# Numerical Simulation of Three-dimensional Unstable Detonation Wave Structures using a Windows Parallel Cluster

**Deok-Rae Cho, Su-Hee Won and Jeong-Yeol Choi ***

Department of Aerospace Engineering
Pusan National University
30 Jangjeon-dong, Geumjeon-gu, Busan, 609-735 Republic of Korea
E-mail:aerochoi@pusan.ac.kr - Web page: http://home.pusan.ac.kr/~apcl/

**Key Words**: Detonation Wave, Instability, Cell Structure, Windows Cluster

## ABSTRACT

Three-dimensional structures of detonation wave propagating in tubes were investigated. Inviscid fluid dynamics equations coupled with a conservation equation of reaction progress variable were analyzed by a MUSCL-type TVD scheme and four stage Runge-Kutta time integration. Variable-$\gamma$ formulation was used to account for the variable properties between unburned and burned states and the chemical reaction was modeled by using a simplified one-step irreversible kinetics model. The computational code was parallelized based on domain decomposition technique using MPI-II message passing library. The computations were carried out using an in-house Windows cluster system with AMD Athlon$^{TM}$ XP and Athlon$^{TM}$ 64-X2 processor cores. The computational domain consisted of through a square-shaped duct with wall conditions on its lateral boundaries. As an initial condition, analytical ZND solution was distributed over the computational domain with small disturbances. The unsteady computational results in three-dimension show the detailed mechanisms of rectangular and diagonal mode of detonation wave instabilities resulting same cell length but different cell width in smoked-foil record.

The unsteady results in three-dimension show the detailed mechanisms of rectangular and diagonal mode of detonation wave instabilities resulting same cell length but different cell width in smoked-foil record. The detonation cell size from 2-D result and 3-D rectangular mode result are equivalent at same flow condition, except the slapping wave pattern in 3-D result. It is understood from the results that the rectangular and diagonal modes are looks different, but the similarity is found by 45° slice cut of the smoked-foil record. Spinning mode of detonation wave propagation has been observed for a mixture of low sensitivity if the detonation cell size is large than the tube diameter. Present numerical results qualitatively agree well with experimental results regardless of the different mixture condition.

## REFERENCES

[1] Fickett, W., and Davis, W.C., Detonation Theory and Experiment, Dover Publications, New York, 2000.

[2] Taki, S., and Fujiwara, T., "Numerical Simulation of Triple Shock Behavior of Gaseous Detonation," Proceedings of the Combustion Institute, Vol. 18, 1981, pp. 1671-1681.

[3] Oran, E.S., Boris, J.P., Young, T., Flanigan, M., Burks, T., and Picone, M., "Numerical Simulations of Detonations in Hydrogen-Air and Methane-Air Mixtures," Proceedings of the Combustion Institute, Vol. 18, 1981, pp. 1641-1649.

[4] Oran E.S., Weber, J.W., Stefaniw, E.I., Lefebvre, M.H., and Anderson, J.D., "A Numerical Study of a Two-Dimensional H2-O2-Ar Detonation Using a Detailed Chemical Reaction Model," Combustion and Flame, Vol. 113, 1998, pp.147-163.

[5] Gamezo, V.N., Desbordes, D., and Oran E.S., "Two-Dimensional Reactive Flow Dynamics in Cellular Detonation Waves," Shock Waves, Vol. 9, 1999, pp. 11-17.

[6] Singh, S., Powers, J.M., and Paolucci, S., "Detonation Solutions from Reactive Navier-Stokes Equations," AIAA Paper 1999-0966, January 1999.

[7] Nikolic, M., Williams, D.N., and Bauwens, L., "Detonation Cell Sizes – A Numerical Study," AIAA Paper 1999-0967, January 1999.

[8] Gavrikov, A.I., Efimenko, A.A., and Dorofeev, S.B., "A Model for Detonation Cell Size Prediction from Chemical Kinetics," Combustion and Flame, Vol. 120, 2000, pp. 19-33.

[9] Sharpe, G.J., "Transverse Waves in Numerical Simulations of Cellular Detonations," Journal of Fluid Mechanics, Vol. 447, 2001, pp. 31-51.

[10] Hu, X.Y., Khoo, B.C., Zhang, D.L., and Jiang, Z.L., "The Cellular Structure of a Two-Dimensional H2/O2/Ar Detonation Wave" Combustion Theory Modeling, Vol. 18, 2004, pp. 339-359.

[11] Choi, J.-Y., Ma, F., and Yang, V., "Numerical Simulation of Cellular Structure of Two-Dimensional Detonation Waves," AIAA Paper 2005-1174, 43rd AIAA Aerospace Sciences Meeting and Exhibit, Jan. 10-13, 2005, Reno, NV.

