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Sensitivity to model parameters and roughness in finite-rate reacting hypersonic flows

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14. ABSTRACT
Computational techniques for the simulation of high-speed flows have outpaced the tools to analyze flow fields they generate. This is even more true for flows that rely on a significant amount of modeling assumptions, such as flows at conditions where non-equilibrium and finite-rate aerothermochemistry effects play a significant role. We propose the development and application of a computational framework for the analysis of fluid systems using adjoint techniques and gradient/sensitivity information. This information will be extracted directly and efficiently from a nonlinear simulation code, with minimal intrusion and involvement of the user. Information gained in this manner will be used, as a start, to analyze large-scale fluid systems as to their sensitivity to model assumptions and geometric modifications on the boundary. The same framework is, however, also applicable to input-output analyses, susceptibility analysis and to control efforts. In our application, we will in particular concentrate on the design of improved models, the reduction of large-scale motion and the influence of roughness on integral output quantities of interest.

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Sensitivity to model parameters and roughness in finite-rate reacting hypersonic flows – Final report 12/2022
EOARD/AFOSR grant FA9550-18-1-0127

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Summary. This final report presents a summary of activities regarding the EOARD/AFOSR grant FA9550-18-1-0127 "Sensitivity to Model Parameters and Roughness in Finite-rate Reacting Hypersonic Flows" supervised by Program Officer Dr. Douglas Smith. It consists of a brief recapitulation of the grant objectives, followed by a description of accomplished tasks and research results.

1. Background and motivation. The hypersonic regime is central to a range of critical flight missions, from reentry vehicles to missile aerodynamics, from high-speed transport to space exploration. It contains some of the most stringent constraints on accurate modelling and simulations which commonly stem from the aero-thermo-chemistry of the ambient gases and from the real-gas effects that arise at extreme temperatures. Simulations that aim for a high predictive capability need to incorporate all pertinent aero-thermo-chemistry and gas dynamics to arrive at forecasts of transition points and heat loads, to name only two of many quantities of interest (QoI). The sensitivity of these QoIs to assumptions and parameters of the underpinning models has been largely neglected or only insufficiently estimated. While these sensitivities are of secondary concern in the lower Mach-number regime, they become increasingly more important – and ultimately dominate the hypersonic regime. These sensitivities manifest themselves as second-order effects. While the first-order statistics (mean flow quantities) displays a rather benign response to real-gas and non-equilibrium gas-effects, it is significant enough to have an order-one effect on physical effects that derive from the first-order statistics. Instability growth rates, transition location, maximum thermal load and peak heat locations can vary by order-one changes, even though the mean flow profiles of the real-gas case are hardly distinguishable from idealized analogues. These sensitivities are important to quantify for many reasons. First, they quantify the uncertainty contained in the simulation results and provide a level of confidence (or error) in the predictions made due to simulations. Second, they establish a guideline for focusing on certain aspects of the real-gas-effect modelling effort. Parts of the model that are identified as particularly prone to influence the quantities of interest need to constructed with far more care and detail than other parts that affect the outcome in a substantially less severe way. Third, sensitivities can have positive attributes as they pinpoint opportunities for effective active and/or passive control strategies. When manipulating heat loads or transition locations by actuator devices, it seems prudent to exploit sensitivities to accomplish a stated objective in an efficient way. In this context, high sensitivities are associated with favorable controllability.

Non-equilibrium models have been the focus of a concerted research effort over the past decade. This effort concentrated on a sophisticated and detailed description of reaction net-

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works, including dissociation, reaction, catalysis and recombination. Excitation of various degrees of vibration in di-atomic and mono-atomic gases, its modelling using gas-dynamic arguments, quantum mechanics or molecular dynamics has made great progress over the years, culminating in impressive libraries for the modelling of real-gas dynamics in and beyond equilibrium under a wide range of environmental circumstances. Difficulties arise when these libraries are coupled to simulation codes via their material-modelling interface. Little attention has been directed towards the influence of model parameters within the library on the output quantities provided by the simulation code.

