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Dr. Philip C. E. Jorgenson
NASA Glenn Research Center
Mail Stop 5-11
Cleveland, OH 44135

Subject:	Final Report
Contract Number:	NASA Glenn, NCC3-580
Contract Title:	Applications of the Method of Space-Time Conservation Element and the Solution Element to Unsteady Chemically Reactive Flows

Dear Dr. Jorgenson,

We are writing to report to you the conclusion and findings of our research activities of the above grant. The goal of the project is the development and application of the method of Space-Time Conservation Element and Solution Element, or the CE/SE method, to simulate chemically reacting flows. The product of the project will be a high-fidelity, time-accurate flow solver analyzing unsteady flow fields advanced propulsion concepts, including the low-emission turbojet engine combustion and flow fields of Pulse Detonation Engines (PDE). Based on the documents and computer software of the CE/SE method that we have received from the CE/SE working group at NASA Lewis, we have focused our research effort on addressing outstanding technical issues related to the extension of the CE/SE method for unsteady, chemically reactive flows. In particular, we have made progresses in the following three aspects:

1. *Derivation of the governing equations for reacting flows.* In order to ensure the accuracy of the model equations for unsteady flows, we re-drive the eigen-system of the governing equations without invoking unnecessary assumptions, which have been routinely used for reactive flows at steady state.

2. *Numerical treatments of stiff source terms*. In the context of the CE/SE method, we have successfully developed an effective numerical treatment for stiff source terms, which occur in the species equations due to chemical reactions.

3. *Detailed simulations of ZND detonation waves.* To demonstrate and validate the above theoretical development, the classical ZND detonations have been employed as the testing ground to assess the accuracy of the numerical calculations.

4. *Development of a 2D Navier Stokes solver.* In the context of the CE/SE method, we have successfully developed an efficient Navier Stokes solver. Numerical algorithms for both structured and mesh unstructured meshes are developed. To calculate the viscous flux terms, a 'midpoint rule' is used. In the setting of space-time flux conservation, two boundary-condition treatments for solid wall are introduced. The Navier Stokes solvers retain all favorable features of the original CE/SE method for the Euler equations, including high fidelity resolution of unsteady flows, easy implementation of non-reflective boundary conditions, and simplicity of computational logic. In addition, numerical results show that the present Navier-Stokes solvers can be used for high-speed flows as well as low-Mach-number flows without preconditioning. The present Navier Stokes solvers are efficient, accurate, and very robust for flows at all speeds. Many technical issues about the boundary condition treatment were resolved. In addition, a NS solver based on the modified CE/SE method using conventional body fitted coordinate system was also developed.

5. *Benchmark tests of the new NS solver*. Code validation of the newly developed NS solvers was conducted. The classical shock/boundary layer interaction was simulated and the numerical results compared well with the experimental data. To demonstrate the all speed feature of the CE/SE method, we have simulated driven cavity flows, buoyant flows in a square closure, and flows over a cylinder.

6. *2D simulation of classical ZND detonations*. Previous simulations of the 1D ZND detonations were extended for 2D detonations. The two-dimensional Euler equations in conjunction with a species equation are solved in a time-accurate manner. The stiff source term is treated by a volumetric integration over a space-time region. Two examples are reported: detonation initiation and two-dimensional propagating detonations. Special flow features of detonations are crisply resolved, including cellular structure, triple points, unburned pocket, and transverse waves. These calculations clearly demonstrate the accuracy of the CE/SE method.

7. *Simulation of detonation wave with detailed finite rate chemistry.* The previously developed stiff source term treatment was implemented to simulate detonation with multiple reaction steps. Chemical reactions of hydrogen/air are modeled by

using nine species and eighteen reaction steps. A systematic approach of identifying the suitable time scale in numerical calculation is developed.

The above development has been summarized in three conference papers, which have been presented in the following international technical conferences:

1. S.J. Park, **S.T. Yu**, S.C. Chang, and P.C.E. Jorgenson "Direct Calculations of Stable and Unstable Detonations by the Space-Time Conservation Element and Solution Element Method," AIAA Paper 98-3212, the 34th AIAA/ASME/SAE Joint Propulsion Conference and Exhibit, July 1989, Cleveland, OH.

2. **S.T. Yu**, A. Himansu, and P.C.E. Jorgenson "Treating Stiff Source Terms in Conservation Laws by the Space-Time Conservation Element and Solution Element Method," the 16th International Conference on Numerical Methods in Fluid Dynamics, June 1998, Arcachon, France.

3. **S.T. Yu**, S.C. Chang, and P.C.E. Jorgenson "Basic Equations of Chemically Reactive Flows for Computational Fluid Dynamics," AIAA Paper 98-1051, the 36th Aerospace Sciences Meeting and Exhibit, January 1998, Reno, NV.

