Comparison and Uncertainty Assessment of CFD Codes for Hypersonic Flow Modeling

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Abstract:

The process of selecting a code for hypersonic simulations is a nontrivial one, especially given the range of CFD software options currently available. In this paper, we give an overview of and compare the codes US3D, SANS, and BuBL to establish their usefulness, limitations, and accuracy. We evaluate state-of-the-art codes that span a range of fidelities, turbulence models, chemistry models, and computational implementations to assess the performance of the codes and the uncertainty associated with their heat flux predictions. A sample transitional, flat plate, experimental case is used for analysis and comparison. Uncertainty metrics for each code are found to be similar for both the laminar and turbulent regions. However, greater uncertainty is found for the turbulent region. Further code considerations including runtime and required expertise are discussed as well. In general, this paper serves as a framework for code comparisons by setting quantitative methodologies for experimental and numerical uncertainty assessments.

Keywords: Hypersonics, Computational Fluid Dynamics, Uncertainty Assessment, Turbulence Modeling, Chemistry Modeling

1 Introduction

The study of hypersonic flows is limited by the lack of reliable experimental data. As such, the use of Computational Fluid Dynamics (CFD) is critical for the prediction of these flows. CFD has had a significant impact in the fields of design, analysis, and optimization of hypersonic engineering systems [1]. Currently, there are a large number of codes that have the ability to carry out high-speed and compressible flows. These codes differ in computational scheme, flow assumption, computer architecture, numerics, flow models, etc. These differences in implementation exist as alternatives for handling the significant challenges associated with hypersonic CFD. Achieving accurate, convergent solutions with low numerical uncertainty using a CFD code can be quite difficult. Many commercially available CFD codes that have wide use for various fluid dynamic simulations are not suitable for hypersonic systems [2]. In general, expert knowledge is required to produce viable hypersonic simulations. To determine if a code is sufficient for a particular context, it is critical to understand how the code itself works and the uncertainty analysis is performed, its documentation is incomplete.

Hypersonics suffers from a lack of accessible comparison data of both the computational and experimental variety. However, hypersonic databases do exist. For example, the National Project for Applications-oriented Research in CFD (NPARC) [2] has validation cases available for a variety of flow regimes, and the Calspan

University at Buffalo Research Center (CUBRC) has experimental results for hypersonic flows [3]. Fernholz and Finley have collected experimental data for compressible turbulent boundary layers [4, 5]. Settles and Dodson also worked to develop a database [6, 7]. This database includes cases for high-speed compressible turbulence. However, each of these databases contain dated findings. Roy and Blottner update the latter database by adding only three new cases [8]. Unfortunately, these resources are far from comprehensive. We seek to add to the catalog of available hypersonic data. In this study, we refer to an experimental and CFD database from NASA that includes reference examples for hypersonic 2-D and axisymmetric cases [9] as a comparison for our CFD results.

Furthermore, chemistry and turbulence (including transition) modeling pose significant challenges in simulating hypersonic flows. At hypersonic speeds, temperatures often become great enough that high-temperature and real gas effects can become non-negligible. There are a range of potential chemistry effects. Activation of the vibrational mode can result in the breakdown of the calorically perfect gas assumption. Furthermore, gases can become reactive and enter thermochemical non-equilibrium in which ab-initio chemistry becomes pertinent. Candler et. al. highlight the significant impact that non-equilibrium chemistry can have through a validation study [10]. In addition, turbulence can be a significant source of uncertainty [2, 11]. There are many models that capture the turbulent behavior of flows along with the transition from the laminar state. A summary of turbulence models for hypersonic flows can be found in Roy and Blottner [8]. In this paper, we will examine and compare both RANS and LES turbulence results along with results for perfect gas and modified fluid viscosity equations.

A key element of code-to-code comparisons is uncertainty quantification. Even predictions from deterministic simulations have uncertainty due to differences in partial differential equation numerics and modeling assumptions. As such, we aim to understand how much uncertainty is associated with each code due to the particulars of their mathematical underpinnings and their implementations. This understanding is important to the overall goal of improving the state-of-the-art in CFD using improved modeling. Whether this improvement be in turbulence, chemistry, or novel reduced-order modeling techniques, a researcher must know the vector contribution of error in order to improve models. Figure 1 gives a graphical example of how modeling uncertainty can be incorrectly approximated. The implications of which are that researcher may be led to believe that a model is accurately capturing the relevant physics when it is not. While there is no method to know the exact numerical uncertainty in a simulation, or experimental uncertainty in a dataset, systematic quantification methods are necessary in fields of research meant to improve CFD models.



Figure 1: Graphical definition of simulation and experiment results and their associated uncertainty, where the true modeling uncertainty is much greater than the assumed modeling uncertainty in the presence of poor experimental characterization and convergence studies

To assess uncertainty, we follow a framework inspired by Roy and Oberkampf and using metrics from Gnoffo et al. [12, 11]. Therefore, our study will employ elements of verification and validation. Verification is the process of characterizing numerical approximation errors in a simulation, and validation is the assessment

of accuracy by comparison with experimental data [12].

Previous studies have performed code-to-code comparisons, many of such studies are accomplished through validation studies. For example, Roy et al. performed a code-to-code comparison with three codes in the process of verifying the SACCARA compressible fluid mechanics code [13]. Maicke provides an assessment of the state of hypersonic codes at the time, evaluating the specialized codes DPLR and VULCAN and the unspecialized codes CFD++ and VULCAN [2]. However, this assessment is general and largely qualitative as opposed to quantitative. DPLR has been the subject of many comparison studies. These studies include the work by Hollis for the context of Mars entry [14], the study by Candler evaluating the state-of-the-art of simulation [15], and Maclean's comparison against the NPARC WIND code [16]. WIND also appears in other comparison studies [1]. The Langley Aerothermodynamic Upwind Relaxation Algorithm (LAURA) Code also appears in these types of studies [17, 14]. Gnoffo et al. use LAURA, DPLR, and VULCAN to assess a variety of turbulence and chemistry models [11]. Unfortunately, many of the subjects of these comparison studies are limited to finite-volume solvers, whereas we include finite-element and finite-difference codes as well. Watermann et al. perform a code comparison, but only for stability codes [18]. Harvey et al. conducted an extensive validation study involving the comparison of 25 mostly Navier-Stokes codes [19]. This study was done for low Reynolds number laminar flows on various geometries. However, the details of the various code implementations are not included. Many of these studies sought to evaluate the leading codes of the time. However, many of these studies are now dated. Although there exist hypersonic code comparison studies that include US3D, a code included in this work, most of these studies given above do not include the diversity in code types included in the present work [20, 15]. Many of these comparisons also do not quantitatively address both experimental and numerical uncertainties. When numerical studies do not provide either a convergence study or a numerical uncertainty approximation, it is unknown what kind of results are provided. Figure 2 shows one example of turbulence modeling for which the author highlights how coarse grid results seem to match the experimental results much better than the results for more resolved meshes [21]. This convergence study for the SA turbulence model is an example that highlights how important it can be to rigorously account for numerical uncertainty.



Figure 2: Comparison of y-velocity profiles downstream of a shock impingement for the SA turbulence model where the grids are numbered by increasing resolution [21]

In this paper, we perform a comparison of three state-of-the-art CFD codes used in academic contexts. The purpose of this work is to understand uncertainty and assess confidence in codes for hypersonic modeling. To do so, we first discuss the implementation of these codes. Then, as a case study, we simulate a standard set of inflow conditions over a flat plate geometry using various numerical and modeling methods. This analysis focuses particularly on the evaluation of modeling uncertainty due to the treatment of governing equations, turbulence, and chemical models. Note that the chemistry modifications in this paper describe any changes to the base equations of state used in any solver, whether it be a change to the ideal gas assumption, specific heats, or viscosity calculations. The Gnoffo and Oberkampf methods guide the uncertainty analysis completed in this study [11, 22].

2 Code Methodology

This section will describe each code and their numerical implementations, as well as their physical models and assumptions used in this study. A summary of these codes is presented at the end of this section in Table 1.

2.1 US3D

UnStructured 3D (US3D) is a tool developed by the University of Minnesota and the NASA AMES Research Center for the simulation of compressible and reacting flows [15]. US3D has been extensively studied and, as such, it is one of the most frequently referenced hypersonic CFD tools in recent literature.

