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Inverse Lax-Wendroff procedure for high order boundary conditions: survey and recent developments

Prof. Yi-Ju Chou

Numerical investigation of convective sedimentation in strongly stratified environment

We conduct numerical simulation to investigate the formation of the leaking pattern in convective sedimentation when a particle-laden fluid layer descends through a sharply stratified ambient flow. This is a phenomenon frequently seen in sedimentation of small suspended particles near the surface of natural water bodies, including sediments, volcanic ashes, and microorganisms. We show that the temporal evolution of the sedimentation process can be divided into three stages, including (in temporal order) Rayleigh-Taylor instability, convection, and dissipation stages. Theoretical argument based on the heat convection problem is provided for the second stage. In the third stage, which becomes the final stationary state, we derive the criterion for the occurrence of the leaking pattern from the scaling argument, which is further confirmed by the present simulation results and previous laboratory experiments.

Inverse Lax-Wendroff procedure for high order boundary conditions: survey and recent developments

Prof. Chi-Wang Shu

We discuss a recent development of a high order finite difference numerical boundary condition for solving hyperbolic Hamilton-Jacobi equations, hyperbolic conservation laws, and convection-diffusion equations on complex geometry using a Cartesian mesh. The challenge results from the wide stencil of the interior high order scheme and the fact that the boundary may not be aligned with the mesh. Our method is based on an inverse Lax-Wendroff procedure for the inflow boundary conditions coupled with traditional extrapolation or weighted essentially non-oscillatory (WENO) extrapolation for outflow boundary conditions. The schemes are shown to be high order and stable, under the standard CFL condition for the inner schemes, regardless of the distance of the first grid point to the physical boundary, that is, the "cut-cell" difficulty is overcome by this procedure. Numerical examples are provided to illustrate the good performance of our method.

Inverse Design: Thermal Management and Control

Prof. George P. G. Huang

Using fuel as a heat sink to manage and control the thermal endurance of aircraft is an area of interest from a fundamental point of view. First, the topology of the fuel line not only can affect the efficiency of the heat release but also can be designed to respond quickly to the change of the environmental heat load conditions. Second, the problem is an inverse design one in which the solution is generally known by the requirements of the aircraft and the design or/and control strategies are optimized to give the best desired solution. In the current work we shall focus on the dynamic optimal solution of the differential equations governing the heat transfer of recirculated fuel flows for the single and dual tank arrangements. It has been observed that the dual tank arrangement can store and release energy faster than the single tank case. Finally, the adjoint method is shown to be a subset of the current solution method and the linear quadratic regulator, the feedback controller, can be derived by linearizing the adjoint equations against the trim point to offer a simple control strategy which can be implemented directly in the feedback control hardware.

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Essence of Shock Capturing

Prof. Taku Ohwada

We will develop a high-performance shock-capturing scheme on the basis of a simple principle and elementary gadgets aiming to reveal the essence of shock capturing. The formal accuracy of the scheme is fourth order in time and fifth order in space. The former accuracy is achieved by the use of the conventional Runge-Kutta method and the latter is done by the conventional polynomial approximation. The scheme is capable of capturing shock waves sharply and has strong resistance against shock anomalies, such as carbuncle phenomenon and post-shock oscillations. This noteworthy capability is brought about by a smooth transformation of the scheme into the first order equilibrium flux method, the numerical flux of which can be interpreted as a variant of the standard one, around shock waves.

The scheme is also capable of capturing stationary contact discontinuities sharply without internal mesh points owing to a smooth transformation of the scheme into the simple upwind scheme around them.

The scheme does not require the local characteristic decomposition and it is less costly than WENO scheme with the same formal accuracy.

Multiphysics Modeling and Computations of Complex Flows in Aerospace Applications

Prof. Yen-Sen Chen

Aerospace sciences and engineering designs require the aid of comprehensive scientific computing in order to enjoy cost-effective development outcomes with more in-depth understanding of the underlying physics and improved performance of the products or test articles. In the area of fluid and thermal dynamics, Navier-Stokes equations solver with physical models that involved multiple disciplines are often required to solve the flow dynamics problems that are closely linked with critical performance parameters of the design. In this work, a Multiphysics computational method has been developed with extensive design validations against many benchmark cases ranging from small-scale tests in the laboratories to mission oriented full-scale flying articles. This computational model features in second-order numerical scheme for all-speed flow regimes, real-gas and real-fluid thermal properties, finite-rate chemistry, turbulence models, multiphase flow models, radiative transfer models, conjugate heat transfer and fluid-solid interactions model, etc. Application test cases include rocket engine combustion and internal flows, hypersonic flows with aerothermodynamics effects and supersonic combustion ramjet physics, high-energy laser plasma propulsion benchmarking, and rocket nozzle side loads with fluid-structure interaction modeling. These multiphysics aerospace test cases are presented and discussed with findings and recommendations for future developments of the numerical model.

