



Numerical Simulation of Chemically Reacting Flows

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This research looks to enhance the solution of chemically reacting systems through a number of computational methodologies. In particular, we have examined methods for solving problems by constraining the temperature and/or species fields; we have developed three-dimensional local gridding techniques and we have utilized velocity-vorticity methods for fluid dynamic modeling of combustion problems. Finally, we have combined high order, high resolution spatial discretization schemes with a robust implicit solution strategy. A central premise of the research discussed in this proposal is that the advancement of computational algorithms and the interaction between computation and experiments can play a role of equal or even greater importance, compared to computational architecture development, in the solution of these critical problems. All the topics were designed to provide a more effective computational/experimental strategy for the solution of problems of interest to the Air Force.

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Numerical Simulation of Chemically Reacting Flows Final Report FA9550-12-1-0157

Overview

To an increasing extent, computational models are being used in the design of chemically reacting flow systems. This trend will continue as models improve, computer power increases, and the alternative of empirical testing becomes more expensive. Of central importance here is a fundamental understanding of high-temperature, high-heat-release systems — namely, flames. Such systems, often nonpremixed and subject to many competing physical effects involving numerous mixture components changing rapidly in space and time, contain the essential features inherent to practical engineered systems. This research looks to enhance the solution of these systems through a number of computational methodologies. In particular, we have examined methods for solving problems by constraining the temperature and/or species fields; we have developed three-dimensional local gridding techniques and we have utilized velocity-vorticity methods for fluid dynamic modeling of combustion problems. Finally, we have combined high order, high resolution spatial discretization schemes with a robust implicit solution strategy. A central premise of the research discussed in this proposal is that the advancement of computational algorithms and the interaction between computation and experiments can play a role of equal or even greater importance, compared to computational architecture development, in the solution of these critical problems. All the topics were designed to provide a more effective computational/experimental strategy for the solution of problems of interest to the Air Force.

Experimentally Constrained Computations

In our development of computational models for one-dimensional burner-stabilized premixed laminar flames, we discovered that it was often difficult to produce accurate comparisons of numerical calculations with experimental data. This was true even for simple fuels such as hydrogen [1]. In addition, convergence difficulties often occurred due to the exponential dependence of the temperature in the Arrhenius chemistry terms. As a result, by specifying the temperature profile, we reduced the convergence difficulties of the Newton-based solution algorithm and we did not have to model distributed heat losses (often radiative). The immediate benefit was that the species comparisons were often dramatically better than when the temperature was computed. This *constrained* approach to premixed flame computations is still an option in the various PREMIX versions that circulate in research labs today [2]. A variant of the concept was also utilized in a paper by Ashurst et al., in which a precomputed velocity field was utilized as an input field in a multidimensional reacting system that approximated a turbulent reacting flow [3]. Generalization of these ideas has not been explored in any significant detail in the solution of flames with more complex chemistry. As part of our research program, we have utilized multidimensional experimental data for the temperature and the chemical

species to constrain the computation. This could be in the form of mole fractions or experimental signals. Several computational issues manifest themselves immediately. Once the constrained numerical solution is generated, we need to iterate the process so as to form revised experimental species and/or experimental signal information. As with one-dimensional premixed flames, a failure to converge implies an inconsistency with the model and the experimental data. We have applied this approach to coflow diffusion flames with simple fuels (methane, ethylene). A comparison between experimental and computational soot volume fractions for a 40% ethylene-air coflow diffusion flame is illustrated in Figure 1.

