Workshop Traitement de Données pour la Mécanique des Fluides

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LRI

Book of Abstracts

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Introduction à la réduction de modèles en Dynamique des Fluides

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Cet exposé présentera les méthodes les plus couramment utilisées en Dynamique des Fluides pour analyser les données de plus en plus massives obtenues expérimentalement ou numériquement par simulations haute-fidélité. L'objectif est d'extraire des modèles simplifiés de dynamique qui capturent
l'essentiel des phénomènes présents dans ces écoulements, dans le but d'améliorer la compréhension physique des phénomènes ou de développer des stratégies de contrôle. Dans une première partie, nous décrirons les méthodes basées uniquement sur des données en commençant par l'approche la plus établie dans la communauté, la Proper Orthogonal Decomposition (POD). Nous introduirons alors la projection de Galerkin qui permet d'obtenir un modèle réduit de dynamique par projection des équations d'état sur une base donnée. Nous poursuivrons avec la description de la Dynamic Mode Decomposition (DMD), plus récemment introduite, et de la Cluster-based Reduced-Order Modelling (CROM) qui repose sur un algorithme d'agrégation d'états (k-means). Dans une seconde partie, nous décrirons les méthodes basées sur l'existence d'opérateurs de propagation dynamique. Nous présenterons alors l'analyse de Koopman, qui généralise l'analyse DMD précédente, puis présenterons rapidement l'analyse de stabilité globale et l'analyse en modes résolvants. Pour terminer, nous étendrons notre description sur les méthodes à noyau en décrivant la Kernel Principal Component Analysis (KPCA).

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Décomposition de données pour la caractérisation des cycles limite en combustion

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Pratiquement toutes les chambres de combustion sont sujettes à des oscillations de pression que l'on tente de maintenir à des niveaux acceptables pour l'utilisation et la durée de vie des équipements. Ces oscillations résultent de couplages multi physique entre l'écoulement, le dégagement de chaleur, l'acoustique et les limites du volume de combustion. Certains couplages sont des sources d'amplification des oscillations de pression, d'autres représentent des puits, leur équilibre conduit à des cycles limites dont l'amplitude et les fréquences caractérisent le niveau de perturbation. Les méthodes de décomposition de données permettent, à partir de données expérimentales ou numériques, (1) de caractériser les cycles limite, (2) de séparer spatialement et temporellement les grandeurs physiques et (3) de mettre en évidence les cohérences pour identifier l'origine des puits et des sources de pression. La présentation propose de mettre en évidence comment les décompositions orthogonales (POD) et dynamiques (DMD) sont utilisées en combustion pour comprendre les couplages en jeu et proposer des pistes de réduction des instabilités de combustion.

Practically all combustion chambers experience pressure oscillations that are attempted to be maintained at acceptable levels for use and service life of equipment. These oscillations result from multiphysics coupling between flow, heat release, acoustics and the limits of the combustion chamber. Some couplings are sources of amplification of the pressure oscillations, others represent wells, their equilibrium leads to limit cycles whose amplitude and frequencies characterize the level of

disturbance. The data decomposition methods allow, from experimental or numerical data, (1) to characterize the limit cycles, (2) to separate spatially and temporally the physical quantities and (3) to highlight the coherences to identify the origin of wells and sources of pressure. The presentation proposes to highlight how orthogonal (POD) and dynamic (DMD) decompositions are used in combustion to understand the couplings in action and propose ways of reducing combustion instabilities.

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Time-resolved analysis of thermo-acoustic instability triggering in a low-swirl burner using simultaneous high-speed laser diagnostics.