US3D relies on the finite-volume method (FVM) to discretize the system of partial differential equations that govern hypersonic fluid flows. Inviscid fluxes are approximated in one of two ways, depending on whether a steady or unsteady solution is desired. For steady flow simulations, a modified Steger-Warming flux-vector splitting scheme is used to approximate the inviscid fluxes at cell faces. This scheme extrapolates upwind-biased data to a cell face using a second-order monotonic upstream-centered scheme for conservation laws (MUSCL) approach and employs a flux limiter in order to ensure a total variation diminishing (TVD) scheme. For unsteady flows, inviscid fluxes are approximated by a fourth-order, kinetic energy consistent (KEC) scheme [23]. Since the KEC scheme is much less dissipative than the modified Steger-Warming scheme, a scaled dissipative flux is added in certain regions of the flow for improved stability, with the scaling factor given by the Ducros sensor [24]:

$$\phi = \frac{(\nabla \cdot \boldsymbol{u})^2}{(\nabla \cdot \boldsymbol{u})^2 + \|\nabla \times \boldsymbol{u}\|^2 + \epsilon}$$
(1)

in which ϵ is set to a small positive value to avoid division by zero. Viscous fluxes at cell faces are approximated through a second-order weighted least-squares fit to the cell-centered flow variable gradients.

Temporal discretization follows either the backward Euler method (for steady flows) or the Crank-Nicolson method (for unsteady flows). In both cases, the implicit system of equations is solved using a pointwise relaxation method [25, 26].

In addition to its numerical capabilities, the US3D software package includes thermochemical modeling of finite-rate chemistry and vibrational relaxation. US3D is still actively being developed and can be customized with plugins and user-implemented subroutines. In this paper, US3D is used to run steady laminar and RANS computations, as well as unsteady LES.

US3D simultaneously solves equations for the conservation of fluid mass, momentum, and energy

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \tag{2}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j}$$
(3)

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho E u_j}{\partial x_i} = -\frac{\partial p u_j}{\partial x_i} + \frac{\partial \sigma_{ij} u_i}{\partial x_i} - \frac{\partial q_j}{\partial x_i} \tag{4}$$

where the following definitions apply

$$E = e + \frac{u_k u_k}{2} \tag{5}$$

$$\sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \tag{6}$$

$$q_i = -k \frac{\partial T}{\partial x_i} \tag{7}$$

For laminar simulations, the governing equations are solved iteratively until a steady-state solution is obtained. For RANS simulations, the above equations are solved in Reynolds-averaged form to reach steady

state. The SA-Catris turbulence model is used to approximate the Reynolds stresses (for more details on the RANS approach, see section 2.2).

LES computations solve the spatially-filtered conservation equations

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_j}{\partial x_j} = 0 \tag{8}$$

$$\frac{\partial \overline{\rho} \widetilde{u}_i}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_i \widetilde{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \widehat{\sigma}_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j} \left[\overline{\rho} \nu_t \left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \overline{\rho} \nu_t \frac{\partial \widetilde{u}_k}{\partial x_k} \delta_{ij} \right]$$
(9)

$$\frac{\partial \overline{\rho} \widehat{E}}{\partial t} + \frac{\partial \overline{\rho} \widehat{E} \widehat{u}_j}{\partial x_j} = -\frac{\partial \overline{p} \widetilde{u}_j}{\partial x_j} + \frac{\partial \widehat{\sigma}_{ij} \widetilde{u}_i}{\partial x_j} + \widetilde{u}_i \frac{\partial}{\partial x_j} \left[\overline{\rho} \nu_t \left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \overline{\rho} \nu_t \frac{\partial \widetilde{u}_k}{\partial x_k} \delta_{ij} \right] - \frac{\partial \widehat{q}_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left[\frac{\overline{\rho} c_p \nu_t}{P r_t} \frac{\partial \widetilde{T}}{\partial x_i} \right]$$
(10)

In the above equations, an overbar denotes a spatially-filtered variable, a tilde denotes a Favre-filtered variable, and an overhat implies that a variable is a function of other resolved variables (e.g., $\hat{a} = \hat{a} \left(\overline{\rho}, \widetilde{\boldsymbol{u}}, \overline{p}, \widetilde{T} \right)$). Note that these filtered variables are not the same as the averaged variables described in the following section.

The Vreman eddy viscosity model [27] is used to account for the sub-grid scale (SGS) stresses. In accordance with the Vreman model, the local eddy viscosity is computed as

$$\nu_t = 2.5 C_s^2 \sqrt{\frac{B_{11}B_{22} - B_{12}^2 + B_{11}B_{33} - B_{13}^2 + B_{22}B_{33} - B_{23}^2}{\frac{\partial \tilde{u_i}^2}{\partial x_j}^2}}$$
(11)

where

$$B_{ij} = \Delta_k^2 \frac{\partial \widetilde{u}_i}{\partial x_k} \frac{\partial \widetilde{u}_j}{\partial x_k} \tag{12}$$

and Δ_i is the local grid spacing in the x_i direction. The Smagorinsky constant is set to $C_s = 0.092$, and the turbulent Prandtl number appearing in the spatially-filtered energy equation is taken to be $Pr_t = 0.9$.

For all computations, the fluid is assumed to be a perfect gas

$$p = \rho RT \tag{13}$$

$$e\left(T\right) = c_v T \tag{14}$$

with a constant Prandtl number given by Eucken's relation

$$Pr = \frac{4\gamma}{9\gamma - 5} \tag{15}$$

and viscosity is assumed to be a function of temperature according to Sutherland's law

$$\mu(T) = \mu_{ref} \left(\frac{T}{T_{ref}}\right)^{3/2} \frac{T_{ref} + T_s}{T + T_s}$$
(16)

For air, we assume specific heat capacities $c_p = 7/2 R$ and $c_v = 5/2 R$, and a gas constant $R = 287 \frac{\text{J}}{\text{kg K}}$. The air-specific gas constants appearing in Sutherland's law take on the values $\mu_{ref} = 1.84645 \times 10^{-5} \frac{\text{kg}}{\text{m s}}$, $T_{ref} = 300 \text{ K}$, and $T_s = 110.4 \text{ K}$.

2.2 SANS

SANS is a high-order unstructured finite element method (FEM) flow solver which utilizes Variational Multi-Scale with Discontinuous subscales (VMSD) discretization [28]. VMSD combines continuous Galerkin (CG) and discontinuous Galerkin (DG) methods while staying adjoint consistent. The adjoint consistency allows for accurate numerical error estimates. SANS is able to adapt grids to reduce discretization error multiple orders of magnitude lower than what is generally achievable using manually generated grids [29, 30]. SANS is advantageous because it ensures that the discretization errors are negligibly small. This allows the code to

be useful in turbulence and chemical model development, as well as code comparison studies. The results of SANS often highlight areas of large numerical error in other simulations and also define areas for improvement in physical modeling. In hypersonic simulations, shocks are anisotropic by nature and are generally a very challenging part of finite volume simulations with structured grids [31]. Since shocks result in very high gradients in physical properties, any numerical method is reduced to virtually first-order accuracy in their vicinity. Any misalignment of the mesh near shocks will introduce non-physical numerical features which propagate throughout the solution and lead to poor prediction of output quantities such as heat transfer [32]. Without solution adaptive grids and numerical error estimates, researchers have found it difficult to produce resolved grids for geometries that result in unpredictable flow features such as separation bubbles on hypersonic compression corners [11]. Furthermore, solution adaptive grids have been proven to be robust across several discretization methods. Galbraith has shown that an output-based mesh produced in a FEM discretization also improved the solution for a separate FEM code and an FVM code [30]. Hu has even shown that adapted meshing for turbulent boundary layers tends to place more nodes in the buffer layer than in the viscous sublayer or log layer [33]. Therefore, while the mesh produced by adaptation may not adhere to normal meshing standards, it can effectively reduce the numerical error when applied in several environments. The progress in unstructured meshes coupled with output-based grid adaptation has proved finite element solvers as a very useful tool not only for engineering prediction but also for model validation without the influence of significant numerical error.

SANS uses output-based adaptation to update the mesh until the error estimate in an integral output quantity, such as drag or heat flux, has reached a minimum for a target number of degrees of freedom (DOF) [34]. The Metric Optimization through Error Sampling and Synthesis (MOESS) algorithm [35, 34] is utilized via the Dual Weighted Residual method [36] to provide a local error estimate. This optimization occurs on a continuous metric field, \mathcal{M} , rather than on the actual mesh. The metric is optimized with respect to a cost model, \mathcal{C} , such that the resulting mesh should have less than or equal to the given target DOF, N. The new optimal metric is found to be the one that minimizes the error model, \mathcal{E} , which, in turn, is made up of local error contributions, η , as shown in Eq. 17.

$$\mathcal{E}(\mathcal{M}) = \int_{\Omega} \eta\left(\mathcal{M}(x), x\right) \, dx. \tag{17}$$

$$\mathcal{M}^* = \underset{\mathcal{M}\in\mathcal{M}(\Omega)}{\operatorname{arg\,min}} \mathcal{E}\left(\mathcal{M}\right), \quad \text{s.t.} \quad \mathcal{C}\left(\mathcal{M}\right) \le N,$$
(18)

Since it is infeasible for one adaptation step to reduce the discretization error to convergence, small steps of grid adaptation are performed to allow for better solver stability. Adaptation starts with an isotropic mesh generated from simple dimensions through the Triangle software [37]. The metric field from the MOESS algorithm is employed by the AVRO software to generate a new mesh over several adaptation steps [38]. An example of this may be starting with an isotropic mesh of approximately 300 DOF, and taking 50 steps to a final adapted mesh of about 16,000 DOF.