Development of a Parallel Direct Simulation Monte Carlo Code (PDSC++) and Its Applications in Aerodynamics and Industry

Prof. Jong-Shinn Wu

Abstract

Non-equilibrium rarefied gas dynamics effect has been playing an important role in several scientific and engineering disciplines. These include high-altitude hypersonic flow, reentry flight from orbit with considerable chemical reactions, vacuum technology, micro and nano-scale gas flows, plume impingement on spacecraft, low-pressure materials processing flow, and comet dust and gas plume, to name a few. These gas flows are either highly rarefied or strongly non-equilibrium, which makes the continuum-based Navier-Stokes equations either breakdown or unsuitable for describing these flow phenomena correctly. Instead, the integro-differential Boltzmann equation can faithfully describe these flows. Unfortunately, not only does it have six phase spaces (three positions and three velocities) but also there is a nearly intractable collision integral term. This makes the direct numerical solution of the Boltzmann equation very difficult even with the advanced modern supercomputer system. An alternative and efficient numerical method, which is the direct simulation Monte Carlo (DSMC) method, is proposed by G.A. Bird [1] for modeling the nonequilibrium rarefied gas flows.

The central idea of DSMC is to reproduce real flow properties with no more than collision kinetics of gas molecules through a large number of pseudo particles that are used to represent real gas molecules. Each pseudo particle represents a fairly large number of real gas molecules. In this paper, a general-purpose parallel DSMC (PDSC++) code based on the C++ language using a 2-D/2D-axis/3-D hybrid unstructured grid has been developed and validated for more than a decade. Some important features of the PDSC++ include hybrid unstructured mesh, variable time-step (VTS) scheme [2], transient adaptive sub-cell (TAS) method [3], domain re-decomposition, convergence scheme, parallel computing technique, and chemical reaction based on TCE model [1]. Many important applications in aerodynamics and industry are presented in the meeting.

References

- [1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford Univ. Press (1994).
- [2] J.-S. Wu, K.-C. Tseng, F.-Y. Wu, "Three Dimensional Direct Simulation Monte Carlo Method Using Unstructured Adaptive Mesh and Variable Time Step", *Comput. Phys. Comm.*, 162, 166-187 (2004).
- [3] C.-C. Su, K.-C. Tseng, H.M. Cave, J.-S. Wu, Y.-Y. Lain, T.-C. Kuo and M.C. Jermy, "Implementation of a Transient Adaptive Sub-Cell Module for the Parallel DSMC Code Using Unstructured Grids", *Comput. Fluids*, 39, 1136-1145 (2010).

Computational Fluid Dynamics Based on The Unified Coordinates

Prof. Wai-How Hui

For material related to this talk, [click here](#).

Numerical Study of Transition-Related Turbomachinery Flows

Prof. Song Fu

For material related to this talk, [click here](#).

Numerical Descriptions of Nonlinear Acoustic Propagations in Homogenous Thermoviscous Media

Dr. Manuel Diaz

Lattice Boltzmann simulations on multi-GPU cluster

Prof. Chao-An Lin

Lattice Boltzmann method (LBM) as an explicit numerical scheme, which requires only neighboring operations, is very suitable for parallel or graphic processing unit (GPU) computations. There are several strategies to further improve the GPU performance, such as reducing the data transaction between host and device, and using efficient memory management, such as shared memory. Another way is adopting different streaming strategy to optimize the data transfer between the GPU global and shared memory. On the other hand, multi-GPU computation can certainly elevate the performance. This can be achieved by using multi GPUs on a single node through OpenMP or POSIX thread. Alternatively, for cross node GPU computations, MPI on cluster of GPUs can be employed, which is adopted here. Several test simulations will be presented to demonstrate the effectiveness of LBM simulations of GPU cluster.

