J}_h$, the Lewis numbers $Le_i$, assumed to be constant, and the reaction rates $\omega_i$. The main assumptions underlying system (1) are, first, the gas mixture is Newtonian, second, heat transport is only determined by conduction and diffusion, and third, a generalization of Fick’s law holds for mass diffusion. As a consequence of the latter two
assumptions, the enthalpy diffusion flux $J_h$ is given by

$$J_h = \frac{\lambda}{c_p} \sum_{i=1}^{N_s-1} \left( \frac{1}{Le_i} - 1 \right) (h_i - h_{N_s}) \nabla Y_i,$$

with $h_i$ the specific enthalpy of the $i$th species. The first two equations in (1) are referred to as the flow equations and the latter two as the combustion equations. Note, that we only have to solve the conservation laws for the first $N_s - 1$ species and that the mass fraction of the last species follows from the constraint $\sum_{i=1}^{N_s} Y_i = 1$.

The conservation equations (1) have to be completed with the caloric equation of state

$$h = h_T + \sum_{i=1}^{N_s-1} h_{i,ref} Y_i, \quad h_T := \int_{T_{ref}}^{T} c_p(T', Y_1, Y_2, \ldots, Y_{N_s}) \, dT',$$

which defines $h$ as a function of the temperature $T$ and the species mass fractions $Y_i$, and the thermal equation of state

$$p_{amb} = \frac{\rho RT}{M}, \quad \frac{1}{M} = \sum_{i=1}^{N_s} \frac{Y_i}{M_i}.$$ 

The variables $h_T$ and $h_{i,ref}$ in (3a) are the specific thermal enthalpy and the specific enthalpies of formation at reference temperature $T_{ref}$, respectively. Furthermore in (3b), $R$ is the universal gas constant, $M$ the average molar mas of the gas mixture and $M_i$ the molar mass of species $i$. The pressure $p$ is set to the ambient pressure $p_{amb}$ in (3b), which is valid for zero-Mach number flows [10].

Using the thermal equation of state (3b), we can express the density $\rho$ as a function of the combustion variables $T$ and $Y_i$. Applying the material derivative $D/Dt := \partial/\partial t + \mathbf{v} \cdot \nabla$ to this relation and eliminating $D\rho/Dt$ from the continuity equation (1a), we obtain a constraint equation of the form

$$\nabla \cdot \mathbf{v} = s,$$

where $s$ describes expansion of the gas mixture due to conduction, diffusion and heat production. It is given by

$$s = \frac{1}{T} \frac{DT}{Dt} - \frac{1}{M} \frac{DM}{Dt}$$

$$= \frac{1}{\rho c_p T} \left( \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h \right) + \nabla \cdot J_h \right) +$$

$$+ \frac{1}{\rho} \sum_{i=1}^{N_s-1} \left( M \left( \frac{1}{M_i} - \frac{1}{M_{N_s}} \right) - h_{i,ref} \frac{1}{c_p T} \right) \left( \frac{1}{Le_i} \nabla \cdot \left( \frac{\lambda}{c_p} \nabla Y_i \right) + \omega_i \right).$$

We have derived the second equality in (4b) by replacing the material derivatives by expressions obtained from the combustion equations (1c), (1d) and the caloric equation
of state (3a). Note that expansion of the mixture due to pressure variations is not taken into account by virtue of the assumption that $p = p_{amb}$ in (3b). Equation (4a) is referred to as the expansion equation and will replace the continuity equation.

Summarizing, our model for laminar flames consists of the momentum equations (1b), the combustion equations (1c) and (1d), the expansion equation (4a) and the equations of state (3).

Finally, we note that we can derive an elliptic equation for the pressure as follows. Writing the Navier-Stokes equations (1b) in convective form, applying the divergence operator and combining the resulting equation with the expansion equation (4a), we obtain

$$\nabla \cdot \left( \frac{1}{\rho} \nabla p \right) = \nabla \cdot \left( \frac{1}{\rho} \nabla \cdot \mathbf{T} \right) - \left( \frac{Ds}{Dt} + s^2 \right) + 2\Phi + \frac{1}{2} |\mathbf{\omega}|^2,$$

(5a)

where the variable $\Phi$ is the second invariant of the deformation tensor $E = (e_{ij})$, defined by [5]

$$\Phi := (e_{11}e_{22} - e_{12}e_{21}) + (e_{11}e_{33} - e_{31}e_{13}) + (e_{22}e_{33} - e_{23}e_{32}),$$

(5b)

and where $\mathbf{\omega} := \nabla \times \mathbf{v}$ is the vorticity.

