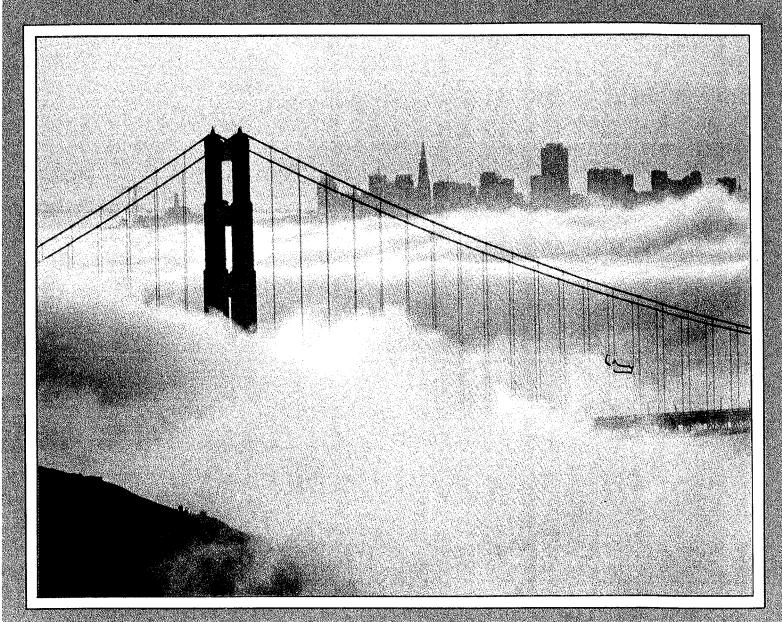
Preliminary Program

SIMM(CONTRIBERING DON) NUMBRICAL COMBUSINON March 9-111, 1987

Conducted with the cosponsorship of INRIA and SMAI

Holiday Inn — Golden Gateway • San Francisco, California



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Adaptive Gridding

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Complex Chemical Kinetics

Use of the Supercomputer

Multidimensional Moving Boundary Problems

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John D. Buckmaster, Cochair, University of Illinois, Urbana and University of Washington, Seattle

D. Scott Stewart, Cochair, University of Illinois, Urbana

Harry Dwyer, University of California, Davis

James G. Glimm, Courant Institute of Mathematical Sciences, New York University

Bernard Larrouturou, INRIA-Sophia Antipolis, France

Roger Temam, Université de Paris-Sud, France

Charles Westbrook, Lawrence Livermore National Laboratory

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SIAM is conducting this conference with the partial support of the Department of Energy and the National Science Foundation.

Photographs graciously provided by the San Francisco Convention and Visitors Bureau.

Invited Presentations

Monday, March 9, 8:30 AM Invited Presentation 1 Numerical Computation of Turbulent Combustion

The probability density function (pdf) method is a statistical approach to solving the equations governing turbulent combustion. The method has been applied successfully in several applications recently. The speaker will discuss the case of a one-point joint pdf of the fluid velocity and composition. Closed form solutions are available in this case for convection and reaction. But even in this highly simplified situation, the joint pdf contains seven independent variables and the standard numerical methods are impractical and have to be replaced by Monte Carlo methods for the determination of the pdf. The speaker will show the results of calculations for both premixed and diffusion flames to show the attributes of the method.

Stephen B. Pope Cornell University

Monday, March 9, 9:15 AM
Invited Presentation 2
Computational Questions that Arise in
Detonation Physics and High Speed

Detonation is a violent, explosive phenomenon that is sometimes desirable (explosives), sometimes not (coal mines, grain elevators). More understanding of detonation is needed in order to design better explosives, and to prevent it from occurring where it is not wanted.

The computational questions that arise in detonation physics and high speed flows are distinct from those of low speed combustion. The main difference is that the combustion field contains regions where the equations are of hyperbolic type. In a typical problem, it is necessary to identify the reactive and nonreactive shocks that develop in the combustion field.

The speaker will describe new theoretical understanding that has led to improved computational tools. For example, recent advances in the asymptotic theory are leading to well-posed moving boundary problems that can be used with new numerical algorithms to reduce the computational effect required in certain classes of problems.

In addition, he will identify problems for which present tools are inadequate. For example, new numerical methods that do not employ artificial viscosity are needed for the calculation of multidimensional detonations and the evolution to detonation.

John B. Bdzil Los Alamos National Laboratory Tuesday, March 10, 8:30 AM Invited Presentation 3

Physical Processes in Combustion Engineering that Require Advanced Numerical Treatment

Industrial researchers routinely are confronted with complex processes and problems that can be elucidated by the application of numerical and analytical techniques. Examples will be discussed from the fields of two-phase flows and combustion. An effort will be made to identify specific topics that require the development of advanced numerical techniques or even the reexamination of the constitutive equations.

Frediano V. Bracco Princeton University

Tuesday, March 10, 9:15 AM Invited Presentation 4

The Use of Analytical Knowledge and Adaptive Gridding in Combustion Problems

It has long been recognized that a priori knowledge of the solution is helpful, and often essential, in numerical computations. Regions in which the solution changes very rapidly must be anticipated or identified, and the grid locally adjusted to provide the required accuracy in those regions. There has been a lack of emphasis on the need for adaptive numerical methods and the proper response of the methods to the asymptotic parameters causing interior boundary regions and scaling problems.

James M. Hyman Los Alamos National Laboratory

Wednesday, March 11, 8:30 AM Invited Presentation 5 Numerical Solution of Moving Boundary

Problems in Combustion Theory

Flames are often thin. If it is known where they go and how they behave, reasonable understanding of the combustion field can be obtained. Such flames define moving boundaries, separating unburnt gas from burnt gas, or fuel from oxidizer.

Combustion theory has long used this approximation. Finding the response of a given combustion system often requires that the reaction zone be tracked as part of the solution of a nonlinear moving boundary problem. Front tracking in one dimension is understood but the best methods are not widely known to the user community. For multidimensional problems, front tracking methods are only now being developed. The speaker will discuss problems in combustion theory that help define the state-of-the-art in numerical front tracking and provide a good testing ground for these methods.

