High-Order Method for Low Mach Number Combustion

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Problem Statement

- We want to effectively model **low Mach number flames** with **complex chemistry**.
- Combustion simulations have important implications for **clean fuels** and **renewable energy**.
- Simulations can obtain results impossible or impractical to obtain via experiment.
- This problem involves **multiple, vastly different time-scales**: we need a method that addresses the **stiffness** of the problem.
- Until now, methods have been **low order** or **unstable** when generalized to higher orders.

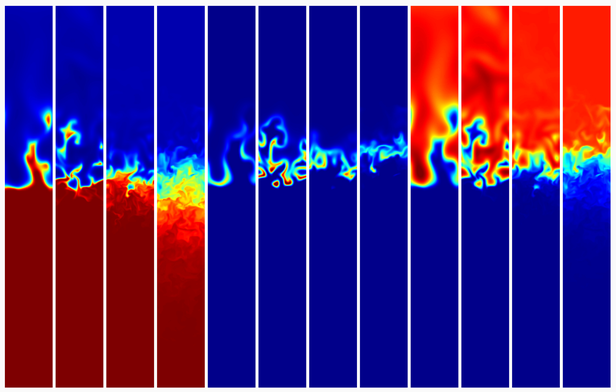


Fig. 1: Simulation of a premixed hydrogen flame (CCSE)

Method

The current state-of-the art low Mach number combustion code[1] uses a modified **multi-implicit spectral deferred correction**[2] method, solving the following "correction equations" at every timestep:

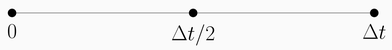
$$\frac{\partial(\rho Y_m)}{\partial t} = Q_{\rho Y_m}(t) + \dot{\omega}_m(Y,T), \tag{1}$$
$$\frac{\partial(\rho h)}{\partial t} = Q_{\rho h}(t), \tag{2}$$

where Q represents the contribution of advection and diffusion.

Stability analysis of the higher-order generalization of this method reveals a **stringent timestep restriction**!

We return to a formulation more "in the spirit" of MISDC that benefit from **highly favorable stability conditions**.

We subdivide one timestep $[0, \Delta t]$ into two **substeps**



according to the **Gauss-Lobatto quadrature rule**.

Instead of solving correction equations (1) and (2), we instead use a Backward Euler discretization

$$(\rho Y_m)^{n+1} = (\rho Y_m)^n + \Delta t(\tilde{Q}_{\rho Y_m} + \dot{\omega}_m(Y,T)) + I_{\rho Y_m} \tag{3}$$
$$(\rho h)^{n+1} = (\rho h)^n + \Delta t(\tilde{Q}_{\rho h}) + I_{\rho h} \tag{4}$$

Because we have three nodes, the quadrature is **fourth-order accurate**.

This **non-linear system of equations** is very **difficult** and **costly** to solve using Newton's method. But, we can use equations (1) and (2) to obtain a **provisional solution**.

This solution is used as the **initial guess** in the Newton solver for equations (3) and (4). We converge to a tolerance of 10^{-18} within only a couple iterations!

Results

With successive iterations, this simple, low-order correction results in a high-order method.

The overall **order of accuracy** p of the method is given by

$$p = \min\{q, k\},$$

where q is the order of the quadrature rule, and k is the number of correction iterations performed

Therefore, to obtain the desired fourth-order accuracy, we need:

Three Gauss-Lobatto nodes Four MISDC iterations

This method has been implemented in the full 1D low Mach number combustion code with complex chemistry.
We have successfully simulated the following flames:

Hydrogen Methane (GRI-Mech) Dimethyl Ether

with up to **53 different chemical species** and **325 chemical reactions.**

Attaining 4th-Order Accuracy

As a **test bed** we solve an A-D-R **model equation**

$$u_t = au_x + \epsilon u_{xx} + ru(u-1)(u-1/2) \tag{5}$$

Implementing the above method, we achieve the desired **overall fourth order accuracy** in **space and time**.

