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Kun Xu
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1 Introduction

There are two distinguishable modelling scales in gas dynamics: kinetic and hydrodynamic scales. The kinetic scale is the scale of particle mean free path and particle collision time. In this scale, the dynamics of particle transport and collision can be modelled separately. The Boltzmann equation keeps the particle free streaming on the left-hand side and takes account of particle collision on the right-hand side. There should have no more than one collision for an individual particle in the kinetic scale in order to validate the particle free transport modelling on the left-hand side of the Boltzmann equation. In the kinetic scale, the particle moves freely and there is no closed and connected fluid element concept. Numerically, deterministic Boltzmann solvers and a stochastic direct simulation Monte Carlo (DSMC) method have been constructed in such a scale. On the other hand, macroscopic fluid dynamic equations are constructed in a hydrodynamic scale. Even though there is no precise definition of the hydrodynamic scale, the macroscopic equations describe the wave phenomena of accumulating movement of a large number of particles in a quasi-equilibrium state. The hydrodynamic scales must have tens or hundreds of particle mean free paths and particle collision times in order to include enough particles for a well-defined accumulating macroscopic particle behaviour. Navier-Stokes (NS) equations are an example of well-defined hydrodynamic equations. Under the continuum mechanics assumption of no-particle penetration between fluid elements, the NS equations are basically the conservation laws for each fluid element with the viscous stress and heat exchange between the elements. In the regime between the hydrodynamic scale NS and kinetic scale Boltzmann equations, there should be a continuously varying length scale for the description of gas dynamics. However, a variational scale has not been clearly defined between the above two limits for fluid modelling. In this Element, in order to fill up the gap between kinetic and hydrodynamic scale flow modelling, a unified framework according to a cell's Knudsen number, which is defined as the ratio of the particle mean free path over the numerical cell size or the ratio of the particle collision time over the numerical time step, will be constructed for the flow simulation in all regimes. In the continuum regime at a small cell's Knudsen number, the unified algorithm will go to an NS flow solver. In the rarefied regime, it will converge to the Boltzmann solver. The flow physics in the transition regime are determined by the accumulating effect of particle transport and collision within a time step scale for the evolution of both macroscopic flow variables and microscopic gas distribution function. The unified algorithm connects the Boltzmann and NS modelling smoothly with the variation-of-cell Knudsen number.

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Due to a continuous scale variation and the difficulty of identifying appropriate flow variables for the description of gas dynamics in the transition regime, no reliable governing equations have ever been proposed. The simplest way is to use brutal force and resolve flow physics down to the particle mean free path scale everywhere. Other attempts try to roughly connect distinguishable NS and Boltzmann solvers through a buffer zone. The flow physics in the buffer zone are assumed to be described correctly by both models. Physically, merging them smoothly is associated with difficulties due to their distinguishable modeling scales. The unified framework is to construct discrete governing equations according to a local cell's Knudsen number and connect different flow regimes seamlessly.

The unified gas-kinetic scheme (UGKS) is an extension of the gas-kinetic scheme (GKS) for the NS solutions. The GKS automatically becomes the limiting scheme of UGKS in the continuum flow regime. As a finite volume flow solver, the GKS only updates macroscopic flow variables through numerical fluxes. Based on the Chapman-Enskog expansion, in the continuum flow regime, the NS gas distribution function is well defined. The GKS uses the integral solution of the kinetic model equation to construct the gas evolution solution from an initial NS distribution function around a cell interface, from which the time accurate numerical flux can be evaluated. In UGKS, in order to capture peculiar non-equilibrium gas distribution function, instead of reconstructing it through the Chapman-Enskog expansion, the gas distribution function is tracked, along with the update of macroscopic flow variables. The same time evolution model is used in UGKS and GKS for the flux evaluation. The integral solution includes the accumulating effect from particle transport and collision within a numerical time step, and it is the key for developing a multi-scale algorithm. Dynamically, it has the similar function as the Riemann solver in establishing CFD for the Euler and NS solutions. The intensity of a particle collision within a time step determines the dynamic equations of the UGKS. In UGKS, both DVM-based gas distribution function and macroscopic flow variables are updated, and the direct modelling algorithm recovers the NS and Boltzmann solution according to the corresponding cell's Knudsen number. Under the UGKS framework, the further extension of the algorithm includes the purely particle-based unified gas-kinetic particle (UGKP) method and the wave-particle-based unified gas-kinetic wave-particle (UGKWP) method. In UGKWP, the gas distribution function is composed of analytic wave and discrete particle, and its evolution is tracked by the same integral solution of the kinetic model equation. According to the cell's Knudsen number $K_{n_c} = \tau/\Delta t$, the number of discrete particles used in the description of the gas distribution function is proportional to $\exp(-1/K_{n_c})$, which varies in different flow regimes. In the highly rarefied hypersonic flow computation, the UGKWP becomes a particle method with notably reduced memory requirements and

