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Non-linear reduced order models for steady aerodynamics

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Abstract

A reduced order modelling approach for predicting steady aerodynamic flows and loads data based on Computational Fluid Dynamics (CFD) and global Proper Orthogonal Decomposition (POD), that is, POD for multiple different variables of interest simultaneously, is presented. A suitable data transformation for obtaining problem-adapted global basis modes is introduced.
Model order reduction is achieved by parameter space sampling, reduced solution space representation via global POD and restriction of a CFD flow solver to the reduced POD subspace. Solving the governing equations of fluid dynamics is replaced by solving a non-linear least-squares optimization problem. Methods for obtaining feasible starting solutions for the optimization procedure are discussed.
The method is demonstrated by computing reduced-order solutions to the compressible Euler equations for the NACA 0012 airfoil based on two different snapshot sets; one in the subsonic and one in the transonic flow regime, where shocks occur. Results are compared with those obtained by POD-based interpolation using Kriging and the Thin Plate Spline method (TPS).

Keywords: Least-Squares Flux Residual Minimization, Global POD, Computational Fluid Dynamics

1. Introduction

Given the large amount of aerodynamic data and load cases that need to be evaluated to achieve aircraft certification, efficient tools for making rapid but accurate predictions of the aerodynamic loads acting on an aircraft throughout its flight envelope and beyond are sought after. The loads can be used in determining preliminary structural sizing and to support wing trade studies, for example. For background information, consult e .g. [1].
Following the approach of LeGresley and Alonso [2], a reduced order model (ROM) for predicting steady aerodynamic flows and loads data has been developed based on Computational Fluid Dynamics (CFD) and global Proper Orthogonal Decomposition (POD), that is, POD for multiple different variables of interest simultaneously. The reader is referred to [3] for a comprehensive introduction to POD.
The method can be summarized as follows: After sampling a design space of interest by computing so-called snapshot solutions at a finite number of parameter combinations (e.g. of Mach number Ma and angle of attack α) with a CFD flow solver, POD is performed to obtain a (possibly reduced) orthogonal representation of the space spanned

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by these snapshots. Subsequently, to predict the flow solution at an unsampled point in the parameter space, the objective is to find the flux-residual minimizing flow solution contained in the POD subspace. For doing so, the DLR CFD flow solver TAU [4, 5] is restricted to the POD subspace and a non-linear least-squares optimization problem is solved. The method will be referred to as POD-subspace restricted least-squares method. While other promising, more sophisticated approaches for non-linear model reduction have been suggested [6, 7], this method has the additional advantage, that it is relatively easy to implement using an existing industrial CFD code, a fact not to be underestimated.

For a CFD-based residual evaluation, it is necessary that each flow solution snapshot contains data for all flow variables associated to the (spatially discretized) governing equations of fluid dynamics at once. Consequently, global POD basis modes have to account simultaneously for a large variety of different information. For example, for the inviscid, compressible Euler equations, the primitive flow variables are density, the velocity components in each coordinate direction and energy and their values may differ by some orders of magnitude.

Moreover, since POD is a mathematical orthogonalization method, there is no reason for the basis modes not to feature e.g. negative density values. In other words, physics might be disrespected in the basis modes, which in turn can result in the inapplicability of the high-fidelity CFD solver to evaluate flux residuals inside the POD subspace.

A data transformation tackling both of the above challenges is applied in order to obtain a global POD representation with balanced influence from all variables. Different approaches of how to compute feasible starting solutions for the optimization procedure are discussed. These issues were not treated in [2].

The method is demonstrated by computing reduced-order solutions to the Euler equations for the NACA 0012 airfoil based on two different snapshot sets; one in the subsonic and one in the transonic regime, where shocks, or, mathematically speaking, discontinuities occur. To the best of the authors' knowledge, this is the first application of the POD-subspace restricted least-squares method to transonic flows. Results are compared with those obtained by POD-based interpolation [8] using Kriging [9, 10] and the Thin Plate Spline method (TPS).

