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Scientific Computing Technologies Devising High-Order Methods and Adaptive Mesh Refinements

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Johnston Hall 338

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Abstract:

Recent paradigm in large-scale scientific computing have motivated investigations into computational fluid dynamics (CFD) and numerical methods that are more suitable for distributed-memory parallel computers. The future evolution of high-performance computing (HPC) will require a highly scalable, accurate and efficient computational algorithm. Accurate numerical schemes are essential to ensure high-fidelity simulations capable of capturing the multi-physical, multi-scale, and complex phenomena. To construct efficient computational meshes for a variety of CFD and numerical methods, adaptive mesh refinement (AMR) with suitable error estimators need to be devised. Scalable performance is necessary to exploit the massively-parallel petascale systems that will dominate HPC for the foreseeable future. The goal of my thrust will be research into implementation of advanced computational technologies through high-order methods - e.g., high-order finite element method (p - FEM); spectral element method (SEM); discontinuous Galerkin methods (DGM) - devised with a scalable parallel computing algorithm. The applicability and efficiency of CFD and numerical methods span a wide variety of scientific and engineering applications. Despite the relative maturity and widespread success of CFD and numerical techniques in science and engineering, there remain open challenges that need to exploit the full potential of current high-performance parallel computers. In order to address some of open issues, my talk will cover some of recent efforts to achieve the goal of my future research. First, I will address parallel computations for emerging engineering applications: the electro-osmotic flow and species transport phenomena in micro-mixer as well as convective heat/mass transfers for an array of electronic cooling devices. The computational codes, which are designed by 2-D triangle and 3-D tetrahedron based methods devising AMR techniques, are written in C/C++ interfacing with Petsc solver through libMesh software package. Second, to develop a scalable conservative dynamical core for the global climate and atmospheric modelings, I will address my role of DOE funded SciDAC project currently participated: extension of an existing 2-D DGM to a scalable 3-D DGM into the NCAR high-order method modeling environment (HOMME), which has currently proven to efficiently scale up to O (1000) parallel processors of IBM Blue Gene/L and IBM POWER5 p575 supercomputers. The code is written in Fortran 90/95 devising hybrid MPI/OpenMP approach interfacing with LAPACK, LINPACK, BLAS, and METIS. Furthermore, the code supports parallel data handing capabilities through the Parallel Network Common Data Form (pNETCDF) library and its scientific visualization is performed by NCAR Command Language (NCL).

Speaker's Bio:

Hae-Won Choi is currently a Post-doctoral research associate in the Department of Computer Science, Computational Science Center, University of Colorado at Boulder. Choi received his Ph.D. in Mechanical Engineering (2005) from the University of Toronto, Canada; his M.A.Sc. in Mechanical Engineering (2001) from the University of Toronto, Canada; and his B.Eng. in Mechanical Engineering (1999) from Pusan National University, Republic of Korea (South Korea). Choi's Research Interests include: Computational Fluid Dynamics (CFD); Numerical Modeling for Microfluidics; Fluid Mechanics & Transport Phenomena; Computational MEMS & BioMEMS; Interdisciplinary, Multi-scale Design & Optimization; Scientific and Engineering Computation; Numerical Methods; High Performance Parallel Computing; Adaptive Mesh Refinement(AMR); Discontinuous Galerkin (DG) Methods; Finite Element Methods (FEM); Spectral Element Methods (SEM); A-Posteriori Error Estimation.

Refreshments will be served.

This lecture has a reception.