While the sensitivities *within* the library have been analyzed, the coupling through a flow solver and their manifestation in QoIs remains to be an open problem. High sensitivities within the library will not necessary translate into output effects, in which case the exact modelling details may allow a larger uncertainty margin. In contrast, even a minute change in the library may invoke a noticeable response in the integral output, which would require a more precise modelling effort. Which parts of the model display a large compound sensitivity was one of the objectives of this project.

In pursuit of this objective, we used a computational framework based on adjoint technology. This platform has proven advantageous in low-speed applications, where it has improved design and control applications for aerodynamic flows. The methodology has been coupled to a nonlinear simulation code and benchmarked on generic but relevant flow configurations.

A second part of the project has been concerned with roughness-induced transition under real-gas effects. While this configuration has been studied in previous investigations, we concentrated on the influence of multiple roughness elements on the overall flow conditions. In particular, a periodic arrangement of the roughness elements is of interest to us, since it represents a commonly observed and favored configuration on many space vehicles. It is acknowledged that periodic arrangements of flow devices have tendency to lock into low-frequency, large-scale fluid motion via a synchronization mechanism. While this phenomenon is well-known, computational techniques to analyze it are largely underdeveloped. During the course of this project, we established a numerical technique that allows the capture of synchronizing instabilities via a Bloch-wave analysis. This type of analysis quantifies the response of locked-in subunits to external forcing. Remarkably, this analysis can be accomplished nearly at the cost of a simulation of a single subunit, while allowing conclusions on the behavior of a periodic array. This efficiency can be coupled in a minimally intrusive manner in simulation codes for roughness-induced transition.

2. The simulation code.

The simulation code has been developed and extended over the duration of this project to accomodate high-enthalpy flows, including the coupling to non-equilibrium libraries. Most significantly, the code includes adjoint capabilities in the form of a solver which, at minimal cost and with minimal intrusion, extracts adjoint information directly from the forward solver via a reserve-mode automatic differentiation approach. This approach has proven highly advantageous in other application and has been validated in numerous applications over the years.

We have extended the code's capabilities to accommodate shocks to study shock-boundary layer interactions. This has been accomplished by a localized artificial viscosity technique, which detects the presence of shocks and locally increases the diffusive terms to avoid ringing

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and other numerical divergences near discontinuities in the solution. While we maintain high-order accuracy in areas of the computational domain that are shock-free, while we sacrifice accuracy for numerical stability at shock positions. The new features in the simulation code have been tested and benchmarked against well-known flow configurations, such as shock-boundary layer interactions. Besides its accurate recovery of known flow dynamics, the implementation has been shown to add only a negligible cost to the computation of shock-driven flow situations. A more complex configuration has been a jet-in-crossflow showing a complex and unsteady bow-shock structure in front of the transverse jet. More importantly, the shock capability integrates seamlessly into the automatic-differentiation framework that builds the core of the sensitivity analysis module. In other words, the discontinuity presented by the shock does not pose any conceptual problem, as the adjoint framework is based on a weak formulation using variational principles.

3. Non-equilibrium aerothermochemistry. The first subtopic of the project is concerned with the coupling of the flow solver with the look-up library for gas-dynamic properties: Mutation++, developed at the von Karman Institute (VKI) in Belgium. For the direct (primal) problem, the current flow state together with the tracked species is passed to the Mutation++ library, which computes the relevant reactions among the tracked species and sends back quantities that go into the forcing terms for the momentum, energy and species equation. These terms properly model the effect of non-equilibrium, dissociation and recombination processes, which collectively are referred to as finite-rate chemistry phenomena. This look-up process is very accurate, even though it is adds to the computational load, on top of the typical time-step. For simulations of generic flow configurations, the coupling to the Mutation++ library for non-equilibrium dynamics can add a factor of 40 to the simulation, making non-equilibrium simulations rather costly. For this reason, an accelerated procedure based on the adaptive build-up of a surrogate model of part of the full library has been tackled.