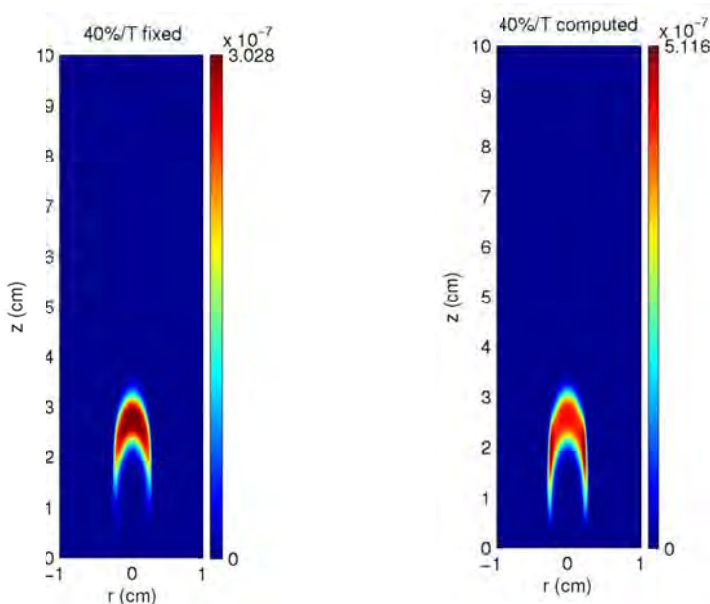


Figure 1. Soot profiles for a 40% ethylene-air coflow diffusion flame. The contours on the left were generated using an experimentally measured temperature profile. The contours on the right were generated in a calculation where the temperature was computed.

Local Grid Refinement

The local rectangular refinement (LRR) solution-adaptive gridding method, which has been used to model numerous laminar flames during the past two decades, has been extended to unsteady reacting applications in three spatial dimensions (LRR3D). Like LRR, LRR3D automatically generates robust unstructured grids by refining individual cells (not patches), uses multiple-scale discretizations, and solves coupled systems of PDEs via a damped modified Newton's method. The grids' unstructured nature produces a nonstandard sparsity pattern within the Newton's method Jacobian, as described in the original LRR3D paper in 2007 [4].

Beginning in 2012, the LRR3D algorithm was updated in several ways, the main one of which was to employ a full Jacobian (not a partial one, as in 2007) and thus take advantage of the quadratic convergence rate of Newton's method. Furthermore, the full Jacobian is implemented in a memory-efficient way, so that the only Jacobian blocks that are evaluated and stored are the ones that potentially may be nonzero, based on the local connectivity of points in the grid. Each time the grid adapts, local connectivity is evaluated just once. This change (partial Jacobian to

full Jacobian) was quite substantial, as it affected several of the major data structures in the code. It paid off in considerably faster convergence of the application problem from the 2007 paper (for one case, the updated code required only 1 Newton iteration, down from 11 in 2007).

More recent updates to LRR3D include the fact that now many quantities appearing frequently in the multiple-scale discretizations are precomputed (each time the grid adapts) to save CPU time later during residual formation, and that additional redundancy has been built into the arrays used to navigate the unstructured LRR3D grids, thus enabling quicker access of quantities needed for residual formation. These improvements, along with the earlier updates, have led to a factor of 100 speedup in the grid adaption process, which enabled LRR3D to be applied finally to unsteady reacting applications --- ones in which the grid adapts every few time steps. Subsequently, two unsteady reacting applications were investigated numerically using LRR3D, as described below.

The first application was a 3D extension of convection-diffusion-reaction problem with an analytical solution, whose purpose was to demonstrate the efficiency and accuracy of LRR3D. This problem was governed by a single nonlinear PDE. The same problem was also solved using a structured-grid code that had discretizations of the same level of accuracy as those in LRR3D, as well as the same Newton solver; however, all data storage and access in the structured-grid code was greatly simplified compared to that in the LRR3D code. The structured grid itself was equispaced and had the same minimum spacing as the LRR3D grid. Conclusions were as follows:

- In plots of spatially averaged error as a function of time, LRR3D results and structured-grid results were indistinguishable.
- LRR3D used approximately 530,000 points (this value is time-averaged, since the number of grid points changed throughout the LRR3D simulation as the grid adapted), while the structured-grid code employed approximately 4.2 million points, which was fixed throughout the calculation.
- LRR3D required approximately one-fourth of the CPU time that the structured-grid calculation took.