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computational costs in comparison with DVM. In the continuum flow regime, with the diminishing of particles, the UGKWP smoothly returns to the GKS for the update of macroscopic flow variables only, where the analytical wave part of the gas distribution function will automatically converge to the Chapman-Enskog expansion of the NS solution. In the transition regime, the contribution from the discrete particle and analytical wave depends on the local cell Knudsen number. For the low-speed micro-flow, the original DVM-based UGKS still has an advantage in terms of obtaining numerical solutions efficiently, due to the absence of noises from particles. The employ of UGKS or UGKWP for the multiscale flow study depends on the specific engineering applications.

1.1 Multi-scale Modelling for Gas Dynamics

The modelling scale of gas dynamics changes significantly from the deterministic molecular dynamics (MD) by following an individual particle, to the Boltzmann equation by statistically modelling particle transport and collision in the kinetic scale, up to the Navier-Stokes (NS) equations by constructing conservation laws in the hydrodynamic scale. The MD equation captures particle trajectory precisely according to Newton's law, e.g., the particle motion under external field from other particles, and the resolution in the MD goes to the molecular diameter. For the Boltzmann equation, the modelling is up-scaled to the particle mean free path and mean particle collision time. In such a kinetic scale, the information about the precise trajectory of an individual particle gets lost. Instead, the particle is described by probability in each velocity range, e.g., the so-called gas distribution function, which is distributed continuously in space and time through mean-field approximation. In the kinetic scale, the particle will not take more than one collision in order to model particle transport and collision separately, such as the uncoupled particle free streaming and binary collision in the Boltzmann equation. The separate representation of particle transport and collision implicitly enforces the kinetic scale in the Boltzmann modelling. The same constraints on the cell size and time step have been adopted in the DSMC method and many direct Boltzmann solvers because they are based on the same kinetic modeling scale in the construction of numerical algorithms. If a particle takes more than one collision, it will not follow the free streaming movement all the time, and the accumulation of multiple collisions has to be taken into account in the equation. At the current stage, there is no such governing equation with the inclusion of multiple particle collisions. Due to the decoupling of particle transport and collision, it should be emphasized that the Boltzmann equation is only valid in the kinetic scale of particle mean free path and collision time. The solution beyond this scale can be

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only obtained through the accumulation of a kinetic scale solution, but with the resolution sticking on the kinetic scale, such as the constraints on the cell size and time step in the DSMC simulation. Beyond the particle mean free path and collision time scales, it is difficult to handle a continuously varying scale mathematically to construct the corresponding dynamics, such as modelling the physics for a scale with several particle mean free path resolutions, where the accumulation of multiple particle collisions with zigzag movement can be hardly described mathematically in partial differential equations, even the flow variables cannot be clearly defined.