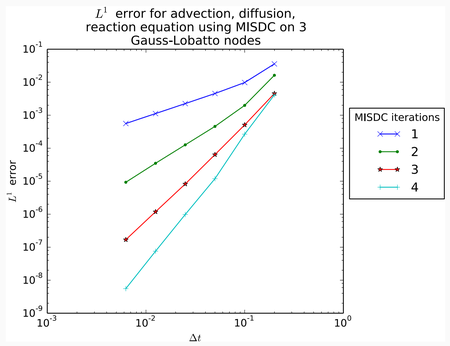


Fig. 3: Convergence results for model PDE

Stability Restrictions

In order for the method to converge, we have to satisfy the **stability criterion**.
The regions are **analytically derived.**

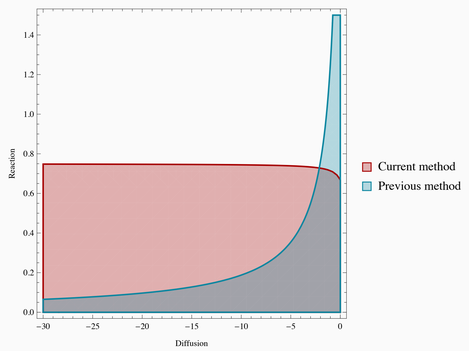


Fig. 4: Stability regions for new (Backward Euler) and previous (correction ODE) methods

Stability Analysis

We can consider the MISDC method as an **iterative scheme**, converging to the solution of the coupled A-D-R processes. In order for the iterations to converge, we require

$$\lim_{k\to\infty} |y^{(k+1)} - y^{(k)}| = 0.$$

Studying the linear ODE

$$y' = ay + dy + ry,$$

where 'advection' is treated explicitly, and 'diffusion' and 'reaction' are treated implicitly, we can write

$$\left|y^{\Delta t,(k+1)} - y^{\Delta t,(k)}\right| \leq \alpha \left|y^{\Delta t/2,(k)} - y^{\Delta t/2,(k-1)}\right| + \beta \left|y^{\Delta t,(k)} - y^{\Delta t,(k-1)}\right|,$$

We see that $\alpha, \beta < 1$ is a sufficient condition for convergence!

Computing explicitly (normalizing a to 1 and denoting $d\Delta t$ and $r\Delta t$ by d and r for convenience),

$$\alpha = \left|\frac{-12dr + 8(r-2)(r+1) + 2d^2(2+r)}{3(d-2)^2(r-2)^2}\right|, \qquad \beta = \left|\frac{-28 + 2d(54-19d) + r(d-2)(41d-44) - 4r^2(3d^2-9d+7)}{12(d-2)^2(r-2)^2}\right|$$

The condition $\alpha, \beta < 1$ leads to the stability region depicted in Figure 4. We notice that these expressions lead to a region which is **asymptotically horizontal**. This property is required because diffusion terms, given by the **eigenvalues of the Laplacian operator scale like** $1/h^2$**.**

In constrast, the previous method, when generalized, results in a coefficient α such that $\alpha \to \infty$ as $d \to -\infty$, for any choice of $r > 0$. The conclusion is that the previous method is **unstable** whenever $\Delta t \sim \Delta x$, and $\Delta x \to 0$.

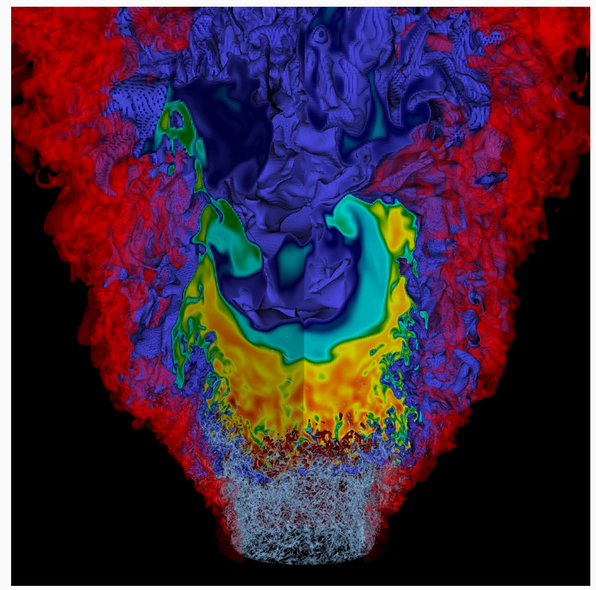


Fig. 5: Simulation of a hydrogen-air mixture burning (CCSE)

Conclusions

- We have provided a **rigorous mathematical analysis** of why the previous methods resulted in instability at higher orders.
- Additionally, we have formulated a numerical method, which is **demonstrably higher-order**, and whose **stability properties** allow us to run with **the same timestep** as the second-order code.
- This method has been implemented in a **1D low Mach number solver**, and results in **fourth order in time** accuracy.

Future Directions

- This method provides a **clear path forward** towards an **overall fourth order** algorithm for low Mach number combustion with complex chemistry.
- The time-stepping scheme easily generalizes to **arbitrary order**.
- Implementing fourth-order spatial operators in multiple dimensions introduces some very interesting and challenging problems.

Literature Cited

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