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The growth of a thermo-acoustic instability is studied in a low-swirl methane-air burner as the equivalence ratio is increased. Using simultaneous high-speed acetone (for fresh gases) and OH (for burnt gases) laser induced fluorescence, it is possible to study the flame and flow motions. Dynamic Mode Decomposition allows to extract the behavior of the flame at the frequency of the thermo- acoustic instability and to confirm that the origin of the instability lies in the periodic detachment of ring vortices, as expected from the literature. To study the growth of the instability , Hilbert transform is used to obtain the temporal evolution of the phase of the fluorescence signal at different points in the burner. It shows that the inner and outer parts of the flame fluctuate more and more in phase as the equivalence ratio is increased. By creating bursts of flame, this is the mechanism for the increase of the amplitude of the instability.

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Surrogate models and reduction methods for UQ and inference in large-scale models

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Uncertainty Quantification (UQ) and Global Sensitivity Analysis (GSA) in numerical models often rely on sampling approaches (either random or deterministic) that call for many resolutions of the model. Even though these computations can usually be carried out in parallel, the application of UQ and GSA methods to large-scale simulations remains challenging, both from the computational, storage and memory points of view. Similarly, Bayesian inference and assimilation problems can be favorably impacted by over-abundant observations, because of overconstrained update problems or numerical issues (overflows, complexity,…), raising the question of observations reduction.

A solution to alleviate the computational burden is to use a surrogate model of the full large scale model, that can be sampled extensively to estimate sensitivity coefficients and characterize the prediction uncertainty. However, building a surrogate for the whole large scale model solution can be extremely demanding and reduction strategies are needed. In this talk, I will introduce several techniques for the reduction of the model output and the construction of its surrogate. Some of these

techniques will be illustrated on ocean circulation model simulations. For the reduction of observations, I will discuss and compare few strategies based on information theoretical considerations that have been recently proposed for the Bayesian framework.

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What problem can you solve with machine learning and how?

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In this lecture I will cover the various families of problems that machine learning can solve. Using examples, primarily on images, I will present various linear and non-linear dimensionality reduction methods (PCA,NMF, T-SNE), I will motivate the use of certain clustering techniques (K-means, DBSCAN) and I will then explain which families of methods exist for building predictive models (linear methods, trees, nearest neighbors). I will insist on the computational aspects explaining the differences between batch and online learning which is necessary when data become too big to fit in RAM. This talk with be a live demo using the scikit-learn software.

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In-situ analysis and visualization of massively parallel computations of transitional and turbulent flows

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Massively parallel simulations generate increasing volumes of large data, whose exploitation requires large storage resources, efficient network and increasingly large post-processing facilities. In the coming era of exascale computations, there is an emerging need for new data analysis and visualization strategies.

Data manipulation, during the simulation and after, considerably slows down the analysis process, now becoming the bottleneck of high performance computing. The traditional usage consists in performing the simulations in order to write output data on disk. When dealing with three-dimensional time-dependent problems computed on thousands of cores, the volume of data generated is big and highly partitioned. As a consequence, their post-processing often requires to decrease the spatial or the time resolution in order to be performed on local platform, with less resources than on the computational machine. Another solution consists in coupling analysis with simulation, so that both are performed simultaneously.

In order to address these questions, a client-server in-situ analysis for massively parallel time-evolving computations has been developed and applied to a spectral code for the study of turbulence and transition. It is shown to have a low impact on computational time with a reasonable increase of resource usage, while enriching data exploration. Large time sequences have been analyzed. This could not have been achieved with the traditional workflow. Moreover, computational steering has been performed with real-time adjustment of the simulation parameters, thereby getting closer to a numerical experiment process.

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Visualisations tridimensionnelles de données issues de simulations numériques à très haute résolution en mécanique des fluides

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Aujourd'hui, la puissance de simulation disponible dans les centres de calcul nationaux et européens permet d'aborder des problèmes de plus en plus complexes, physiquement et géométriquement. Les maillages, utilisés pour discrétiser ces géométries dans nos simulations numériques d'écoulements turbulents, franchissent allègrement le milliard de points de calcul quand ce n'est pas la dizaine de milliards. Post-traiter et visualiser ces simulations sont devenus un enjeu important, surtout lorsque l'on souhaite y associer simplicité d'utilisation et disponibilité des outils ou de la ressource de calcul nécessaire.
Nous présenterons le workflow qui a été mis en place au LEGI, basé sur des solutions de logiciels libres comme Paraview, et qui permet, à partir d'un poste de travail élémentaire, de mobiliser des ressources distantes pour manipuler et visualiser ces grands volumes de données.