4. **S.T. Yu**, S.C. Chang, and P.C.E. Jorgenson, " Direct Calculation of Detonation with Multi-Step Finite-Rate Chemistry by the Space-Time Conservation Element and Solution Element Method," AIAA Paper 99-3772, AIAA 30th Fluid Conference and Exhibit, Jun 1999, Norfolk, VA.

5. Z.C. Zhang, **S.T. Yu**, S.C. Chang, A. Himansu, and P.C.E. Jorgenson, "A Modified Space-Time Conservation Element and Solution Element Method for Euler and Navier-Stokes Equations," AIAA Paper 99-3327, AIAA CFD Conference, Norfolk, VA, June 1999

6. S.J. Park, **S.T. Yu**, M.C. Lai S.C. Chang, and P.C.E. Jorgenson, "Numerical Calculations of Two-Dimensional Unstable Detonations by the Space-Time CE/SE Method," AIAA Paper 99-0491, the 37th Aerospace Sciences Meeting and Exhibit, January 1999, Reno, NV.

7. Z.C. Zhang and **S.T. Yu,** "Shock Capturing without Riemann Solver – A Modified Space-Time CE/SE Method for Conservation Laws," AIAA Paper 99-0904, the 37th Aerospace Sciences Meeting and Exhibit, January 1999, Reno, NV.

8. Himansu, S.C. Chang, **S.T.Yu**, X.Y. Wang, C.Y. Loh, and P.C.E. Jorgenson, " High-Resolution Genuinely Multidimensional Solution of Conservation Laws by the Space-Time Conservation Element and Solution Element Method," AIAA Paper 99-1006, the 37th Aerospace Sciences Meeting and Exhibit, January 1999, Reno, NV.

Many of the above papers can be directly downloaded from our web page www.cfd.eng.wayne.edu. We are also in the process of compiling additional results and drafting several papers to be submitted to journals.

In what follows, we summarize our innovative inventions and new technology developed during the course of the NASA supported project.

Basic Equations of Unsteady Reactive Flows

Basic equations for chemically reacting flows have been analyzed to clear up the confusion of their characteristics for numerical solution using modern CFD methods. Chemical reactions are modeled by finite rate chemistry, and species equations are incorporated with the momentum and energy equations to model reactive flows. Various forms of the governing equations have been derived, including the conservative, the non-conservative, and the characteristic forms. The transformation between different equation forms and the associated transformation matrices were also derived. *The Jacobian matrix of the equation set, its eigenvalues, and the associated eigenvector matrices have been systematically derived without any unnecessary assumptions.* The homogeneity of the flux vector as a function of the unknown vector was verified. The theoretical model has been presented in a step-by-step manner from first principles.

Treatments of Stiff Source Terms

Due to the finite-rate chemistry employed in governing equations of reactive flows, stiff source terms exist in the species equations. In the context of the space-time CE/SE method, a treatment for the stiff source term based on a volumetric integration over a space-time region has been developed. In particular, we assumed that the flow properties in macroscopic scales would not be significantly influenced by the integral effect of the stiff source terms. As a result, we proposed to redistribute the shape of the space-time conservation element such that all source term effect would hinge on the flow solution at the new time step. As such, the so called "amplification effect" caused by the stiff source term has been avoided. The numerical treatment is robust and very effective. As a contrast to the modern upwind schemes, no modulated Riemann solver or splitting method is used. Thus the logic of the present scheme is much simpler.

Direct Calculation of ZND Detonations

We have performed numerical calculations of stable and unstable ZND detonation waves by the extended CE/SE method. Due to its richness of flow physics and highly unstable characteristics, ZND detonations have been chosen as the testing ground for the above numerical development. The structure of a typical ZND detonation is composed of three parts: a pure gas dynamic *shock*, followed by *a flame zone*, and *the equilibrium states* of the burnt and unburned gases before the shock and after the flame zone. A sufficient numerical resolution of the flame zone is critical to the success of ZND calculations. We have established that only five mesh nodes are needed to resolve a half of the reaction zone when using the CE/SE method. Numerical accuracy of the result has assessed by detailed comparisons between the theoretical solutions and the numerical results for both stable and unstable ZND waves. The superb resolution shown by the CE/SE method is comparable to the most sophisticated CFD method specially developed for detonations and yet the CE/SE method is much simpler in logic and rational and thus much more efficient. For two-dimensional ZND waves, all salient features were crisply resolved, including the unstable triple points, unburned pocket, and transverse instability.

The proposed tasks in the project have been successfully performed. The resultant numerical methods and software are available to the NASA researchers. The results of the works show a new direction of high performance simulations of propulsion and combustion by using the space-time CE/SE method.

Sincerely,

Sheng-Tao Yu
Associate Professor