On the macroscopic level, the Navier-Stokes (NS) equations were constructed by applying Newton's law to the macroscopic fluid element with the implementation of a constitutive relationship and Fourier's law. The hydrodynamic scale for the NS equations, such as the size of a fluid element, has never been precisely defined, which is usually claimed as microscopically large and macroscopically small. It is commonly agreed that the hydrodynamic scale should at least be about one or two orders of magnitude larger than the particle mean free path. The hydrodynamic scale should be large enough to include a very large number of particles within each fluid element, and the mass exchange between neighbouring elements can be ignored. The NS equations describe the wave phenomena from collective particle motion in the quasi-equilibrium state with intensive collisions. In such a scale, each fluid element is assumed to be a closed particle system with the same amount of mass along its movement, and the NS equations provide the conservation laws for each fluid element under force interaction and heat exchange between the elements. Even with volume change along the trajectory of the fluid element, the mass exchange between neighbouring elements is prohibited in the modelling in order to implement the thermodynamic equation of state which is built upon a closed system. The hydrodynamic time scale is the time interval for a wave propagating through an element. Furthermore, the hydrodynamic modelling needs a continuous connection between neighbouring fluid elements, i.e., the so-called continuum mechanics assumption. The Lagrangian formulation of the Euler and NS equations clearly indicates that the connection among neighbouring elements never breaks down. As a result, at the hydrodynamic level, there is actually no non-equilibrium transport mechanism related to the particle penetration. The continuum mechanics assumption for fluid elements in the NS equations, as well as in other extended hydrodynamic equations, will break down gradually with a change of scale from hydrodynamic to kinetic one. Many unsolved problems in fluid mechanics, such as the turbulence, separating flow, and laminar-turbulent transition, may stem from the intrinsic continuum mechanics assumption in the NS formulation, where the non-equilibrium transport mechanism and the abundant discontinuities within the

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fluid are absent in the mathematical formulation. The breaking down of connected fluid elements and the associated non-equilibrium transport may become important for the description of turbulent flow, such as the rapid emerging of a large amount of degrees of freedom in the laminar turbulence transition. But, the NS-based turbulence modelling has only a quasi-equilibrium transport mechanism with a diffusive process, even with enhanced turbulence viscosity. In the mathematical formulation, there is not much difference between NS gas dynamics equations and equation for the elastic body deformation. There may have intrinsic weakness in the hydrodynamic modelling for the non-equilibrium turbulence flow.

The physical modelling among MD, Boltzmann, and NS equations is associated with a reduction of information in a flow description through a coarse-graining process. Theoretically, the gas evolution can be fully captured through MD formulation without going to the Boltzmann and NS equations at all. However, in reality, it is not practical and possible to follow a large number of particles in the MD resolution, and it is legitimate to find the most efficient and appropriate way to describe flow dynamics in the corresponding regime. For example, for a re-entry problem, the dynamics provided by the Boltzmann equation through the DSMC are accurate, and the method is efficient for the flight simulation above 80 kilometres. At an altitude lower than 40 kilometres, the NS equations can be applied faithfully. Therefore, efficient and distinguishable governing equations are preferred in different flow regimes. The current study is to find out a method which can produce an accurate and efficient description in all flow regimes with adaptive physical modelling. In practice, for hypersonic flow, one single flight may be associated with the existence of multiple flow regimes, such as the compressible high density flow at leading edge and the rarefied one at trailing edge. The development of a unified algorithm is to solve this kind of multi-scale problem.

In order to develop a CFD method for both rarefied and continuum flow simulation, the flow modelling in both kinetic and hydrodynamic scales has to be bridged dynamically with the variation of scale, such that both the Boltzmann and NS equations should become the limiting equations automatically. In the kinetic scale, there are mainly two kinds of numerical methods to solve the Boltzmann equation: the stochastic particle method and the deterministic kinetic solver. Both methods are widely used in academic research and engineering applications. The stochastic method employs discrete particles to simulate the statistical behaviour of molecular gas dynamics. The direct simulation Monte Carlo (DSMC) method is the most successful particle simulation method for rarefied flow (Bird 1994; Oran et al. 1998). The consistency of the DSMC method and the Boltzmann equation has been established mathematically (Wagner 1992). Similar to many direct Boltzmann solvers, the mesh size and time step in the DSMC method are constrained by the particle mean free path and mean collision