2. Theoretical Background

Considering the compressible Euler or Navier-Stokes equations [11], spatially discretized on a computational grid of size $n \in \mathbb{N}$ around a given aerodynamic body, let $v \in \mathbb{N}$ be the corresponding number of flow variables. For example, for the Euler equations, the primitive flow variables are density, the velocity components in all spatial directions and energy; thus, $v = 4$ for 2D Euler problems and $v = 5$ for 3D Euler problems. Let $n_t = vn$ denote the total dimension of the discretized flow solution vector. The differential equation for steady flows to be solved in pseudo-time reads

$$\partial_t W + R(W) = 0, \tag{1}$$

where W is the vector of primitive variables and $R : \mathbb{R}^{n_t} \to \mathbb{R}^{n_t}$ is the (highly non-linear) flux residual [11]. Hence, the steady state is attained if the time derivative vanishes, i.e. if

$$0 = R(W) \in \mathbb{R}^{n_t}. \tag{2}$$

Note that the flux residual features n_t free unknowns and equation (2) is thus also of this precise order.

2.1. Proper Orthogonal Decomposition

We will briefly review POD in finite dimensional euclidean vector spaces. Theoretical details can be found in [12] and references therein. Let each superscript $i = 1, ..., m$ denote a certain combination of independent (flow) parameters, e.g. $i \hat{=} (Ma_i, \alpha_i)$ and let $W^1, ..., W^m \in \mathbb{R}^{n_t}$ be the corresponding steady CFD solutions to the flow problem at hand, in the following called snapshots. Then the snapshot matrix is defined by

$$Y = (W^1, ..., W^m) \in \mathbb{R}^{n_t \times m}.$$

Choosing suitable flow parameter combinations for snapshot computation is a very important issue of its own, yet beyond the scope of this work.
The objective of POD is to represent the space spanned by the snapshots by mutually orthogonal basis modes ordered by information content. Precise mathematical formulation leads to an optimization problem, which in turn can be reduced to solving the $n_t \times n_t$-dimensional eigenvalue problem

$$YY^T U^j = \lambda_j U^j \in \mathbb{R}^{n_t}, \quad j = 1, ..., m. \tag{3}$$

In order to reduce the computational effort, the eigenvectors U^j, $j = 1, ..., m$, also called POD basis modes, can be obtained by solving the usually much smaller $m \times m$-dimensional eigenvalue problem

$$(Y^T Y)V^j = \lambda_j V^j \in \mathbb{R}^m, j = 1, ..., m. \tag{4}$$

This is the so-called method of snapshots [14]. The basis modes can then be computed via

$$U^j = (\sqrt{\lambda_j})^{-1} Y V^j \in \mathbb{R}^{n_t}, \quad j = 1, ..., m. \tag{5}$$

The relative information content of the jth mode is defined as the ratio $r_j = \lambda_j \left(\sum_{i=1}^m \lambda_i\right)^{-1}$ and the relative information content (RIC) of the first $\tilde{m} \leq m$ basis modes is given by

$$RIC(\tilde{m}) = \sum_{i=1}^{\tilde{m}} r_i.$$

The space spanned by the first $\tilde{m} \leq m$ POD basis modes is the best order-$\tilde{m}$-representation of the initial snapshot space with respect to the underlying scalar product. A common choice is to take $\tilde{m}$ such that $RIC(\tilde{m}) \geq 0.999$, that is, such that the first $\tilde{m}$ modes contain 99.9% of the information provided by the snapshots.
Remark: For the results presented here, not the snapshot matrix Y itself, but the transformed matrix $T(Y)$ was decomposed, see next section.
The POD basis may also be obtained via Singular Value Decomposition (SVD), yet the authors' implementation of the method of snapshots using the eigenvalue routines as presented in [15] turned out to be faster by a factor of 4 than the LAPACK[16] SVD, while still maintaining sufficient accuracy.

