ENHANCING THE COMPUTATIONAL EFFICIENCY OF THE SOLUTION OF CHEMICALLY REACTING FLOWS

Mitchell D. Smooke
Department of Mechanical Engineering
Yale University
New Haven, CT 06520-8284
Two-Part Contract

**Part I:** Enhancing the Computational Efficiency of the Solution of Chemically Reacting Flows  
**Program Manager:** Dr. Chiping Li (new start)

**Part II:** Development of Implicit-Compact Methods with Application to Chemically Reacting Flows  
**Program Manager:** Dr. Fariba Fahroo (renewal)
Research Plan - Part I

Overview:

Numerical simulations are used as an experimental tool to explore qualitatively key combustion phenomena to obtain fundamental understanding and to identify rate-controlling processes and scales in different ranges of flow (including turbulence) and fueling conditions

- Experimentally constrained combustion computations
- Reduction strategies for laminar flames based upon on-the-fly chemical mechanism reduction with a Directed Relation Graph (DRG)
- Implementation of adaptive methods in three dimensional flames
- Investigating the use of these approaches in time-dependent combustion using high order methods to help facilitate a first principles understanding of aspects of turbulent combustion
If an experimental temperature profile is available, substituting this profile for the energy equation may produce a solution of the species equations that is a better representation of the chemistry actually occurring in the flame.

Under real burning conditions, there can often be distributed heat losses (usually radiative) which may not be considered by the model.

Can use species profiles other than the temperature.

Calculating NO Mole Fraction

- NO LIF data is used to form a two-dimensional mole fraction field that is held fixed by the computation – Isolate specific chemical effects
- Can be used with other measured species including soot volume fraction
Directed Relation Graphs

1. Introduce a measure for the direct coupling between the unknowns in the problem
2. Use the measure to define a directed relation graph which connects the unknown in the problem
3. Define a set of *important* unknowns
4. “Search” the graph and sort the species according to “how much they connect” with the important species
5. Eliminate “loosely connected” species
DRG: On-the-Fly Methane

Methane 16-species 47-reactions, $123 \times 149$ gridpoints, $\varepsilon = 0.10$

- Reduction is present despite small mechanism size
- The $\text{CH}_3 \rightarrow \text{CHO}$ chain is affected
Multiresolution Methods

Multiresolution – adaptive grid refinement based on wavelet transform (approximation theory)


- High memory reduction
- Rigorous mathematical background
- Robust and accurate (error estimate)
- Straightforward extension to 2D, 3D
- Requires sophisticated data structures

- Applications
  - Reacting fronts
  - High speed flows

(Duarte et al., 2012)
3-D Local Mesh Refinement in an Implicit Setting

Options:

i) Compute all nodes together

ii) Use Local Defect Corrections and work with one grid at a time

iii) Compressed Storage algorithms

N.B. Over 400 ways in which a three-dimensional refinement implementation can be locally unstructured at a given point (35 ways in 2D)
Overview

Development of a fully coupled, parallel, implicit algorithm with high-order spatial discretization validated on time-dependent flames with detailed transport and finite-rate multi-step chemistry and soot formation

• Initial focus on forced and unforced (flickering) laminar flames – an important intermediate configuration between steady-state laminar and turbulent flames

• Current focus is on flame vortex interaction leading to first principles understanding of aspects of combustion related to flame stretch, local extinction and ignition

• Joint computational and experimental (DOE) program
• Problems with conventional methods:
  – Artificial diffusion and poor resolution of short length scales in standard low order (LO) methods leads to spuriously damped flame behavior
  – Tensor-product meshes presume a single localized “region of interest” and are not suited to the dynamic tracking of many complicated multiscale phenomena

• Possible solutions:
  – Local adaptive mesh refinement: AMR, LRR, Multiresolution (MR)
  – High order spatial discretization: WENO, Compact Schemes (CS)
  – Ideally, both would be desirable for combustion

Bennett, Smooke (LRR)
Implicit-Compact Methods

• Compact spatial discretization:
  – finite difference method
  – high accuracy in a classical sense, i.e., low truncation error
  – “spectral-like” resolution of shorter length scales
  – arbitrary boundary conditions
  – prior track record in flame calculations (e.g., Poinset)