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Logiciels libres et Python pour l'acquisition, la gestion et le traitement de grosses données expérimentales, exemple d'une campagne sur la plate-forme Coriolis.

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Les techniques de mesure de pointe en mécanique des fluides expérimentale impliquent souvent la gestion de grande quantité de données. Je présenterai le cas d'une série d'expériences avec PIV scannée sur la plate-forme Coriolis.

D'un autre côté, les méthodes de l'open-source d'aujourd'hui sont pour la recherche une opportunité encore inexploitée. On peut aujourd'hui imaginer une recherche où les développements logiciels sont partagés, pris au sérieux et de qualité.

Je montrerais comment les logiciels libres et Python ont été utilisés pour le contrôle des expériences et l'acquisition, la gestion et le traitement des données. Ces méthodes nous ont permis d'utiliser efficacement les clusters du labo et de développer dans le cadre du projet Fluiddyn des codes Python libres et de bonne qualité utilisables par toute la communauté de mécanique des fluides expérimentale.

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Challenges computationnels de l'étude de l'incertitude dans les simulations numériques

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Plusieurs simulations (parfois plusieurs milliers) sont nécessaires pour calculer des statistiques pertinentes pour l'analyse de sensibilité globale. La pratique actuelle consiste à exécuter toutes les simulations nécessaires avec des paramètres d'entrée différents, à stocker les résultats sur disque, pour les lire plus tard et finalement calculer les statistiques requises. La quantité de stockage nécessaire peut rapidement devenir écrasante, avec un temps de lecture associé très long qui fait que le calcul statistique prend un temps excessif. Pour éviter ce problème, les scientifiques réduisent la taille de leur études en exécutant des simulations à basse résolution ou en sous-échantillonnant les données de sortie dans l'espace et le temps. Aujourd'hui, les machines petascale et demain exascale offrent des capacités de calcul qui permettraient des études de sensibilité à grande échelle. Mais ils ne sont malheureusement pas réalisables en raison de ce problème de stockage. Dans cette présentation, nous explorerons ce problème et discuterons de nouvelles approches qui pourraient être utilisées à l'avenir.

T. Terraz, A. Ribes, Y. Fournier, B. Iooss, and B. Raffin. 2017. Melissa: Large Scale In Transit Sensitivity Analysis of Model Outputs Avoiding Intermediate Files. In Proceedings of Super Computing conference, Denver, Colorado USA, November 2017 (SC'17)

A. Ribes "Computing Ubiquitous Statistics: Computational Challenges", Keynote at ISAV (In Situ Infrastructures for Enabling Extreme-scale Analysis and Visualization), November, 12th 2017. Denver, USA.

T. Terraz, B. Raffin, A. Ribes, Y. Fournier. "In Situ Statistical Analysis for Parametric Studies". Proceedings of the In Situ Infrastructures for Enabling Extreme-scale Analysis and Visualization (ISAV), Salt Lake City, USA, November 2016.

A. Ribes, B. Lorendeau, J. Jomier and Y. Fournier. "In-Situ Visualization in Computational Fluid Dynamics Using Open-Source tools: Integration of Catalyst into Code_Saturne", chapter in "Topological and Statistical Methods for Complex Data – Tackling Large-Scale, High-Dimensional, and Multivariate Data Sets", Springer. Pages 21-37 (2015) ISBN 978-3-662-44899-1.