SANS solves the Reynolds-averaged Navier-Stokes (RANS) equations to complete 2D laminar and turbulent RANS simulations. These equations are represented below, where the fluctuation terms are zero when running a laminar simulation.

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \hat{u}_j}{\partial x_j} = 0 \tag{19}$$

$$\frac{\partial \bar{\rho} \hat{u}_i}{\partial t} + \frac{\partial \hat{u}_i \bar{\rho} \hat{u}_j}{\partial x_i} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \overline{\sigma_{ij}}}{\partial x_i} - \frac{\partial \bar{\rho} u'_i u'_j}{\partial x_i}$$
(20)

$$\frac{\partial \overline{\rho} \hat{E}}{\partial t} + \frac{\partial \hat{u}_j \overline{\rho} \hat{H}}{\partial x_j} = \frac{\partial (\overline{\sigma_{ij}} \hat{u}_i + \overline{\sigma_{ij} u_i'})}{\partial x_j} - \frac{\partial (\overline{q_j} + c_p \overline{\rho u_j' T'} + \hat{u}_i \tau_{ij} + \frac{1}{2} \overline{\rho u_i' u_i' u_j'})}{\partial x_j}$$
(21)

When completing a turbulent simulation, we follow the Boussinesq hypothesis for linear eddy viscosity and use the SA-CatrisCons [39, 40] turbulence model to represent the eddy viscosity. In these equations \bar{u} represents a Reynolds ensemble-averaged velocity, \hat{u} represents a Favre-averaged velocity, and all other variables are as defined by NASA TMR [39]. This model has been shown to perform well for the simulation

of 2D hypersonic flat plates and compression corners [11, 40]. SA-CatrisCons is used in both steady RANS simulations of US3D and SANS in this study.

$$\frac{\partial \rho \tilde{\nu}}{\partial t} + \frac{\partial \rho u_j \tilde{\nu}}{\partial x_j} - \rho \tilde{\nu} \frac{\partial u_j}{\partial x_j} = \rho c_{b1} (1 - f_{t2}) \tilde{S} \tilde{\nu} - \rho \left(c_{w1} f_w - \frac{c_{b1}}{\kappa^2} f_{t2} \right) \left[\frac{\tilde{\nu}}{d} \right]^2 \\ + \frac{1}{\sigma} \left[\frac{\partial}{\partial x_j} \left(\rho (\nu + \tilde{\nu}) \frac{\partial \tilde{\nu}}{\partial x_j} + \frac{\tilde{\nu}^2}{2} \frac{\partial \rho}{\partial x_j} \right) + \rho c_{b2} \frac{\partial \tilde{\nu}}{\partial x_i} \frac{\partial \tilde{\nu}}{\partial x_i} \right] + \frac{c_{b2}}{\sigma} \left(\tilde{\nu} \frac{\partial \rho}{\partial x_i} \frac{\partial \tilde{\nu}}{\partial x_i} + \frac{1}{4} \frac{\tilde{\nu}^2}{\rho} \frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_i} \right)$$
(22)

In this study, SANS simulations are run with further assumptions, such as gradient diffusion heat flux with a constant turbulent Prandtl number. Two viscosity coefficient models are used: one assumming a perfect gas with viscosity calculated by Sutherland's law, and the other, a kinetic theory approach using collision integrals. A Lennard-Jones-like phenomenological intermolecular potential model for collision integrals [41] is used in conjunction with the Armaly-Sutton mixing rule [42, 43] to calculate the equilibrium air mixture viscosity coefficient directly from kinetic theory from 50K to 2,000K. It should be noted that the Nitrogen and Oxygen mole fractions for equilibrium air change by less than 1% over this range of temperatures, indicating it is reasonable to neglect any gas composition effects. For computational efficiency, the results are curve-fit in the form of equation (23):

$$\mu(T) = \exp(C) T^{(A \ln(T) + B)},$$
(23)

where A = -0.064482, B = 1.5591, and C = -15.286.

2.3 BuBL

BuBL is a steady, laminar, compressible boundary layer code for 2D geometries developed in the MIT Hypersonics Research Lab [44, 45]. BuBL is the lowest fidelity and least computationally expensive solver that is explored in this study. BuBL manages its computational speed-up by using fluid boundary layer equations and the inviscid Euler equations rather than the full Navier-Stokes equations. The boundary layer equations are useful here, as we are not concerned with the full flowfield. Rather, our aim is to model quantities at the surface of our geometry. BuBL solves the compressible boundary layer equations in a transformed coordinate system. The resulting equations are known as the Lees-Dorodnitsyn boundary layer (LDBL) equations [46]. The coordinate transformation is given by:

$$\xi = \int_0^x \rho_e u_e \mu_e \, dx \tag{24}$$

$$\eta = \frac{u_e}{\sqrt{2\xi}} \int_0^y \rho_e \, dy \tag{25}$$

where the subscript 'e' denotes the edge of the boundary layer.

The LDBL are a set of equations derived from the Thin Shear Layer approximations to the Navier-Stokes Equations [47] and are given below:

$$(Cf'')' + ff'' = \frac{2\xi}{u_e} \left[(f')^2 - \frac{\rho_e}{\rho} \right] \frac{du_e}{d\xi} + 2\xi \left(f' \frac{\partial f'}{\partial \xi} - \frac{\partial f}{\partial \xi} f'' \right)$$
(26)
$$\frac{\partial p}{\partial \rho} = 0$$
(27)

$$\frac{\partial p}{\partial \eta} = 0 \tag{27}$$

$$\left(\frac{C}{Pr}g'\right)' + fg' = 2\xi \left[f'\frac{\partial g}{\partial\xi} + \frac{f'g}{h_e}\frac{\partial h_e}{\partial\xi} - g'\frac{\partial f}{\partial\xi} + \frac{\rho_e u_e}{\rho h_e}f'\frac{du_e}{d\xi}\right] - C\frac{u_e^2}{h_e}(f'')^2 \tag{28}$$

where f is a stream function, g is an enthalpy ratio, and C is the Chapman-Rubesin factor [46]. BuBL uses a non-linear Newton-Raphson iterative solver to evaluate a second order finite-difference method (FDM)

discretization of the LDBL equations [47]. This discretization is a compact, implicit, "box" computational stencil as described in [48].

While BuBL is primarily a boundary layer solver, external flow conditions are required as a boundary condition for the boundary layer calculations. These external flow calculations comprise a separate set of flow pre-calculations that take place prior to the solution of the boundary layer. As an input, they take a prescribed pressure gradient, which must be found or computed a priori, and solve the Euler inviscid flow equations. The Euler inviscid equation for the edge of the boundary layer is

$$dp_e = -\rho_e u_e du_e \tag{29}$$

This gives

$$\frac{dp_e}{d\xi} = -\rho_e u_e \frac{du_e}{d\xi} \tag{30}$$

in the LDBL coordinate system. The Euler equations are paired with isentropic relations, transformed into the LDBL coordinate system, and solved as a 1-D, boundary-value, FDM problem. The solution of the system is then used as the edge boundary condition for the main boundary layer solver.

An important feature of BuBL is that it has the capability to model temperature dependence in flow properties namely viscosity, specific heat, Prandtl number, and thermal conductivity. By allowing for these variable quantities, BuBL can accurately treat calorically and thermally perfect gases. It does so using the Vincenti and Kruger harmonic oscillator model for diatomic molecules such as air, which is modeled as a mixture of Nitrogen and Oxygen [49] resulting in (31) for the specific heat of air. Sutherland's law (16) is used for viscosity with $T_{ref} = 288K$, $T_S = 110K$, and $\mu_{ref} = 1.789 \times 10^{-5} \frac{\text{kg}}{\text{ms}}$. In BuBL, various models can be used to find thermal conductivity and then subsequently to find the Prandtl number [44]. However, in this work, the thermal conductivity is set based on a constant value Prandtl number of 0.72.

$$c_{p,air} = R_{N_2} m_{N_2} \left(\frac{7}{2} + \left(\frac{\frac{\Theta_{vib,N_2}}{2T}}{\sinh \frac{\Theta_{vib,N_2}}{2T}} \right)^2 \right) + R_{O_2} m_{O_2} \left(\frac{7}{2} + \left(\frac{\frac{\Theta_{vib,O_2}}{2T}}{\sinh \frac{\Theta_{vib,O_2}}{2T}} \right)^2 \right)$$
(31)

BuBL achieves solutions for a flat plate by assuming zero variation in flow quantities at the edge of the boundary layer. Namely, the boundary layer is taken to have zero pressure gradient. BuBL will be used to run 2D laminar simulations for both calorically perfect and thermally perfect gas assumptions.

