Computer Physics Communications 184 (2013) 2378–2390

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

A true-direction reconstruction of the quiet direct simulation method for inviscid gas flows

Y.-J. Lin [a], M.R. Smith [b,c], F.-A. Kuo [a,c], H.M. Cave [a,d], J.-C. Huang [e], J.-S. Wu [a,*]

[a] Department of Mechanical Engineering, National Chiao Tung University, Hsinchu, Taiwan
[b] Department of Mechanical Engineering, National Cheng Kung University, Tainan, Taiwan
[c] National Center for High-performance Computing, Hsinchu, Taiwan
[d] Department of Mechanical Engineering, University of Canterbury, Christchurch, New Zealand
[e] Department of Merchant Marine, National Taiwan Ocean University, Keelung, Taiwan

ARTICLE INFO

Article history:
Received 1 December 2012
Received in revised form
4 April 2013
Accepted 8 May 2013
Available online 20 May 2013

Keywords:
QDSMC
QDS
Euler equations
TDEFM
CFD
Kinetic theory of gases

ABSTRACT

In this paper, a true-direction flux reconstruction of the second-order quiet direct simulation (QDS-2N) Smith et al. (2009) [3] as an equivalent Euler equation solver, called QDS-N^2, is proposed. Because of the true-directional nature of QDS, where volume-to-volume (true-direction) fluxes are computed, as opposed to fluxes at cell interfaces as employed by traditional finite volume schemes, a volumetric reconstruction is required to reach a totally true-direction scheme. The conserved quantities are permitted to vary (according to a polynomial expression) across all simulated dimensions. Prior to the flux computation, QDS particles are introduced using properties based on weighted moments taken over the polynomial reconstruction of the conserved quantity fields. The resulting flux expressions are shown to exactly reproduce the existing second-order extension for a one-dimensional flow, while providing a means for true multi-dimensional reconstruction. The new reconstruction is demonstrated in several verification studies. These include a shock–bubble interaction problem, an Euler-four-shock interaction problem, and the advection of a vortical disturbance. These results are presented, and the increased computation time and the effect of higher-order extension are discussed in this paper. The results show that the proposed multi-dimensional reconstruction provides a significant increase in the accuracy of the solution. We show that, despite the increase in the computational expense, the computational speed of the proposed QDS-N^2 method is several times higher than that of the previously proposed QDS-2N scheme for a fixed degree of numerical accuracy, at least, for the test problem of the advection of vertical disturbances.

1. Introduction

There are a number of approaches for the simulation of gas flows, depending on the nature and level of rarefaction of the flow. Computational fluid dynamics (CFD) typically uses the finite volume method to solve a set of discretized governing equations, usually the Euler or Navier–Stokes equations for continuum flows. Contemporary finite-volume CFD divides the computational domain into a grid of cells, and fluxes of mass, momentum, and energy are calculated through the interfaces between these cells. This technique may suffer from the major disadvantage that the poor alignment of the grid with the flow field may result in large errors for some important flows (e.g., explosive blast wave), since fluxes can only occur between cells that share an interface, i.e., no reflection of the true-direction nature of the gas flow. Thus, CFD requires a careful grid design to ensure accurate results, convergence, and stability.

Since the development of direct simulation Monte Carlo (DSMC) by Bird [1] for statistically solving the Boltzmann equation, a large number of continuum kinetic theory-based schemes have emerged following a similar spirit. In 1980, Pullin [2] proposed the equilibrium flux method (EFM) as an analytical equivalent to the equilibrium particle simulation method (EPSM), which is a direct simulation method where particles are forced to assume the Maxwell–Boltzmann equilibrium velocity probability distribution function instead of performing collisions. Later, Smith et al. [3] proposed a general form of the EFM method known as the true-direction equilibrium flux method (TDEFM), which captures relatively accurately the transport mechanism employed by EPSM. Fluxes calculated by TDEFM represent the true analytical solution to the molecular free flight problem, under the assumptions of thermal equilibrium and uniformly distributed quantities in each cell.

* Corresponding author. Tel.: +886 3 573 1693; fax: +886 3 611 0023.
E-mail address: chongsin@faculty.nctu.edu.tw (J.-S. Wu).

0010-4655/$ – see front matter © 2013 Published by Elsevier B.V.
http://dx.doi.org/10.1016/j.cpc.2013.05.007

Albright et al. [4] developed a numerical scheme for the solution of the Euler equations, known as the quiet direct simulation Monte Carlo (QDSMC) method. In this method, the integrals encountered in the TDEFM formulation are replaced by approximations using Gaussian numerical integration, effectively replacing the continuous velocity distribution function with a series of discrete velocities. The method was later renamed the quiet direct simulation (QDS) method, because of the lack of stochastic processes, and was extended to second-order spatial accuracy [5]. The lack of complex mathematical functions results in a computationally very efficient scheme with a considerably higher performance than EFM while maintaining the advantages of true-directional fluxes like TDEFM.

Because of the assumption of unrestricted motion during free flight, each of the abovementioned kinetic solvers has a large amount of (cell-size-based) numerical diffusion. To combat this dissipation, a common strategy, employed in conventional finite volume methods, is to apply the higher-order reconstruction of properties or fluxes. Macrossan [6] applied EFM using higher-order spatial extensions, while Smith [7] attempted the analytical inclusion of gradients into true-direction volume-to-volume fluxes, only to find that the complete analytical inclusion of gradient terms in the TDEFM flux expressions is impossible. Smith et al. [5] reduced the numerical diffusion by applying "simplified" flux reconstruction at the interface that improves the original QDS to be almost second order in spatial accuracy; this method is called QDS-2N.