[12] Williams, D. N., Luc Bauwens and Oran, E. S., "Detailed Structure and Propagation of Three-Dimensional Detonations," Proceedings of the Combustion Institute, Vol. 26, 1997, pp. 2991-2998.

[13] Zhang, Z.-C., Yu, S. T. J. and Chang, S.-C., "A Space-Time Conservation Element and Solution Element Method for Solving the Two- and Three-Dimensional Unsteady Euler Equations Using Quadrilateral and Hexahedral Meshes," Journal of Computational Physics, Vol. 175, 2002, pp.168-199.

[14] Tsuboi, N., Katoh, S. and Hayashi, A. K., "Three-Dimensional Numerical Simulation for Hydrogen/ Air Detonation: Rectangular and Diagonal Structures," Proceedings of the Combustion Institute, Vol. 29, 2002, pp. 2783–2788.

[15] Deiterding, R., "Numerical Structure Analysis of Regular Hydrogen-Oxygen Detonations," Proc. of fall '03 meeting of Western States Section of The Combustion Institute, Oct. 20-21, 2003.

[16] Eto, K, Tsuboi, N. and Hayashi, A. K., "Numerical Study on Three-dimensional C-J Detonation Waves: Detailed Propagating Mechanism and Existence of OH Radical," Proceedings of the Combustion Institute, Vol. 30, 2005, pp. 1907-1913.

[17] Hayashi, A. K., Eto, K. and Tsuboi, N., "Numerical Simulation of Spin Detonation in Square Tube," 20th ICDERS, Jul.31-Aug.5, McGill University, Montreal, Canada.

[18] Tsuboi, N., Eto, K. and Hayashi, A. K., "Three-Dimensional Numerical Simulation of H2/Air Detonation in a Circular Tube: Structure of Spinning Mode," 20th ICDERS, Jul.31-Aug.5, McGill University, Montreal, Canada.

[19] Deledicque, V. and Papalexandris, M. V., "Computational Study of Three-Dimensional Gaseous Detonation Structures," Combustion and Flame, Available online 15 November 2005, to be appeared 2006.

[20] Austin, J. M., Pintgen, F. and Shepherd, J.E., "Reaction Zones in Highly Unstable Detonations," Proceedings of the Combustion Institute, Vol.30/2, 2005, pp. 1849-1858.

[21] Choi, J.-Y., Jeung, I.-S. and Yoon, Y., "Computational Fluid Dynamics Algorithms for Unsteady Shock-Induced Combustion, Part 1: Validation," AIAA Journal, Vol. 38, No. 7,

July 2000, pp.1179-1187.

[22] Choi, J.-Y., Jeung, I.-S. and Yoon, Y., "Computational Fluid Dynamics Algorithms for Unsteady Shock-Induced Combustion, Part 2: Comparison," AIAA Journal, Vol. 38, No. 7, July 2000, pp.1188-1195.

[23] Lee, J.H., Soloukhin, R.I., and Oppenheim, A.K., Astronautica Acta., Vol. 14, pp.565-584, 1967.