The second application was a 3D extension of an unsteady 2D solid-solid alloying problem studied in the mid-1980s [5]. The problem describes a reactor containing a mixture of solid particles of aluminum and palladium (Figure 2). The particle radius varies, with larger particles close to the reactor's central axis, smaller particles close to the exterior walls, and a gradual variation in between. The problem's physics are governed by two coupled nonlinear PDEs involving two unknowns: temperature and solid fraction. Values of material properties appearing in the equations are taken from measurements by Birnbaum and co-workers [6,7]. Initially the aluminum and palladium are cold and unreacted. The bottom wall of the reactor is then gradually heated, causing a diffusion-controlled alloying front to propagate through the domain. The simulation terminates when the alloying is complete.

Because this application problem has four-fold symmetry, only one-fourth of the physical domain was modeled. As can be seen in the figure, the alloying front (purple) is non-planar

because the local reaction rate depends on particle size. The LRR3D grid consists of the base (equispaced) grid plus four levels of refinement; the finest grid spacings automatically occur in the region of highest gradients: surrounding the alloying front. To preserve readability of the figure, only 2D slices through the 3D grid are shown. The application was also studied using the same structured-grid

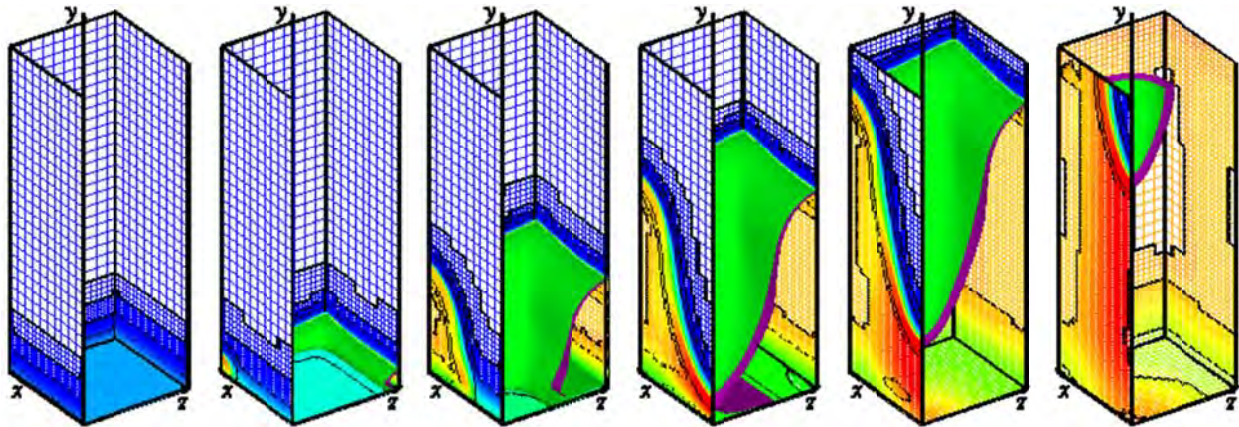


Figure 2. In the unsteady solid-solid alloying application, shown is the computed solution at six instances in time. The alloying front is visualized by the purple surface, which is where the solid fraction equals 0.99 locally. Isotherms (other colors) are superimposed on four 2D slices of the LRR3D grid.

code mentioned above. For this application, LRR3D's overall level of accuracy and efficiency compared to the structured-grid code was similar to its level of performance observed for the first application. Recent efforts have focused on deriving in 3D Cartesian coordinates the governing equations for a vorticity-velocity formulation that includes non-constant physical properties (density, viscosity, etc.). Now that these equations have been successfully derived, the next challenge lies in developing multiple-scale discretizations of the cross-derivative terms --- in particular, discretizations that are as conservative as possible within the constraint of using only "allowed" points in the stencil.