Numerical issues on some interfacial problems with fluid flows

Ming-Chih Lai

In this talk, we shall introduce some numerical issues arising from 3D simulations for the interfacial flows with surfactant and vesicle problems. In particular, the major numerical challenges to study those problems mainly fall into the geometrical modeling of 3D surface representations and its computations on geometrical quantities and the derivatives along the surface. We will explain the mathematical models and the numerical methods in detail.

A Characteristic-based AUSMD Scheme to Solve the Shock and Droplet Flow Problems

Prof. Yang-Yao Niu

For material related to this talk, [click here](#).

CFD Simulation of Serpentine S-Duct with Flow Control

Prof. Lie-Mine Gea

For material related to this talk, [click here](#).

Laser-induced cavitation bubbles: Mathematical models & simulations

Prof. Keh-Ming Shyue

For material related to this talk, [click here](#).

An Optimal Analysis on Collision-Pair Search Algorithm in Lagrangian Particle Tracking Method

Prof. Keh-Chin Chang

For material related to this talk, [click here](#).

Dynamic Discrete Ordinate Method in Solving Boltzmann Equation for Gas Flows

Chin-Tsau Hsu and Kelvin K.F. Sin

¹ Professor Emeritus, Department of Mechanical and Aerospace Engineering, Hong Kong University of Science and Technology, Hong Kong.

² Consultant, Ove Arup & Partners Hong Kong Ltd. (ARUP), Hong Kong

Abstract

Boltzmann equation based on gas kinetic theory has been well accepted as an alternative formulation of gas flows, with wider regime than Navier-Stokes equation. However, the high computational cost rendered numerically solving Boltzmann equation unaffordable and impractical for engineering applications. The main hurdle in traditional numerical implementation appeared in the evaluation of macroscopic quantities by taking hydrodynamic moments with a quadrature method in physical domains. This difficulty amplified particularly for flows at high Mach number and with large thermal inhomogeneity, where huge number of quadrature points is required to cover a large range of velocity space for numerical accuracy. Recently, a Dynamic Quadrature Scheme (DQS)

was proposed [1] for removing this hurdle. The novel feature of DQS is that the hydrodynamic moment integrals are transformed into non-dimensional forms before taking a quadrature procedure. As a result, the required number of quadrature points for numerical accuracy in taking hydrodynamic moments is independent of macroscopic quantities and the numerical error occurs only at the second order of small Knudsen number which is the common case of gas flows encountered in engineering problems.

In this paper, the salient features of DQS and the implementation of DQS to Discrete Ordinate Method, referred as "Dynamic Discrete Ordinate Method" (DDOM), are briefly reviewed. To show the computational efficiency of DDOM, 1D and 2D DDOM codes were developed based on the BGK collision model with Maxwell equilibrium distribution for Boltzmann equation and validated with the benchmark flows of 1D and 2D Riemann problems, backward-step problem, as well as cavity flows. It was found that only 3 quadrature points are needed in each velocity dimension by DDOM for all tested flows. An efficiency of 20-times faster in computational-time is achieved by DDOM than by traditional DOM for 2D flows, while 5 times faster for 1-D problems. For 3D simulations, a 3D DDOM parallelized code along with a 2D DDOM parallelized code were developed and tested preliminarily with the enhancement of CUDA and Graphic Processing Unit (GPU) cluster. The results of tests show an over 90% parallel efficiency. With a Quad-GPU cluster, the speedup of 780 times was achieved versus the identical process running on a single thread of CPU.

[1]. Hsu, C.T., Chiang, S.W., and Sin, K.F., (2012), "A novel dynamic quadrature scheme for solving Boltzmann equation with discrete ordinate and lattice Boltzmann methods", *Communications in Computational Physics*, 11 (4), 1397-1414.

Unified Gas-kinetic Scheme for Multiscale Transport

Prof. Kun Xu

For material related to this talk, [click here](#).

What we have done with Godunov scheme in the past?

Prof. Feng Xiao

For material related to this talk, [click here](#).

Towards Large Eddy Simulation for Turbomachinery Flows

Prof. Z. J. Wang

For material related to this talk, [click here](#).

High-Order Conservative Asymptotic-Preserving Schemes for Modeling Rarefied Gas Dynamical Flows with Boltzmann-BGK Equation

Prof. Min-Hung Chen

For material related to this talk, [click here](#).

New aspects of internal and boundary friction for the onset of dense granular mass

Prof. Fu-Ling Yang

For material related to this talk, [click here](#).