3 SEMI-DISCRETE FORMULATION

We apply the transverse method of lines [22], i.e., discretise the time derivatives first, to derive a set of boundary value problems for velocity, pressure and all combustion variables. Moreover, we employ the pressure correction method to decouple the velocity and pressure computation.

Consider the governing equations (1b)-(1d) in convective form, together with the expansion equation (4a). Introducing the species mass fraction vector $\mathbf{Y} := (Y_1, \ldots, Y_{N_s-1})^T$ and the combustion variables vector $\mathbf{\psi} := (T, Y_1, \ldots, Y_{N_s-1})^T$, these equations can be written in the symbolic form

$$\frac{\partial \mathbf{v}}{\partial t} = \mathbf{F}_1[\mathbf{v}, \mathbf{\psi}] - \rho^{-1}(\mathbf{\psi})\nabla p,$$

(6a)

$$\frac{\partial h(\mathbf{\psi})}{\partial t} = \mathbf{F}_2[\mathbf{v}, \mathbf{\psi}],$$

(6b)

$$\frac{\partial \mathbf{Y}}{\partial t} = \mathbf{F}_3[\mathbf{v}, \mathbf{\psi}],$$

(6c)

$$\nabla \cdot \mathbf{v} = s(\mathbf{\psi}),$$

(6d)

where $\mathbf{F}_1$, $\mathbf{F}_2$ and $\mathbf{F}_3$ are spatial differential operators. Note that we have explicitly denoted the dependence of $\rho$, $h$ and $s$ on the combustion variables $\mathbf{\psi}$. Obviously, these equations should be coupled to the equations of state (3). System (6a)-(6c) is very stiff, mainly due to the chemical source terms, implying we should use an implicit time integration method. Moreover, we have to enforce the expansion equation (6d) at each time.
level. For time accurate computations, IMEX multistep methods are very suitable; see [19]. However, in this paper we apply the method of false transient [22] to compute the steady solution of (6), for which the implicit Euler method is most appropriate.

Thus, applying the implicit Euler time integration method to (6) we have

$$\frac{1}{\Delta t}(v^{n+1} - v^n) - \mathcal{F}_1[v^{n+1}, \psi^{n+1}] + \rho^{-1}(\psi^{n+1})\nabla p^{n+1} = 0, \quad (7a)$$

$$\frac{1}{\Delta t}(h(\psi^{n+1}) - h(\psi^n)) - \mathcal{F}_2[v^{n+1}, \psi^{n+1}] = 0, \quad (7b)$$

$$\frac{1}{\Delta t}(Y^{n+1} - Y^n) - \mathcal{F}_3[v^{n+1}, \psi^{n+1}] = 0, \quad (7c)$$

$$\nabla \cdot v^{n+1} = s(\psi^{n+1}), \quad (7d)$$

where $v^n$ denotes the semi-discrete approximation of $v(x, t^n)$ at the time level $t^n := n\Delta t$, with $\Delta t > 0$ the time step; etc. Note that (7) is a system of PDEs independent of the time $t$. One of the difficulties associated with this system is the coupling between the velocity field $v^{n+1}$ and the pressure field $p^{n+1}$ in equation (7a). Therefore, we apply a pressure correction technique to (7) as follows; see e.g., [20]. First, we define a predictor $v^*$ for the velocity field $v^{n+1}$ by replacing $p^{n+1}$ in (7a) by $p^n$. This way we obtain for $v^*$ and $\psi^{n+1}$ the following system

$$\frac{1}{\Delta t}(v^* - v^n) - \mathcal{F}_1[v^*, \psi^{n+1}] + \rho^{-1}(\psi^{n+1})\nabla p^n = 0, \quad (8a)$$

$$\frac{1}{\Delta t}(h(\psi^{n+1}) - h(\psi^n)) - \mathcal{F}_2[v^*, \psi^{n+1}] = 0, \quad (8b)$$

$$\frac{1}{\Delta t}(Y^{n+1} - Y^n) - \mathcal{F}_3[v^*, \psi^{n+1}] = 0. \quad (8c)$$

Next, we replace the term $\mathcal{F}_1[v^{n+1}, \psi^{n+1}]$ in (7a) by its predictor $\mathcal{F}_1[v^*, \psi^{n+1}]$, defining the corrector for $v^{n+1}$. Denoting this by $v^{n+1}$ as well, we find

$$\frac{1}{\Delta t}(v^{n+1} - v^n) - \mathcal{F}_1[v^*, \psi^{n+1}] + \rho^{-1}(\psi^{n+1})\nabla p^{n+1} = 0. \quad (9)$$