Vorticity-Velocity Fluid Dynamic Modeling

Since 2012, a novel vorticity-velocity formulation of the Navier-Stokes equations — the Mass-Conserving, Smooth (MC-Smooth) vorticity-velocity formulation — has been developed. The governing equations of the MC-Smooth formulation include a new second-order Poisson-like elliptic velocity equation, along with the vorticity transport equation, the energy conservation equation, and N_{spec} species mass balance equations. Compared to the two pre-existing vorticity-velocity formulations (e.g., the Original (ORIG) vorticity-velocity formulation [8] and the Modified (MOD) vorticity-velocity formulation [9]), the MC-Smooth formulation can ensure mass conservation and solution smoothness over a broader range of flow conditions, and it requires the least CPU time to converge.

During the development of the MC-Smooth formulation, we have employed two axisymmetric coflow laminar diffusion flames as a testbed to evaluate the performance of MC-Smooth and two pre-existing vorticity-velocity formulations. The first flame is a confined flame, and the second

flame is an unconfined flame. These two flames are selected because they cover a broad spectrum of operating conditions and the conclusions drawn from them are useful for future applications.

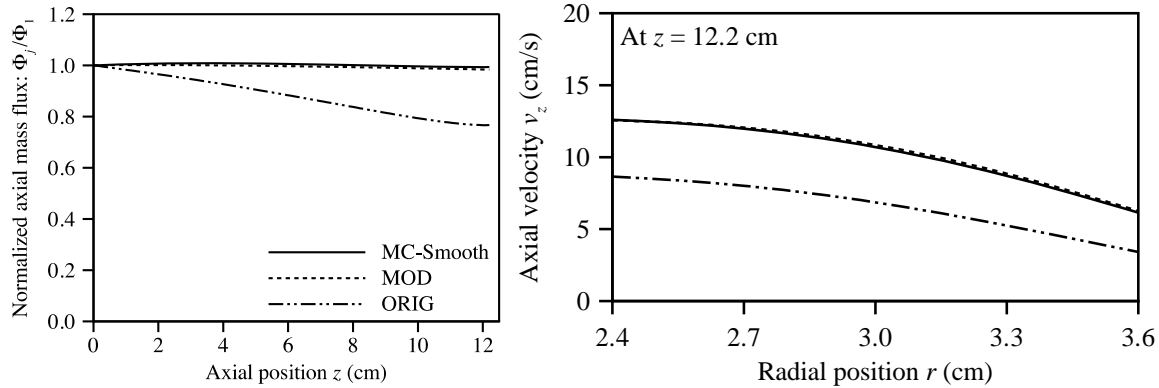


Figure 3. Left: Normalized axial mass flux of the confined flame as a function of the axial position. At $z = z_{\max} = 12.2$ cm, $\Phi_j/\Phi_1 = 0.994$ for the MC-Smooth formulation, $\Phi_j/\Phi_1 = 0.984$ for the modified formulation, and $\Phi_j/\Phi_1 = 0.766$ for the original formulation. Right: One-dimensional profiles of axial velocity in the confined flame in a portion of the computational domain at $z = z_{\max} = 12.2$ cm. At $r = 2.96$ cm, $v_z = 10.9$ cm/s for the MC-Smooth formulation, $v_z = 11.0$ cm/s for the modified formulation, and $v_z = 7.0$ cm/s for the original formulation.

To quantify the mass conservation performance of each formulation in the confined flame, we have computed the normalized axial mass flux Φ_j/Φ_1 along the axial direction, and the results are shown in the left half of Figure 3. As can be seen from this plot, when $z = z_{\max} = 12.2$ cm, the MC-Smooth solution loses 0.6% of its mass, the MOD solution loses 1.6% of its mass, and the ORIG solution loses 23.4% of its mass. This result indicates that MC-Smooth and MOD can ensure mass conservation but ORIG cannot. In the right half of Figure 3, the corresponding one-dimensional distribution of axial velocity at $z = z_{\max} = 12.2$ cm are depicted. From this plot, it is clearly observed that losing mass can significantly change the prediction of the velocity field, and that ensuring mass conservation is a crucial condition in obtaining a correct prediction of the velocity field.