3.1. Data analysis and machine learning for extracting a lighter version of Mutation++. The procedure builds on an input-output map that is represented in a high-dimensional phase space, tracing out a convoluted manifold for the Mutation++ mapping. This surrogate surface is obtained by applying training techniques from library snapshots.

The goal of the training is to obtain an efficient and accurate surrogate model g of the library f. With $\mathbf{X} \in \mathbb{R}^{N\times D}$ as a set of N scaled inputs to the library and $\mathbf{Z} \in \mathbb{R}^{N\times D_Z}$ as the corresponding outputs, the objective is to find g, such that $\hat{\mathbf{Z}} = g(\mathbf{X})$, and $\|\mathbf{Z} - \mathbf{Z}\|$ is minimized. The training of the data-driven model is performed in three steps. In the first step, dimensionality reduction, the input vector $\mathbf{X}$ is encoded into a low-dimensional space that accounts for most of the features of the output space through an input/output encoder (IO-E). The IO-E architecture consists of two sequential deep neural networks. The first network, the encoder, projects the inputs of the library into a latent space of dimension $d < D$. The second network, the decoder, predicts the outputs of the library from this latent space. The training is done through back-propagation of the L_2-norm of the error $\|\hat{\mathbf{Z}} - \mathbf{Z}\|^2$ through the full IO-E, where $\hat{\mathbf{Z}}$ denotes the prediction of the network. However, only the encoder part of the network is used. A radial basis function networks has been chosen owing to its higher accuracy. In the second step, clustering, the low-dimensional representation of the input vector, $\mathbf{Y} \in \mathbb{R}^{N\times d}$, is clustered using Newman's algorithm. This algorithm detects

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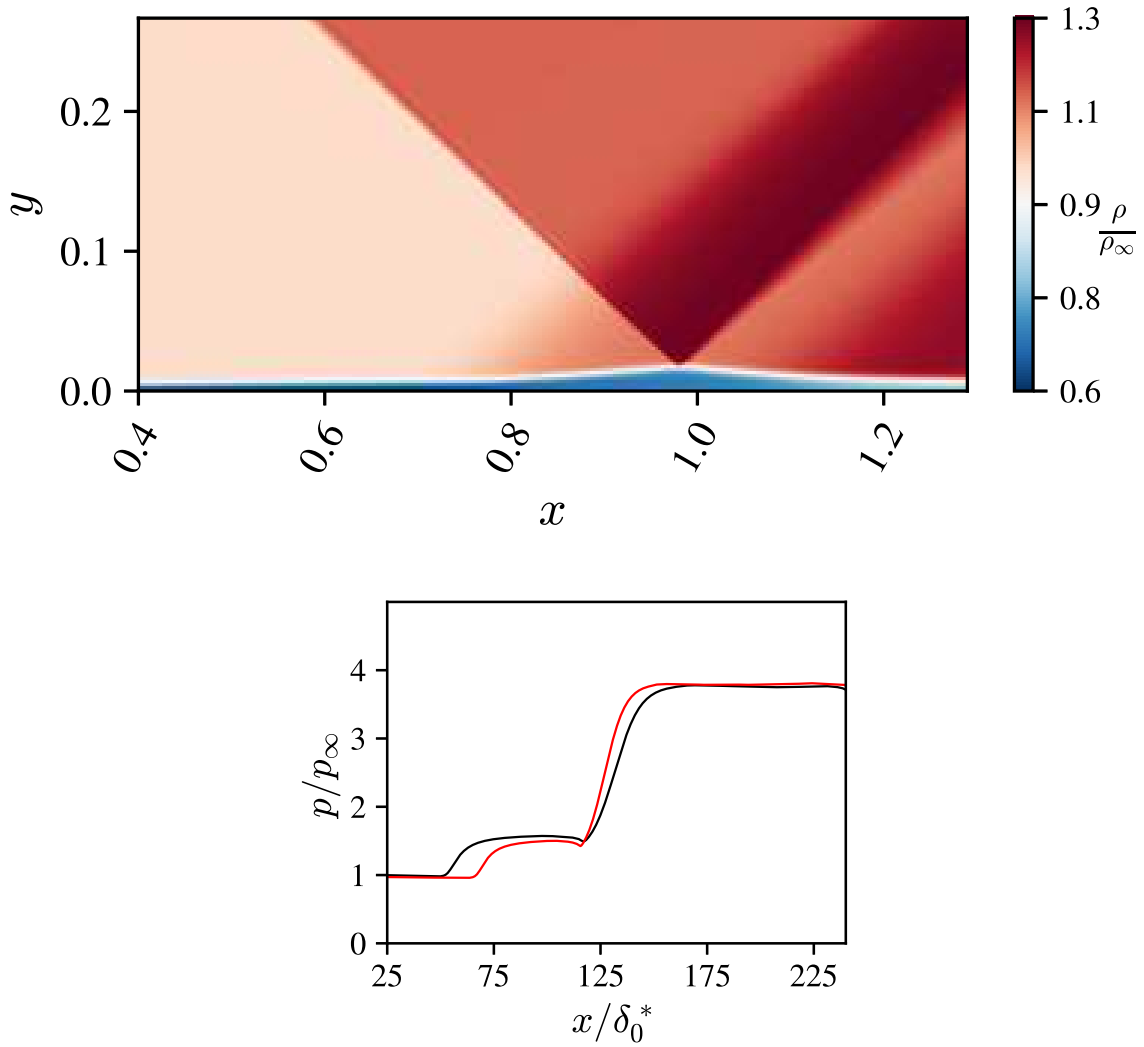

