Research Statement/Interest/Future Plan
High-performance computing techniques for multidisciplinary Problems

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Outlines:

- High Performance Computing Techniques
- Numerical Methods, Analysis and Computation
- Particle (Vortex Methods, Level Set Methods) and Grid(FDM, FVM, FEM) Methods
- Computational Fluid Dynamics (Numerical Simulation and Numerical Experiment)
- Turbulence Modeling (LES, DES, RANS) (**Ongoing**)
- Application of Numerical Software to Science & Engineering
- Commercial Softwares: ANSYS Fluent, Gambit, Star CCM+, OpenFOAM (**Ongoing**)
- Mathematical Programming (Non/Linear), Optimization

1. Introduction

High Performance Computing (HPC) is the field that concentrates on developing supercomputers and software to run on supercomputers. A main area of this discipline is developing parallel processing algorithms and software. HPC is about big problems which needs lots of memory, many cpu cycles and big hard drives. No matter what fields it works in, perhaps the research would benefit by making problems larger through transferring from 2D to 3D, to generate fine mesh and to increase number of elements in the simulation. The great challenges of HPC are simulations of physical phenomena such as weather forecasting, black holes colliding, oil reservoir management, economic modeling, computer-aided design, drug design, exploring the origins of the universe, searching for extra-terrestrial life, computer vision and nuclear power and weapons simulations. The following topics are specializations and interest of my research.

2. Fast Vortex Method (Pure Lagrangian Method)

A mathematical formulation for the 3D vortex method has been developed for calculation using a special-purpose computer MDGRAPE-2. A rigorous assessment of this hardware has been made for a few representative problems and compared the results with and without it. The error arising from the approximation is evaluated by calculating three pairs of vortex rings impinging to themselves. Consequently, acceleration of about 100 times is achieved by MDGRAPE-2 while the error in the statistical quantities such as kinetic energy and enstrophy remain negligible.

MDGRAPE-3, successor of MDGRAPE-2, has been applied to the same calculations and the improvement in speed was 1000 times faster when compared with the host PC for $N=10^6$. The simultaneous use of the fast multipole method (FMM) with MDGRAPE-2 and MDGRAPE-3 has been successfully applied to the same calculations to investigate the possibility of further accelerations. The various forms of FMM and their performance on MDGRAPE-2 and MDGRAPE-3 have been investigated. With the help of these acceleration techniques the dynamics of two colliding vortex rings have been studied and the computation time has been reduced by a factor of 2000 compared to a direct calculation on a standard PC. The global kinetic energy and enstrophy have been investigated to address the numerical accuracy. The reconnection of the vortex rings was clearly observed, and the discretization error became nearly negligible for the calculation using 10^7 elements.

3. Parallel Mesh Algorithm (Finite Element Method)

The advancements of parallel mesh generation and adaptation tools are important in current CFD research. In fact there are lots of problems related to mesh generation and adaptivity remain open. Finite element and finite volume methods could largely benefit by proposing solutions to the remaining issues. Among the challenges that are still to be taken up, we will mention the adaptation for curvilinear meshes, the anisotropic mesh adaptation with high aspect ratios, the gradation control on highly anisotropic meshes, the automatic generation and adaptation of boundary layer meshses, the handling of complex CAD models, issues in mesh optimization like fully robust sliver elimination, and adaptively for very large meshes.

We identify and propose solutions for several issues encountered when designing a mesh adaptation package, like mesh-to-mesh projections and mesh database design, and we describe an algorithm to integrate a mesh adaptation procedure in a physics solver. The open source MAdLib package is presented as an example of such a mesh adaptation library. A new technique combining global node repositioning and mesh optimization in order to perform arbitrarily large deformations is also proposed. We then present several test cases to evaluate the performances of the proposed techniques and to show their applicability to fluid-structure interaction problems with arbitrarily large deformations.