For the unconfined flame, the two-dimensional distributions of the axial velocity field predicted by the MC-Smooth formulation and the modified formulation are shown in the left part of Figure 4. From this contour, we can observe that the modified formulation is unable to ensure the smoothness of the velocity field, and that the nonsmoothness in its velocity field will propagate vertically to the downstream. The right part of Figure 4 shows the one-dimensional profiles of the axial velocity at $z = 3.0$ cm. From this plot, it is also observed that the velocity field of the modified formulation indeed has significant nonsmoothness. Containing nonsmoothness in the velocity field is not negligible, because it can further affect derived quantities such as the residence time and the soot volume fraction. The MC-Smooth formulation, on the other hand, can always ensure the smoothness of the velocity field, and this improvement is confirmed by the two plots in Figure 4. The MC-Smooth formulation also requires the least CPU time to converge. Specifically, for the simulations related to the confined flame (Figure 3), the CPU time required by MC-Smooth is 26% and 16% lower than those required by MOD and ORIG, respectively; for the simulations related to the unconfined flame (Figure 4), the CPU time required by MC-

Smooth is 39% and 18% lower than those required by MOD and ORIG, respectively. Consequently, MC-Smooth not only has a wider applicability than MOD and ORIG, but it also requires a lower computational cost.

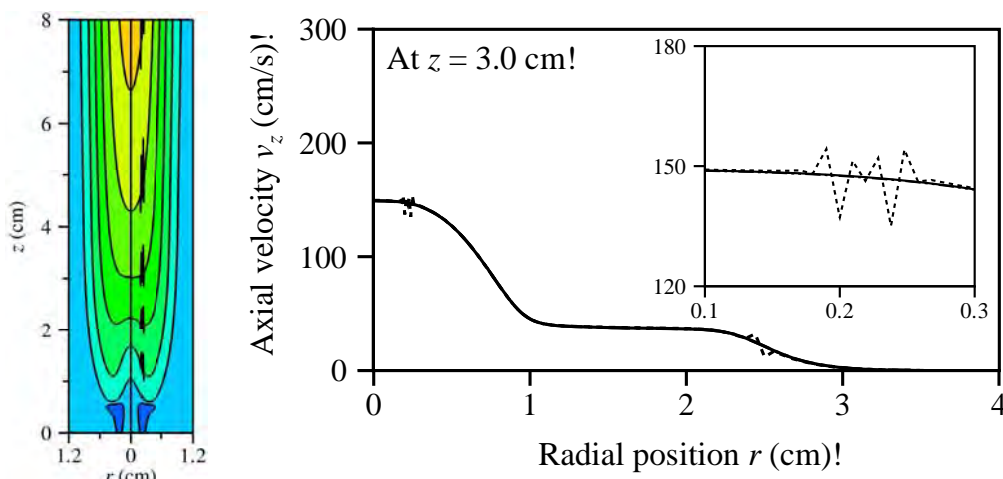


Figure 4. Left: Computed axial velocity distribution of the unconfined flame in a portion of the computational domain. The left half of the plot contains results from the MC-Smooth formulation, and the right half of the plot contains results from the modified formulation. Right: One-dimensional axial velocity profiles of the unconfined flame in a portion of the computational domain. In this plot, the solid line is the MC-Smooth prediction, the dashed line is the MOD prediction, and the dash-dot-dot line is the ORIG prediction. For the data shown above, the three lines mostly overlap with each other. The inset highlights small differences among the curves.

In addition to the improvements discussed above, other important advantages of the MC-Smooth formulation include: (1) it does not require the use of a staggered grid, and (2) it does not require excessive grid refinement to ensure mass conservation. With all these attractive features, the MC-Smooth formulation is a computationally feasible approach that can effectively extend the applicability of the vorticity-velocity formulation. Since 2012, the MC-Smooth formulation has been employed to simulate a wide spectrum of flames, including flames at microgravity, flames at elevated pressure, flames with soot formation, and flames with advanced radiation model. For most flames, the MC-Smooth formulation can generate accurate predictions of the flame structure, and very good to excellent agreement between simulations and measurements has been obtained. In addition to combining MC-Smooth with advanced numerical techniques such as adaptive grid refinement, future work will likely focus on the application of MC-Smooth to time-dependent sooting flames.

