

Visitor Research Report

Visitor Name: Professor Tsin-Fu Jiang
National Chiao-Tung University

Area of Research: Numerical Computation of 3D Time-Dependent
Schrodinger Equations Using the CESE Method

Period of Visit: April 9, 2008 through April 18, 2008

Goal:

During the visiting period, the visitor stays at NIA office room and has daily discussions with Dr. Chau-Lyan Chang of Langley Research Center. The visitor is a professor of theoretical physics and is interested in developing a practical computation method for realistic quantum mechanical problems, especially for the quantum dynamics of intense laser on atoms, molecules or clusters. Dr. Chang is a senior researcher of NASA Computational Aerosciences Branch. He and Dr. Sin-Chung Chang of NASA Glenn Center are pioneers of the CE/SE (conservation element/solution element) method which was first developed by Dr. Sin-Chung Chang in 90's. They have successfully developed the CE/SE applications to Navier-Stokes equation which is far more complicated than the Schrodinger equation of quantum mechanics. On the other hand, the numerical methods that can simulate real experiments of intense laser on atoms or molecules in reasonable short time are still demanding. CE/SE method shows especially promising capability in solving higher dimensional time-dependent partial differential equations. The visitor and Dr. Chang aim to work together for the development of the CE/SE method for quantum mechanical problems.

Strategy:

To build the numerical experience of solving the time-dependent Schrodinger equation by CE/SE method, the visitor starts from the beginning a-scheme of the simplest wave equation. Because the a-scheme is non-dissipative numerically, c-scheme is necessary for the convection-diffusion equation and nonlinear systems. The visitor practiced the two schemes on simple systems successfully. The next step is to learn the technique of Courant number insensitive (CNI) scheme and the spatial 2-dimensional, 3-dimensional methods. Then, we will be ready for research problems.

Accomplishments:

The visitor has finished the study of a-scheme, c-scheme. And the important non-reflecting boundary condition method. Those are under the instructive helps of Dr. Chang. Dr. Chang also explained the Courant number insensitive scheme and the higher dimensional techniques to the visitor in details. It will be hard to accomplish without the intensive talks during the visit.

Future Work:

The visit is made possible through the MoU between NIA/NARL. The face-to-face discussions are extremely helpful. In the near future, the visitor will keep studying the CNI scheme and the higher dimensional methods. Then, the visitor's group and Dr. Chang will be able to work together on the current interested research topics. The behalf of the visitor now just finish the first stage study. The next stage of higher dimensional method is even more complicated. Further mutual visits in the future would speed up the development of realistic quantum dynamics by CE/SE method. In the intense field physics problems, the information in the truncated coordinate space is also important. For instance, the photoelectron spectra are measured in the experiments of intense laser on atoms or molecules. The visitor developed a momentum space computation for hydrogen photoelectron spectrum as delivered in the seminar talk. Combine with the CE/SE, the calculation of general nonperturbative time-dependent quantum system will be another developing direction in addition to the conventional coordinate space CE/SE method.

Pending Publications: N/A

Seminar Presented:

"Computation of Hydrogen Atom Photoelectron Spectra in Momentum Space",
April 17, 2008, 2 pm, NIA Room 137