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Learning-based strategies for the modeling and reconstruction of dynamical systems

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Data-driven strategies for the modeling and reconstruction of dynamical systems emerge as promising alternatives to classical model-driven frameworks, especially when dealing with computationally-demanding models and modeling uncertainty. Data-driven strategies provide novel means to benefit from large-scale observation and/or simulation datasets.
In this talk, we will review data-driven representations of dynamical systems and their applications to the resolution of inverse problems (data assimilation). The focus will be given to analog and neural network representations and address applications to high-dimensional systems. Besides numerical experiments for chaotic systems, we will illustrate applications to the reconstruction of sea surface dynamics from satellite observations.

Some references:

R. Lguensat, P. Tandeo, P. Aillot, R. Fablet. The Analog Data Assimilation. Monthly Weather Review, 2017.
R. Fablet, P. Viet, R. Lguensat. Data-driven Methods for Spatio-Temporal Interpolation of Sea Surface Temperature Images. IEEE Trans. on Computational Imaging, 2017.
R. Lguensat, P. Viet, M. Sun, G. Chen, F. Tenglin, B. Chapron, R. Fablet. Data-driven Interpolation of Sea Level Anomalies using Analog Data Assimilation. https://hal.archives-

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Quantifying uncertainties in large eddy simulations of pollutant dispersion using surrogate models

Authors: Mélanie Rochoux[1]; Géraldine Rea[1]; Matthias De Lozzo[1]; Olivier Vermorel[2]

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Accurately predicting the unsteady short-to-medium range plume dynamics and dispersion induced by emission source(s) remains a challenge for air quality prediction and health impact quantification. Large eddy simulation has been identified as a promising tool to tackle this challenge. At the scale of micro-meteorology, simulating the near field is a multi-physics multi-scale problem since pollutant concentrations can vary by orders of magnitude in time and space due to the complex flow dynamics induced by the presence of obstacles (e.g. buildings) in a urban district or an industrial site as well as time-transient meteorological conditions. We thus need to analyze how uncertainties affect pollutant concentration predictions. Since large eddy simulations are computationally expensive, we have access to a limited number of simulations. To overcome this issue, we investigate the use of a surrogate model to quantify concentration uncertainties and analyze concentration sensitivity with respect to inlet flow conditions. Two surrogate strategies are compared, Polynomial Chaos and Gaussian Process, in terms of approximation of statistical moments and Sobol' sensitivity indices. The methods will be illustrated in the framework of the MUST (Mock Urban Setting Test) field-scale experiment 1 corresponding to an idealized urban environment. The MUST experiment was simulated using the large eddy simulation code YALES2-AE (CERFACS/CORIA) 2. An ensemble of 30 large eddy simulations was carried out, each simulation corresponding to a different inlet wind scenario, and form the training set for the surrogate models.

References
1 Yee, E., Biltoft, C. A., 2004. Concentration fluctuation measurements in a plume dispersing through a regular array of obstacles. Boundary-Layer Meteorology 111 (3), 363–415.
2 G. Rea, M.C. Rochoux, F. Auguste, O. Vermorel, A. Lopez Gascon & D. Cariolle: Model intercomparison in micro-scale meteorology and pollutant dispersion: large eddy simulations of the MUST experiment, Atmospheric Environment, in preparation.

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TLT : a new fast compression approach. Application to physics data.

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Une nouvelle méthode de compression de données sans perte a été développée conjointement par Olivier Thomine, Guillaume Latu et Mathieu Thevenin (CEA/DEN, CEA/DRF et CEA/DRT. Cette méthode ultra-rapide possède de multiples applications, allant de l'optimisation des codes de calcul à l'amélioration de la vitesse de transmissions de données (appareils photo, détecteurs divers, télécommunications, etc.). La méthode habituellement utilisée consiste à transférer d'une part les données compressées avec perte, et d'autre part l'erreur induite par cette compression avec perte. Cette nouvelle méthode consiste à utiliser une estimation continue des données non transférées pour se soustraire de la nécessité de transmission des données compressées.