Figure 2.1. *(top) Density contour for the $Ma_\infty = 2$ laminar shock-boundary layer interaction (SBLI) case. The impinging and reflected shockwaves are visible, as well as the recirculation bubble and other relevant flow features. (bottom) Normalized wall pressure stream- wise distribution for the $Ma_\infty = 5.92$ SBLI. Comparison of thermally perfect gas (black lines) and chemical non-equilibrium (red lines) results.*

N_c coherent thermodynamic communities within the low-dimensional subspace. In the third step, surrogate model construction, a radial basis function network is trained with N_R kernels to predict the outputs of the library (i.e. $\hat{\mathbf{Z}}$) on the low-dimensional subspace spanned by each cluster.

We see encouraging speed-ups compared to the standard Mutation++ simulations, and we are optimistic that non-equilibrium simulations can be performed accurately and with a more reasonable computational overhead. Further improvements will be made beyond the

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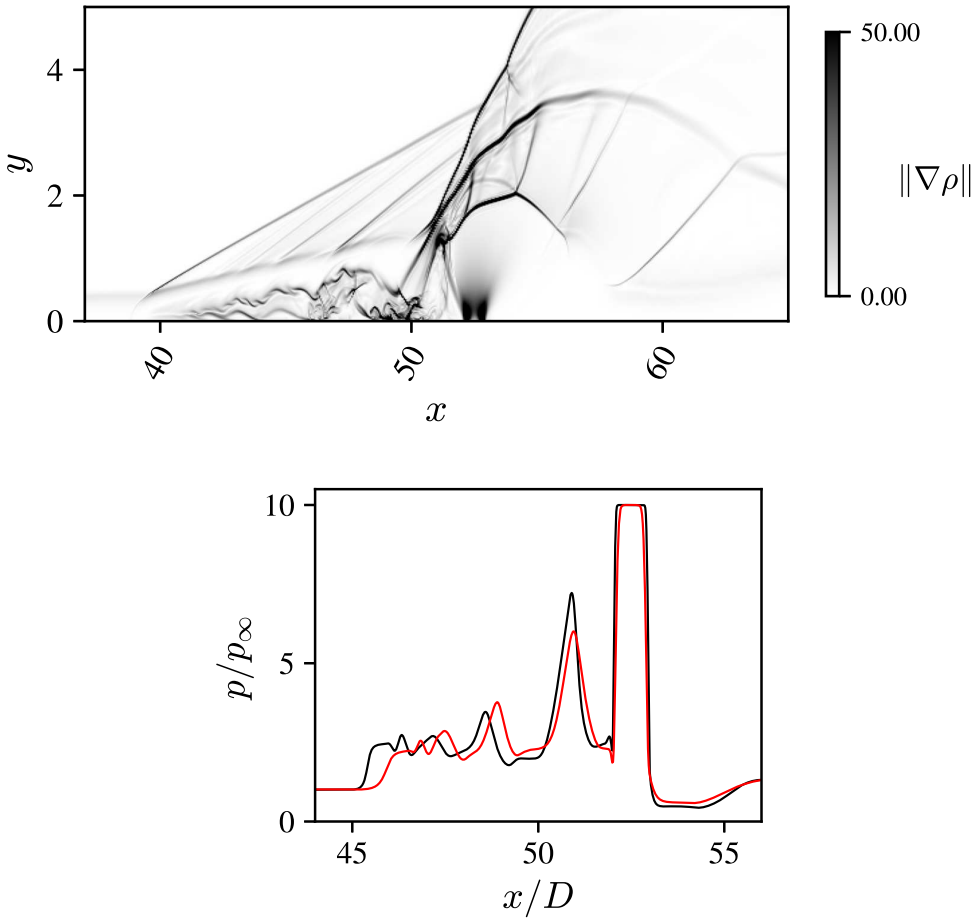