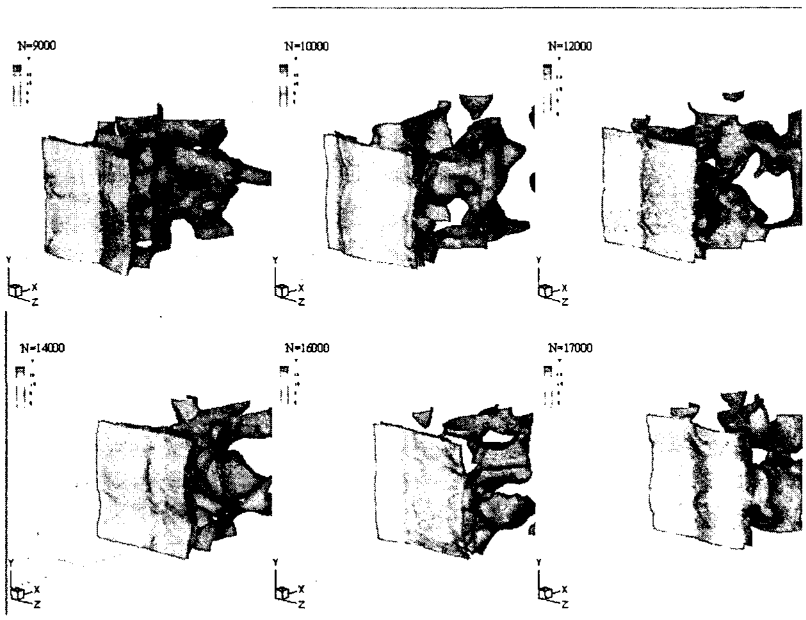


Fig. 1 Rectangular mode instability of 3D detonation wave

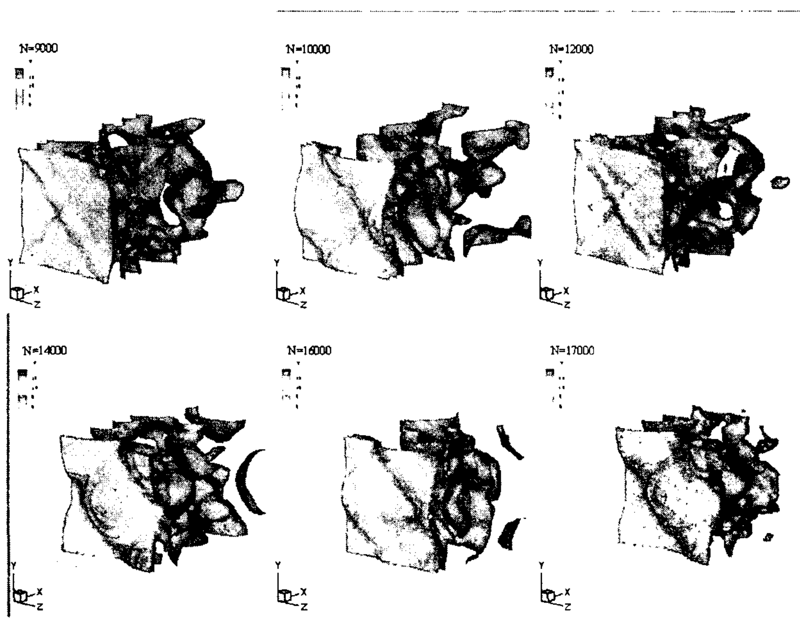


Fig. 2 Diagonal mode instability of 3D detonation wave

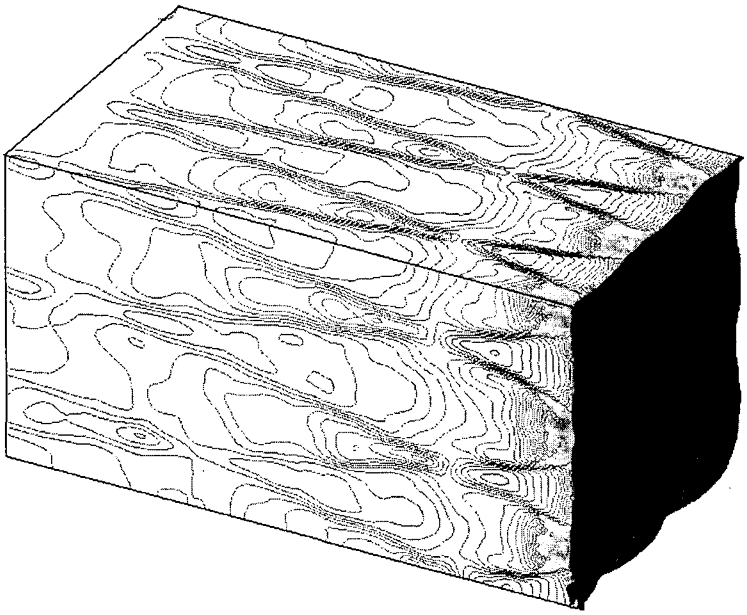

Fig. 3 Wave front and pressure contours of diagonal mode instability

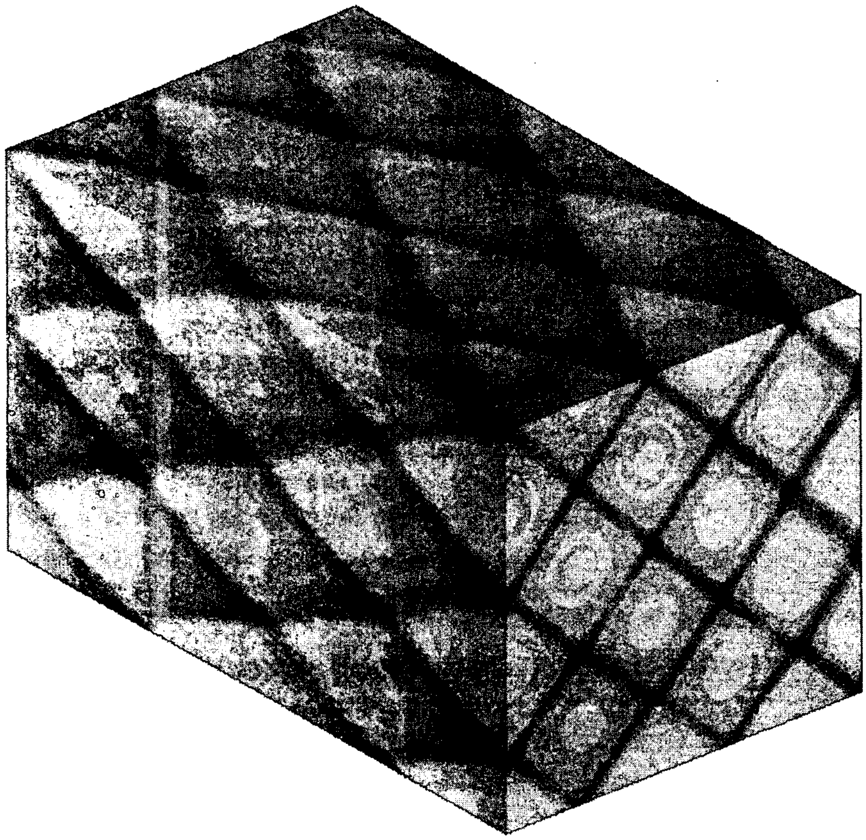