• Implicit time discretization:
  – time steps chosen based on the physics of the flame
  – no stability limitations from CFL, chemical time scales
  – time scale disparity in real flames \( \sim 10^{10} \) (Oran & Boris)
  – benefit vs. explicit: steps can be orders of magnitude larger
  – benefit vs. semi-implicit: robustness, no splitting errors
Compact Schemes

• Uniform grids: Lele (1992)
• Nonuniform grids: Gamet et al. (1994)
• Idea: construct a linear algebraic relationship between the values of a function and of its derivative on a grid
  – For example, in one dimension we could write

\[
\alpha_{i-1} u'_{i-1} + \alpha_i u'_i + \alpha_{i+1} u'_{i+1} = \beta_{i-2} u_{i-2} + \beta_{i-1} u_{i-1} + \beta_i u_i + \beta_{i+1} u_{i+1} + \beta_{i+2} u_{i+2}
\]

  – The unknown coefficients (\(\alpha\)'s and \(\beta\)'s) are constant for a given grid, and are determined by matching terms in 8 Taylor series
Compact Schemes

• Implementation:
  – the $\alpha$’s are written as elements in a tridiagonal matrix ($A$), and the $\beta$’s define a pentadiagonal matrix ($B$)

\[
A \cdot u' = B \cdot u
\]

  – this system is solved efficiently by the Thomas algorithm

• “Composite grids”:
  – if uniform grid spacing ($h$) is feasible in the region of interest, then 6th order accuracy can be attained where it matters most (in the interior of the domain)

\[
LTE_1 = \frac{1}{1260} h^6 u^{(7)}(\xi) \quad LTE_2 = -\frac{23}{55440} h^6 u^{(8)}(\xi)
\]

(first derivative) (second derivative)
Nonlinear Solver Algorithms

• Newton methods
  – Time discretization by BDF methods leads to large systems of coupled nonlinear algebraic equations; L-stable integrators preferred (stiffness)
  – Inexact, damped, modified Newton methods; “Newton-like” (Deuflhard)

• Jacobian options
  – Jacobian-free Newton-Krylov method (JFNK)
    • PRO: facilitates use of high order Jacobian at every iteration without storage challenges; streamlines task of parallelization
    • CON: ill-suited to problems with “sharp nonlinear solution structure” (addressed by proper nondimensionalization); issues with small species
  – Low order finite difference Jacobian within a “modified, Newton-like” framework, with residuals computed using the high order method
    • PRO: proven technology for low order implicit solvers and steady problems; analogies with established deferred correction methods
    • CON: Jacobian is only approximate for high order discretization; efficient “modified” approach may affect accuracy of time-dependent solutions
• **Jacobian linear systems**
  – Compact differentiation matrices are not sparse, leading to large, relatively nonsparse Jacobians – direct solution is not an option
  – For combustion applications these are also nonsymmetric and highly indefinite, possibly ill-conditioned, non-normal, etc.

• **Krylov methods**
  – Jacobian-vector product can be computed/approximated efficiently in various ways
  – GMRES (Saad, Schultz): more robust than Bi-CGSTAB but less memory efficient; robustness enhanced further via reorthogonalized modified Gram-Schmidt
  – Krylov subspace built up in GMRES can be exploited to estimate the conditioning of the linear system, permitting control of the solver
Time-Dependent Forced Laminar Diffusion Flame

- For high forcing frequencies and large velocity perturbations, such flames provide an important configuration between laminar and turbulent systems.

- The acoustic forcing is periodic and carefully controlled, so the system is well characterized.

- The effect of the forcing of the fuel is modeled by an inlet boundary condition on the axial velocity of the following form:

\[ V_z(r,t) = V_z^{steady}(r) \cdot (1 + b \sin(2\pi f t)) \]

where \( b \) is the size (%) of the perturbation relative to the steady profile and \( f = 20 \text{ Hz} \).
Low Order vs. Compact Method:
Temperature evolution (50% perturbation)
Low Order vs. Compact Method:
Flame surface on temperature (100% forcing)

The mixture in the pinch-off region burns for at least 15% of a period longer in the CS solution.
Hydrodynamically unstable “flickering” jet diffusion flames are a reacting flow system of considerable theoretical and practical interest