Ainsi, seule l'erreur est communiquée, réduisant ainsi le volume de données à transférer. Des tests préliminaires ont été effectués. Le premier concerne le code de simulation GYSELA, développé à

la DRF, dont le but est de simuler l'évolution des plasmas dans les tokamaks, tel que ceux présents dans Tore-Supra (Cadarache) et à l'avenir, dans ITER. Cette méthode a permit une réduction de 20 % du temps de transfert des données, incluant le temps de compression. Cette méthode a aussi été implémentée dans un code de CFD massivement parallèle (Asphodele), et a permi une réduction significative des écritures fichier et des transferts MPI.

Son domaine d'application va donc de la simulation (HPC) aux mesures expérimentales, où un des enjeu actuel est de permettre le stockage ou le transfert d'un nombre de données croissant, et qui constitue un verrou technologique identifié actuellement.

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Analysis of spatial and spatio-temporal coherence of engine flows. Statistical tools, short note on Lagrangian approaches.

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One key challenge with present engine development is the modeling, understanding and control of cycle to cycle variations (CCV). This cyclic variability is understood here as a large scale cycle to cycle variation that ultimately controls the gas motion and composition in the vicinity of the spark plug and at the time of ignition. This industrial and environmental challenge has triggered a large amount of research work. Recent developments in measurement technology now enable the study of both spatial and temporal coherence of in-cylinder flows using high speed PIV. On the modeling side, large eddy simulation (LES) or hybrid RANS/LES methodologies are becoming attractive. For such complex geometries, it is already a challenge to obtain reliable experimental or numerical results and to gather data bases relevant for statistical analysis. However, one should not forget that analyzing the large amount of data generated is also very challenging. For engine flows, but also for a very large class of internal and external aerodynamic flows, such analysis techniques should provide: (i) key flow patterns responsible for CCV including flow structure, kinetic energy and mixing ; (ii) objective guidelines to compare unsteady computations to experiments – a posteriori validation ; (iii) pertinent indications to turbulence modeling and rigorous tests of associated closures – a priori validation ; (iv) information to new modelling routes like reduced-order models or cluster-based reduced order models.

The main part of this talk will be devoted to a presentation of the use of proper orthogonal decomposition (POD) and extended POD in this context, including some practical concerns. We will particularly insist on spatio-temporal strategies: phase invariant POD will be used to propose a conditional statistical study of the breakdown of a tumbling motion. Moreover, we will define and illustrate a cluster-based analysis of cycle-to-cycle variations for the same flow. A part of the talk will consider another route, namely Lagrangian Coherent Structure eduction techniques. These methods are seen here as a natural extension of topology based analysis for unsteady flows. One difficulty is to apply them to high Reynolds turbulent flows but they are believed to be promising ways to explore the spatial and temporal coherence of in-cycle flows.

These methodologies are applied here to engine flow but can of course clearly be valuable for any periodically driven fluid flows at large Reynolds numbers. Such approaches can be used for the very large set of data generated by PIV or LES, using any kind of informations (velocity, concentration, …) in any region of space.

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Introduction à l'assimilation de données

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Le terme « assimilation de données » désigne l'ensemble des techniques mathématiques qui visent à combiner de façon optimale (dans un sens à préciser) des informations de natures diverses sur un système dynamique, afin de reconstituer aussi précisément que possible son état ou d'en estimer une quantité particulièrement intéressante.
On dispose ainsi d'informations diverses, souvent partielles et très hétérogènes en nature et en qualité : équations mathématiques (modèle) traduisant le comportement plus ou moins idéalisé du système, mesures quantitatives de précisions variées, observations qualitatives, images, données statistiques… La notion d'optimalité dans la combinaison de ces informations reste alors à définir, et c'est notamment le sens qu'on lui donnera qui mènera à différentes approches (bayesiennes, variationnelles…).
Cet exposé dressera une présentation générale de ces méthodes d'assimilation, en tentant notamment d'expliquer leurs fondements et leurs liens.