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	Method	Laminar	RANS	LES	Chemistry	Total Simulations
BuBL	FDM	LDBL	-	-	$c_p(T)$	2
SANS	FEM	NS	SA-CatrisCons	-	$\mu(T)$ Collision Integrals	3
US3D	FVM	NS	SA-CatrisCons	Wall-Resolved	-	3

3 Uncertainty Quantification

We employ an approach to uncertainty quantification inspired by Roy and Oberkampf [12] and consistent with Gnoffo et al. [11]. Here, it is important to clarify a distinction in our definition of uncertainty, namely how it differs from error. Both lead to a loss of accuracy, but errors are knowable and correctable, whereas uncertainty is due to a genuine lack of knowledge [50]. For this work, we focus primarily on uncertainty, but also approximate the amount of error in the simulations.

We identify three sources of uncertainty: numerical approximation, model form, and experimental error [12]. Numerical approximation uncertainty is due to errors introduced by the mathematical implementation of the simulation. It has three sources: iterative error, discretization error, and round-off error [12]. We neglect numerical round-off and iterative error as we can reasonably expect their magnitudes to be small

compared to that of the discretization error. This latter type of error can be characterized using knowledge of the codes and through convergence studies, which are also a form of code verification. Convergence studies are also used to estimate the numerical error in the results section of this paper.

Model form error, E_{mod} , is the degree to which the mathematical model represents the reality of the physical system. E_{mod} can be quantified using the following procedure: first, the codes are compared by running the test case (see Section 4) at a sufficiently high resolution as a two-dimensional (2D) simulation [51]. Heat flux outputs compared to the experimental data give a benchmark comparison between the codes for solving the 2D laminar Navier-Stokes (NS) equations in the hypersonic regime. Next, different levels of chemical modeling are tested on the laminar case to identify how modeling assumptions such as assuming a calorically perfect gas, a thermally perfect gas, or a real gas impact the solution for a flat plate. We then compare each code to assess how they predict heat flux over the hypersonic flat plate with a turbulent boundary layer using a methodology similar to the laminar cases. This is completed using Reynolds-Averaged Navier-Stokes (RANS) simulations with the SA-CatrisCons turbulence model [40, 39], along with a comparison to a 3D wall-resolved Large Eddy Simulation (LES). This turbulent boundary layer study will focus on quantifying the uncertainty in the heat flux to the surface when compared to the experimental data.

Finally, the experimental uncertainty, E_{exp} , is comprised of measurement error E_{meas} , error due to inaccuracies in measuring the experimental data, and model input uncertainty, E_{inp} . Model input uncertainty, E_{inp} , is the uncertainty due to the parameters used in the model and the data describing the surroundings of the system of interest [12]. In this case, model input refers to uncertainty in the experimental conditions. This type of uncertainty can be found through a sensitivity study which will be described in further detail later in this paper.

3.1 Uncertainty Metrics

To move from a qualitative to a quantitative approach for uncertainty analysis and code comparison, this study uses uncertainty metrics. These metrics provide a quantifiable means to anticipate how different numerical and modeling approaches affect a computational solution. Such insight can inform an engineer of the important factors to include when performing design simulations.

Coarse grained uncertainty quantification utilizes two main types of metrics to simply quantify the uncertainty in hypersonic flows [11]. All of these metrics compare surface values as functions of the xcoordinate along the geometry, since this is the most common method for supplying experimental data. The first metric type compares statistical quantities of the experimental and CFD datasets with each other and is denoted by E(F). For example, E(F) can compare the mean of experimental and simulated heat fluxes over the x-direction of a flat plate. The second finds the difference between the interpolated CFD values and the corresponding experimental points to compute a statistical quantity, and is denoted by E(f). An example of calculating an E(f) value would be finding the relative difference between the function values at three experimental points and the predicted CFD function values at the same x locations and then determining the average of these differences. In summary, E corresponds to a statistical uncertainty metric, F corresponds to comparing statistical quantities of different data sets' distributions, and f corresponds to comparing individual points of each data set and finding the statistical quantities from these differences. More specifically, $f_{\rm CFD}(x_{\rm exp})$ corresponds to pointwise surface CFD predictions at experimental x-locations. In the code, we use the later metric, E(f), as it is less sensitive to extreme values. When quantifying the modeling uncertainty in our results, we use $E(f_{avg})$ as the metric to understand how the simulation modeling assumptions affected the solution across the entire domain of interest. This choice is due to the flat plate geometry, where the prediction of a quantity over the entire plate is more important than having the lowest uncertainty at one point on the plate. For the overall uncertainty metric, we take the conservative approach of assuming that all errors are additive. We use the $E(f_{avg})$ metric as the modeling uncertainty metric for all cases in this study.

Uncertainty Metric Type	Simplified Equation
Average of compared points: $E(f_{avg})$	$\operatorname{mean}\left(\left \frac{f_{\operatorname{CFD}}(x_{\exp}) - f_{\exp}(x_{\exp})}{f_{\exp}(x_{\exp})}\right \right) * 100$
Maximum of compared points: $E(f_{\text{max}})$	$\max\left(\frac{f_{\rm CFD}(x_{\rm exp}) - f_{\rm exp}(x_{\rm exp})}{f_{\rm exp}(x_{\rm exp})}\right) * 100$
Overall Error Metric [11]	$E_{\text{all}} = E(f_{\text{avg}})_{\text{num}} + E(f_{\text{avg}})_{\text{mod}} + E(f_{\text{avg}})_{\text{exp}}$

Table 2: Uncertainty metric definitions

4 Test Case



Figure 3: Flat plate geometry with Holden[52] input conditions

As a case study, we examine the Mach 11.1 Holden flat plate test case [9, 51]. The experimental conditions are summarized in Table 3. The generalized boundary conditions for the simulation are shown in Figure 3. Note that these boundary conditions are slightly modified for each solver, as BuBL only produces a boundary layer solution, and US3D does not require an exit symmetry wall for solution stability. This flat plate test case is a benchmark experiment which includes regions of laminar and turbulent flow. A flat plate is one of the most simple geometries for laminar and turbulent predictions, as many self-similar solutions to the problem can also be formed [53]. The lowest uncertainty metrics are expected for this type of geometry since the flow does not involve any other complex, hypersonic flow features such as (Shockwave-Boundary-Layer Interaction) SBLI or shock interactions. This case allows us to compare both fully laminar and fully turbulent solutions against each other to assess how the predictions of each code differ. In addition, we can perform analysis for a simulation that directly captures the laminar-turbulent transition.

Table 3: Test case conditions from the Holden experiment [9, 51]

Description	M_{∞}	$ ho_{\infty}(kg/m^3)$	$T_{\infty}(K)$	$T_{\mathrm{stag}}(K)$	T_w	Fluid
Holden Flat Plate	11.1	0.09483	64	1641	300	Air

5 Results

Quantitative results of the uncertainty assessment are presented in this section for the test case. The codes of focus in this study have a wide range of experience and equipment needed for successful simulation. These are important considerations in engineering design. Therefore, in addition to modeling uncertainty metrics, the user and computational cost of each code are also discussed.

5.1 Sensitivity Study

We are interested in quantifying the bias in the experimental outputs due to model input uncertainty, E_{inp} . A sensitivity study is a means of assessing the impact of input parameters on the output of a model [54]. To perform a sensitivity study, we first characterize the uncertainty of the model as epistemic. Epistemic uncertainty is defined as uncertainty due to a lack of knowledge or ignorance of the relevant factors [55]. Without further information on the experimental setup, we cannot assume that uncertainty in model inputs can be modeled with a probability distribution. Instead, we treat the uncertainty as an interval. Then, we use interval analysis to find for a particular set of input intervals the corresponding interval in the output [56]. An additional benefit of these studies is that they allow us to identify the most relevant input parameters, a critical part of CFD validation [2].