Subtracting equation (8a) from (9) we find the relation

$$\frac{1}{\Delta t}(v^{n+1} - v^*) + \rho^{-1}(\psi^{n+1})\nabla q^n = 0, \quad q^n := p^{n+1} - p^n. \quad (10)$$

Finally, applying the divergence operator to (10) and using the constraint (7d), we obtain the following elliptic equation for the pressure increment $q^n$

$$\nabla \cdot (\rho^{-1}(\psi^{n+1})\nabla q^n) = \frac{1}{\Delta t}(\nabla \cdot v^* - s(\psi^{n+1})). \quad (11)$$
We will refer to this equation as the pressure equation. Note that it is similar to equation (5a) for the pressure.

Summarizing, we have the following algorithm.

PC algorithm

1. Solve system (8) for the predictor velocity $v^*$ and the combustion variables $\psi^{n+1}$.
2. Solve equation (11) for the pressure update $q^n$. 
3. Update the pressure and compute the corrector velocity $v^{n+1}$ from (10).

4 MULTI-LEVEL LDC

In this section we present an outline of multi-level LDC; for a more detailed account see, e.g., [2, 3, 13]. Thus, consider on a simply connected domain $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) the boundary value problem (BVP)

\[
\mathcal{N}[u] = 0, \quad x \in \Omega, \\
\mathcal{B}[u] = g, \quad x \in \partial \Omega,
\]

where $\mathcal{N}$ is a nonlinear elliptic differential operator and $\mathcal{B}$ a boundary operator, either of Dirichlet or Neumann type. We cover $\Omega$ with a global uniform coarse grid $\Omega_{h_0}$, of grid size $h_0$, and apply a discretisation method resulting in the nonlinear system

\[
\mathcal{N}_{h_0}[u_{h_0}] = f_{h_0}, \quad x \in \Omega_{h_0},
\]

where $u_{h_0}$ is the grid function representing all unknowns on $\Omega_{h_0}$ and where the right-hand side $f_{h_0}$ contains the boundary data $g$. Applying an iterative solution method to (13), we obtain the approximation $u_{h_0}^0$.

Suppose, the solution $u$ of (12) changes very rapidly in a small subdomain of $\Omega$, the so-called high activity region, whereas outside this region $u$ is very smooth. In this high activity region, the grid size $h_0$ is definitely too coarse to capture the detailed structure of $u$. Therefore, we introduce a local subdomain $\Omega_\ell \subset \Omega$ enclosing the high activity region and cover $\Omega_\ell$ with a sequence of nested, local uniform grids $\Omega_{\ell,h_k}$ of grid size $h_k$ ($k = 1, 2, \ldots, k_{\text{max}}$) as shown in Figure 1. Obviously, $h_0 > h_1 > \ldots > h_{\text{max}}$, otherwise the refinement factors $\sigma_k = h_k/h_{k-1}$ ($k = 1, 2, \ldots, k_{\text{max}}$) are arbitrary. Let $\Gamma_{h_k}$ be the set of boundary points of $\Omega_{\ell,h_k}$, that are not on the Dirichlet boundary. We will subsequently solve discrete BVPs on $\Omega_{\ell,h_k}$ for $k = 1, 2, \ldots, k_{\text{max}}$, that are defined by the discretisation of equation (12a) on $\Omega_{\ell,h_k}$, possibly the boundary condition on $\partial \Omega_\ell \cap \partial \Omega$ and the interface condition on $\Gamma_{h_k}$, i.e.,

\[
\begin{align*}
  u &= b_{h_1} := \mathcal{P}^{h_1,h_0}[u_{h_0}], \quad x \in \Gamma_{h_1}, \\
  u &= b_{h_k} := \mathcal{P}^{h_k,h_{k-1}}[u_{\ell,h_{k-1}}], \quad x \in \Gamma_{h_k}, \quad (k = 2, 3, \ldots, k_{\text{max}}),
\end{align*}
\]
Figure 1: A global coarse and three local fine grids.