James G. Glimm Courant Institute of Mathematical Sciences New York University Wednesday, March 11, 9:15 AM Invited Presentation 6

Using Asymptotics to Define Numerical Experiments in Combustion

In defining a numerical problem one can try to include everything that is likely to be of physical importance, or one can "model", deliberately discarding ingredients in order to better understand the effect of those that are kept. The first approach is necessary if the goal is to obtain numbers that must be compared with the physical world. The second is of great value when the goal is physical understanding.

Asymptotics can be used to define interesting models of combustion. In some cases the result of the asymptotics is a field equation, a simple paradigm for the "exact" equations. The Kuramoto-Sivashinsky equation is an example. In other cases, the asymptotics suggests approximations that lead to great simplification. For example, flame sheet models can be useful even when there is no formal asymptotic justification for them.

John D. Buckmaster University of Illinois, Urbana and University of Washington, Seattle

1. Detonation Physics and High Speed **Flows**

Andrew Majda Princeton University

2. Computation of Systems with Complex Chemical Kinetics Robert J. Kee

Sandia National Laboratories Livermore, CA

3. Applications of Adaptive Gridding Methods to Combustion Problems Bernard Larrouturou INRIA-Sophia Antipolis, France

4. Numerical Solution of Engineering **Problems in Combustion**

T. Daniel Butler Los Alamos National Laboratory

5. Impact of Supercomputers on the Solution of Combustion Problems Harry A. Dwyer University of California, Davis, CA

6. The Role of Asymptotics in Computational Combustion D. Scott Stewart

University of Illinois, Urbana

7. Multidimensional Moving Boundary **Problems**

Gunter H. Meyer Georgia Institute of Technology

8. Turbulent Combustion

Jay P. Boris Naval Research Laboratory

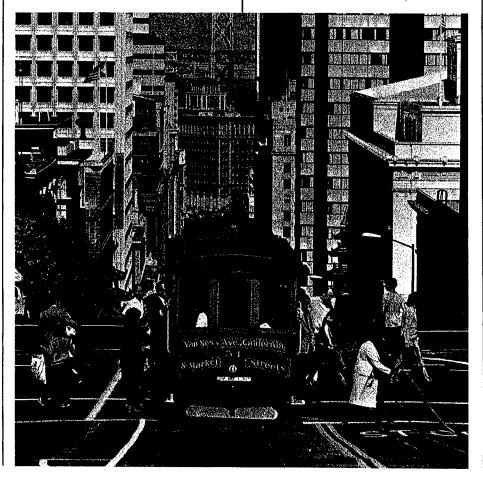
Minisymposia

Special Functions

Welcoming Reception Sunday, March 8, 8:00 PM - 10:00 PM Crystal Room

Beer Party

Monday, March 9, 8:00 PM – 10:00 PM Crystal Room



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M Short Course and Conference on

Optimization Hotel Intercontinental Houston, T.

SIAM Short Course and Conference on Applied Geometry: Geometric Modeling, Computational Geometry, Tiling, and Robotics

Albany Hilton Albany, NY

October 12+15, 1987 SIAM Annual Meeting Marriott Hotel - City Center Denver, CO

PROGRAM-AT-A-GLANCE

Sunday, March 8/PM

5:00 PM/Emerald Room

Registration Opens

8:00 PM/Crystal Room

Welcoming Reception

10:00 PM/Emerald Room

Registration Closes

Monday, March 9/AM

7:00 AM/Emerald Room

Registration Opens

8:15 AM/Emerald Room Opening Remarks

8:30 AM/Emerald Room

Invited Presentations 1 and 2

Chair: David Kassoy

University of Colorado, Boulder

8:30 AM

Numerical Computation of Turbulent

Combustion

Stephen B. Pope Cornell University

9:15 AM

Computational Questions that Arise in Detonation Physics and High Speed Flows

John B. Bdzil

Los Alamos National Laboratory

10:00 AM/Coffee

10:30 AM/CONCURRENT SESSIONS

Minisymposium 1/Emerald Room

Detonation Physics and High Speed Flows

Chair: Andrew J. Majda Princeton University

Minisymposium 2/Washington Room

Computation of Systems with Complex Chemical Kinetics

Chair: Robert J. Kee

Sandia National Laboratories

Minisymposium 8/Nevada Room

Turbulent Combustion

Chair: Jay P. Boris

Naval Research Laboratory

Monday, March 9/PM

12:30 PM/Lunch

2:00 PM/CONCURRENT SESSIONS

Contributed Presentations 1/Emerald Room

Finite Element Methods

Chair: Bernard Larrouturou INRIA-Sophia Antipolis, France

Contributed Presentations 2/Washington

Room

Detonation Stability

Chair: John Buckmaster University of Illinois, Urbana and University of Washington, Seattle