High Order Compact Methods

Two key numerical challenges with compact methods have manifested themselves during recent work on forced flames with detailed chemistry, one concerning the linear solver, and the other, the Newton method. We have worked on overcoming these challenges by focusing on block-based generalized saddle point preconditioners and novel numerical techniques for compressed Jacobian storage and operations. Ultimately, a hybrid parallelization strategy incorporating both task-based and domain-based algorithms will make it feasible to extend the validation of the

solver to three-dimensional problems while retaining, for the time being, the global approximation on which the high order compact finite differences are based. Concurrent work in the combustion diagnostics portion of the research has provided indispensable support for the validation and continued development of the numerical methods.

One critical issue that arose in the C1 flame calculations was a form of preconditioner instability that made it very difficult to recover from a rejected time step by simply reducing the stepsize. Further work using a time-dependent “flame sheet” model considerably clarified the diagnosis of the problem. The relative simplicity of the flame sheet model has allowed us to determine that the preconditioner instability is related to certain features of the fluid dynamical subproblem, in particular (1) the presence of the time derivative of density in the continuity equation, and (2) the absence of pressure in the same. Since the flames we are studying burn in a very low Mach number regime where the flow is hydrodynamically incompressible, the most natural set of primitive variables includes the pressure at the expense of the density, and hence this time derivative involves time derivatives of temperature and of all of the mass fractions via the ideal gas law. Moreover, in a fully implicit, pressure-based formulation of the problem, the pressure unknown is associated with the continuity equation, which is, of course, independent of the pressure. Accordingly, every row in the Jacobian matrix corresponding to the continuity equation has not only many strong off-diagonal entries of size related to the inverse of the time step but also a zero on the diagonal. The effect of this is potentially destabilizing on any standard incomplete factorization algorithm applied to the low order approximate Jacobian in the preconditioner formation process, and it gets worse as the time step gets smaller and the departure from diagonal dominance increases. In some cases, such as in our calculations of the one-step flames with the finite-rate Arrhenius chemistry model, the preconditioners constructed in this way could be made sufficiently tractable for a satisfactory range of time steps by various stabilization techniques, and the computations could be completed; in others, it proved very difficult or impossible to form or maintain a sufficiently stable and accurate preconditioner, without which the Newton-Krylov method could not converge.

Over the past several years we have developed a detailed understanding of this difficulty, as well as a plan for leveraging an important body of recent (and ongoing) research in numerical linear algebra in order to address it [10]. The key point is that the discrete form of the linear systems which arise in the implicit-compact solution process has strong similarities with the form of so-called saddle point linear systems, which have received a great deal of attention from numerical analysts in the past decade [11]. Typical examples of saddle point problems come from constrained optimization, PDE-constrained optimal control, and incompressible fluid dynamics. The common thread here is the presence of a constraint. In an incompressible flow, the pressure field is fixed by the divergence-free constraint on the velocity field. Similarly, in the low Mach number limit, the governing equations of chemically reacting flows describe a constrained mechanical system in which the tiny hydrodynamic pressure can be interpreted as a Lagrange multiplier that imposes the proper divergence constraint on the velocity field. It can be shown that the only sources (S) of nonzero divergence of the velocity in an open vessel are due to the diffusion of heat and its production by means of the chemical reaction, e.g., [12]. Hence, it is possible to formulate a low Mach number combustion problem as a kind of incompressible flow problem with additional conservation equations for the species and a generalized divergence constraint on the velocity field. This insight is fundamental to some well-known splitting