where $\mathcal{P}^{h_k} (k = 2, 3, \ldots, k_{\text{max}})$ is an interpolation operator that maps the local grid function $u_{\ell,h_k}$ onto a grid function on $\Gamma_h$; a similar definition holds for $\mathcal{P}^{h_0}$. The discrete BVPs on $\Omega_{\ell,h_k}$ then read

$$\mathcal{N}_{\ell,h_k} [u_{\ell,h_k}; b_{h_k}] = f_{\ell,h_k}, \quad x \in \Omega_{\ell,h_k}, \quad (k = 1, 2, \ldots, k_{\text{max}}),$$  \hspace{1cm} (15)

where $u_{\ell,h_k}$ is the local grid function of unknowns on $\Omega_{\ell,h_k}$ and $f_{\ell,h_k}$ is the grid function containing the boundary data $g$ on $\partial \Omega_{\ell} \cap \partial \Omega$. Note that the dependence of $u_{\ell,h_k}$ on the solution $u_{\ell,h_{k-1}}$ at one coarser level is explicitly denoted by the interface condition $b_{h_k}$. We denote the numerically computed solutions of (15) by $u_{\ell,h_k}^0 (k = 1, 2, \ldots, k_{\text{max}})$.

Next, we use the fine grid solutions $u_{\ell,h_k} (k = 1, 2, \ldots, k_{\text{max}})$ to improve the accuracy of the global coarse grid solution $u_{h_0}$. To this end we have to estimate the local discretisation error of the coarse grid problem (13) and of the fine grid problems (15) for $k = 1, 2, \ldots, k_{\text{max}} - 1$, which are defined as, respectively,

$$d_{h_0} := \mathcal{N}_{h_0} [u] - f_{h_0},$$  \hspace{1cm} (16a)

$$d_{h_k} := \mathcal{N}_{\ell,h_k} [u ; b_{h_k}] - f_{\ell,h_k}, \quad (k = 1, 2, \ldots, k_{\text{max}} - 1),$$  \hspace{1cm} (16b)

where $u$ is the exact solution of (12) and where the interface conditions $b_{h_k}$ are computed from (14) with $u_{h_0}$ replaced by $u$. Therefore, we replace $u$ in (16) by the fine grid solution $u_{\ell,h_{k+1}}^0$ at one level finer, wherever available, restricted to $\Omega_{\ell,h_k}$. This way we obtain the local defects $\mathcal{D}[u_{h_0}^0; u_{\ell,h_1}^0]$ and $\mathcal{D}[u_{\ell,h_k}^0; u_{\ell,h_{k+1}}^0] (k = 1, 2, \ldots, k_{\text{max}} - 1)$ as approximations of the local discretisation error on $\Omega_{\ell,h_0} := \Omega_{\ell} \cap \Omega_{h_0}$ and $\Omega_{\ell,h_k} (k = 1, 2, \ldots, k_{\text{max}} - 1)$, respectively. At grid points of $\Omega_{\ell,h_k}$ where the (restriction of the) solution $u_{\ell,h_{k+1}}^0$ is not available, we set $\mathcal{D}[u_{\ell,h_k}^0; u_{\ell,h_{k+1}}^0] = 0$. Once we have computed the defects, we add these to the corresponding systems, to get for $i = 0$,

$$\mathcal{N}_{h_0} [u_{h_0}] = f_{h_0} + \mathcal{D}[u_{h_0}^0; u_{\ell,h_1}^i], \quad x \in \Omega_{h_0},$$  \hspace{1cm} (17a)

$$\mathcal{N}_{\ell,h_k} [u_{\ell,h_k}; b_{h_k}] = f_{\ell,h_k} + \mathcal{D}[u_{\ell,h_k}^0; u_{\ell,h_{k+1}}^i], \quad x \in \Omega_{\ell,h_k} (k = 1, 2, \ldots, k_{\text{max}} - 1).$$  \hspace{1cm} (17b)
We subsequently solve (17) iteratively for $k = k_{\max} - 1, k_{\max} - 2, \ldots, 0$, to find the approximations $u_{h_0}^1$ and $u_{\ell,h_k}^1 (k = 1, 2, \ldots, k_{\max} - 1)$, that are presumably better approximations than their zeroth order counterparts. These solutions can again be used to compute interface conditions, new fine grid solutions; etc.

This procedure gives rise to the following algorithm; see also Figure 2.