3:30 PM/Coffee

4:00 PM/CONCURRENT SESSIONS

Contributed Presentations 3/Emerald Room

Detonations

Chair: Antoni Oppenheim

University of California, Berkeley

Contributed Presentations 4/Washington Room

Turbulence

Chair: Jay P. Boris

Naval Research Laboratory

Contributed Presentations 5/Nevada Room

Complex Chemistry

Chair: D. Scott Stewart University of Illinois, Urbana

8:00 PM/Crystal Room

Beer Party

Tuesday, March 10/AM

8:30 AM/Emerald Room

Invited Presentations 3 and 4

Chair: Ronald Rehm National Bureau of Standards

Gaithersburg, MD

8:30 AM

Physical Processes in Combustion Engineering that Require Advanced

Numerical Treatment

Frediano V. Bracco Princeton University

9:15 AM

The Use of Analytical Knowledge and Adaptive Gridding in Combustion

Problems

James M. Hyman Los Alamos National Laboratory

10:00 AM/Coffee

10:30 AM/CONCURRENT SESSIONS

Minisymposium 3/Emerald Room

Applications of Adaptive Gridding

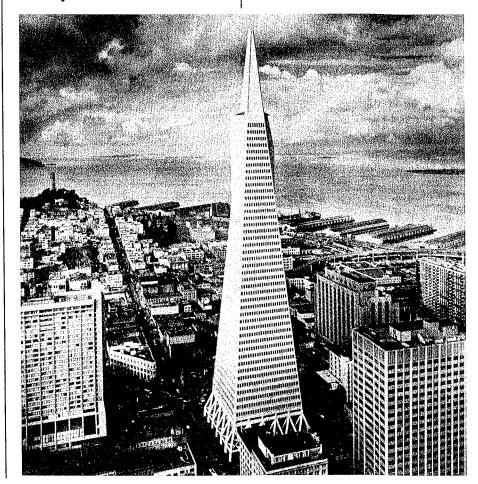
Methods to Combustion Problems

Chair: Bernard Larrouturou INRIA-Sophia Antipolis, France

Minisymposium 4/Washington Room

Numerical Solution of Engineering Problems in Combustion

Chair: T. Daniel Butler Los Alamos National Laboratory



Tuesday, March 10/PM

12:30 PM/Lunch

2:00 PM/CONCURRENT SESSIONS

Contributed Presentations 6/Emerald

Room

Inviscid Flows/Flames in Chambers

Chair: Ashwani Kapila

Rensselaer Polytechnic Institute

Contributed Presentations 7/Washington

Room

Drops and Sprays

Chair: Howard Baum

National Bureau of Standards

Gaithersburg, MD

Contributed Presentations 8/Nevada Room

Plane Flames Chair: Guy Joulin

C.N.R.S., France 3:30 PM/Coffee

4:00 PM/CONCURRENT SESSIONS

Contributed Presentations 9/Emerald Room

Flame Vortex Interaction

Chair: George Kosaly

University of Washington, Seattle

Contributed Presentations 10/Washington Room

New Numerical Methods

Chair: Claudine Schmidt-Laine École Centrale de Lyon, France

Contributed Presentations 11/Nevada

Room

Coal Combustion

Chair: John Buckmaster

University of Illinois, Urbana and University of Washington, Seattle

Wednesday, March 11/AM

8:30 AM/Emerald Room
Invited Presentations 5 and 6

Chair: Stephen Margolis Sandia National Laboratories

8:30 AM

Numerical Solution of Moving Boundary Problems in Combustion Theory

James G. Glimm

Courant Institute of Mathematical

Sciences

New York University

9:15 AM

Using Asymptotics to Define Numerical Experiments in Combustion

John Buckmaster

University of Illinois, Urbana and University of Washington, Seattle

10:00 AM/Coffee

10:30 AM/CONCURRENT SESSIONS

Minisymposium 5/Emerald Room Impact of Supercomputers on the Solution of Combustion Problems

Chair: Harry Dwyer

University of California, Davis

Minisymposium 6/Washington Room The Role of Asymptotics in

Computational Combustion Chair: D. Scott Stewart University of Illinois, Urbana

Wednesday, March 11 PM

12:30 PM/Lunch

2:00 PM/CONCURRENT SESSIONS

Contributed Presentations 12/Emerald Room

Vector Parallel Processing

Chair: Sisira Weeratunga Avco Research Laboratory

Minisymposium 7/Washington Room Multidimensional Moving Boundary

Chair: Gunter H. Meyer Georgia Institute of Technology

3:30 PM/Coffee

4:00 PM/CONCURRENT SESSIONS

Contributed Presentations 13/Nevada Room

Theoretical Problems

Chair: Arje Nachman

Air Force Office of Scientific Research

Contributed Presentations 14/Emerald Room

Modeling of Laminar Flames

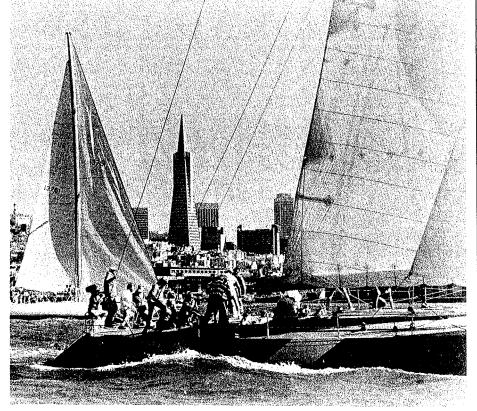
Chair: Peyman Givi Flow Research Company

Special Notice to Contributed Presentation Authors and Chairmen of Contributed Presentation Sessions:

Fifteen minutes are allowed for each contributed presentation. Presenters are requested to spend a maximum of 12 minutes for their presentation, and 3 minutes for questions and answers.

Please note:

For presentations with more than one author, an <u>underlineation</u> is used to denote the <u>author who will</u> present the paper.



Monday, March 9/10:30 AM
Minisymposium 1/Emerald Room
DETONATION PHYSICS AND HIGH
SPEED FLOWS

Recent work involving both numerical modeling and asymptotics on a variety of problems will be discussed including the following: the development of exothermic hot spots and their role in initiation of detonation; the decaying mechanisms and their effects on detonation velocity in expanding geometries, and theories for the regular spacing of Mach Stems in reacting shock waves.

CHAIR AND ORGANIZER Andrew J. Majda Princeton University Princeton, NJ

A Theory for Regular Spacing of Reacting Mach Stems (to be presented by the chair)

Numerical Modeling Initiation of Reacting Shock Waves Victor Roytburd

Victor Roytburd Rensselaer Polytechnic Institute Troy, NY

Detonation Wave Initiation by Energy Deposition at a Boundary

D. R. Kassoy
University of Colorado, Boulder
Boulder, CO
and
J. F. Clarke
Cranfield Institute of Technology
Cranfield, England
and
N. Riley
University of East Anglia
Norwich, England

Some Theoretical and Numerical Results for Diverging Detonations

Bruce Bukiet and <u>James Jones</u> Los Alamos National <u>Laboratory</u> Los Alamos, NM

Monday, March 9/10:30 AM Minisymposium 2/Washington Room COMPUTATION OF SYSTEMS WITH COMPLEX CHEMICAL KINETICS