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time (Alexander et al. 1998). Otherwise, due to the operator splitting treatment of particle transport and collision, the numerical dissipative coefficient being proportional to the time step Δt would take over the physical one, which is on the order of the particle collision time τ. On the other hand, since the required number of simulation particles is independent of the Mach and Knudsen numbers, the stochastic particle method seems to use the best adaptive technique in the discretization of particle velocity space. The DSMC method requires low computational memory to cover the whole velocity space and gains high efficiency in rarefied flow computation, especially for the multidimensional high-speed flow. As a particle method, the DSMC suffers from statistical noise due to an insufficient number of particles. It becomes very difficult to simulate low-speed flow and capture small temperature variation. Moreover, with the increase of flow density, such as flight simulation at an altitude below 80 kilometres, the computational cost in 3D DSMC calculation grows dramatically and nonlinearly. The DSMC's intensive particle collision and small cell size requirement make it impossible to simulate flow in the continuum and near continuum regime. In order to address the stiffness problem in the continuum regime, asymptotic preserving (AP) Monte Carlo methods (Pareschi & Russo 2000; Ren et al. 2014) were developed so that the Euler solution can be obtained in the hydrodynamic limit without constraints on the time step and mesh size, as required by the traditional DSMC method. Unfortunately, these AP schemes can only use the Euler limit instead of an NS one in the continuum flow regime. As a result, the accuracy of AP-DSMC in the near continuum regime, when the cell size and time step are larger than the particle mean free path and collision time, is questionable. The stochastic particle methods based on kinetic model equations, such as the Bhatnagar-Gross-Krook (BGK), the ellipsoidal statistical BGK (ES-BGK) models (Gallis & Torczynski 2000; Macrossan 2001; Tumuklu et al 2016; Fei et al. 2020), and the Fokker-Planck (FP) model (Jenny et al. 2010; Gorji & Jenny 2015), have been constructed for further improvement of computational efficiency. In order to recover the NS solution in the continuum flow regime, instead of AP property, the schemes have to satisfy the unified preserving (UP) property (Guo et al. 2020), where the coupled discretization of particle transport and collision within a time step becomes necessary.

The deterministic methods employ a discrete distribution function to solve the kinetic equations. The discrete velocity methods (DVM) for Boltzmann and kinetic model equations have been extensively studied in the last several decades (Chu 1965; Yang & Huang 1995; Aristov 2012; Tcheremissine 2005; Li & Zhang 2004; Wu et al. 2015), which have great advantages for simulating low-speed microflow (Huang et al. 2013; Wu et al. 2014). In order to improve

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the efficiency and remove time-step limitations on the deterministic kinetic solvers, AP schemes (Larsen et al. 1987; Jin 1999) and kinetic-fluid hybrid methods (Degond et al. 2010) have been proposed and constructed. Accurate solutions can be obtained without statistical noises, and high efficiency can be achieved using numerical acceleration techniques, such as implicit (Mieussens 2000; Zhu et al. 2017a, 2019a), multigrid (Zhu et al. 2017b), high-order/low-order (HOLO) decomposition (Chacon et al. 2017); memory reduction techniques (Chen et al. 2017); a fast spectral method for the full Boltzmann collision term (Mouhot & Pareschi 2006; Wu et al. 2013); and an adaptive refinement method (Chen et al. 2012). For both stochastic and deterministic methods, once the gas evolution process is split into collisionless particle transport and instant collision, a numerical dissipation that is proportional to the time step will be introduced implicitly. Therefore, the mesh size and the time step in many kinetic solvers need to be less than the particle mean free path and collision time. The analysis of the dissipative mechanism in the kinetic flux vector splitting scheme and the Lattice Boltzmann method (LBM) will be presented in several places in this Element.

Besides the methods starting from the kinetic equation and being extended to the continuum regime, other approaches are coming from the NS side. Based on the hydrodynamic formulation, the extended hydrodynamics and moment equations developed in the continuum flow regime are pushed to the transition and rarefied flow. Based on the Chapman and Enskog expansion, the Euler, Navier-Stokes, Burnett, and super-Burnett equations can be derived (Chapman et al. 1990). In shock-wave calculation, the Burnett and super-Burnett equations are subject to numerical instabilities, and the equations need to be regularized (Zhong et al. 1993). Another interesting approach is the moment method (Grad 1949), where the distribution function is expanded in terms of a complete set of orthogonal polynomials, e.g., the Hermite polynomials, with the coefficients corresponding to the velocity moments. This expansion is truncated up to a certain order, resulting in a closed set of moment equations. Although the Grad moment approach has been widely used, it is best suited for problems where the velocity distribution function can be expressed as a perturbation of the equilibrium state, i.e., the near continuum flow. Recently, the Chapman-Enskog expansion and the Grad moment methods have been combined in the development of regularized methods (Levermore 1996), such as the well-defined R13 and R26 (Struchtrup 2005; Struchtrup & Torrihon 2003; Gu & Emerson 2009). The success of these methods in low-speed microflow with a modest Knudsen number has been confirmed. For high-speed flow, on the basis of Eu's generalized hydrodynamics (Eu 2016), the balanced closure has been recently developed (Myong 2001) and the hypersonic rarefied flow