**Multi-level LDC algorithm**

a. Initialization, $i = 0$

- Solve the basic coarse grid problem (13) for $u_{h_0}^i$
- For $k = 1, 2, \ldots, k_{\max}$ do
  - Compute the interface condition (14) for $u_{\ell,h_k}$
  - Solve the fine grid problem (15) for $u_{\ell,h_k}^i$

b. Iteration, $i = 1, 2, \ldots$

- For $k = k_{\max} - 1, k_{\max} - 2, \ldots, 0$ do
  - Compute the defect $D[u_{\ell,h_k}^{i-1}, u_{\ell,h_k+1}^{i-1}]$ or $D[u_{h_0}^0, u_{\ell,h_1}^0]$.
  - Solve the updated problem (17) for $u_{\ell,h_k}$ or $u_{h_0}$.
- For $k = 1, 2, \ldots, k_{\max}$ do
  - Compute the interface condition (14) for $u_{\ell,h_k}$
  - Solve the fine grid problem (15) for $u_{\ell,h_k}^i$

Convergence of this algorithm is very fast, usually only one or two iterations are needed for convergence [3]. The final solution is the composite grid solution, i.e., the solution at the finest level available.

To demonstrate the feasibility of LDC, consider the following two-point BVP

\begin{align*}
  u'' + f(u) &= 0, \quad 0 < x < 1, \quad (18a) \\
  u(0) &= u_{\ell}, \quad u(1) = u_r, \quad (18b)
\end{align*}

with $f(u) := 2\alpha^2 u(1-u)(u - \frac{1}{2})$. The solution of (18) is of the form

\[ u(x) = \frac{1}{2} \left( 1 + \tanh(\alpha(x - x_0)) \right), \]

characterised by an interior layer at $x = x_0$ when $\alpha \gg 1$. We have computed a numerical solution of (18) for the parameter values $x_0 = 0.33$ and $\alpha = 25$. For space discretisation we use the standard central difference scheme. We have computed a global coarse grid solution with $H = 1/16$ and a local fine grid solution on $\Omega_\ell := (0.2, 0.5)$ with $h = 1/64$ to resolve the interior layer, the results of which are shown in Figure 3. The left figure
shows the results before defect correction. Clearly, the coarse grid solution is poor in the entire domain, and consequently, the interface conditions for the fine grid solution are very inaccurate. The fine grid solution does not really improve the accuracy of the coarse grid solution. However, in $\Omega_\ell$ the structure of the fine grid solution is a fair approximation of the interior layer, although the absolute errors are still large. The right figure shows the composite grid solution after one iteration step. Obviously, this solution is much better than the one before defect correction. More LDC iterations are not needed. Actually, we can show that in this case further iterations do not improve the solution [14].

Figure 2: Schematic representation of the initialization procedure and one iteration step of the four-level LDC method. The meaning of the identifiers is as follows: $S$ stands for solve discrete system, $I$ for computation interface conditions, $D$ for defect computation and $C$ for solve updated system.

Figure 3: Numerical solution of the two-point BVP (18) before (left) and after (right) defect correction.
5 LDC FOR LAMINAR FLAMES

In this section we will combine the PC algorithm from Section 3 with the multi-level LDC algorithm from Section 4. In the PC algorithm, we have to solve two BVPs, i.e., one corresponding to system (8), to compute \( \mathbf{v}^*, \psi_h^{n+1} \), and one corresponding to the pressure equation (11), to compute \( q^n \). We will subsequently solve both BVPs using the LDC algorithm.

For (space)discretisation of (8) we use the cell-centred finite volume method on a staggered grid in combination with an exponential scheme for the computation of the numerical fluxes; for more details see [17, 18]. Moreover, for the pressure gradient at the cell boundaries we take the central difference scheme. We apply these discretisation schemes on a global coarse grid \( \Omega_{h_0} \) of typical grid size \( h_0 \), and on a sequence of local fine grids \( \Omega_{\ell,h_k} \) of typical grid size \( h_k \). This way, we obtain for (8) a nonlinear algebraic system on \( \Omega_{h_0} \), which can be symbolically written as

\[
\mathcal{N}_{h_0}[\mathbf{v}^*_{h_0}, \psi_{h_0}^{n+1}] = \mathbf{f}_{h_0}, \quad x \in \Omega_{h_0},
\]

where \( \mathbf{v}^*_{h_0}, \psi_{h_0}^{n+1} \) and \( \mathbf{f}_{h_0} \) are (vector-valued) grid functions on \( \Omega_{h_0} \). Likewise, we have on \( \Omega_{\ell,h_k} \) the fine grid discretisations

\[
\mathcal{N}_{\ell,h_k}[\mathbf{v}^*_{hk}, \psi^{n+1}_{hk}, \mathbf{v}^*_{hk-1}, \psi^{n+1}_{hk-1}] = \mathbf{f}_{hk}, \quad x \in \Omega_{\ell,h_k}, \quad (k = 1, 2, \ldots, k_{\max}).
\]