- their unforced oscillations exhibit a monochromatic frequency response essentially independent of Re (experiments show $f_0 \sim 11.5$ Hz for a CH4/air flame)
- such oscillations could possibly be employed to control thermoacoustic instability in engines (M. Juniper et al., *Proc. Combustion Institute*, 2008)

The nature of the instability mechanism is still not totally understood today

- Kelvin-Helmholtz- vs. buoyancy-induced
- “convective” vs. “absolute”
- role of diffusion (Lewis Number), fuel composition
Unforced, Flickering Flame

Temperature (K)

Position on centerline: \( z=1\text{cm}, z=3\text{cm}, z=5\text{cm}, z=7\text{cm} \)

Time series

Spectral analysis

Normalized Fourier coefficient

\( f_0 = 11.54 \text{ Hz} \)

\( f_0 = 11.60 \text{ Hz} \)

\( z=1\text{cm} \)

\( z=7\text{cm} \)
Flickering Coflow Jet Diffusion Flame: compact vs. low order method

A small initial velocity perturbation is imposed to trigger the instability, leading to an initial temperature perturbation ~ 5 K.

The low order spatial discretization produces a classic damped oscillation.

Position on centerline: $z=3\,\text{cm}$, $z=5\,\text{cm}$, $z=7\,\text{cm}$
Diffusion Flame in a Vortex: Overview

- Flame/Vortex Interaction
  - Canonical configuration facilitating a first-principles understanding of aspects of turbulent combustion (e.g., flame stretch, local extinction, and even soot production)

- Numerical Challenges
  - Strong coupling of flow and combustion, complicated evolution of very fine spatial structures, boundary conditions for laboratory systems
  - Formidable memory requirements for conventional implicit solvers
Diffusion Flame in a Vortex: Model

• Configuration
  – Lamb-Oseen vortex with initial core radius of 10^{-1}
  – Characteristic speed of rotation given by Re
  – Fuel (F) in top half plane, oxidizer (O) in bottom
  – Ignition problem: hot air/cold fuel, characteristic ignition delay time

• Cases
  – LO quasi-uniform grid with Δx ≈ 0.008
  – CS quasi-uniform grid with Δx ≈ 0.008
  – adaptive MR (10 levels) Δx_{min} ≈ 0.002

Flame-Vortex (Re = 600)
Conventional LO vs. CS (fixed grid)

quasi-uniform grid with $\Delta x \approx 0.008$

4th order convection (up to 6th order on uniform grid)
Flame-Vortex (Re = 600)
Conventional LO vs. CS (fixed grid)

LO, t=3.00d-4

CS, t=3.00d-4

quasi-uniform grid $\Delta x \approx 0.008$

4th order convection (up to 6th order on uniform grid)
Flame-Vortex (Re = 600)

Conventional LO vs. MR (dynamic grid)

LO, t=3.00d-4

MR, t=3.00d-4

quasi-uniform grid, $\Delta x \approx 0.008$

adaptive in space and time, 10 levels, $\Delta x_{\text{min}} \approx 0.002$
Flame-Vortex (Re = 600) High order and local adaptivity

• Both the high order scheme on the fixed grid (CS) and the low order scheme on the dynamically adapted grid (MR) give a huge improvement over the conventional approach

• Small differences between CS and MR solutions are currently under investigation – still too premature to say which one is “better”

• High order scheme needs ~ 1/4 of the points of the MR to resolve thinnest structure; adaptive method needs ~ 1/10 of the points to solve the problem
Future Work on Numerical Methods for Time-Dependent Combustion

• Implicit MR-based adaptive low order method
  – Jacobian algorithms for unstructured MR data structures
  – Inexact Newton with preconditioned Krylov methods

• Implicit-compact high order method
  – Jacobian-free Newton and/or Jacobian-based compression algorithms to overcome memory limitations of high order Jacobians
  – Preconditioning generalized saddle point problems (Navier-Stokes)

• Eventual merging of these approaches
  – High order adaptive method for stiff multiscale problems with strong coupling between global flow structures and highly localized fronts

• Applications to time-dependent combustion
  – Forced jets, Flame-Vortex interactions at higher Reynolds numbers
  – Three-dimensional systems
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