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The main rsults of this grant is a hybrid high order algorithm for the study of 2-D detonation waves, and the development of an adaptive wavelet ADI method as a direct or as a preconditioner for implicit time depedent integration of viscous Navier Stokes equations. Convergence acceleration using the wavelet ADI as a preconditioner is studied for the reaction diffusion equations. Also parallel implementation of the wavelet ADI preconditioner is investigated.

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FINAL TECHNICAL REPORT

Multi-resolution Wavelet Methods for the Simulation of Flames

Grant (Contract) Number AFOSR # F49620-96-1-0412

Period: 15 September 1996 - 14 September 14, 1999

Principal Investigator: Wei Cai

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1 Objectives:

Development of high order methods for detonation waves and efficient Wavelet ADI methods for reacting compressible viscous Navier Stokes equations and direct numerical simulations of multi-dimensional premixed Flame Propagations and deflagration to detonation transitions (DDT).

2 Status of effort:

We have studied adaptive wavelet ADI method for the 2-D reacting compressible Navier-Stokes equation for the simulation of premixed flames, and high order methods for 2-D detonation waves. During the three year period of the grant, we have investigated the stability of two dimensional detonation waves, and the role of using wavelet ADI as a direct solver or as a preconditioner to achieve an efficient time integrator for implicit time integration of Navier Stokes equations.

3 Research Accomplishments/New findings

The main accomplishment for this grant is a hybrid high order algorithm for the study of 2-D detonation waves, and the development of an adaptive wavelet ADI method as a direct solver or as a preconditioner for implicit time integration of Navier Stokes equations. Convergence acceleration using wavelet ADI as a preconditioner is studied for reaction diffusion equations. Also parallel implementation of the wavelet ADI preconditioner is investigated.

Cellulr Structure of Detonation Waves

Partially supported in this project, we completed the development of high order hybrid numerical simulation of two dimensional detonation waves. The major finding of this work was that the cellular structure of detonation waves depended very sensitively on the numerical dissipation of the algorithms representing detonation fronts. Further studies of the work in three dimensional cases were needed to understand the three dimensional effects of detonation waves.

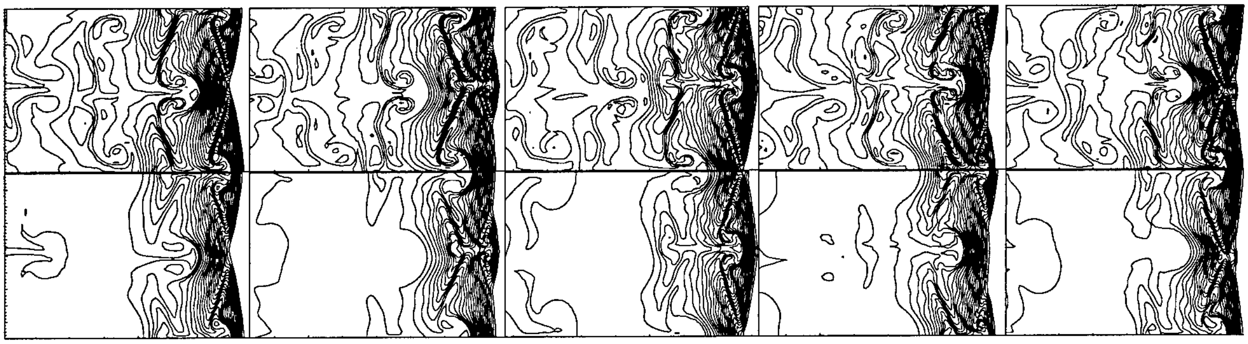


Figure 1: Two dimensional detonation wave Five snapshots of temperature, mass fraction of reactant

Wavelet ADI Schemes for Multidimensional Reacting Navier Stokes Equations

We have concentrated on the construction and implementation of the wavelet ADI methods based on Beam Warming approximate factorization of viscous Navier Stokes equations for two dimensional premixed flames. The wavelet ADI methods can be used as an efficient preconditioner for implicit time integration.