Note that we use a slightly different notation than in Section 4 to denote the dependence of \( \mathcal{N}_{\ell,h_k} \) on the grid functions \( \mathbf{v}^*_{hk-1}, \psi^{n+1}_{hk-1} \) at one coarser level through the interface condition. After solving the nonlinear systems (19) we can compute the corresponding defects on the grids \( \Omega_{\ell,h_k} \) \((k = 0, 1, \ldots, k_{\max} - 1)\), which we denote by \( \mathcal{D}[\mathbf{v}^*_{hk}, \psi^{n+1}_{hk}; \mathbf{v}^*_{hk+1}, \psi^{n+1}_{hk+1}] \).

For space discretisation of (11) we use the finite volume method as well, this time combined with central differences to approximate the fluxes. This way, we obtain \( k_{\max} + 1 \) linear algebraic systems, which can be symbolically written as

\[
\mathcal{L}_{h_0}(\psi_{h_0}^{n+1})[q^n_{h_0}] = g_{h_0}, \quad x \in \Omega_{h_0},
\]

\[
\mathcal{L}_{\ell,h_k}(\psi_{hk}^{n+1})[q^n_{hk}; q^n_{hk-1}] = g_{hk}, \quad x \in \Omega_{\ell,h_k}, \quad (k = 1, 2, \ldots, k_{\max}),
\]

where the notation \( \mathcal{L}_{h_0}(\psi_{h_0}^{n+1}) \) indicates that the linear differential operator \( \mathcal{L}_{h_0} \) depends on the combustion variables \( \psi_{h_0}^{n+1} \); likewise for \( \mathcal{L}_{\ell,h_k} \). From the numerical solutions of (20) we can compute the defects \( \mathcal{D}[q^n_{hk}; q^n_{hk+1}] \).

Next, we add the defects to the corresponding systems, to give

\[
\mathcal{N}_{h_0}[\mathbf{v}^*_{h_0}, \psi_{h_0}^{n+1}] = \mathbf{f}_{h_0} + \mathcal{D}[\mathbf{v}^*_{h_0}, \psi_{h_0}^{n+1}; \mathbf{v}^*_{h_1}, \psi_{h_1}^{n+1}],
\]

\[
\mathcal{N}_{\ell,h_k}[\mathbf{v}^*_{hk}, \psi_{hk}^{n+1}; \mathbf{v}^*_{hk-1}, \psi_{hk-1}^{n+1}] = \mathbf{f}_{hk} + \mathcal{D}[\mathbf{v}^*_{hk}, \psi_{hk}^{n+1}; \mathbf{v}^*_{hk+1}, \psi_{hk+1}^{n+1}],
\]

\[
(k = 1, 2, \ldots, k_{\max} - 1),
\]

\[
\mathcal{L}_{h_0}(\psi_{h_0}^{n+1})[q^n_{h_0}] = g_{h_0} + \mathcal{D}[q^n_{h_0}; q^n_{h_1}],
\]

\[
\mathcal{L}_{\ell,h_k}(\psi_{hk}^{n+1})[q^n_{hk}; q^n_{hk-1}] = g_{hk} + \mathcal{D}[q^n_{hk}; q^n_{hk+1}] \quad (k = 1, 2, \ldots, k_{\max} - 1),
\]

(21a)
from which we can subsequently compute the updated solutions at the levels \( k = k_{\text{max}} - 1, k_{\text{max}} - 2, \ldots, 0 \). These updated solutions are subsequently used to determine interface conditions, compute fine grid solutions, etc.

In the following we suppress the superscripts \( n, * \) and \( n+1 \) indicating a time level, in order to keep the notation tractable. Thus we have \( v = v^*, \psi = \psi^{n+1} \) and \( q = q^n \). Instead, we add as superscript the iteration level. Combining the PC-algorithm and the LDC-algorithm and putting everything together, we obtain the following algorithm.