There are many approaches to sensitivity studies. Perhaps the most popular is Monte Carlo sampling [12]. With the uncertainties characterized, two Monte Carlo methods can be used to quantify how uncertainty propagates through our system. Both methods are types of orthogonal array studies [54]: Latin Hypercube sampling [57, 58] and a full factorial design study [56]. These methods use sampling of the input/feature space to inform the interval analysis. Latin hypercube sampling is a form of stratified random sampling that selects points in a distributed fashion over the feature space. Conversely, the full factorial design not only allows us to examine the extreme edges of the feature space, but also allows us to determine main effects and potential parameter interaction effects. For the full factorial study, we neglect higher-order interaction effects due to their low likelihood of occurrence. Schematics of these two sampling methods are given in Figure 4.



Figure 4: Schematics of orthogonal array sampling designs, (a) is given with increased resolution due to its sparsity

While there may be additional relevant parameters, we chose to focus on the specific factors whose uncertainty is quantified in or derived from the original study. Marvin et. al. provide that there is experimental uncertainty in the measured Mach number M_{∞} , stagnation enthalpy h_0 , and the dynamic pressure p_{∞} [9]. These uncertainties are 1.5%, 5%, and 5% respectively. To convert the dynamic pressure q_{∞} into a more convenient quantity for our calculations, we use isentropic relation (32a) rearranged into (32b), combining Mach number and dynamic pressure to find an estimate for the uncertainty in the static pressure. Subsequently, the parameters used for the sensitivity study are Mach number, static pressure, and total enthalpy.

$$q_{\infty} = \frac{\gamma}{2} p_{\infty} M_{\infty}^2 \tag{32a}$$

$$p_{\infty} = \frac{2}{\gamma} \frac{q_{\infty}}{M_{\infty}^2} \tag{32b}$$

From the isentropic relation (32b), it is determined using standard uncertainty metric combination properties that p_{∞} has a 5% + (2 × 1.5%) = 8% uncertainty.

For tractability, we perform the sensitivity study with BuBL, the lowest fidelity but fastest running code

examined in this study. We also perform this study for the simple case of a laminar flow with a calorically perfect gas. To minimize computational expense, simulations are conducted for a slightly unresolved grid after verifying that these results are expected to be within 0.2% of the finer grid solution. Because the results for this case are found to be so similar to those of the higher-fidelity CFD codes, we assume that the trends found generalize to those codes as well. Heat transfer outputs are generated for the five x-locations corresponding to the laminar experimental data points.

For both sampling procedures, sample sizes were selected by examining trade-offs between granularity of input space and computational/time requirements, as it is not possible to directly estimate the sample sizes required for exact results [54]. 300 samples were generated for the Latin Hypercube and 5 levels or $5^3 = 125$ samples were selected for the full factorial experiment. More samples were required for the Latin hypercube design given its sparsity (Figure 4). The results of the Latin hypercube and full factorial experiments are given by the box-and-whisker plots in Figure 5. It is observed that the two orthogonal array studies had similar values for their ranges and medians. Furthermore, these medians were nearly identical to the heat flux values predicted using the nominal values of Mach number, stagnation enthalpy, and static pressure. However, the full factorial design resulted in a slightly wider range of heat transfer values and slightly lower medians. Notably, all of the experimental data points fall within the range of the calculated model input uncertainty.



Figure 5: Summary of the sampling results using both the Latin Hypercube design and the full factorial design. Experimental values are also included.

Each of the outputs for the five data locations exhibits similar trends. Figure 6, which is for data point 1 but is indicative of the results found for all five outputs, shows that heat transfer is positively correlated with Mach number, stagnation enthalpy, and static pressure. The correlation is slight for Mach number and most pronounced for stagnation enthalpy. This indicates that the input parameters have an order of significance is static pressure, then stagnation enthalpy, then freestream Mach number. We also note that no significant interaction effects were found during the orthogonal vector study. However, in the production of those values for the study, an important result is found. When the parameter combinations representing the extremes of the parameter input space are calculated, the worst-case uncertainty bounds for the model input are found. This is expected given the results of the main effects analysis. For each of the laminar data points the upper bound on the input uncertainty, E_{inp} , is +11.4% and the lower bound is -10.9% – a slightly asymmetric result. We note that Gnoffo et al. calculate a value of 7.6% using an alternative methodology derived from energy calculations [11].



Figure 6: Results of main effects analysis for data point 1

5.2 Laminar Comparison

Table 4: Modeling uncertainty metric, E_{mod} , results for the laminar flow portion of the Holden [51] data (0.0508 m < x < 0.1778 m)

Uncertainty Metric	BuBL	BuBL-C	SANS	SANS-C	US3D	US3D-L
$\mathbf{E}(\mathbf{f}_{\mathrm{avg}})$	4.81	5.22	4.93	10.73	4.68	7.20
$\mathbf{E}(\mathbf{f}_{\max})$	7.03	7.71	7.29	14.22	7.44	12.93

The first analysis of the test case is the comparison of BuBL, SANS, and US3D in the laminar portion of the flat plate flow. Each of these codes are compared with the five experimental data points closest to the leading of the Holden geometry. We expect relatively small uncertainty metric values for this laminar section because of the few modeling assumptions made when simulating laminar flow compared to turbulent flow. The main sources of uncertainty in hypersonic laminar simulations come from numerical error in the simulation, the simplification of the Navier-Stokes equations using assumptions based on geometry, the equation discretization, and the modeling of the fluid chemistry. The chemical modeling aspect is unique to high speed flows. The default assumptions in many solvers include a constant ratio of specific heats, $\gamma = 1.4$ for air, a constant thermal conductivity, and a fluid viscosity based on Sutherland's law. In the Holden experiment [51], the freestream fluid temperature falls below 100K, and the fluid temperature near the stagnation region of the flat plate can reach nearly 1600K. From chemical experiments, we know that the specific heats of air can vary in this temperature range by more than 20% [44].

For this reason, this study has investigated several chemical models to examine how varying fluid viscosity or specific heat according to more physically accurate models (as discussed in Section 2) can impact results. The base steady solvers of BuBL, SANS, and US3D use very similar chemical modeling assumptions. As such, they have very similar uncertainty metric results in the laminar region, as shown in Table 4¹. These codes also have lower uncertainty predictions than the SANS, BuBL, and US3D simulations that used more advanced chemical modeling processes or modeled unsteadiness. Specifically, by modeling the fluid viscosity with collision integrals rather than Sutherland's law, the average error between the simulation data and the Holden experimental data increased from 4.93% to 10.73%. In this case, collision integrals led to a higher fluid viscosity prediction than those predicted using Sutherland's law, as shown in Figure 7. An increased

¹Where "-C" stands for a chemical modeling modification, and "-L" stands for the LES

prediction of heat flux resulted due to its positive correlation with viscosity [49]. In general, the changes in viscosity modeling led to a freestream viscosity prediction difference of 15% and a maximum viscosity prediction difference of 20%.



(a) Sutherland's law viscosity

(b) Collision integral viscosity

Figure 7: Difference in viscosity predictions over the leading edge of the Holden flat plate plate for the different SANS viscosity models where $\mu_{FreestreamSutherland} = 4.29e-06$ Pa-s

A similar result was observed with the BuBL solver. Allowing relations for a varying specific heat resulted in simulation results that were slightly less representative of the experimental results. This is unexpected given that, in reality, the specific heat is a function of temperature. The specific heat of diatomic gases generally increases with temperature, and these increases lead to a specific heat that is larger in magnitude than the constant approximation. Therefore, it would be reasonable to assume that simulations that account for this variation in specific heat, whether through collision integrals or the harmonic oscillator model, would be more accurate. However, these solutions tend to overpredict the experimental data. This result is consistent with the increase in specific heat, given that specific heat positively correlates with heat transfer.

During this study, a simulation in US3D with equilibrium chemistry was another expected result. However, the addition of chemical reactions creates additional challenges in finding time scales to resolve a steady simulation, especially near the leading edge. For this reason, this study was unable to compare chemically reacting US3D results with BuBL or SANS.



Figure 8: Holden laminar heat flux experimental data comparison

To fully explain the discrepancies between expectation and the observed experimental results, more information would be needed on the experimental test case, or other similar experimental test cases could be used. One simple explanation is that this is the worst case scenario in which the modeling error associated with the simulations (see Table 4) happens to constructively add to the other types of error. In coarse grained uncertainty metrics quantification we assume that error sources are orthogonal and adding them together produces a conservative, but feasible, uncertainty approximation. We also assume that the experimental results are accurate. Instead, our analysis suggests that the measured experimental values may underpredict the heat flux for the reported experimental setup, and it is possible that the cases with the more involved chemical modeling are the more accurate representations of the flow physics. This is just one hypthesis, though, and higher-fidelity simulations are required to confirm or deny this thought. Moreover, if we account for a a true worst-case scenario and include the model input uncertainty (-10.9%/+11.4%) determined from the sensitivity study (see Section 5.1), it becomes impossible to make a definitive assessment of the accuracy of these laminar simulations. In short, our results suggest that the experiment is not sufficiently precise in this region, and any of the laminar simulations could be the most accurate.