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simulations have been presented (Jiang et al. 2019b). The uncertainty in the extended hydrodynamic and moment equations is the absence of any clear definition of modelling scale in the construction of these equations. They are basically derived from equation to equation, not from the direct modelling in different scales. The number of flow variables that is suitable for a valid description of non-equilibrium flow is also unclear. Intrinsically, all macroscopic flow variables are space-averaged quantities on the hydrodynamic scale, which is far beyond kinetic scale modelling. Theoretically, these equations lack the non-equilibrium transport mechanism due to the underlying continuum mechanics assumption, where the no-penetration and unbreakable connection between neighbouring fluid elements are intrinsically rooted in these models. As a result, these equations can cope with the diffusive and dispersive process for the description of quasi-equilibrium state evolution. In fact, it becomes hard to capture the non-equilibrium transport, even though the dissipative coefficients can be enlarged and have a delicate dependence on the flow variables. In the continuum flow regime, the intensive particle collisions merge an individual particle's movement into a collective 'wave' behaviour, and their dynamic evolution can be described by a few flow variables, such as the mass, momentum, and energy in the NS equations. With the increase of rarefaction, the individual particle's contribution to the flow dynamics becomes important, where the closed fluid element assumption breaks down. In a highly rarefied flow, individual particle movement becomes gradually independent with free penetration. The flow physics from continuum to rarefied is associated with a dramatic increase of information with the change of modelling scale, which can be hardly described by a few predefined macroscopic flow variables. Extending this modelling process continuously from hydrodynamic to kinetic scale is difficult due to the following reasons. First, it is unclear how to define a continuous variation of modelling scale between the kinetic and hydrodynamic one and to get the corresponding equations under such a varying scale. Second, it is unclear what kind of flow variables are appropriate for describing the flow physics between these two limits. Third, there is no clear scale separation in the transition regime. Conventional mathematical tools, such as asymptotic expansion, may not be applicable to cover the whole regime. In the NS equations, there are only five flow variables. For the Boltzmann equation, the particles are basically independent, and there is a theoretically infinite number of degrees of freedom for capturing the gas distribution function. Between the hydrodynamic and kinetic limits, it is essentially unclear how many flow variables and what kinds of variables are appropriate in the moments and extended hydrodynamic equations. But, these questions need to be properly answered in the construction of a unified algorithm. The existing extended and

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irreversible thermodynamics mainly focus on the study of the flow close to equilibrium. There is not much knowledge available regarding how to describe non-equilibrium properties through a macroscopic thermodynamic formulation. The flow physics between the kinetic and hydrodynamic scales have not been properly explored theoretically. A direct task for the unified algorithm is to clearly define a modelling scale and construct the gas dynamics in such a scale.