In recent years there has been considerable progress modeling complex chemical kinetics processes in combustion. This minisymposium will focus both on the ways in which chemical kinetics models are used to understand combustion processes and on new mathematical and computational methods for modeling chemical kinetics. Examples of the former include the detailed understanding of premixed and diffusion flame structure, optimization of methods for reduction of pollutants, and applications to turbulent combustion via laminar flamelet theory. Examples of the latter include numerical methods for the solution of stiff differential equations (including parameter estimation) and the reduction of large reaction mechanisms via the constrained equilibrium approach. CHAIR AND ORGANIZER Robert J. Kee Sandia National Laboratories

Chemical Kinetics and Flame Modeling

James A. Miller Sandia National Laboratories Livermore, CA

Large-Scale Simulation and Parameter Identification in Chemical Kinetics
Ule Nowak

Konrad-Zuse Zentrum fur Informâtionstechnik Berlin, Federal Republic of Germany

Laminar Flamelets and Stretched Flames

Juergen Warnatz Universität Karlsruhe Karlsruhe, W. Germany and Universität Heidelberg Heidelberg, W. Germany

Constrained-Equilibrium Approach to Chemical Kinetics Modeling

James C. Keck Massachusetts Institute of Technology Cambridge, MA

Tuesday, March 10/10:30 AM
Minisymposium 3/Emerald Room
APPLICATIONS OF ADAPTIVE
GRIDDING METHODS TO COMBUSTION
PROBLEMS

The solutions of many combustion problems exhibit sharp gradients in very thin regions. Therefore an adaptive gridding method, which concentrates the computational nodes in these regions of high spatial activity is necessary for an accurate numerical simulation of these phenomena at a reasonable cost. Several of these adaptive techniques will be described, for transient and steady-state problems, for one-dimensional and two-dimensional geometries. The accuracy and the effectiveness of the resulting numerical methods will be discussed for different physical phenomena.

CHAIR AND ORGANIZER Bernard Larrouturou INRIA-Sophia Antipolis Valbonne, France

Some Adaptive Numerical Methods for One- and Two-Dimensional Combustion Problems

(to be presented by the chair)

Static and Dynamic Regridding in Extrapolation Integrators for Reaction-Diffusion Systems

U. Nowak Konrad-Zuse Zentrum für Informationstechnik Berlin, Federal Republic of Germany

On the Use of Adaptive Methods for Combustion Problems with Complex Chemistry

Mitchell D. Smooke Yale University New Haven, CT Tuesday, March 10/10:30 AM Minisymposium 4/Washington Room NUMERICAL SOLUTION OF ENGINEERING PROBLEMS IN COMBUSTION

This series of papers deals primarily with the application of computer programs for the analysis of transient, multidimensional combusting flows. Such numerical models are apprehensive in nature requiring detailed descriptions for the coupled fluid dynamics, mixing, heat transfer, chemical reactions, and fuel spray dynamics. Imperfections in the physics and chemical sub-models embodied in the codes exist. Nevertheless, applications of the codes to practical combustion systems are providing valuable insight and detailed understanding of the processes that occur. The authors will present example solutions to a broad spectrum of problems to illustrate the power of the solution methods.

CHAIR AND ORGANIZER T. Daniel Butler Los Alamos National Laboratory Los Alamos, NM

Numerical Simulations of Reactive Flows

Elaine Oran Naval Research Laboratory Washington, DC

(title to be announced)
Keith Meintjes
General Motors Research Laboratories
Warren, MI

Two Recent Applications of the KIVA Computer Program

Peter J. O'Rourke Los Alamos National Laboratory Los Alamos, NM

Numerical Simulation of Flame Acceleration in Large-Confined Channels

Kenneth D. Marx Sandia National Laboratories Livermore, CA

Wednesday, March 11/10:30 AM Minisymposium 5/Emerald Room IMPACT OF SUPERCOMPUTERS ON THE SOLUTION OF COMBUSTION PROBLEMS

The purpose of this symposium is to present to the applied mathematics community a series of speakers who both develop methods for and use supercomputers in their research studies on combustion. The scientists who will be speaking have had or have access to supercomputers on a regular basis, and are very familiar with the capabilities and limitations of the available numerical algorithms in their areas of specialization. The presentations will include examples of their current research investigations, as well as discussions of their future research directions and plans. CHAIR AND ORGANIZER Harry A. Dwyer University of California, Davis Davis, CA

Livermore, CA

Simulation of Supersonic Chemically Reacting Mixing Layers

J. Philip Drummond and M. Y. Hussaini NASA Langley Research Center Hampton, VA

Numerical Aspects in Computing Hyperbolic Conservation Laws with Stiff Source Terms

Helen C. Yee NASA Ames Research Center Moffett Field, CA

Numerical Simulation of Turbulent Premixed Flame Structure

William T. Ashurst
Sandia National Laboratories
Livermore, CA
and
N. Peters
Institute für Allgemeine Mechanik
Aachen, W. Germany
and
Mitchell D. Smooke
Yale University
New Haven, CT

Analysis of Combustion Instability in Liquid-Fueled Ramjets

William A. Sirignano University of California, Irvine Irvine, CA

Adaptive Pseudo-Spectral Computation of Combustion Problems on Supercomputers

A. Bayliss Northwestern University Evanston, IL

B. J. Matkowsky
Northwestern University
Evanston, IL
and
Argonne National Laboratory
Argonne, IL
and
M. Minkoff
Argonne National Laboratory
Argonne, IL

Wednesday, March 11/10:30 AM Minisymposium 6/Washington Room THE ROLE OF ASYMPTOTICS IN COMPUTATIONAL COMBUSTION

This minisymposium will focus on numerical problems that have been formulated by the asymptotic theory of combustion. The issue of using asymptotically derived information to enhance direct combustion simulations will be discussed.