methods for reacting flow problems [13-15], yet the connection to saddle point problems is not clearly articulated in the combustion literature, precisely because most practitioners of computational combustion still avoid fully coupled numerical methods. In the field of incompressible fluid dynamics, however, where implicit solvers have been used for decades, the past fifteen years have seen the advent of new, highly efficient saddle point preconditioning algorithms for the fully coupled solution of the steady Navier-Stokes equations [16-19]. Notably, these algorithms have also been used in conjunction with a Newton solver [20], and recast in an easily parallelizable form [21]. More recently, they have been applied to time-dependent problems [22], and used to study more complicated physics, such as buoyancy driven flow [23]. Most importantly of all, various generalizations of these algorithms have been devised for linear systems which deviate from the canonical saddle point form in one way or another [24, 25]. The time derivative of density in the continuity equation is just one element of the reacting flow problem which leads to problems with generalized saddle point structure (we note that problems with off-diagonal time derivatives have been solved previously with numerical methods of the kind we propose to develop [26]).

We have begun development of these methods in Matlab [27], where the existence of ILUx routines allow detailed comparison with our current algebraic preconditioning approach in a controlled environment. The time-dependent flame sheet problem provides a compelling test of their performance on a small-scale flame problem. Applications to more realistic flames can follow as soon as suitably efficient Schur complement approximations can be devised for problems with strong, localized source terms. One possibility is to use block diagonal approximations for the chemistry terms (like in some operator splitting methods) and multigrid for the flow variables.

As already mentioned, the preliminary C1 flame calculations undertaken were made possible by replacing the JFNK method with a Newton-like method that employs a time-lagged, low order Jacobian matrix. Although “modified” Newton is an established strategy for the efficient computation of steady flames by “time-dependent” methods [28, 29], our numerical experiments have revealed that time-lagging of the Jacobian can lead to inaccurate results for unsteady flames, even when the refresh rate of the Jacobian is relatively fast compared to the characteristic dynamical time scale of the flame evolution. Given that the modified Newton iteration is not a robust approach for true time-dependent simulations and that JFNK has difficulties with small chemical species which cannot be resolved well on grids of modest size and complexity, better Jacobian options for the nonlinear solver will be explored in the future. Automatic Differentiation is not a realistic option, since the residual function that needs to be differentiated is actually a complicated hierarchy of subroutines that involves Chemkin and other third-party software for the various physical submodels. A more promising approach may be to revisit the “Jacobian component” methodology, which was first introduced in [30] and implemented in the implicit-compact primitive variable solver for nonreacting flows that was developed in the earliest stage of our AFOSR sponsorship. This is best understood as a novel data compression scheme for Jacobian matrices arising in the nonlinear solution of PDE problems. Using the “component form,” a full (nonsparse) high order Jacobian can be decomposed into a mere two arrays using less memory than is required to store a nine blockdiagonal (sparse) low order Jacobian. Moreover, this high order Jacobian can be applied to a vector — the key operation of any iterative linear solver based on Krylov subspaces — in $O(N)$ operations, where N is the

dimension of the Jacobian. Although incredibly promising on paper, the effectiveness of this numerical approach was thought to be dependent on the accurate analytical derivation of the elements in the two “component” arrays. For nonreacting flow problems, the robustness of this process was secured by an in-house code generator based on the symbolic computing capabilities of Mathematica [31]. However, it proved extremely challenging to extend this software in such a way that it could reliably derive the correct “Jacobian components” for combustion problems with detailed kinetics. We believe that this approach may be able to be salvaged, albeit at marginally greater computational cost and with some (acceptable) loss of accuracy, by replacing all analytically generated quantities with numerically estimated ones. This change should pose no more problems than the switch from an analytical Jacobian matrix to a numerical Jacobian matrix — which, in most normal circumstances, is not considered critical to the performance of a Newton method [32].