**Multi-level PC LDC algorithm**

1. Compute the predictor velocity \( v \) and the combustion variables \( \psi \).
   a. Initialization, \( i = 0 \)
      - Solve the coarse grid problem (19a) for \( v^i_{h_0} \) and \( \psi^i_{h_0} \).
      - For \( k = 1, 2, \ldots, k_{\text{max}} \) do
         - Compute the interface conditions for \( v_{h_k} \) and \( \psi_{h_k} \).
         - Solve the fine grid problem (19b) for \( v^i_{h_k} \) and \( \psi^i_{h_k} \).
   b. Iteration, \( i = 1, 2, \ldots \)
      - For \( k = k_{\text{max}} - 1, k_{\text{max}} - 2, \ldots, 0 \) do
         - Compute the defect \( D[v^i_{h_k}; \psi^i_{h_k}; v^i_{h_{k+1}}; \psi^i_{h_{k+1}}] \)
         - Solve the updated problem (21a) or (21b) for \( v_{h_k} \) and \( \psi_{h_k} \)
      - For \( k = 1, 2, \ldots, k_{\text{max}} \) do
         - Compute the interface conditions for \( v_{h_k} \) and \( \psi_{h_k} \).
         - Solve the fine grid problem (19b) for \( v^i_{h_k} \) and \( \psi^i_{h_k} \).
   c. Converged solution: \( v_{h_k}, \psi_{h_k} (k = 0, 1, \ldots, k_{\text{max}}) \).

2. Compute the pressure increment \( q \).
   a. Initialization, \( i = 0 \)
      - Solve the coarse grid problem (20a) for \( q^i_{h_0} \).
      - For \( k = 1, 2, \ldots, k_{\text{max}} \) do
         - Compute the interface conditions for \( q_{h_k} \).
         - Solve the fine grid problem (20b) for \( q^i_{h_k} \).
   b. Iteration, \( i = 1, 2, \ldots \)
      - For \( k = k_{\text{max}} - 1, k_{\text{max}} - 2, \ldots, 0 \) do
         - Compute the defect \( D[q^i_{h_k}; q^i_{h_{k+1}}] \)
         - Solve the updated problem (21c) or (21d) for \( q_{h_k} \).
– For $k = 1, 2, \ldots, k_{\text{max}}$ do
  • Compute the interface condition for $q_{h_k}$.
  • Solve the fine grid problem (20b) for $q_{h_k}^k$.

3. Converged solution: $q_{h_k} (k = 0, 1, \ldots, k_{\text{max}})$.

Note that in the algorithm above, $\mathbf{N}_{\ell,h_0}$ and $\mathbf{L}_{\ell,h_0}$ should be interpreted as $\mathbf{N}_{h_0}$ and $\mathbf{L}_{h_0}$, respectively.

For all nonlinear systems we use block-Gauss-Seidel iteration (outer iteration) in combination with quasi-Newton iteration (inner iteration) and we use GMRES to solve all linear systems. The PC-LDC algorithm is carried out each time step until all (discrete) time derivatives are smaller than $10^{-6}$.

6 NUMERICAL RESULTS AND DISCUSSION

We apply the multi-level PC LDC algorithm to simulate a two-dimensional methane/air flame on (a section of) a slit burner, the domain of which is shown in Figure 4. Reference solutions for the methane mass fraction and the pressure, computed on a very fine uniform grid of approximately 50,000 control volumes, are also shown in this figure. The boundary

Figure 4: Section of a slit burner as computation domain (left) and the reference solution for the methane mass fraction (middle) and the pressure (right), computed on a uniform fine grid.
Figure 5: The methane mass fraction on the global coarse grid (left), the local finest grid (middle) and the composite grid (right).

conditions for this problem are as follows:

\begin{align*}
\text{inflow (I)} & \quad u = 0, \quad v = v_0 \left(1 - \left(\frac{x}{d}\right)^2\right), \quad T = T_{in}, \quad Y_j = Y_{j,in}, \\
\text{outflow (O)} & \quad \frac{\partial f}{\partial n} = 0 \quad (f = u, v, T, Y_j), \quad p = p_{amb}, \\
\text{symmetry (S)} & \quad u = 0, \quad \frac{\partial f}{\partial n} = 0 \quad (f = v, T, Y_j), \\
\text{wall (W)} & \quad u = v = 0, \quad T = T_{wall}, \quad \frac{\partial Y_j}{\partial n} = 0,
\end{align*}

where \(v_0 = 2.6 \text{ m/s}, \ d = 1.5 \text{ mm}, \ T_{in} = T_{wall} = 400 \text{ K},\) and where the inlet species mass fractions \(Y_{j,in}\) correspond to an equivalence ratio \(\varphi = 0.95.\) The one-step model for methane/air combustion is used [21].