CHAIR AND ORGANIZER D. Scott Stewart University of Illinois Urbana, IL

Numerical Simulation of Buoyancy Induced Motion of a Hydrogen Flame Bubble

Sisira K. Weeratunga
Avco Research Laboratory, Inc.
Everett, MA and
John D. Buckmaster
University of Illinois, Urbana and
University of Washington
Seattle, WA and
Robert E. Johnson
University of Illinois
Urbana, IL

Further Numerical Results from Detonation Theory

G. S. S. Ludford Cornell University Ithaca, NY and C. Schmidt-Laine Ecole Centrale de Lyon France

The Role of Asymptotics in Detonation Initiation Calculation

Ashwani K. Kapila Rensselaer Polytechnic Institute Troy, NY and University of Minnesota Minneapolis, MN

Computation of Criticality in Combustion

Karl Gustafson University of Colorado Boulder, CO

Wednesday, March 11/2:00 PM Minisymposium 7/Washington Room MULTI-DIMENSIONAL MOVING BOUNDARY PROBLEMS

Moving and free boundary problems arise naturally and as a simplifying approximation in combustion and detonation theory. Threshold assumptions, reactions of fractional order and the propagation of detonation waves can be modeled as free boundary problems, while high activation energy asymptotics for laminar combustion collapses reaction zones to free surfaces. The resulting multi-dimensional free boundary problems are quite complex and largely unresolved numerically. This minisymposium will introduce some representative classes of moving boundary problems and detail some possible approaches to their solution.

CHAIR AND ORGANIZER Gunter H. Meyer Georgia Institute of Technology Atlanta, GA

Higher-Order Bifurcation Phenomena in Premixed Combustion

Stephen B. Margolis
Sandia National Laboratories
Livermore, CA

Modeling Combustion and Detonation with Free Boundaries

D. Scott Stewart University of Illinois Urbana, IL

Diffusive Systems with Free Boundaries (to be presented by the chair)

Gradient Method for Modeling Interface Propagation

Kenneth J. Laskey Carnegie-Mellon University Pittsburgh, PA and Elaine S. Oran and Jay P. Boris Naval Research Laboratory Washington, DC

Monday, March 9/10:30 AM Minisymposium 8/Nevada Room TURBULENT COMBUSTION

Turbulent Combustion depends on the interactions between turbulent fluid dynamic convection, molecular diffusion which must mix the fuel and oxidizer, and chemical reactions which provide kinetic and bouyant energy to drive further turbulent convection. Thus, there are many additional physical effects and variables in turbulent combustion that do not appear in incompressible low Mach number constant density shear mixing. The three papers in this minisymposium consider turbulent combustion in the low, intermediate, and high Mach number regimes.

CHAIR AND ORGANIZER Jay P. Boris Naval Research Laboratory, Washington, DC

${\bf Turbulence\text{-}Combustion\ Interactions\ in} \\ {\bf Shear\ Flow}$

Ahmed Ghoniem Massachusetts Institute of Technology Cambridge, MA

Simulations of the Reactive Flowfield in a Combustor

K. Kailasanath, J. H. Gardner, Elaine S. Oran, and J. P. Boris Naval Research Laboratory Washington, DC

Onset of Instability in Supersonic Shear Layers

R. Guirguis, Berkeley Research
Associates, Springfield, VA and T. Young,
K. Kailasanath, E. Oran, and J. P. Boris,
Naval Research Laboratory, Washington,
DC

CONTRIBUTED PRESENTATIONS

Monday, March 9/2:00 PM Contributed Presentations 1/Emerald Room

FINITE ELEMENT METHODS

An Upwind Finite-Element Method for Steady Planar Flames

M. Ghilani and M. Sermange, INRIA-Sophia Antipolis, France

Finite-Element Investigation of Two-Dimensional Compressible Reacting Flows

A. Dervieux, B. Larrouturou, A. Habbal, H. Guillard, F. Benkhaldoun, INRIA-Sophia Antipolis, France

Finite Element Techniques for Combustion Problems

T. J. Chung, J. L. Sohn and Y. M. Kim, The University of Alabama in Huntsville, Huntsville, AL

The Moving Finite Element Method. 1-D and 2-D Gas Dynamics Standard Applications

Gilles Rusaouen, Jean Noel, and Denis Jeandel, Laboratoire de Mecanique des Fluides, Ecully Cedex, France

Monday March 9/2:00 PM Contributed Presentations 2/Washington Room

DETONATION STABILITY

Numerical Simulation of a Standing Oblique Hydrogen-Air Detonation Wave David T. Pratt and Dennis E. Glenn, Aerojet Propulsion Research Institute, Sacramento, CA

Effect of Chemical Reaction Parameters on the Regularity of the Cellular Structure of Detonations

R. Guirguis, Berkeley Research Associates, Springfield, VA, and K. Kallasanath and E. S. Oran, Naval Research Laboratory, Washington, DC

Stability of Self-Similar Spherical Detonations

<u>David L. Book</u> and Ira B. Bernstein, Naval Research Laboratory, Washington, DC

Effect of Reversible Reactions on One-Dimensional Detonation Stability

P. A. Thibault, Combustion Dynamics Ltd, Alberta, Canada, and J. E. Shepherd, Rensselaer Polytechnic Institute, Troy, NY

Numerical Simulation of Detonation Wave Corner-Turning Effect

Morton Lutzky, and Kibong Kim, Naval Surface Weapons Center, Silver Spring, MD

The Effect of Numerical Study of Ignition External Corner Geometries of a Reactive Solid

Loelke G. Vorsteveld, <u>Clarke E. Hermance</u>, University of Vermont, <u>Burlington</u>, <u>VT</u>

Monday, March 9/4:00 PM Contributed Presentations 3/Emerald Room

DETONATIONS

Numerical Modeling of Detonation Waves in Heterogeneous Solid Explosives

Craig M. Tarver, Lawrence Livermore National Laboratory, Livermore, CA

The Effect of An Imbedded Void Upon the Detonation Initiation

Gabi Luttwak, Rafael Ballistics Center, Haifa, Israel

Moving Mesh Forest Fire: A Computational Method for Detonations W. David Barfield, Los Alamos National Laboratory, Los Alamos, NM

A Model for the Short-Pulse-Duration Shock-Initiation of Explosives

John Starkenberg, U.S. Army Ballistics Research Laboratory, Aberdeen Proving Ground, MD

A Study of Shock-Induced Reaction Processes in Heterogeneous High Explosives

Pier K. Tang, Los Alamos National Laboratory, Los Alamos, NM

A Numerical Model of Combusting Two-Phase Flow in Interior Ballistics

Garry D. Tong, Computational Fluid Mechanics International, South Australia, Australia