2.2. Data Transformation

The demands on global POD basis modes in the present context are manifold. They have to account for variables in different units and ranges of values, they have to capture the main solution features for each flow variable simultaneously, and ideally, any linear combination of modes should give a physically feasible solution. In order to come close to these requirements, the snapshot data is transformed as outlined in the following.
Let $f_1, ..., f_v$ denote the given flow variables, e.g. $f_1 = \rho =$ density. The snapshot matrix Y is devided into sub-blocks $Y^T = \left((Y^{f_1})^T, ..., (Y^{f_v})^T\right)$, where $Y^{f_k} \in \mathbb{R}^{n \times m}$ contains the snapshot data associated to the flow variable f_k, $k = 1, ..., v$. Note that $Y^T Y = \sum_{k=1}^v (Y^{f_k})^T Y^{f_k}$. If one flow variable f_{k_0} dominates the remaining ones by some orders of magnitude, as it is the case for pressure in fluid flow problems, then $Y^T Y \approx (Y^{f_{k_0}})^T Y^{f_{k_0}}$. Hence, the POD eigenmodes will essentially be f_{k_0}-modes with minor influnce from the remaining variables.
In order to arrive at a balanced decomposition, for each flow variable, the mean value over all available snapshot data is computed. Let s_k be the mean value of the data for variable f_k, i.e. $s_k = \frac{1}{nm} \sum_{i=1}^n \sum_{j=1}^m Y_{ij}^{f_k}$ and define the scaling matrix

$$S = diag\left(s_1^{-1} I, ..., s_v^{-1} I\right) \in \mathbb{R}^{n_t \times n_t},$$

where each $I \in \mathbb{R}^{n \times n}$ denotes a unit matrix diagonal block.
To support physical feasibility of linear combinations of POD modes, the data is centred by subtracting the row-wise snapshot mean values. This results in an affine POD subspace representation, as suggested in [17]. Defining $A = (avg_1, ..., avg_{n_t})^T \in \mathbb{R}^{n_t}$ via $avg_i = \frac{1}{m} \sum_{j=1}^m Y_{ij}$, the complete (non-orthogonal) data transformation reads

$$T : \mathbb{R}^{n_t \times m} \to \mathbb{R}^{n_t \times m}, Y \mapsto S(Y - A \underbrace{(1, ..., 1)}_{m}). \tag{6}$$

Orthogonal decomposition as described in section 2.1 is performed for the transformed snapshot matrix $\hat{Y} = T(Y)$. For a given vector a of POD coefficients, the corresponding flow solution is constructed as follows:

$$W(a) = S^{-1}\left(\sum_{k=1}^{\tilde{m}} a_k U^k\right) + A = \sum_{k=1}^{\tilde{m}} a_k S^{-1} U^k + A. \tag{7}$$

Hence, for computing an approximate flow solution in the reduced space at a certain parameter combination, it is sufficient to compute the associated coefficient vector a. The constant mean flow vector A shifts the mathematical construction back to the range of physical values.

Remark: Generally, sub-blocks of global POD modes will not form orthogonal sub-bases.
If a dominated POD is desirable, this can be achieved by adjusting the scaling factors s_k.

2.3. POD-based interpolation

Writing the transformed snapshot matrix as $\hat{Y} = \left(\hat{W}^1, ..., \hat{W}^m\right) \in \mathbb{R}^{n_t \times m}$, it holds

$$\hat{W}^j = \sum_{k=1}^{m} a_k^j U^k, \quad a_k^j = \langle \hat{W}^j, U^k \rangle = (\hat{W}^j)^T (\sqrt{\lambda_k})^{-1} Y V^k = \sqrt{\lambda_k} V_j^k,$$

where V_j^k is the jth component of $V^k = (V_1^k, ..., V_m^k)^T$, see (4). Therefore, the projection of the snapshot vectors on the affine POD-subspace is given by

$$\Pi(W^j) = \sum_{k=1}^{\tilde{m}} a_k^j S^{-1} U^k + A = \sum_{k=1}^{\tilde{m}} \sqrt{\lambda_k} V_j^k S^{-1} U^k + A,$$

Note that if $\tilde{m} = m$, then $\Pi(W^j) = W^j$. Let $p^j = (p_1^j, ..., p_d^j)$ denote the flow parameter combinations corresponding to the snapshot solutions $W^j = W(p^j)$, e.g. $d = 2$ and $W^j = W(Ma^j, \alpha^j)$.
An approximate flow solution $W^* = W(p^*) = \sum_{k=1}^{\tilde{m}} a_k^* S^{-1} U^k + A$ at conditions p^* can be obtained via interpolating each scalar coefficient $a_k^* = a_k(p^*)$ based on the sample points $a_k^1 = a_k(p^1), ..., a_k^m = a_k(p^m)$ for $k = 1, ..., \tilde{m}$. This is by far more efficient than direct component-wise interpolation of the snapshot vectors, where n_t interpolation procedures, each considering m sample points are due. Details can be found in [8].
For the results presented in this paper, Kriging [10, 13], and the Thin Plate Spline Method (TPS) [13], were applied for multi-dimensional interpolation.

