Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2024-0022

Vol. **39**, No. 2, pp. 448-474
February 2026

A Determinant Aided Fixed Point Method for Nonlinear Coupled Constitutive Relation of Rarefied Nonequilibrium Flows

Chengming Zeng[1], Dongjun Jiang[1] and Qibing Li[2,*]

[1] *Department of Engineering Physics, Tsinghua University, Beijing 100084, China.*
[2] *Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China.*

Communicated by Kun Xu

Received 25 January 2024; Accepted (in revised version) 8 July 2024

Abstract. The Nonlinear Coupled Constitutive Relation (NCCR) model is derived from the generalized hydrodynamic equations of Eu and has the capability to describe some significant characteristics of rarefied flows. However, the NCCR model is a complicated nonlinear system, and previous iterative methods for solving the NCCR equations have been observed to be associated with unphysical solutions and instability in some unfavourable conditions. In this study, a new numerical method for solving NCCR equations is proposed to enhance the reliability of the NCCR model. An objective function for a single variable is employed within a fixed point perspective to determine the solution, and the NCCR equation system is reorganized into a smaller linear matrix system for iterative processes. The determinant of the matrix system is used to search the valid solution region, ensuring the method's robustness. Three typical flow problems in transition regimes are conducted to validate the numerical performance of the proposed method. Results show that the computational time of the proposed method is only approximately 2 to 6 times that of the NS solution, representing efficiency at the same magnitude order of NS solvers and enabling broader engineering applications.

AMS subject classifications: 76K05, 76P05, 82B40
Key words: Rarefied flow, nonlinear coupled constitutive relation, fixed-point method, unstructured grid.

1 Introduction

The conventional Navier-Stokes-Fourier (NS) equations have been proved inadequate for accurately characterizing the behaviour of the nonequilibrium flows. The adjustment

*Corresponding author. *Email addresses:* `lqb@tsinghua.edu.cn` (Q. B. Li), `zcm21@mails.tsinghua.edu.cn` (C. Zeng), `jiangdj@tsinghua.edu.cn` (D. Jiang)

of slip boundary conditions is also insufficient to address the fundamental flaw of the NS solution in simulating high-Knudsen nonequilibrium flows. Consequently, numerous effective numerical methods have been proposed based on the Boltzmann equation, and they can be divided into two main categories: the stochastic particle method and the deterministic method. Direct simulation Monte Carlo (DSMC) [1] is one of the typical stochastic particle methods and it is frequently employed as a benchmark for rarefied nonequilibrium flows. However, it requires time steps and cell sizes that are smaller than the particle collision time and the mean free path, resulting in significant computational expenses in continuum flow conditions. The issue of stochastic fluctuation also constrains the precision and efficiency of the method. The deterministic method mainly comprises two parts. One is founded on discrete velocity space, such as Unified Gas-Kinetic Scheme (UGKS) [2–4], Discrete Unified Gas Kinetic Scheme (DUGKS) [5–7], and Gas-Kinetic Unified Algorithm (GKUA) [8]. These approaches can yield satisfactory outcomes that align with DSMC results and effectively address the cross-regime flow problem. However, the prohibitive computational expenses stemming from velocity space discretization pose a significant barrier to their widespread adoption in engineering applications. The other part involves high-order moment methods, such as Burnett-type equations [9], Grad's moment equations, and regularized 13-moment equations (R13) [10]. They are methods based on macroscopic variables similar to the NS equations and therefore with much lower computational cost, but they may present stability issues in the solution and require complex higher-order boundary conditions.

The Nonlinear Coupled Constitutive Relation (NCCR) model proposed by Myong [11] is based on the Generalized Hydrodynamic Equations (GHE) of Eu [12]. Its capacity to capture the major characteristics of nonequilibrium effects, especially in the near-continuum flow regime, including the slip regime and part of the transition regime, has been evaluated across various cases [13–16]. Additionally, the absence of high-order spatial derivatives in the model contributes to its stability and simplifies the implementation of boundary conditions. In practical engineering applications, the efficiency of a method with certain accuracy is crucial. Therefore, the essentially low-cost property of NCCR as a macroscopic method and its acceptable ability to describe the nonequilibrium flow behaviours provide the NCCR model with significant potential for engineering applications. The combination with second-order boundary conditions [17], and the extensions to gas-particle problems [18] and multiphase flows [19] also present its improvement and advantages in physical modelling. Nevertheless, the determination of stress and heat flux in the NCCR model necessitates the resolution of a complex nonlinear system, thereby creating a significant demand for an efficient solution algorithm for NCCR.

The earliest practical and popular solution algorithm is a decomposed solving method introduced by Myong [20]. Myong's method simplifies the three-dimensional coupled equations into three one-dimensional independent equations in the x, y, and z directions, effectively avoiding the complexities of the coupled system. However, this simplification of coupled directions results in unphysical deviations in multidimensional problems and computational instability, such as the negative-density phenomenon. Jiang