Fig. 4 Thee-dimensional smoked foil record showing surface and cross section structure

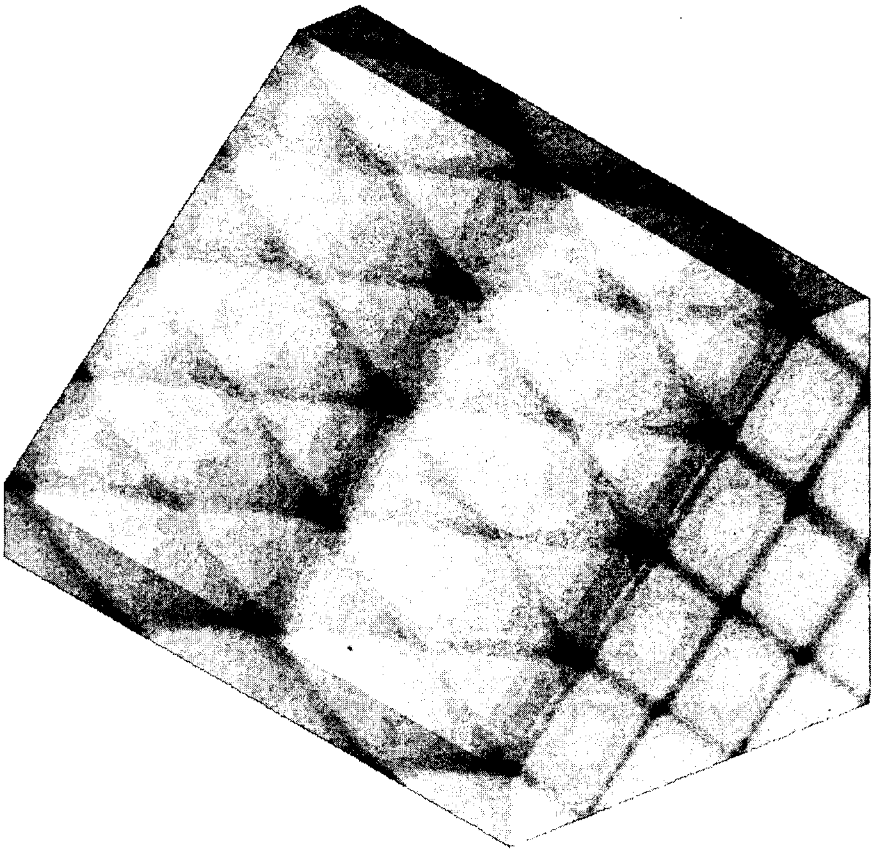

Fig. 5 Diagonal cut of thee-dimensional smoked foil record showing slapping mode history

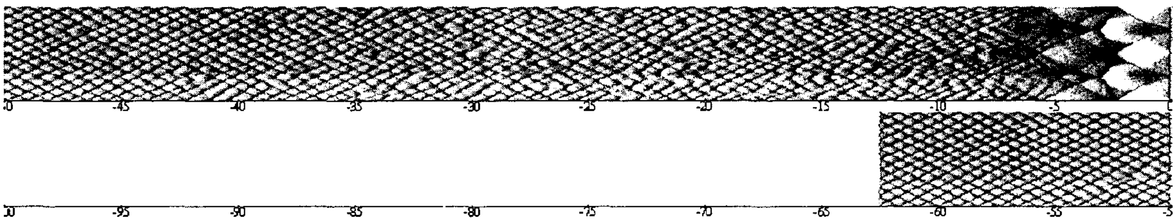

Fig. 6 Surface smoked foil record at every four sides of the rectangular duct.