2.4. Reduced Order Modelling

While in the previous section a purely mathematics-based approach of obtaining POD coefficients was outlined, we now present a method which takes flow physics into account. To this end the coefficients of the reduced solution are determined by minimizing the associated flux residual as suggested in [2], which is evaluated using the DLR CFD solver TAU [4, 5]. Precise mathematical formulation of the unconstrained optimization problem gives

$$\min_{a=(a_1,...,a_{\tilde{m}})} \|R(W(a))\|^2 = \sum_{i=1}^{n_t} R_i(W(a))^2, \tag{8}$$

which is a non-linear least squares problem. Of all flow solution vectors, which allow for a representation of the form of (7), i.e. all flow solution vectors contained in the POD subspace, the solution to (8) is closest to a converged CFD solution for the given parameter combination.
In this way, solving the order-n_t equation system (2) is replaced by solving the order-$\tilde{m}$ optimization problem (8). In order to achieve appropriate optimization performance, the gradient-based Levenberg-Marquardt method [18] is applied. Hence the Jacobian of the flux residual with respect to the POD coefficients is required. For the results presented here, the Jacobian is obtained using finite difference approximation and rank-one Broyden updates [18]. The associated step sizes are weighted by the eigenvalues corresponding to the POD coefficients.
We suggest three ways of initialing the optimization procedure:

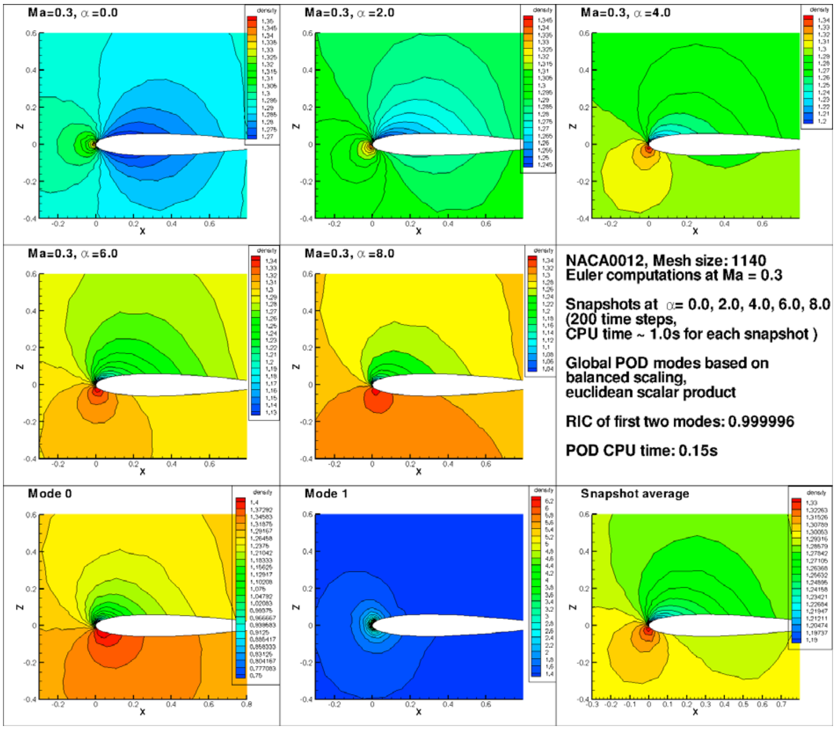

Figure 1: Snapshot set and POD modes used for building the ROM at Mach 0.3. Density fields.

- Start from the highest energy POD basis mode: $a^{init} = (1.0, 0.0, ..., 0.0)$, $W^{init} = S^{-1}U^1 + A$
- Start from the snapshot average $a^{init} = (0.0, 0.0, ..., 0.0)$, $W^0 = A$
- Start from an interpolated solution according to section 2.3.