In this paper, we extend the second-order QDS algorithm (QDS-2N) [5] to higher-order reconstruction through the true-direction polynomial multi-dimensional reconstruction of conserved properties across each cell width; this method is called QDS-N^2. The net fluxes are computed through the individual contributions of QDS particles, computed by taking moments over the polynomial reconstruction. The particle properties are updated, considering the average value of the conserved quantity between the region bounds, which are required in translational directions and the application of splitting. The fluxes of conserved properties are calculated by a sum of weighted moments over the polynomial spatial reconstruction of mass, momentum, and energy across the cell width. The verification simulations of four two-dimensional cases are carried out to show the improved accuracy of the proposed QDS-N^2 scheme for inviscid gas flow simulations.

2. Numerical method

2.1. Quiet direct simulation (QDS)

The normal random variable $N(0, 1)$ is defined by the probability density:

$$p(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}}. \tag{1}$$

By using a Gaussian quadrature approximation, the integral of Eq. (1) over its limits can be approximated by:

$$\int_{-\infty}^{\infty} \frac{e^{-x^2/2}}{\sqrt{2\pi}} f(x)dx \approx \sum_{j=1}^{N} w_j f(q_j) \tag{2}$$

where w_j and q_j are the weights and abscissas of the Gaussian quadrature (also known as the Gauss–Hermite parameters), and N is the number of terms. The abscissas are the roots of the Hermite polynomials, which can be defined by the recurrence equation:

$$H_{n+1}(q) = 2qH_n - 2nH_{n-1} \tag{3}$$

where $H_{-1} = 0$, and $H_0 = 1$. The weights can be determined from:

$$w_j = \frac{2^{n-1} n! \sqrt{\pi}}{n^2 \left[H_{n-1}(q_i)\right]^2}. \tag{4}$$

The net fluxes of mass, momentum and energy of a cell are given by the sum of individual flux contributions from all the particles flowing in and out as follows:

$$\begin{aligned} F_{MASS} &= \left(\sum_{J=1}^{M} F^J_{MASS}\right)_{in} - \left(\sum_{J=1}^{N} F^J_{MASS}\right)_{out}, \\ F_{MOM} &= \left(\sum_{J=1}^{M} F^J_{MOM}\right)_{in} - \left(\sum_{J=1}^{N} F^J_{MOM}\right)_{out}, \\ F_{ENG} &= \left(\sum_{J=1}^{M} F^J_{ENG}\right)_{in} - \left(\sum_{J=1}^{N} F^J_{ENG}\right)_{out} \end{aligned} \tag{5}$$

where F^J_{MASS}, F^J_{MOM} and F^J_{ENG} is the individual mass flux, individual momentum flux and individual energy flux from particle J respectively, M and N is the number of inflow and outflow particles respectively into the cell under consideration. Each of the individual contributions (with first order spatial accuracy) can be described by the expressions, e.g., in one-dimensional case:

$$\begin{aligned} F^J_{MASS} &= \frac{v_J \Delta t}{\Delta x} m_J \qquad F^J_{MOM} = \frac{v_J \Delta t}{\Delta x} m_J v_J \\ F^J_{ENG} &= \frac{v_J \Delta t}{\Delta x} m_J \left[\frac{1}{2} v_J^2 + \varepsilon_J\right] \end{aligned} \tag{6}$$

where the particle mass m_J, particle velocity v_J, and particle internal energy ε_J are expressed as:

$$\begin{aligned} m_J &= \frac{\rho \Delta x w_J}{\sqrt{\pi}} \qquad v_J = u + \sqrt{2}\sigma q_J \\ \varepsilon_J &= \frac{(\xi - \Omega)\sigma^2}{2} \end{aligned} \tag{7}$$

where ρ is the density, u is the bulk (or mean) flow velocity, and $\sigma = (RT)^{1/2}$ in a given source cell. Note R is the universal gas constant, and T is the gas temperature. The total number of degrees of freedom ξ is defined as $\xi = 2(\gamma - 1)^{-1}$ where γ is the specific heat ratio ($= C_p/C_v$), and Ω is the number of simulated degrees of freedom (e.g., $\Omega = 1$ for one dimensional flow). In the existing QDS-2N [5], the values of ρ, u, and σ employed in QDS particle initialization are taken from reconstructions based on linear variations between neighbor cells. Despite fluxes being true direction in nature, the reconstructions performed in previous implementations are directionally decoupled—i.e. a flux is computed through the product of (separate) fluxes previously computed (for 2D flow) in the x and y directions. For the 2D case, the particle mass and velocities in Eq. (7) become:

$$\begin{aligned} m_{JK} &= \frac{\rho \Delta x \Delta y w_J w_K}{\pi} \qquad v_J = u_x + \sqrt{2\sigma^2} q_J \\ v_K &= u_y + \sqrt{2\sigma^2} q_K \end{aligned} \tag{8}$$

where there are $K = 1, \ldots, M$ particles in the y-direction and the definition of other variables are the same as those in 1D case. The internal energy remains identical to the 1-D case, allowing for a corresponding increase in Ω to account for the extra simulated dimension. The fluxes from sources cell to any arbitrary destination cell can be calculated by the particle position distributions. The fluxes of mass, momentum and energy, which are based on the proportion of the overlapped area to the area of the original cell, are given by:

$$\begin{aligned} F_{MASS} &= \frac{A}{A_s} m_{JK} \qquad F_{MOM-X} = \frac{A}{A_s} m_{JK} v_J \\ F_{MOM-Y} &= \frac{A}{A_s} m_{JK} v_K \\ F_{ENG} &= \frac{A}{A_s} m_{JK} \left[\frac{1}{2}(v_J^2 + v_K^2) + \varepsilon_{JK}\right] \end{aligned} \tag{9}$$