Achievements

Progress of adaptive finite element (FE) method in solving nonlinear partial differential equation (PDE)

Scientific computation is widely used in multiple cross-disciplinary areas. Most of the issues coming from this area finally result in solving PDE. In the process of solving PDE, the meshes are firstly generated within the area where PDE is functional; then, the methods of FE, Finite Difference (FD), and Finite Volume (FV) are applied on the meshes to solve the PDE. Because of the unknown results of the PDE, the traditional methods for the mesh generation are experiential. This strategy mostly results in the low efficiency in the complicated engineering computing environment especially for those nonlinear problems, and confines the application scope of these discretized methods.

Adaptive Finite Element (AFE) method is a discretized method that automatically coordinates the finite element mesh to optimize the computation complexity according to the convergent accuracy of the results and the characteristics of the solutions. This method is based on the theory of posteriori error analysis, can be widely used and programmed by software, and becomes one of the focuses of scientific computation. With the consistent support from NSFC, especially the support from the fund for National Distinguished Young Scholars, Prof. Zhiming Chen from Academy of Mathematics and Systems Science, CAS, progressed in their research in the nonlinear problems of posteriori error analysis and adaptivity in the topics of elliptical calculus of variations, superconductivity, continuous casting, electromagnetic scattering and the Richards equation for the mobility of non-saturated water:

1. The scientific computation on the unconfined area for electromagnetic scattering became an important subject with extensive considerations. The global research focused on the trace to solve electromagnetic scattering problems casting on the technique of the perfectly matched layer (PML), which was firstly proposed in 1994 using FE method. Prof. Chen and his research team further developed and published Adaptive PML for grating problems and 2D acoustic scattering problems, namely, utilized the theory of posteriori error analysis to define the parameters of PML. They overcame the deficiency from experientially defined parameters in engineering computation. And this method possesses prosperous application future and theoretical significance.

2. Nonlinear conductive-diffusive equation is widely utilized in the scientific computation of fluid mechanics. Prof. Chen obtained new results, which could not be solved by traditional numerical methods, in allusion to nonlinear Richards' equations for the mobility of non-saturated water, by applying the famous Kruzkov method of posteriori error analysis in nonlinear balance equation to nonlinear parabolic equation with boundary conditions. Prof. Chen further improved their AFE method with *Method of Line* (AML) to solve the nonlinear conductive-diffusive equation based on the previous approach. A majority computation results showed that this new improved algorithm had the optimized computation complexity for evolutionary problems. Although the fact that AFE method had the optimized computation complexity for the elliptic problems, for the evolutionary problems, AML was not recognized and deeply studied in its optimized computation complexity before Prof. Chen's work. Prof. Chen's innovation clarified that AML method of parabolic equation had better optimized computation complexity than AFE.

Prof. Chen gained praising evaluation from international colleagues on the innovative research of AFE, and was invited to present a 45-min lecture on the 2006 International Congress of Mathematicians held in Spain.

Controlling the electromagnetism of single ion by "molecular surgery"

Controlling and modifying the magnetic property of a single molecule is the frontier for the development of molecular science. With the funding support from NSFC, Scientific Innovation Program of CAS as well as 973 from Ministry of Science and Technology of China, Prof. Jianguo Hou (Member of CAS) and Prof. Jinlong Yang from National Laboratory for Physical Sciences at the Microscale of University of Science & Technology of China, together with Prof. Qingshi Zhu (Member of CAS), made an artifice surgical operation to a single CoPc