Figure 2.2. *(top) Instantaneous numerical Schlieren field for the sonic jet in $Ma_\infty = 5$ hypersonic crossflow. Jet location is at $x = 52.5$. (bottom) Instantaneous streamwise distribution of wall pressure for the sonic jet in $Ma_\infty = 5$ crossflow simulation. Comparison of thermally perfect gas (black lines) and chemical non-equilibrium (red lines) results.*

course of this projects, such as adding adaptivity and a more efficient representation of the surrogate surface. Internal sensitivity measures, directly extracted from the surrogate surface, will also be assessed as to their accuracy for a composite sensitivity analysis.

The accelerated Mutation++ library has been benchmarked using a similarity solution for high-speed boundary layer flow. This solution is particularly efficient in building the surrogate model and has been used as a starting point for more sophisticated flow configurations that do not follow a similarity law. First results are very promising, and additional avenues spawned by this effort will be pursued in the coming years.

4. Roughness-induced transition. The second theme is concerned with the assessment of stability and frequency response characteristics for flow around periodic arrays of roughness elements. In particular, we are interested in the manner in which neighboring subunits syn-

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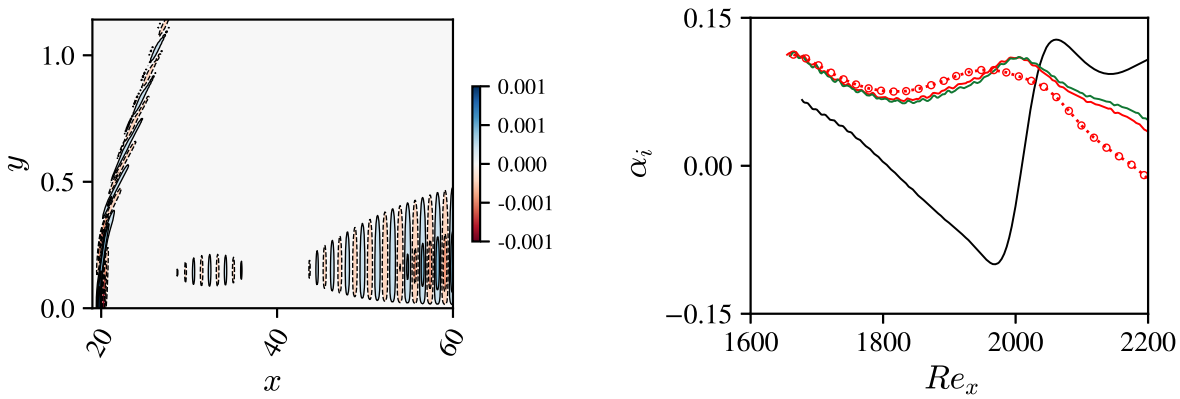