Our multi-level LDC method uses a global uniform coarse grid (level 0) of 780 control volumes and three nested local uniform fine grids of 240 (level 1), 720 (level 2) and 2048 (level 3) control volumes, respectively, that tightly enclose the flame front in the lower left corner of the domain. The grid size of the finest local grid (level 3) is the same as the grid size of the global fine grid for the reference solutions. We carried out only one LDC iteration. The computation of the numerical solution on the finest grid is the most time consuming part of the algorithm, since this grid contains the largest number of control volumes. The numerically computed methane mass fraction is shown in Figure 5. From this figure we conclude the following. The global coarse grid solution is fairly accurate.
outside the flame front, where all variables are virtually constant, however, it clearly does not capture the detailed structure of the flame front. The solution on the finest grid gives an accurate representation of the flame in the flame front. Finally, the composite grid solution closely resembles the reference solution, however, computed with approximately 13 times less control volumes, leading to a significant reduction in CPU time. The same conclusions hold for the numerically computed pressure, shown in Figure 6.

We have compared our LDC algorithm with the Local Uniform Grid Refinement (LUGR) method [27]. Roughly speaking, LUGR is a multi-level solution method for time dependent PDEs that combines a global coarse grid solution with local fine grid solutions. Unlike LDC, the fine grid solutions are not used in a defect correction step. Time integration on the local grids is carried out with a time step smaller than the one used for the global grid. Since we are only interested in steady solutions, we use only one time step for all grids. This version of LUGR is in fact the initialisation procedure of the LDC algorithm; see Figure 2. For the flame problem above, we found hardly any difference between the LDC and the LUGR solutions. The reason for this is that the interface condition provided by the initial coarse grid solution is already accurate enough to guarantee accurate solutions on the local fine grids. Thus, for this problem the defect correction steps are actually not necessary.

The performance of LDC iteration depends critically on the quality of both the global coarse grid solution and the local fine grid solutions. In a proper application of LDC, the coarse grid size $h_0$ should be small enough to resolve all scales outside the flame front, however, it is definitely too large for a correct approximation of the detailed solution in

Figure 6: The pressure on the global coarse grid (left), the local finest grid (middle) and the composite grid (right).
the flame front (preheat zone, inner layer and oxydation layer). This is taken care of by the local fine grids, which should tightly enclose the flame front. If the initial coarse grid solution provides the correct interface condition on $\Gamma_{h0}$, then defect correction is in fact not necessary anymore. This can occur if we choose the refinement region far to wide, which is of course not very wise to do, or if we have an accurate initial solution, as often happens in a time stepping procedure using a small time step. In fact, we can prove that LDC iteration has converged once the interface conditions have converged [2]. On the other hand, when the initial interface condition on $\Gamma_{h0}$ is not correct, a defect correction is needed. This might happen, for example, if we have a poor initial guess or when we want to compute solutions close to quenching or blow off. In these situations, LDC iteration will improve the LUGR method. Consequently, LDC is more robust than LUGR, since it does not rely on accurate interface conditions, allowing to compute a numerical solution from a poor initial guess, provided all nonlinear systems still can be solved. Therefore, a robust nonlinear solver in combination with LDC is an efficient numerical tool for laminar flame simulation.

To conclude, LDC is a general solution strategy for laminar flames, applicable to different models (simple/complex chemistry and/or transport). It can be combined with any discretisation method and (iterative) solution method. Simple structured grids should be used, allowing accurate discretisations and efficient (iterative) solution methods. Our version of LDC is only applicable to steady problems. Its extension to time dependent PDEs is described in [23].

7 CONCLUSIONS

In this paper we have combined the PC method, to decouple the velocity and pressure computation, with the LDC method, to solve BVPs characterised by a high activity region. The PC method is based on the expansion equation as constraint, rather than the continuity equation. The basic idea of LDC is to compute a global coarse grid solution and a local fine grid solution, and subsequently use the latter to improve the coarse grid solution in a defect correction manner. The method is extended recursively to include several levels of refinement. Moreover, this procedure can be repeated iteratively, however, usually one iteration step is sufficient for convergence. The main advantage of this approach is that we can use structured grids, possibly even uniform, allowing accurate discretisation methods resulting in algebraic systems for which efficient iterative solution methods are available.

We have applied a four-level LDC method to compute a methane/air flame on a slit burner. Our LDC solution has the same accuracy as a reference solution computed on a much finer grid, containing 13 times more control volumes. We have also carried out a numerical simulation with the LUGR method, and have virtually found no difference between the two solutions.
REFERENCES