Since these laminar heat flux predictions generated by BuBL, SANS, and US3D are so similar to each other, the choice of which tool to use comes down to the user's goals. If the focus is on simpler geometries, the Naiver-Stokes equations can be simplified into equations that can be more easily solved. A tool like BuBL does just that and is very useful for fast and accurate 2D, hypersonic, laminar boundary layer solutions. SANS is advantageous for more complicated geometries, especially in situations where meshing must change with successive simulations, such as in a trade study with a deflection of a control surface. This is because SANS's output-based adaptation ensures a negligibly small numerical error. US3D is a useful baseline for all simulations, since it is capable of reliably finding steady and unsteady laminar and turbulent solutions.

5.3 RANS Comparison

The RANS uncertainty metrics are expectedly much larger than their laminar counterparts. Previous studies have detailed several reasons for uncertainty in RANS modeling, including the form of the equations and the assumptions involved in Reynolds stress modeling such as those in the Boussinesq hypothesis [40, 59, 58]. This section compares the results between the steady RANS solvers in SANS and US3D. The uncertainty metric results show very similar simulated heat flux predictions, with differences in the maximum and average predictions only being a few percentage points. This difference could be due to the implementation of the turbulence model itself. Discrepancies are common in the implementation of turbulence models, as users find that small modifications often lead to better results. This has been especially true in the SA-CatrisCons model, where researchers sometimes modify coefficients or neglect production or destruction terms in their

Table 5: Uncertainty metric results for the turbulent flow portion of the Holden [51] data (0.4064m $< {\rm x} < 1.2718 {\rm m})$

Uncertainty Metric	SANS	SANS-C	US3D	US3D-L
$\mathbf{E}(\mathbf{f}_{\mathrm{avg}})$	22.25	24.10	21.17	21.16
$\mathbf{E}(\mathbf{f}_{\max})$	37.62	40.31	35.93	-50.04

implementations [11, 40]. With the small discrepancies in our study, it is unlikely that turbulence modeling varies much between the codes. It is more likely that the implementation of other numerical aspects such as flux limiters, shock capturing algorithms, grid resolution, or simply the differences in finite element and finite volume discretization leads to the few percentage point differences in the results.

In general, RANS results suffer in accuracy for transitional cases because of differences in boundary layer thickness compared to those in experiments. In this test case, the RANS simulations assume a turbulent flow from the beginning of the plate, while the experiment experiences a transition near the x = 0.3m location. This difference leads to very different boundary layer profiles in the downstream turbulent flow. A better test for a high-speed turbulence model would involve turbulence modeling with a separate equation or method for boundary layer transition specification. This would allow for a similar turbulent boundary layer thickness to be present at the comparison locations downstream on the plate. While the uncertainties in the RANS simulations are greater than those in the laminar case, this study has resulted in a useful comparison between SANS and US3D in turbulent simulations.



Figure 9: Plot of turbulent heat flux predictions within the turbulent section of the Holden flat plate

5.4 LES Comparison

LES simulations are very similar in functional form to RANS simulations, except that their accurate capture of larger kinetic energy scales allows for a time-accurate simulation capable of predicting laminar-turbulent transition. As such, LES simulations have boundary layer thicknesses comparable to those of the experi-

ment downstream of transition, unlike the previous RANS simulations. This paper examines using an LES simulation in US3D as the highest fidelity simulation in the code comparison.



Figure 10: US3D LES results over the length of the Holden flat plate

The LES simulation in US3D is comparable to the results obtained in both the steady laminar and turbulent results of the previous section. The only difference being that it required only one simulation to capture both the laminar and turbulent flow behavior and also includes a prediction of the laminar-turbulent transition location. The US3D simulation had slightly higher uncertainty in the laminar section when compared to the steady solver results without the chemistry modifications, and had very similar uncertainty quantities predicted compared to the RANS turbulent results. If an engineer needed to estimate the physical transition location over a vehicle while also finding a reasonable estimate of laminar and turbulent heat flux, an LES simulation may be a good place to start to better inform future steady simulations. However, one problem with the results of this LES simulation is that it significantly underestimates the maximum heat flux to the surface by almost 50%. This is different from the normal behavior of high-speed RANS predictions, which tend to overpredict heat flux to the surface [8]. This underprediction can be partially accounted for by the later transition location prediction in comparison to the experimental data. As we can see from the RANS data, early turbulent flow along the flat plate results in a higher maximum heat flux downstream of the leading edge. One more important result of the LES simulation is the comparison in run times between the RANS and LES simulations. While the RANS simulation took 950 CPU-hours to complete a low-numerical error solution, the LES simulation took 13500 CPU-hours to complete a simulation with significantly higher numerical uncertainty.

5.5 Uncertainty Summary

From the Holden experiment, we know that the experimental uncertainty, E_{meas} , is estimated to be 5%, and we approximate E_{inp} as 11.15%, the average of the upper and lower bounds (see Section 5.1). We also assume that E_{inp} generalizes to the turbulent case. Thus, we define $E_{\text{all}_{Lam}}$ and $E_{\text{all}_{Turb}}$ using the definition of E_{all} (see Section 3.1) for each code's respective simulation area. These results are summarized in Table 6.

 Table 6: Performance summary for the three codes without additional chemistry modeling

Code	Simulation Time	$\mathbf{E_{num}}$	$\mathbf{E}_{\mathrm{all}_{\mathbf{Lam}}}$	$\mathbf{E}_{\mathrm{all}_{\mathbf{Turb}}}$
BuBL	$\ll 1~{\rm CPU-hrs}$	0.2%	21.16%	-
SANS	250 CPU-hrs	0.1%	21.18%	38.5%
US3D	950 CPU-hrs	0.1%	20.93%	37.42%
US3D-L	13500 CPU-hrs	3.0%	26.35%	40.31%

The uncertainty metrics are very similar between the three codes. One of the largest differences in uncertainty is in the numerical error estimate. The output-based grid adaptation involves a more detailed error estimation process, which ensures that the discretization error is very small in the final solution. Several convergence studies were performed in SANS to ensure that this final heat flux result had a negligible numerical error, E_{num} , contribution. It is more difficult to quantify the numerical error in the results from the other simulations. Convergence studies for the two other codes were performed to ensure "grid independent" solutions. However, the term "grid independent" can have different meanings when comparing different solvers against each other, especially in regards to the acceptable magnitude of numerical error. To find the numerical error estimate for BuBL and US3D, this study looks at the most resolved grid and the grid one step below for each solver. We then compare the heat flux predictions for these simulations, and the $E(f_{\text{max}})$ value is what we take as a numerical error estimate. This methodology follows in the same spirit of coarse grained uncertainty quantification for which estimates are generally very conservative. This leads to a numerical error estimate of approximately 0.1% for the steady solutions of SANS and US3D, and 3.0% for the LES US3D results in this study. BuBL has a comparable numerical error estimate to that of SANS due to its much more simplified finite difference discretization scheme and the ability to run very fine meshes at a low computational cost. US3D-L, on the other hand, has an order of magnitude greater numerical error estimate due to user decisions for meshing, especially near the leading edge region, and because of the much greater computational cost of running the LES simulation on a grid that is finer than those required for the other flow solvers.

Simulation times in terms of CPU-hrs are also included. These times provide context for the simulation calculations. BuBL has an almost negligible run time compared to the other codes. The laminar and RANS solutions from SANS and US3D require substantially more time, and the LES simulation requires several orders of magnitude more CPU-hrs than the former solutions. These times only include the time and computational requirements required for the simulation itself. There is no consideration of the resources required to generate the computational meshes used for the simulations. The time and effort required to produce a grid for BuBL is almost negligible given that it is a uniform grid for a FDM method whereas SANS and US3D would require much more time and expertise to develop a satisfactory grid.

6 Conclusion

In this paper, we compare three hypersonic codes: SANS, US3D, and BuBL. Using coarse-grained uncertainty metrics, we have assessed the uncertainty in simulations of a hypersonic flow over a flat plate geometry. We found similar levels of modeling uncertainty in the laminar section of the geometry for each of the three codes. This was also the case for the turbulent results, although the uncertainty values were higher. Furthermore, the overall uncertainty is significantly affected by the uncertainty of the experimental input parameters. These findings suggest that it is not sufficient to quantify uncertainty using this particular experiment, although it is regarded as a benchmark case [9]. A significant amount of uncertainty is related to the experiment itself, the exact operating conditions, and the measurement errors. Reducing these uncertainties would substantially improve our ability to use CFD to predict experimental results.