Figure 3.1. *(left) Contours of wall-normal velocity field for an adiabatic wall for chemical non-equilibrium flow. (right) Streamwise growth rate, α_i, of the linear perturbation in the adiabatic boundary layer with respect to Re_x. Current results (solid lines) are compared to Marxen et al. (dotted lines with sym- bols) for different gas models: thermally perfect gas (black), chemical non-equilibrium with the Stefan-Maxwell multicomponent diffusion model (red), chemical non-equilibrium with Ramshaw's simplified dif- fusion model (green).*

chronize and lock into a cross-unit flow pattern. These patterns are known to occur at lower frequencies and, based on a phase-velocity argument, are associated with large-scale structures that span more than one subunits before periodically continuing. A classical example of behavior like this is the onset of rotating stall in the compressor stage of turbomachines where multiple blade-passages lock together and slowly rotate in a retrograde direction.

From a mathematical point of view, n-periodic configurations can be described by a Bloch-wave ansatz. This formalism is based on a decoupling step of a block-circulant system matrix using a root-of-unity concept and allows the computation of trans-unit interactions at the cost of a single-unit calculation. The interaction between neighboring (or all) subunits is accounted for by dephasing the boundary conditions between all units. Physically, this allows for the synchronization across multiple units and the rise of low-frequency response features for periodic arrays of roughness elements. In our case, the periodicity arises from a geometric feature (the roughness-element array), but even saturated primary instabilities, as observed in crossflow vortices with a characteristic spanwise spacing, would be amenable to this type of analysis. A spin-off project is currently underway to explore this opportunity.

4.1. Matrix-free algorithm. Initially, the framework was developed under the assumption of direct access to the system matrix. It has been applied to linear compressor cascades where it has unveiled the locking of blade-passages across multiple units. As part of the project, this methodology has been generalized to applications where only matrix-vector products are available via a linearized version of a simulation code. This step would open possibilities of performing flow analysis with simulation codes of various degree of fidelity (RANS, DES, LES, DNS) when dealing with periodicity in the system. The execution of a single-unit simulation over a given time horizon would be sufficient to draw quantitative conclusions about the fluid dynamics for a system consisting of an arbitrary assembly of single, identical subunits. The step from matrix-based to matrix-vector-product-based execution of the Bloch-wave analysis

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has been instrumental in investigating sophisticated and realistic configurations, as found in vehicle designs for the hypersonic (but also the low-speed) regime. A key ingredient of the matrix-free method is based on a recasting of the full problem in terms of an artificial three-unit system that is 'pinged' by an input vector. The responses in the top and bottom units extract the response due to the linkage between the units, while the middle unit captures the intrinsic unit-dynamics. With these three units, we can tile the full system matrix for any unit configuration by weighing the three solutions (top, middle, bottom) by the appropriate root-of-unit and its inverse. This latter step only requires minimal computational resources.

The search for a test case to illustrate the flexibility and capability of this n-periodic analysis technique has not been straightforward. We are currently considering inclined jets in cross-flow that interact with the boundary layer in a sufficiently strong manner while influencing each other in the spanwise direction. In addition, we are collaborating with a research group at DynFlow, Paris to implement and test-drive the full three-unit implementation to study the synchronization of spanwise periodic streaks caused by an array of streamwise vortices. While this configuration has been extensively studied for a single unit, the synchronization across multiple units has not been treated so far, even though experimental observations point towards phase-locking effects for low-frequency external forcings.

5. Roughness-induced high-speed boundary-layer transition using machine learning. A numerical investigation of disturbance amplification in a Mach-4.8 flat-plate bound- ary layer is performed, for which a two-dimensional discrete roughness has been placed on the surface. The effect of this roughness on disturbance behavior is quantified by comparing the disturbance amplification of a flat plate with and without the roughness. In addition to the perturbation frequency, the height, width and downstream location of the roughness are varied.