The 3-D reacting compressible Navier-Stokes Equations with a one-step reaction are written in the conservation-law form as follows

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}+\frac{\partial G(U)}{\partial y}+\frac{\partial H(U)}{\partial z}=\frac{\partial F_v(U)}{\partial x}+\frac{\partial G_v(U)}{\partial y}+\frac{\partial H_v(U)}{\partial z}+\Omega(Y,T) \tag{1}$$

where vector of conserved vector is $U=(\rho,\rho u,\rho v,\rho w,e,\rho Y)^T$ and $F(U), G(U)$, $H(U)$ are the inviscid fluxes and $F_v(U,\bigtriangledown U)$, $G_v(U,\bigtriangledown U)$, $H_v(U,\bigtriangledown U)$ are the viscous fluxes , $\bigtriangledown U=(U_x,U_y,U_z)$ and $\Omega=(0,0,0,0,0,Q(Y,T))^T$ is the chemical reaction source term and T is the temperature and Y is the mass fraction of the reactant.

The Beam-Warming factorization scheme for (1) without the source term Ω is based on a second order two level implicit time discretization and the source term can be treated separately by a Strang-type operator splitting procedure where a stiff ODE solver is used.

$$\left(1+\Delta t\theta(D_x^1A^n+D_y^1B^n+D_z^1C^n)\right)\Delta U^n=-\Delta tR^n \tag{2}$$

where D_x^1, D_y^1 and D_z^1 denote the wavelet derivative matrices along x, y and z coordinate direction, respectively and the solution increment $\Delta U^n=U^{n+1}-$

U^n and $A^n = \frac{\partial(F-F_v)}{\partial U}$, $B^n = \frac{\partial(G-G_v)}{\partial U}$ and $C^n = \frac{\partial(H-H_v)}{\partial U}$ are the Jacobian matrices for the flux vectors, the residual $R^n = D_x(F - F_v)^n + D_y(G - G_v)^n + D_z(H - H_v)^n$ and $\theta = 0.5$.

The ADI factorization with extra stability enhancement terms for 3-D for (2) will be based on

$$\begin{aligned}(1 + \theta\Delta t D_x^1 A^n - \epsilon_i V_x)(1 &+ \theta\Delta t D_y^1 B^n - \epsilon_i V_y)(1 + \theta\Delta t D_z^1 C^n - \epsilon_i V_z)\Delta U^n \\ &= -\Delta t R^n + \epsilon_e V_e \end{aligned} \tag{3}$$

where the extra V_x, V_y, V_z are second order implicit numerical viscosities and V_e is an explicit numerical viscosity to ensure the linear stability of the ADI scheme, which are especially needed for 3-D problems.

3.1 Relevance to the AF's mission and Applications

The understanding of detonation waves and the process of the deflagration to detonation transitions (DDT) have military and civil applications in the following areas and efficient adaptive wavelet algorithms will enable the development of simulation tools for those applications:

- Pulsed Detonation Engine (PDE) powered propulsion System for missile launches. The understanding of DDT process and the detonation waves will produce insights on the initiation of detonation waves and the cycle time of detonation engines to achieve appropriate cycling frequency while maintaining high specific thrust.
- The safe handling of explosives in military and industrial environments.

4 Personnel Supported

Wei Cai, faculty, PI - total 2.5 summer months.

5 Publications

The following reviewed publications are supported by this AFOSR project:

[1] High-order Hybrid Numerical Simulations of Two Dimensional Detonation Waves, AIAA J. Vol. 33, No. 7, pp 1248-1255, (July, 1995).

[2] Direct numerical calculation of neutral stability curve for one dimensional detonations, (with W.H. Oh, Y.L. Zhu), *SIAM J. Scientific Computing* Vol. 17, No. 4, pp. 814-829, July, 1996.

[3] Adaptive Wavelet Collocation Method for the Initial Value Boundary Problem of Nonlinear PDE's, (with J.Z. Wang), *SIAM Numerical Analysis*, Volume 33, Number 3, June 1996.

[4] Cai, W., and Zhang, W., An Adaptive Spline Wavelet ADI method for two dimensional reaction diffusion equations, Journal of Computational Physics, Vol. 139, 1-35, (1998).

[5] A fast wavelet collocation method for high speed circuit simulation (with Dian Zhou), IEEE transaction on circuits and systems, 1999.

[6] An adaptive wavelet method for nonlinear circuit simulation (with Dian Zhou and W, Zhang) IEEE transaction on CAD, 1999.

6 Interactions/Transitions

(a) Conferences

(b) Contact with DoD Personnels

[1] Dr. Michael Nusca at ARO lab at Arberdeen approving ground, MD on the possibility of extending our research on detonation waves and wavelet methods in the study of reacting flows inside a gun barrel.