4. Multigrid Algorithm for Cell Centered Finite Difference Methods

In recent years, it has become increasingly obvious that iterative methods provide the only feasible technique for solving the large systems of algebraic equations which arise from large scale scientific simulations modelled by partial differential equations. Multigrid methods often represent the most efficient strategy for iteratively solving these systems. For this reason, the multigrid method has been subject to intensive theoretical and computational investigation. Elliptic differential equations with discontinuous coefficients arise from many areas of applications and are difficult to handle, numerically or analytically. Of many such problems, a few examples are flows through porous media with different porosity, electric currents through material of different conductivities and heat flows through heterogeneous materials. The numerical methods treating such problems are important areas of research. Among them, the CCFD is a finite volume type of method and has been used by many engineers for solving elliptic problems with discontinuous diffusion due to its simplicity and local conservation. CCFD methods, however, have certain accuracy limitations on irregular grids.

5. Future Research Plan

HPC in Computational Fluid Dynamics (Turbulence Modelling): Computational fluid dynamics (CFD) is by far the largest user of high-performance computing (HPC) in engineering. The main scientific challenge is the need to gain a greater understanding of turbulence and its consequences for the transfer of momentum, heat and mass in engineering applications, including aerodynamics, industrial flows and combustion systems. Availability of HPC has led to significant advances in direct numerical simulations (DNS) of turbulence and turbulent combustion. Simulation of turbulent flows over complex geometries represents a challenge for a computational fluid dynamics (CFD) code. Computing at the Petascale raises a number of significant challenges for parallel computational fluid dynamics codes. The unstructured mesh has been successfully used in the Reynolds-averaged Navier-Stokes (RANS) and most recently the Large-eddy simulation (LES) applications; it is still not suitable for direct numerical simulation (DNS), in which a higher order numerical scheme is essential in order to capture small-scale turbulent flow motions, particularly in the near wall region.

Large, Periodic and BL Meshes with Deformation: We will do experiments about large deformations, geometry handling and Boundary Layer (BL) mesh adaptation for 'academic' test cases. Introduction of the periodic transformations and the evaluation of the anisotropic unstructured meshes for turbulent boundary layers will be performed. Then, we will turn to do adaptation of meshes for aero elastic computation for 3D wing with 1st bending mode along with BL mesh. In addition, the present algorithm can be applied to adaptive BL mesh, Ocean Modelling and Fluid Structure Interaction (FSI) problems.

Ocean Modelling: The Ocean is a geophysical fluid. The goal of the ocean modelling is to reproduce numerically the dynamics of the ocean. Dynamics of the ocean include: mean and time varying circulation, waves, turbulence, instabilities, convection, mixing, jets etc. The oceans play a crucial role in our climate. Because of the high heat capacity of water (2.5 m of the upper ocean is equivalent to the entire troposphere) and the oceans' large extent (they cover over 70% of the Earth's surface), oceans act as a gigantic thermal flywheel, mitigating the fluctuations of our long-term weather. They are also huge reservoirs of CO_2 (containing about 60 times the amount of CO_2 in the atmosphere) and have a long memory. Oceans therefore play a pivotal role in determining the climatic conditions on our planet on a large variety of timescales. However, we still do not understand well the intricate details of their circulation and their interaction with the atmosphere. Furthermore, the oceanographers are data-poor in general. For predicting the future state of the oceans, and hence of the climate, numerical models are indispensable. There are several numerical models are developed such as OGCM, POM, MOM, MICOM, HICOM, OPA, MITgcm, SEOM, FEOM, FVCOM etc. Our objective is to develop a high performance computing model for oceanography either use existing method or modify to use for large scale simulations.

Highly Scalable Computing: The advent of multicore CPUs and many core GPUs means that mainstream processor chips are now parallel systems. The challenge is to develop application software that transparently scales its parallelism to leverage the increasing number of processor cores, such as 3D graphics applications transparently scale their parallelism to many core GPUs with widely varying numbers of cores. It is a well known fact that dense matrix factorisation scales well and can be implemented efficiently on parallel computers. We will present the fast algorithms to factor a wide class of sparse matrices (including those arising from two- and three-dimensional finite element problems) that are asymptotically as scalable as dense matrix factorisation algorithms on a variety of parallel architectures. Our algorithms will incur less communication overhead and are more scalable than any previously known parallel formulation of sparse matrix factorisation. We will also use some commercial software such as ANSYS FLUENT, Gambit, Star CCM+, OpenFOAM to application in various engineering simulations.

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