The choice of appropriate approaches is problem dependent. The first approach is recommended when it is expected that the first mode already captures the main features of the solution and the flow has to be estimated at a parameter combination far in the extrapolatory regime, where interpolation methods are bound to fail. The second approach is fail safe, since physical feasibility is guaranteed by construction. In fact, the main reason for the centering by the average is to shift the data into the range of physically feasible values. Yet, the average flow vector might be far from the optimum. The third approach is recommended for predictions in the interpolatory regime, where POD based interpolation[8] is known to give good results and thus is expected to provide a good starting guess.
Note that the solution to (8) is constructed relying entirely on the information contained in the initial snapshot set. Therefore, order reduction as well as reduction error is introduced by both POD mode reduction and snapshot-based sampling of the parameter space. The method described above is referred to as *POD-subspace restricted least squares method*.

3. Results

The method introduced above will be demonstrated by computing reduced-order solutions to the compressible Euler equations for the NACA0012 airfoil based on two different snapshot sets; one in the subsonic and one in

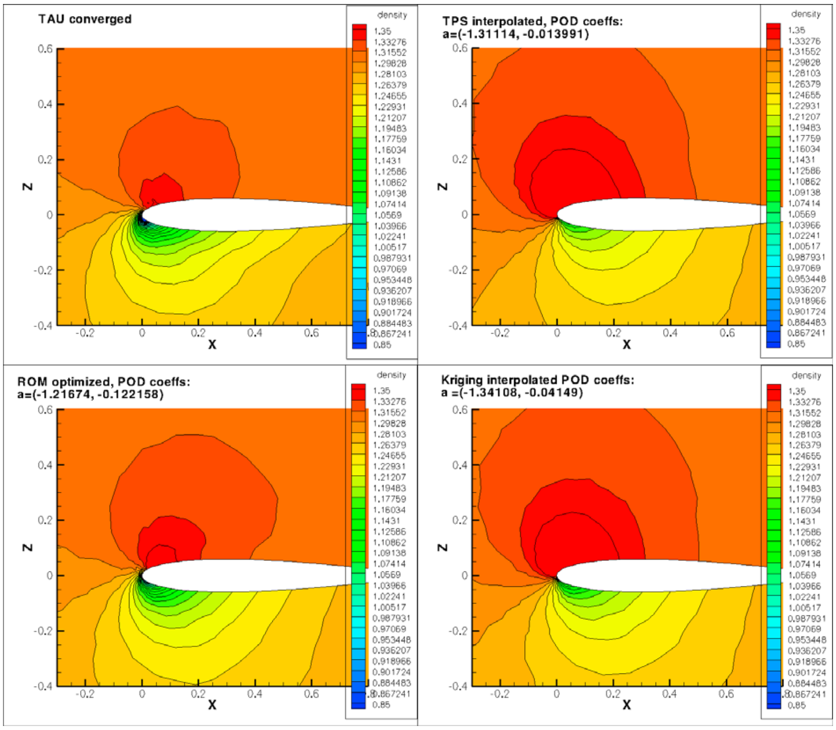

Figure 2: Comparison of the flow approximations via TPS extrapolation, Kriging extrapolation and POD-based ROM with converged reference TAU CFD solution. Subsonic case, Mach 0.3, angle of attack $\alpha = -14.0°$.

the transonic regime. More precisely, the first data set consists of five flow solutions at $Ma = 0.3$ and $\alpha = 0.0°$, $2.0°$, $4.0°$, $6.0°$, $8.0°$, whereas the second one consists of flow solutions at the same set of angles of attack but at a transonic Mach number of $Ma = 0.73$. The unstrutured computational grid features 1,140 points and is shown in Fig. 3. Results will be compared with those obtained by POD-based interpolation using Kriging and the Thin-Plate Spline (TPS) method.

We emphasize that in both test cases, the data transformation according to (6) proved to be essential in order to obtain physical solutions throughout the optimization procedure. Hence, a comparison of results with and without applying (6) is simply not possible, since in the latter case, no results were obtained.

In the optimization routine, the flux residual, see eqs. (1), (2), is scaled by a factor of $\frac{10^6}{n} = \frac{10^6}{1{,}140}$ in order to avoid numerical problems due to too small numbers. Since the residuals feature about the same order of magnitude for all flow variables, it is sufficient to apply a global factor. The scaled residual is denoted by R^{ROM}.

In this section, the POD modes are numbered starting from 0.