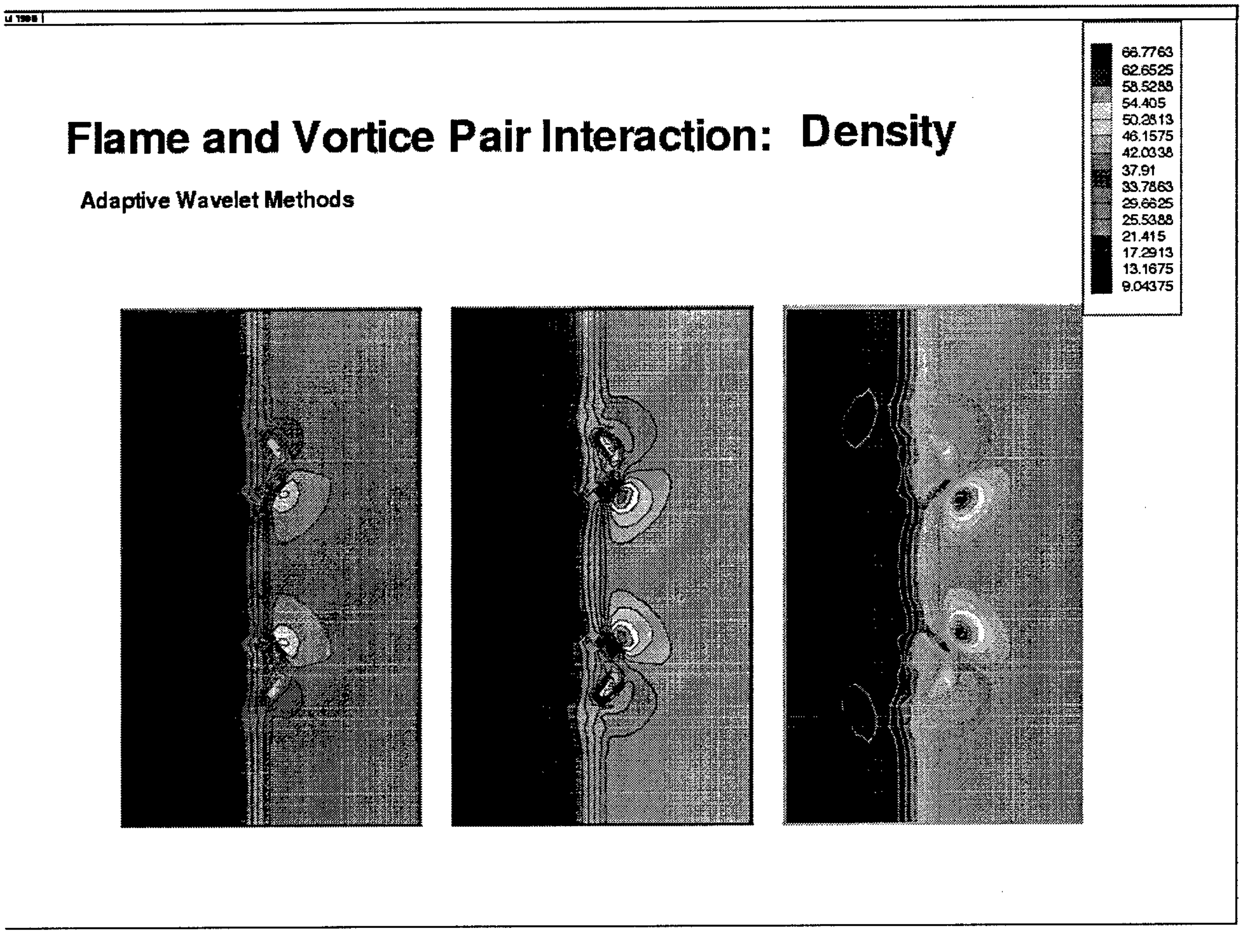
[2] Dr. Datta Gaitonde (937-255-7127) at Wright Patterson AFB regarding our results results on the flame and vortex simulations with wavelet ADI methods.

[3] Dr. Jerome T. Tzeng, Weapons Technology Directorate, Army Research lab on detonation issues in gun barrels. Tel. 410-306-0843.

(c) Transitions

(d) Patent
None

7 Honors and Awards



Flame and Vortice Pair Interaction: Density

Adaptive Wavelet Methods

Figure 2: Adaptive Wavelet ADI Methods for Reacting Navier-Stokes Equations: Flame-Vortices Interaction