1

Quantifying and reducing shape and topological uncertainties in front-tracking problems

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In this talk, we will present a front shape similarity measure adapted to the framework of data assimilation, where uncertainties in the quantities of interest are not only of amplitude-type but also associated with shape and topological uncertainties. The front shape similarity measure derives from image processing and is based on the Chan-Vese contour fitting functional. It can be successfully applied to quantify uncertainties in the quantities of interest, to analyze input-output sensitivities through the use of a Polynomial Chaos surrogate, and to reduce uncertainties through the use of data assimilation, in particular via a joint state-parameter estimation algorithm.
The front shape similarity measure will be illustrated through the example of wildfire [REF], where a front paradigm is used to represent the evolution of the burning area delimitation that moves, undergoes shape and topological changes under heterogeneous orography, biomass fuel and micrometeorology. In this context, the measure is promising to directly assimilate mid-infrared images and design data-driven wildfire modeling strategies.

[REF] M.C. Rochoux, A. Collin, C. Zhang, A. Trouvé, D. Lucor & P. Moireau: Front shape similarity measure for front position sensitivity analysis and data assimilation, ESAIM: Proceedings and Surveys, under review.

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Forward and backward uncertainty quantification for atmospheric reentry flows

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Simulation of aerospace applications, such as atmospheric entries of spacecraft, are challenging problems involving many complex physical phenomena, including rarefied gas effects, aerothermochemistry, radiation, and the response of thermal protection materials to extreme conditions. Reliable predictions require sophisticated physico-chemical models as well as a systematic and comprehensive treatment of model calibration and validation, including the quantification of a very large set of uncertainties inherent in such models. In fact, several sources of uncertainties have to be considered: chemistry model parameters and freestream conditions have to be considered as uncertain input parameters in the forward problems. Moreover, in reacting flows, several constitutive relations are required to describe the chemical mechanism characterizing the gas mixture, each of which contains a large number of parameters. Another challenge is to handle experimental data, since some could be difficult to obtain, especially in-flight measurements of entering space vehicles. For example, during the reentry trajectory of a space vehicle, it is extremely challenging to obtain direct measurements of freestream quantities (velocity and thermodynamic state of the atmosphere), due to the presence of a strong bow shock in front of the vehicle nose. However, these quantities are of relevant importance in both post-flight analysis, to get accurate values of the actual flight trajectory and atmospheric conditions, and during the flight to be able to make adequate real-time corrections in case of manned flights.

The focus of the study presented here is to assess the interest in using heat flux measurements, which are available in recent space missions, for rebuilding freestream conditions, requiring the set-up of multiple numerical tools for tackling several issues which are analyzed and cured here. In this talk, we will first introduce and apply two techniques for tackling this problem featuring a large number of uncertainties and expensive high-fidelity numerical simulation. The first technique relies on a sparse Polynomial Dimensional Decomposition approach. Due to the intimate connection between the PDD and the Analysis of Variance (ANOVA) approaches, PDD is able to provide a simpler and more direct evaluation of the Sobol' sensitivity indices, when compared to the Polynomial Chaos expansion (PC). The second technique is based on the construction of an Active Subspaces, in order to find a low-dimensional dependence structures in the input-to-output map of the forward numerical solver. Here, we will present a different angle on the active subspace-based approach. Instead of using the gradient of the log-likelihood to define the active subspace, we find an independent subspace for each of the parameter-to-observable maps, that we combine for a data-informed subspace. Finally, a Bayesian calibration of the free stream parameters of a hypersonic flow will be performed using both experimental and synthetic data, by exploiting active subspaces for the reduction of the dimensionality of the input space. Bayesian inversion will be then used to assess the feasibility in using measurements of pressure and heat flux at the stagnation point for rebuilding freestream velocity and density.