Other popular numerical algorithms for both continuum and rarefied flow simulations are the hybrid methods. The hybrid methods, such as the combination of the NS and the DSMC or NS and direct Boltzmann solver (Schwartzentruber & Boyd 2007; Degond et al. 2006; Tiwari 1998; Wijesinghe & Hadjiconstantinou 2004), have been used in engineering applications. Since the Boltzmann solver is much more expensive than the NS solver, the NS solver should be applied in a domain as large as possible. In most hybrid methods, a buffer zone is designed to couple different approaches with the exchange of information from different solvers. These methods may depend sensitively on the location of the interface, where many criteria have been proposed to define the buffer zone with the requirement of applicability of both methods in this region. Two well-known hybrid methods are the CFD/DSMC and CFD/Boltzmann solver (Schwartzentruber et al. 2008; Burt et al. 2011). For example, it is commonly stated that in the buffer zone, the flow can be described by both NS equations and kinetic solvers. In fact, this is exactly where the difficulty arises with applying the DSMC in the NS regime. For example, in order to avoid numerical dissipation from the DSMC solution, the cell size in the buffer zone has to be less than the particle mean free path and the buffer zone needs to be located in the kinetic regime. On the other hand, once the cell size in the buffer zone is on the particle mean free path scale, the assumptions in modelling NS are no longer valid. For the DSMC/CFD hybrid method, another difficulty concerns how to overcome the statistical fluctuation in DSMC. A CFD solver may be sensitive to the noise introduced through the boundary and become numerically unstable. Another hybrid method is the combination of the CFD and Boltzmann solver, where a gas-kinetic scheme (GKS) is used as a CFD solver (Kolobov et al. 2007). Recently, in order to improve the efficiency of numerical computation, a hybrid approach is formulated by combining the multi-scale unified gas-kinetic scheme (UGKS) and GKS (Xiao et al. 2020), and the success of this hybrid method is from the multi-scale nature of the UGKS, which is valid in any flow regime but can be replaced by a more efficient method in the continuum flow regime. Distinguished from the above hybrid method, a general synthetic iterative scheme (GSIS) has been developed in recent years. The ingredient of GSIS is that macroscopic synthetic equations are simultaneously solved with gas kinetic equations, from which the

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macroscopic flow properties are obtained to guide the evolution of a gas molecular system. Due to the direct use of macroscopic governing equations, the GSIS asymptotically preserves the Navier-Stokes equations at the continuum limit, so that the restriction on spatial grid cell size is eliminated. (Su et al. 2020; Zhu et al. 2021).

1.2 Unified Gas-Kinetic Schemes

For the high-speed flow around a vehicle in near space flight, flow physics of different regimes may appear simultaneously in a single computation, such as the highly non-equilibrium shock layer, high density leading edge, low density trailing edge, and wake flow. Figure 1 presents the local Knudsen number around a vehicle at Mach number 4 and Reynolds number 59,373, which is calculated by the DVM-based unified gas-kinetic scheme (UGKS). As shown in this figure, the local Knudsen number can cover a wide range of values, from 10^{-5} to 10 with six orders of magnitude difference. A single governing equation, such as the Boltzmann or NS equations, can hardly be applied efficiently in all regions to obtain a reliable physical solution. A unified algorithm to cover all regimes from the compressible NS solution to the free molecular flow is necessary. In fact, a large portion of the flow around the vehicle stays in the transition regime, which connects hydrodynamic and kinetic ones smoothly. In this calculation, it is impossible to use a cell size that is less than the particle mean free path everywhere, and it is unlikely to define a buffer zone to bridge

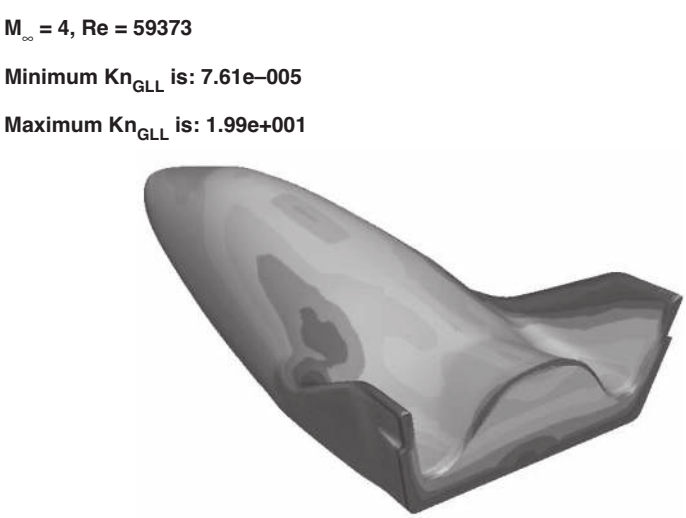

Figure 1 A local Knudsen number around a vehicle at Mach number 4 and Reynolds number 59,373. Courtesy of D.W. Jiang (Jiang et al. 2019a).

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