Monday, March 9/4:00 PM Contributed Presentations 4/Washington Room TURBULENCE

Computation of Turbulent Diffusion Flames with Radiation

P. L. Viollet, D. Garreton and N. Mechitoua, Electricite de France, Chatou, France

Reactive In-Cylinder Flow Simulation by an Implicit Finite-Difference Method

Chia-Chun Hsiao and Fa-Yan Su, Science Applications International Corporation, San Diego, CA

Computation of Turbulent Combustion Characteristics

Essam Eldin Khalil, Cairo University, Cairo, Egypt

The Prediction of Density Fluctuation Influences in High Temperature Axisymmetric Turbulent Jet

P. G. Huang, Michigan Technological University, Houghton, MI and M. A. Leschziner, University of Manchester Institute of Science and Technology, Manchester, England

Investigation of the Modeling of Turbulent Molecular Mixing

G. Kosaly, University of Washington, Seattle, WA and P. Givi, Flow Research Company, Kent, WA

Monday, March 9/4:00 PM Contributed Presentations 5/Nevada Room COMPLEX CHEMISTRY

A Four-Step Chemical Kinetics Mechanism for High Temperature Propane Flames

Thomas M. Kiehne, United States Military Academy, West Point, NY and Ronald D. Matthews, University of Texas at Austin, Austin, TX

An Efficient Code for General Chemical Kinetics and Sensitivity Analysis Computations

Krishnan Radhakrishnan and David A. Bittker, NASA Lewis Research Center, Cleveland, OH

Vector Computers and Complex Chemistry

Vincent Giovangigli, Laboratoire EM2C du CNRS, Chatenay-Malabry, France, and Laboratoire de Mecanique Theorique, Paris, France, and Nasser Darabiha, Laboratoire EM2C du CNRS, Chatenay-Malabry Cedex, France

Self-Stabilizing Methods for the Computation of Reacting Flows with Nonlinear Kinetics

J. Barry Greenberg, Technion-Israel Institute of Technology, Haifa, Israel

A Program for Calculating Constrained Equilibrium Gas Compositions

Robert Law, and Mohamad Metghalchi, Northeastern University, Boston, MA and James C. Keck, Massachusetts Institute of Technology, Cambridge, MA

Patterns of Growth in Chemical Kinetic Models

Charles K. Westbrook, and William J. Pitz, Lawrence Livermore National Laboratory, Livermore, CA

Tuesday, March 10/2:00 PM Contributed Presentation 6/Emerald Room INVISCID FLOWS/FLAMES IN CHAMBERS

Acoustic-Mean Flow Interactions In Combustion Chambers

Joseph D. Baum, Naval Research Laboratory, Washington, DC

Some Performance Comparisons for a Fluid Dynamics Code

Daniel W. Lozier, and Ronald G. Rehm, National Bureau of Standards, Gaithersburg, MD

Numerical Analysis of Combustion Fields In Enclosures

Antoni K. Oppenheim, Maciej Z. Pindera and Douglas A. Rotman, University of California, Berkeley, CA

Numerical Modelling of Flames

Maciej Z. Pindera, University of California at Berkeley, Berkeley, CA

A Numerical Study of Turbulent Reactive Flows in Combustion Chambers

Gaffie D. Hebrard P, ONERA-CERT DERMEX, Toulouse, Cedex, France

Tuesday, March 10/2:00 PM Contributed Presentations 7/Washington Room

DROPS AND SPRAYS

Numerical Combustion of Multi-Phase Fluids

Pak Yan-Liang, Rockwell International Corporation, Canoga Park, CA

Dispersion During Evaporation of Drops in Clusters

Josette Bellan and Kenneth G. Harstad, Jet Propulsion Laboratory, Pasadena, Ca

Mixed Spectral Finite Element Method in Spray Combustion

T. J. Chung, and S. K. Lee, The University of Alabama in Huntsville, Huntsville, AL

Droplet Deformation and Breakup in Shear Flows

D. E. Fyfe, and E. S. Oran, Naval Research Laboratory, Washington, DC Tuesday, March 10/2:00 PM Contributed Presentations 8/Nevada Room **PLANE FLAMES**

Modified Equation Methods for Laminar Flame Calculations

J. I. Ramos, Carnegie-Mellon University, Pittsburgh, PA

Thick Flames with Localised Heat Loss Andrew C. McIntosh, The University of Leeds, Leeds, England

Computation of Laminar Burning Velocity of Hydrogen-Enriched Methane-Air Mixture

Shimshon Refael and Eran Sher, Ben-Gurion University of The Negev, Beer-Sheva, Israel

Travelling Combustion Waves in a Porous Medium

Andrew Stuart, Oxford University, Oxford, England

Extinction of Strained Premixed Laminar Flames with Complex Chemistry

Vincent Giovangigli, Universite Paris VI and Ecole Centrale des Arts et Manufactures, France, and Mitchell D. Smooke, Yale University, New Haven, CT

Partial Extinction of Strained Premixed Laminar Flames with Complex Chemistry

Nasser Darabiha, Laboratoire EM2C du CNRS, Chatenay-Malabry, France, Vincent Giovangigli, Laboratoire EM2C du CNRS, Chatenay-Malabry, France and Laboratoire de Mecanique Theorique, Paris, France, and Sebastien Candel, Laboratoire EM2C du CNRS, Chatenay-Malabry, France also ONERA, Chatillon, France

Calculated Extinction Limits for Diluted, Laminar Propane/Air Flames Richard J. Blint, General Motors Research Laboratories, Warren, MI

Tuesday, March 10/4:00 PM Contributed Presentations 9/Emerald

FLAME VORTEX INTERACTION

A Numerical Analysis of a Diffusion **Flame-Vortex Interaction**

Alan Laverdant, ONERA, Chatillon. France and Sebastien Candel, ONERA, Chatillon France and E. M2. C. Ecole Centrale, Chatenay Malabry

An Implicit Numerical Procedure for Multispecies Diffusion in Chemical Laser Flows

Victor Quan, Rockwell International, Canoga Park, CA

Calculations of a Two-Dimensional Flame in a Vortex Field

Ronald G. Rehm, Daniel W. Lozier, and Howard R. Baum, National Bureau of Standards, Gaithersburg, MD