Our findings are not uncommon, as both Gnoffo et al. and Roy and Blottner arrive at the same conclusion [11, 8]. It is critical that future research focus on producing precise experimental data that can be used for

CFD validation. Accurate data are still needed for modeling turbulence. Initiatives such as the Hypersonic Vehicle Simulation Institute (HVSI) aim to address these shortcomings and improve researchers' ability to simulate hypersonic flow [60]. HVSI has determined that there is particular importance in developing improved turbulence models, including those based on experiments. With such experiments, analyses such as the one included in this paper would be able to produce more concrete results.

With uncertainties not definitively quantified, other, more qualitative aspects of running these simulations become increasingly important. A key result of this analysis is the impact of the experience required to run these codes. Running these simulations and producing accurate, convergent results requires a particular experience due to the varying levels of complexity in the codes' implementations. The lack of results for the chemistry case in US3D is indicative of this. One must weigh the difficulty of using each code when deciding which solver to use. Generally, complexity is also associated with longer run times. In this study, the code with the simplest implementation was found to be able to produce results similar to those of the other codes in the laminar region while only requiring a fraction of the time. Depending on the requirements of the engineering application, it may not be necessary to use the highest fidelity code. In summary, these findings support the view that selecting CFD codes for hypersonic simulations requires a level of discretion and that further studies of this type are required before CFD can cement itself as a viable alternative to experiments and flight tests.

Furthermore, this study suggests there may be benefit in running simulations using multiple codes with a range of fidelities as the capabilities of each code my offer insight another does not. For example, the laminar base flow can be captured by BuBL, while SANS could provide a correction for imperfect gas effects, and US3D could offer a transition location. Experiments can inform simulations, but the opposite is also true as experiments are not always perfectly controlled. For instance, it is possible the US3D prediction of the transition location is accurate but it is being compared to an experiment in which transition is accelerated by ambient noise. In short, no one code is definitively better than the others, especially when time is of concern. As such, CFD solvers should include clear definitions of strengths and weaknesses to assist in efficient engineering applications. Additionally, this study highlights the need to increase the focus on quantification of experimental and numerical uncertainty. For future experiments, we recommend that more effort be put toward wind tunnel characterization, including instrumentation to capture flow conditions for each run. For future CFD simulation studies, more effort should be put towards convergence studies and quantitative estimates for numerical uncertainty. With these types of change, the validation of CFD models will become more effective as the associated uncertainties become smaller.

- C. J. Roy, C. C. Nelson, T. M. Smith, and C. C. Ober, "Verification of Euler/Navier-Stokes codes using the method of manufactured solutions," *International Journal for Numerical Methods in Fluids*, vol. 44, no. 6, pp. 599–620, 2004.
- [2] B. A. Maicke and J. Majdalani, "Evaluation of CFD codes for hypersonic flow modeling," 46th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, no. July, pp. 1–12, 2010.
- [3] M. S. Holden and T. P. Wadhams, "A Database of Aerothermal Measurements in Hypersonic Flow "Building Block" Experiments," in 41st Aerospace Sciences Meeting and Exhibit, vol. 2003-1137, 2003.
- [4] H. H. Fernholz and P. J. Finley, "A Critical Compilation of Compressible Turbulent Boundary Layer Data," tech. rep., Advisory Group for Aerospace Research and Development Neuilly-Sur-Seine (France), 1977.
- [5] H. H. Fernolz, P. J. Finley, and V. Mikulla, "A further compilation of compressible boundary layer data with a survey of turbulence data.," tech. rep., Advisory Group for Aerospace Research and Development Neuilly-Sur-Seine (France), 1981.
- [6] G. S. Settles and L. J. Dodson, "Hypersonic shock/boundary-layer interaction database," AIAA 22nd Fluid Dynamics, Plasma Dynamics and Lasers Conference, 1991, 1991.
- [7] G. S. Settles and L. J. Dodson, "Supersonic and hypersonic shock/boundary-layer interaction database," AIAA Journal, vol. 32, no. 7, pp. 1377–1383, 1994.
- [8] C. J. Roy and F. G. Blottner, "Review and Assessment of Turbulence Models for Hypersonic Flows: 2D/Axisymmetric Cases," in 44th AIAA Aerospace Sciences Meeting and Exhibit, 2006.
- [9] J. G. Marvin, J. L. Brown, and P. A. Gnoffo, "Experimental Database with Baseline CFD Solutions: 2-D and Axisymmetric Hypersonic Shock-Wave/Turbulent-Boundary-Layer Interactions," tech. rep., NASA, 2013.
- [10] G. V. Candler, I. Nompelis, M. C. Druguet, M. S. Holden, T. P. Wadhams, I. D. Boyd, and W. L. Wang, "CFD validation for hypersonic flight: Hypersonic double-cone flow simulations," 40th AIAA Aerospace Sciences Meeting and Exhibit, no. c, 2002.
- [11] P. A. Gnoffo, S. A. Berry, and J. W. Van Norman, "Uncertainty Assessments of 2D and Axisymmetric Hypersonic Shock Wave - Turbulent Boundary Layer Interaction Simulations at Compression Corners," in 42nd AIAA Thermophysics Conference, 2011.
- [12] C. J. Roy and W. L. Oberkampf, "A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing," *Computer Methods in Applied Mechanics and Engineering*, vol. 200, no. 25-28, pp. 2131–2144, 2011.
- [13] C. J. Roy, M. A. McWherter-Payne, and W. L. Oberkampf, "Verification and validation for laminar hypersonic flowfields," *Fluids 2000 Conference and Exhibit*, no. June, 2000.
- [14] B. R. Hollis and D. K. Prabhu, "Assessment of laminar, convective aeroheating prediction uncertainties for mars-entry vehicles," *Journal of Spacecraft and Rockets*, vol. 50, no. 1, pp. 56–68, 2013.
- [15] G. V. Candler, H. B. Johnson, I. Nompelis, P. K. Subbareddy, T. W. Drayna, V. Gidzak, and M. D. Barnhardt, "Development of the US3D code for advanced compressible and reacting flow simulations," 53rd AIAA Aerospace Sciences Meeting, pp. 1–25, 2015.
- [16] M. MacLean and M. Holden, "Validation and comparison of wind and dplr results for hypersonic, laminar problems," AIAA Paper, no. January, pp. 5163–5179, 2004.
- [17] D. H. Rudy, J. L. Thomas, A. Kumar, P. A. Gnoffo, and S. R. Chakravarthy, "Computation of laminar hypersonic compression-corner flows," AIAA Journal, vol. 29, no. 7, pp. 1108–1113, 1991.
- [18] V. Wartemann, A. Wagner, R. Wagnild, F. Pinna, F. M. Miró, and H. Tanno, "Code to code comparison on hypersonic high enthalpy transitional boundary layers," *AIAA Aerospace Sciences Meeting*, 2018, no. 210059, pp. 1–14, 2018.
- [19] J. K. Harvey, M. S. Holden, and T. P. Wadhams, "Code validation study of laminar shock/boundary layer and shock/shock interactions in hypersonic flow - Part B: Comparison with Navier-Stokes and DSMC solutions," 39th Aerospace Sciences Meeting and Exhibit, 2001.
- [20] D. Hash, J. Olejniczak, M. Wright, D. Prabhu, M. Pulsonetti, B. Hollis, P. Gnoffo, M. Barnhardt, I. Nompelis, and G. Candler, "FIRE II calculations for hypersonic nonequilibrium aerothermodynamics code verification: DPLR, LAURA, and US3D," *Collection of Technical Papers - 45th AIAA Aerospace Sciences Meeting*, vol. 11, no. January, pp. 7322–7339, 2007.