The simulation data are used to train a neural network that is shown to be able to quickly predict the effect of roughness on disturbance amplification. The trained neural network is found to achieve good accuracy at a fraction of the cost of the simulations, although these remain nec- essary to provide training data. In addition, an autoencoder approach is applied to the simulation data in order to gain insight into the mechanism underlying amplification in the presence of roughness. The results indicate that the two parameters, disturbance frequency and roughness location, influence amplification in such a way that both can likely be combined into a single parameter. Physical arguments discussed in the litera- ture suggest that such a correlation should indeed exist, but the autoencoder is able to indicate such a correlation without any prior knowledge of the physics of the problem. Therefore, such an approach can be used to reduce the dimensionality of the parameter space and discover underlying correlations.

More specifically, a neural-network-based prediction tool has been implemented with three layers and 25, 20 and 15 neurons per layer, respectively. A nonlinear sigmoid activation function has been chosen. For training, the postprocessed data set (disturbance frequency, roughness height, length and location, together with ΔN, the difference in amplification between flat-plate flow and flow in the presence of a roughness, as an output variable) is fed into an autoencoder. As a start, the autoencoder was trained with a reduced data set, where only data for varying disturbance frequency and roughness length have been used for a fixed roughness

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height and location.

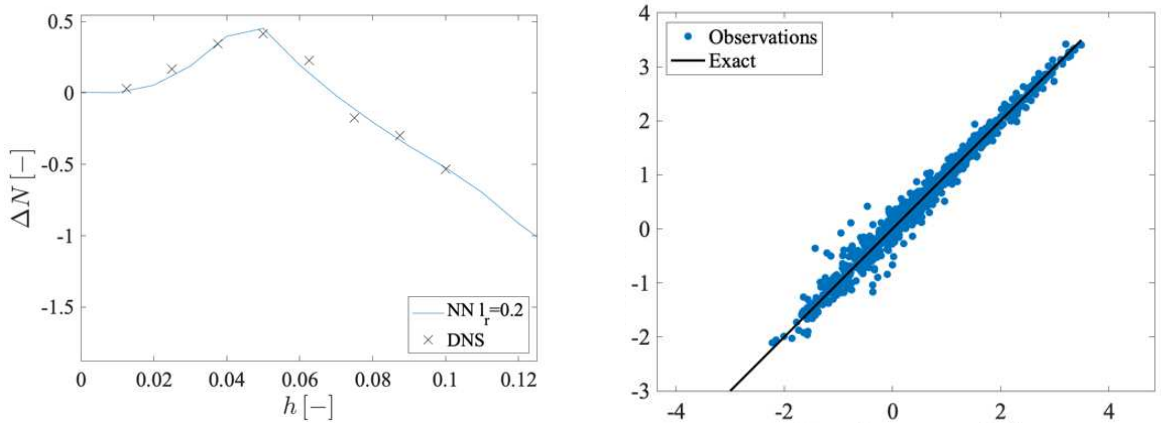

Figure 5.1. *(left) Comparison of DNS results and neural-network (NN) prediction for fixed frequency, fixed roughness length and location but varying height. (right) Validation of the neural network approach by plotting the ΔN response predicted by the neural network (labeled Observations) versus the true response (DNS data), with the black line indicating the exact case.*

6. Computer resources. For the development of the above tools, various computational resources have been used. The UK National Supercomputing Service (ARCHER) has provided support during the first part of the project. Towards the end of the project the installation of ARCHER 2 caused a great deal of delays and an extensive down-time during the installation, porting of software and benchmark runs. For this reason, computational resources from our French partner (T. Sayadi, Sorbonne University) have been used to remedy the lack of access to high-performance computer resources. In addition, recently the supercomputing facilities at KAUST (Shaheen II) have been used as a convenient backup. Despite these opportunities, each porting of the code has been associated with some difficulties and benchmarking needs.

7. Personnel. Besides the three PIs (Sayadi, Marxen, Schmid) with their various expertise, the project supported one graduate student, Athanasios Margaritis, who is enrolled in the PhD Program at the Department of Mathematics at Imperial College London. He is expected to conclude his research in the winter of 2022/2023, is simultaneously writing his dissertation and will defend his thesis in early spring 2023.