Transient Combustion in a Turbulent Eddy

Howard R. Baum, Daniel M. Corley and Ronald G. Rehm, National Bureau of Standards, Gaithersburg, MD

Analysis of Heat Release During Flame-Vortex Pair Interactions

Bose V. S. Manda, and Ann R, Karagozian, University of California at Los Angeles, Los Angeles, CA

Direct Numerical Simulation of Scalar Dissipation in a Turbulent Mixing Layer P. A. McMurtry, University of Washington, and P. Givi, Flow Research Company, Kent, WA

Tuesday, March 10/4:00 PM Contributed Presentations 10/Washington Room

NEW NUMERICAL METHODS

Lagrangian Flame Modelling Using

Adaptive Gridding
K. Kailasanath, P. D. Ronney, E. S. Oran and J. P. Boris, Naval Research Laboratory, Washington, DC

Second Order Scheme for Reacting Flow Application to Detonation

A. Bourgeade, Cel-V, CEA Villeneuve St. Georges, France

A Second-Order Random-Choice Algorithm for Hyperbolic Systems of Equations

P. L. Roe, E. F. Toro, Cranfield Institute of Technology, United Kingdom

BIC-FEM-FCT For Combustion Problems R. Lohner and G. Patnaik, Berkeley

Research Associates, Springfield, VA and Naval Research Laboratory, Washington,

Effect of Boundary Conditions in Computational Flame Simulation

S. Nakamura, The Ohio State University, Columbus, OH

Multiquadrics: A New Tool For Accurate **Hydrodynamic Simulations**

Edward J. Kansa, Lawrence Livermore National Laboratory, Livermore, CA

Tuesday, March 10/4:00 PM Contributed Presentations 11/Nevada Room

COAL COMBUSTION

A Comprehensive Single Particle Char **Combustion Model**

Yam Yee Lee, University of Mississippi, University, MS

Mathematical Modeling of Coal Dust Explosions

John C. Edwards, and J. Edmund Hay, U.S. Bureau of Mines Pittsburgh Research Center, Pittsburgh, PA

Equilibrium Composition for Coal Flames Including Condensed Phases as Nonideal Solutions

Francis E. Spencer, Jr., David J. Wildman and James C. Hendrie, Jr., Pittsburgh Energy Technology Center, Pittsburgh, PA

Estimation of Standard Enthalpy for Coal from ASTM Heating Value via Linear Programming

Francis E. Spencer, Jr., and David J. Wildman, Pittsburgh Energy Technology Center, Pittsburgh, PA

Simplified Model of Coal Particle Combustion

M. J. Lyell and Ismail Celik, West Virginia University, Morgantown, WV and Thomas J. O'Brien, Morgantown Energy Technology Center, Morgantown, WV

Application of Single Char Particle Model to the Combustion of Portuguese Anthracites

Joao Fernando Pereira Gomes, OPPI. SARL Lisbon, Portugal

Wednesday, March 11/2:00 PM Contributed Presentations 12/Emerald Room

VECTOR/PARALLEL PROCESSING

Vectorizing "Bit-Twiddling" Algorithms David S. Dodson, Convex Computer Corporation, Richardson, TX

Scramjet Simulation on the CEDAR **Multiprocessor Supercomputer** Richard Roloff, University of Illinois. Urbana, II.

Parallelization of an Elliptic Solver for Reacting Flows

David E. Keyes, and Mitchell D. Smooke, Yale University, New Haven, CT

Optimization of Householder Transformations Part I: Linear Least Squares

Jim Armstrong, Convex Computer Corporation, Richardson, TX

Wednesday, March 11/4:00 PM Contributed Presentations 13/Nevada

THEORETICAL PROBLEMS

Shock Waves in the Inviscid Limit of the ld Navier-Stokes Equations for Compressible Flow

David Hoff, Indiana University, Bloomington, IN, and Tai-Ping Liu, University of Maryland, College Park, MD

Contributed Presentations

The Application of Symmetry and Bifurcation Theory to the Study of Burner-Stabilized Flames

Barbara Keyfitz, University of Houston, Houston, TX

The Existence and Behavior of Viscous Structure For Plane Detonation Waves David H. Wagner, University of Houston, Houston, TX

Catastrophic Instabilities in Square Wave Models of Detonation

Rodolfo R. Rosales, Massachusetts Institute of Technology, Cambridge, MA

Critical Behavior of an Ignition Model in Chemical Combustion

Peter J. Tonellato, Marquette University, Milwaukee, WI and Paul C. Fife, University of Arizona, Tucson, AZ

The Calculations of the Derivative of Second Virial Coefficients Based on exp-6 Intermolecular Potential Wu Xiong, Xian Modern Chemistry Research Institute, Xian, China

Wednesday, March 11/4:00 PM Contributed Presentations 14/Emerald

MODELING OF LAMINAR FLAMES

Spontaneous Gas-Phase Ignition of Solids

P. D. Gandhi, and L. J. Przybyla, Underwriters Laboratories, Inc., Northbrook, IL

Variable Density Versus Constant
Density Models for Point Source
Ignition of Premixed Gaseous Reactants
M. Champion, B. Deshaies, and G. Joulin,
E.N.S.M.A., Cedex, France

Analytic Model of Combustion in a Catalytic, Fiber-Mat Burner

Clarence M. Ablow, SRI International, Menlo Park, CA., and Hiroki Sadamori, Osaka Gas Co., Ltd., Osaka, Japan

Numerical Modeling of Laminar Diffusion Flames

R. W. Davis, E. F. Moore and H. R. Baum, National Bureau of Standards, Gaithersburg, MD and R. J. Santoro, The Pennsylvania State University, University Park, PA

A Numerical Study of Flame Spread Extinction

Colomba Di Blasi, Silvestro Crescitelli, and Gennaro Russo, Universita di Napoli, Naples, Italy

Burner-Affected Landau Instability of Premixed Flames

Guý Joulin, Laboratoire d'Energetique et de Detonique, Poitiers Cedex, France

TRANSPORTATION INFORMATION

By Air

PARKWAY TRAVEL has been selected to be the official agent for the conference and will guarantee the lowest fares available to San Francisco. Calling hours are 8:30 am-5:30 pm (EST) Monday through Friday. Call toll-free from the U.S. 1-800-235-6500. If calling from abroad, phone 1-215-977-9666. Be certain to mention that you are attending the March SIAM Conference on Numerical Combustion in San Francisco. Parkway Travel will mail you your tickets upon flight confirmation.