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Publications and Presentations:

1. M. D. Smooke, "The Computation of Laminar Flames," Proceedings of the Combustion Institute, 34, 2013.
2. S. Cao, B.A.V. Bennett, and M.D. Smooke, "MC-Smooth: A mass-conserving, smooth vorticity-velocity formulation for multi-dimensional flows," *Combust. Theory Model.*, in press, (2015).
3. S. Cao, B. Ma, D. Giassi, B.A.V. Bennett, M.B. Long, and M.D. Smooke, "Effects of pressure and fuel dilution on coflow laminar methane-air diffusion flames: A computational and experimental Study," in preparation.
4. S. Cao, B. Ma, B.A.V. Bennett, D. Giassi, D.P. Stocker, F. Takahashi, M.B. Long, and M.D. Smooke, "A computational and experimental study of coflow laminar methane/air diffusion flames: Effects of fuel dilution, inlet velocity, and gravity," *Proc. Combust. Inst.*, 35 (2015) 897–903.
5. S. Cao, B.A.V. Bennett, B. Ma, M.B. Long, and M.D. Smooke, "Effects of fuel dilution and pressure on coflow laminar methane-air diffusion flames: A computational and experimental investigation," 9th U.S. National Technical Meeting of the Combustion Institute, Cincinnati, OH, May 17–20, 2015.
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11. S. Cao, B.A.V. Bennett, B. Ma, M.B. Long, and M.D. Smooke, "Effects of pressure and fuel stream dilution on the structure of axisymmetric coflow methane-air laminar diffusion flames: A computational and experimental study," 14th International Conference on Numerical Combustion (ICNC), San Antonio, TX, April 7–10, 2013.

12. B.A.V. Bennett and M.D. Smooke, "Local rectangular refinement in three dimensions (LRR3D) with application to unsteady combustion problems," 14th International Conference on Numerical Combustion (ICNC), San Antonio, TX, April 7-10, 2013.

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14. M. D. Smooke, "The Computation of Laminar Flames," Plenary Lecture, 34th International Symposium on Combustion, Warsaw, Poland, August 2012.

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1. Report Type

Final Report

Primary Contact E-mail**Contact email if there is a problem with the report.**

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Primary Contact Phone Number**Contact phone number if there is a problem with the report**

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Organization / Institution name

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Grant/Contract Title**The full title of the funded effort.**

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Grant/Contract Number**AFOSR assigned control number. It must begin with "FA9550" or "F49620" or "FA2386".**

FA9550-12-1-0157

Principal Investigator Name**The full name of the principal investigator on the grant or contract.**

Mitchell D. Smooke

Program Manager**The AFOSR Program Manager currently assigned to the award**

Dr. Chiping Li

Reporting Period Start Date

06/01/2012

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Abstract

To an increasing extent, computational models are being used in the design of chemically reacting flow systems. This trend will continue as models improve, computer power increases, and the alternative of empirical testing becomes more expensive. Of central importance here is a fundamental understanding of high-temperature, high-heat-release systems — namely, flames. Such systems, often nonpremixed and subject to many competing physical effects involving numerous mixture components changing rapidly in space and time, contain the essential features inherent to practical engineered systems. This research looks to enhance the solution of these systems through a number of computational methodologies. In particular, we have examined methods for solving problems by constraining the temperature and/or species fields; we have developed three-dimensional local gridding techniques and we have utilized velocity-vorticity methods for fluid dynamic modeling of combustion problems. Finally, we have combined high order, high resolution spatial discretization schemes with a robust implicit solution strategy. A central premise of the research discussed in this proposal is that the advancement of computational algorithms and the interaction between computation and experiments can play a role of equal or even greater importance, compared to computational architecture development, in the solution of these critical problems. All the topics were designed to provide a more effective computational/experimental strategy for the solution of problems of interest to the Air Force.

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Archival Publications (published) during reporting period:

1. M. D. Smooke, "The Computation of Laminar Flames," Proceedings of the Combustion Institute, 34, 2013.
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Changes in research objectives (if any):

None

Change in AFOSR Program Manager, if any:

None

Extensions granted or milestones slipped, if any:

None

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, \$K)

	Starting FY	FY+1	FY+2
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