- [21] R. F. Vieira and J. L. F. Azevedo, "RANS Simulations of Flows with Shock Wave-Boundary Layer Interaction," in 51st AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition 2013, 2013.
- [22] W. L. Oberkampf and M. F. Barone, "Measures of agreement between computation and experiment: Validation metrics," *Journal of Computational Physics*, vol. 217, no. 1, pp. 5–36, 2006.
- [23] P. Subbareddy and G. Candler, "A fully discrete, kinetic energy consistent finite-volume scheme for compressible flows," *Journal of Computational Physics*, vol. 228, pp. 1347–64, 2009.
- [24] F. Ducros, V. Ferrand, F. Nicoud, C. Weber, D. Darracq, C. Gacherieu, and T. Poinsot, "Large-eddy simulation of the shock/turbulence interaction," *Journal of Computational Physics*, vol. 152, pp. 517–49, 1999.
- [25] G. Candler, M. Wright, and J. McDonald, "Data-parallel lower-upper relaxation method for reacting flows," AIAA Journal, vol. 32, pp. 2380–6, Dec. 1994.
- [26] M. Wright, G. Candler, and M. Prampolini, "Data-parallel lower-upper relaxation method for the navierstokes equations," AIAA Journal, vol. 34, pp. 1371–7, July 1996.
- [27] A. Vreman, "An eddy-viscosity subrgid-scale model for turbulent shear flow: Algebraic theory and applications," *Physics of Fluids*, vol. 16, pp. 3670–81, Oct. 2004.
- [28] A. C. Huang, H. A. Carson, S. R. Allmaras, M. C. Galbraith, D. L. Darmofal, and D. S. Kamenetskiy, "A Variational Multiscale Method with Discontinuous Subscales for Output-Based Adaptation of Aerodynamic Flows," in AIAA Scitech 2020 Forum, pp. 1–31, 2020.
- [29] C.-I. Ursachi, M. C. Galbraith, S. R. Allmaras, and D. L. Darmofal, "Output-Based Adaptive Reynolds-Averaged Navier–Stokes Higher-Order Finite Element Solutions on a Multielement Airfoil," AIAA Journal, pp. 1–14, 2021.
- [30] M. C. Galbraith, C. I. Ursachi, D. Chandel, S. R. Allmaras, D. L. Darmofal, R. S. Glasby, D. L. Stefanski, J. T. Erwin, K. R. Holst, E. A. Hereth, J. Mukhopadhaya, and J. J. Alonso, "Comparisons of HPCMP CREATE-AV Kestrel-COFFE, SU2, and MIT SANS RANS Solutions using Output-Based Adapted Meshes for a Multi-Element Airfoil," in AIAA Scitech 2021 Forum, 2021.
- [31] G. V. Candler, P. K. Subbareddy, and J. M. Brock, "Advances in computational fluid dynamics methods for hypersonic flows," *Journal of Spacecraft and Rockets*, vol. 52, no. 1, pp. 17–28, 2015.
- [32] G. E. Barter, Shock Capturing with PDE-Based Artificial Viscosity for an Adaptive, Higher-Order Discontinuous Galerkin Finite Element Method. PhD thesis, Massachusetts Institute of Technology, 2008.
- [33] Y. Hu, C. Wagner, S. R. Allmaras, M. C. Galbraith, and D. L. Darmofal, "Application of Higher-Order Adaptive Method to Reynolds-Averaged Navier-Stokes Test Cases," *AIAA Journal*, vol. 54, no. 9, pp. 2626–2644, 2016.
- [34] H. A. Carson, Provably Convergent Anisotropic Output-Based Adaptation for Continuous Finite Element Discretizations. PhD thesis, Massachusetts Institute of Technology, 2020.
- [35] M. Yano, An Optimization Framework for Adaptive Higher-Order Discretizations of Partial Differential Equations on ARCHIVES Anisotropic Simplex Meshes. PhD thesis, Massachusetts Institute of Technology, 2012.
- [36] R. Becker and R. Rannacher, "An optimal control approach to a posteriori error estimation in finite element methods," Acta Numerica, vol. 10, no. May 2021, pp. 1–102, 2001.
- [37] J. R. Shewchuk, "Triangle: Engineering a 2D Quality Mesh Generator and Delaunay Triangulator," Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), vol. 1148, pp. 203–222, 1996.
- [38] P. C. Caplan, R. Haimes, D. L. Darmofal, and M. C. Galbraith, "Extension of local cavity operators to 3d + t spacetime mesh adaptation," *AIAA Scitech 2019 Forum*, 2019.
- [39] B. Smith, C. L. Rumsey, and G. Huang, "Turbulence Modeling Resource Website (https://turbmodels.larc.nasa.gov/)," 2020.
- [40] C. J. Waligura, B. L. Couchman, M. C. Galbraith, S. R. Allmaras, and W. L. Harris, "Investigation of Spalart-Allmaras Turbulence Model Modifications for Hypersonic Flows Utilizing Output-Based Grid Adaptation," AIAA Science and Technology Forum and Exposition, AIAA SciTech Forum 2022, 2022.
- [41] A. Laricchiuta, G. Colonna, D. Bruno, R. Celiberto, C. Gorse, F. Pirani, and M. Capitelli, "Classical transport collision integrals for a Lennard-Jones like phenomenological model potential," *Chemical Physics Letters*, vol. 445, no. 4-6, pp. 133–139, 2007.
- [42] B. F. Armaly and K. Sutton, "Viscosity of Multicomponent Partially Ionized Gas Mixtures.," AIAA

Paper, 1980.

- [43] G. E. Palmer and M. J. Wright, "Comparison of methods to compute high-temperature gas viscosity," Journal of Thermophysics and Heat Transfer, vol. 17, no. 2, pp. 232–239, 2003.
- [44] C. N. Onyeador, "Simulation of Lees-Dorodnitsyn Hypersonic Laminar Boundary Layers with Temperature-Dependent Properties," S.M. Thesis, Massachusetts Institute of Technology, Department of Aeronautics and Astronautics, 2021.
- [45] C. N. Onyeador, A. Hodge, and W. L. Harris, "A Robust Computational Approach to Lees-Dorodnitsyn Laminar Hypersonic Boundary Layers with Temperature-Dependent Properties," *Manuscript in Progress*, 2022.
- [46] J. D. Anderson Jr., *Hypersonic and High-Temperature Gas Dynamics, Second Edition.* Reston, VA: American Institute of Aeronautics and Astronautics Inc, AIAA, 2nd ed., 2006.
- [47] M. Drela, Aerodynamics of Viscous Fluids. Cambridge, MA: Unpublished Manuscript, 2019.
- [48] H. B. Keller and T. Cebeci, "Accurate numerical methods for boundary-layer flows. II: Two-dimensional turbulent flows," AIAA Journal, vol. 10, no. 9, pp. 1193–1199, 1972.
- [49] W. G. Vincenti and C. H. Kruger, Introduction to Physical Gas Dynamics. Malabar, Florida: Robert E. Krieger Publishing Co., Inc., 1965.
- [50] J. L. Brown, "Hypersonic shock wave impingement on turbulent boundary layers: Computational analysis and uncertainty," *Journal of Spacecraft and Rockets*, vol. 50, no. 1, pp. 96–123, 2013.
- [51] M. S. Holden, T. P. Wadhams, and M. MacLean, "A review of experimental studies with the double cone and hollow cylinder/flare configurations in the lens hypervelocity tunnels and comparisons with Navier-Stokes and DSMC computations," 48th AIAA Aerospace Sciences Meeting Including the New Horizons Forum and Aerospace Exposition, 2010.
- [52] M. Holden, M. MacLean, T. Wadhams, and E. Mundy, "Experimental Studies of Shock Wave/Turbulent Boundary Layer Interaction in High Reynolds Number Supersonic and Hypersonic Flows to Evaluate the Performance of CFD Codes," in 40th AIAA Fluid Dynamics Conference, no. July, 2010.
- [53] H. Schlichting and K. Gersten, Boundary-Layer Theory. Berlin, Heidelberg: Springer, 8th ed., 2000.
- [54] J. Zhang, J. Yin, and R. Wang, "Basic framework and main methods of uncertainty quantification," 2020.
- [55] W. L. Oberkampf, J. C. Helton, and K. Sentz, "Mathematical representation of uncertainty," 19th AIAA Applied Aerodynamics Conference, no. April, 2001.
- [56] L. P. Swiler, T. L. Paez, and R. L. Mayes, "Epistemic uncertainty quantification tutorial," Conference Proceedings of the Society for Experimental Mechanics Series, 2009.
- [57] C. J. Sallaberry, J. C. Helton, and S. C. Hora, "Extension of Latin hypercube samples with correlated variables," *Reliability Engineering & System Safety*, vol. 93, pp. 1047–1059, 7 2008.
- [58] H. Xiao and P. Cinnella, "Quantification of model uncertainty in RANS simulations: A review," Progress in Aerospace Sciences, vol. 108, no. June 2018, pp. 1–31, 2019.
- [59] K. Duraisamy, G. Iaccarino, and H. Xiao, "Turbulence Modeling in the Age of Data," Annual Review of Fluid Mechanics, vol. 51, no. 357-77, 2019.
- [60] United States Air Force Academy, "Hypersonic Vehicle Simulation Institute." 2022 [Online]. Available: https://www.usafa.edu/research/research-centers/hypersonic-vehicle-simulation-institute/.