7.1. Challenges. The past two years have presented a great deal of challenges and difficulties that had a noticeable impact on the progress towards the project's objectives. Besides the difficulty in transitioning from ARCHER to ARCHER 2 (see above), the main issue was related to the COVID pandemic. Isolation in the home-office and home-country and the lack of a personal exchange and supportive environment caused a significant slowing in terms of accomplishments. After being isolated in his home country, Thanos spent a few productive months with our partner in Paris, where the more relaxed French Covid restrictions allowed a more supportive group work at Sorbonne University. Lately, Thanos has spent considerable time at KAUST to work in close proximity with me on open research issues as well as

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manuscript preparation.

Added to the difficulty of later part of the project was also my leaving Imperial College London for a new position at KAUST. However, this move has been taken as an opportunity for Thanos to join me at my new location and take advantage of the resources it offers.

In spring of 2021, a no-cost extension was graciously granted, which allowed us to bring the project to a good conclusion.

8. Output and follow-up. Two publications (Phys. Rev. Fluids for the light-version Mutation++ algorithm and application, and Theor. Comp. Fluid Dyn. for the incorporation of non-equilibrium effects into a large-scale simulation code for hypersonic flow) are currently under review. Two further publications will result from Thanos's dissertation and will be submitted to archival journals.

- C. Scherding, G. Rigas, D. Sipp, P.J. Schmid, T. Sayadi: Data-driven framework for input/output lookup tables reduction – with application to hypersonic flows in chemical non-equilibrium, *Phys. Rev. Fluids*, 2022 (under review).
- A.T. Margaritis, C. Scherding, O. Marxen, P.J. Schmid, T. Sayadi: Development of a high-fidelity computational tool for chemically reacting hypersonic flow simulations, *Theor. Comp. Fluid Dyn.*, 2022 (under review).
- A.T. Margaritis, T. Sayadi, O. Marxen, P.J. Schmid: A parallelizable mathematical framework for linearized analysis of flows in the presence of n-periodic structures, *AIAA SciTech 2021 Forum*, p. 1094, 2021.
- O. Marxen, A.T. Margaritis, P.J. Schmid, T.J. Flint, G. Iaccarino: Investigation and prediction of a roughness-induced, high-speed boundary-layer transition using machine learning, *Proc. CTR Summer Progr.*, 2022
- A.T. Margaritis, T. Sayadi, O. Marxen, P.J. Schmid: Sensitivity of reacting hypersonic boundary layers to n-periodic surface roughness, *IUTAM Laminar-Turbulent Transition*, p. 599-612, 2022.

The EOARD/AFOSR-funded project will continue to spawn follow-up projects. The light and accelerated version of Mutation++ will be extended to include advanced adaptivity strategies to further streamline the non-equilibrium capabilities when coupled to a simulation code. This effort will ameliorate the extra effort of finite-rate chemistry simulations, and allow even more complex flow situations. This effort will be in collaboration with Prof. Thierry Magin from the von Karman Institute in Belgium, one of the key architects of the Mutation++ library. An additional effort will be spent on incorporating gas-surface interactions, such as reaction, ablation and catalysis, into large-scale simulation codes.

Machine-learning techniques will be explored to identify and extract scaling relations in transitional flows. The collapse of roughness characteristics into subgroups has been encouraging to look into similar scenarios in other highly parameterized flows. This hands-off extraction can help in the discovery of hidden mechanisms, scaling laws and similarity solutions.

We will also continue to advance the n-periodic Bloch-wave analysis and develop a version that, instead of using the three-unit core analysis, extracts the relevant information for nearest-neighbor coupling from a single subunit by dephasing the boundary conditions in the coupling direction.

Finally, despite difficulties and challenges, the project has been intellectually rewarding

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and has led to a great many avenues to pursue in its wake. The flexible and generous funding of the EOARD/AFOSR has been instrumental, and the patient and reassuring support of the program managers (both EOARD and AFOSR) is greatly appreciated.

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