SPECIAL DISCOUNTS

United Airlines has been chosen as the official carrier for the conference and they have agreed (through Parkway Travel) to offer up to 40% off of regular coach fares, or 5% off the lowest applicable fare. These special fares will not be available through any agency other than Parkway Travel and we suggest that you call them before making other arrangements. Parkway will give you the lowest fare regardless of which carrier you choose. In order to get the flight of your choice, we suggest making reservations as soon as possible.

BY CAR FROM THE AIRPORT

Take 101 North until the freeway splits. Go left towards the Golden Gate Bridge. Follow the Golden Gate signs to the end of the freeway until it becomes Franklin Street. Proceed three blocks to Post Street and turn right. Continue to the intersection of Van Ness Avenue and turn left. The hotel will be three blocks up, on the right.

BY PUBLIC TRANSPORTATION FROM THE AIRPORT

Take Lorries Airport Service, located on the island on the arrival level of the airport. The shuttle departs every twenty minutes, and costs \$8.00. A taxi will cost \$25.00

By Car

FROM LOS ANGELES

Take highway 5 North to 580 West to the Bay Bridge. Take the Main Street exit on the right. Proceed to Market Street and turn left, and then take the first right onto Pine Street. Continue on Pine Street to Van Ness Avenue; the hotel is at 1500 Van Ness Avenue.

CAR RENTAL

BUDGET has been selected as the official car rental agency for the SIAM Conference on Numerical Combustion. The following rates will apply:

Type of Car	Rate	Rate
Economy	\$27	\$149
Compact	\$29	\$160
Intermediate	\$31	\$171
Full Size	\$33	\$182
Premium	\$35	\$193
Luxury	\$39	\$249

- We encourage you to make an advance reservation, as on-site availability cannot be guaranteed. Call 1-800-772-3773.
- Cars may be picked up at the airport, or at the 1301 Van Ness Street location downtown, just two blocks from the conference site.

- Cars must be picked up and dropped off at the same location.
- You will be given 100 free miles per day (cumulative) and charged \$0.20 per mile thereafter.
- You must be 21 years of age to rent a car and have a valid drivers' license.
- You must have one of the following credit cards to rent a car: AMEX, Master Card, VISA, Diners Club, Sears.
- The prices quoted do not include refueling services, tax, optional collision damage waiver, and personal accident insurance.
- Be certain to mention that you are attending the March 9-11, 1987
 SIAM conference in San Francisco.

HOTEL INFORMATION

SIAM is holding a block of rooms at the conference site, the Holiday Inn-Golden Gateway. These rooms are being held on a first come, first served basis at \$68/single and \$80/double. These rooms will be held for our exclusive use only until February 14, after which date reservations will depend on availability.

We urge you to make your reservations as soon as possible. You may do so by telephoning (415) 441-4000, or via the Hotel Reservation Form on the inside back page of this brochure (domestic mail only). When making reservations by telephone, be certain to obtain the discounted rate by identifying yourself as an attendee at the SIAM Conference on Numerical Combustion.

Late Arrival Policy: If you plan to arrive after 6:00 pm, you must guarantee one nights payment by AMEX, VISA, MC or Diners Club.

Check-in 2:00 PM, check-out 12:00 noon If you need to change or cancel your reservation, please be certain to contact the hotel by 4:00 PM on your stated day of arrival.

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Please complete the Advance Registration Form, found on the inside back cover of this brochure, and return it to SIAM in the envelope provided (domestic mail only).

The registration desk will be located in the Emerald Room on the Lobby Level of the hotel, and will be open as listed below:

Sunday, March 8/5:00 PM - 10:00 PM Monday, March 9/7:00 AM - 8:00 PM Tuesday, March 10/8:00 AM - 6:00 PM Wednesday, March 11/8:00 AM - 6:00 PM

Registration Fees

	Member	Member	Student
Advance	\$75	\$ 95	\$10
On-Site	\$95	\$115	\$10

Beer Party

Monday, March 9, 8:00 PM Crystal Room \$10.00

NON SIAM MEMBERS

Non-member registrants are encouraged to join SIAM in order to obtain the member rate for conference registration and all the other benefits of SIAM membership.

SIAM CORPORATE MEMBERS

Non-member attendees who are employed by the following institutions are entitled to the SIAM member rate:

Aerospace Corporation Amoco Production Company AT&T Bell Laboratories **Boeing Company** Cray Research, Inc.
Culler Scientific Systems Corporation E.I. Du Pont de Nemours and Company Eastman Kodak Company Exxon Production Research Company

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Science and Engineering (ICASE) IMSL, Inc. MacNeal-Schwendler Corporation Marathon Oil Company

Martin Marietta Energy Systems Mathematical Sciences Research Institute Standard Oil Company of Ohio (SOHIO) Supercomputing Research Center, a

division of Institute for Defense Analyses Texaco, Inc. United Technologies Corporation

CREDIT CARDS

SIAM is now accepting credit cards for the payment of registration fees and special functions. When you complete the Advance Registration Form, please be certain to indicate the type of credit card, the number, and the expiration date.

SPECIAL NOTE

There will be no prorated fees. There will be no refunds after the conference

To Advance Registrants

Please be certain to process your advance registration form yourself. If this task is delegated to an employee, quite often the form does not reach SIAM by the deadline, and oftentimes not at all.

If SIAM does not receive your advance registration form by the stated deadline, you will be asked to give us a check or a credit card number at the conference. We will not process either until we have ascertained that your registration form has gone astray. In the event that we receive your form after the conference, we will return your check or credit card slip.

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SIAM Conference on Numerical Combustion Holiday Inn-Golden Gateway, San Francisco, California March 9-11, 1987

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