3.1. NACA0012 Euler Computations at Mach 0.3

Fig. 1 shows the density fields of the snapshots used to build the reduced order model (ROM). POD results in an orthogonal representation where the first two modes contain 0.999702% + 0.00029464% > 0.999996% of the total information content. Only these two modes and the mode of averaged flow data are used for the ROM and for the POD coefficient interpolation; the corresponding density fields are also displayed in Fig. 1 . Since the flow average is a constant vector that is not subject to any estimation/optimization procedure, the associated ROM is of order 2, hence, *the initial flow problem of order* $n_t = 4 \cdot 1{,}140 = 4{,}560$ *is reduced to an order-*2 *optimization*

problem.
Converged snapshots were computed with the number of iterations (in pseudo time) limited to 200. All computations were performed on a serial desktop computer. Approximate flow solutions were computed at $\alpha = -14.0°$, using TPS, Kriging and the POD-based ROM. The reference solution computed with the DLR TAU code converged after 229 iterations at these conditions. Since the NACA0012 airfoil is symmetric, it is expected that the chosen snapshot set contains sufficient information to predict the flow at this condition. In regard of the interpolation methods, however, this point is far in the extrapolation regime. The highest-energy mode was used as a starting point for the ROM optimization procedure. The initial residual was $R^{ROM}\left(W^{init}\right) = 25.921$.
The ROM solution was obtained after 13 TAU CFD residual evaluations; during the optimization the residual was decreased by three orders of magnitude, the final residual being: $R^{ROM}(W^{opt}) = 0.1260$.
Corresponding density fields and POD coefficients are given in Fig. 2. The ROM solution is observed to be in better agreement with the converged TAU solution than the interpolation-based results. The corresponding surface pressure distributions are displayed in Fig. 5, left side. Note that the ROM solution is in best agreement with the converged reference TAU solution while the interpolation-based solutions underpredict the suction peak on the upper side of the airfoil and overpredict the overpressure on the lower side. The following table summarizes the computational expenses.

Procedure	Effort (computation time)[s]	CFD residual evaluations
Snapshot computation	1.10	200
POD (reading of data incl.)	0.15	-
ROM	0.3	13
Kriging extrapolation	< 0.001	-
TPS extrapolation	< 0.001	-

3.2. *NACA0012 Euler Computations at Mach 0.73*

Fig. 3 shows the density fields of the snapshots used to build the ROM in the transonic flow regime. POD results in an orthogonal representation where the first four modes capture the complete information contained in the snapshot set. The precise information content of the sorted modes is $r_0 = 0.989633, r_1 = 0.008376, r_2 = 0.0014540, r_3 = 0.000537$. All four modes and the mode of the averaged flow data are used for the ROM as well as for the POD coefficient interpolation; the corresponding density fields are shown in the same figure. Since the flow average is a constant vector that is not subject to any estimation/optimization procedure, the associated ROM is of order 4, hence, *the initial flow problem of order* $n_t = 4,560$ *is reduced to an order-*4 *optimization problem.*
As before, converged snapshots were computed with the number of iterations limited to 200. All computations were performed on a serial desktop computer. Approximate flow solutions were computed at $\alpha = 11.0°$, using TPS, Kriging and the POD-based ROM. The TAU reference solution at these conditions converged after 201 time steps. The TPS-interpolated solution was used as a starting point for the ROM optimization. The initial residual was: $R^{ROM}(W^{TPS}) = 34.104$.
The ROM solution is obtained after 13 TAU residual evaluations, the final residual being: $R^{ROM}(W^{opt}) = 2.956$.
Density fields are given in Fig. 4, the associated surface pressure distributions are displayed in Fig. 5, right side. While all approximate solutions predict the correct shock location, the ROM solution is in best agreement with the converged reference TAU solution in terms of the pressure levels upstream of the shock. By coincidence, the computational expenses are the same as listed in the table in section 3.1.

4. Conclusions

A reduced order model (ROM) for solving the governing fluid flow equations, called POD-subspace restricted least squares model, has been developed based on the DLR CFD solver TAU. Preliminary tests of the method were carried out for building ROMs of the Euler equations based on two different sets of flow solutions for the NACA0012 airfoil computed with the DLR TAU code, one in the subsonic and one in the transonic flow regime.

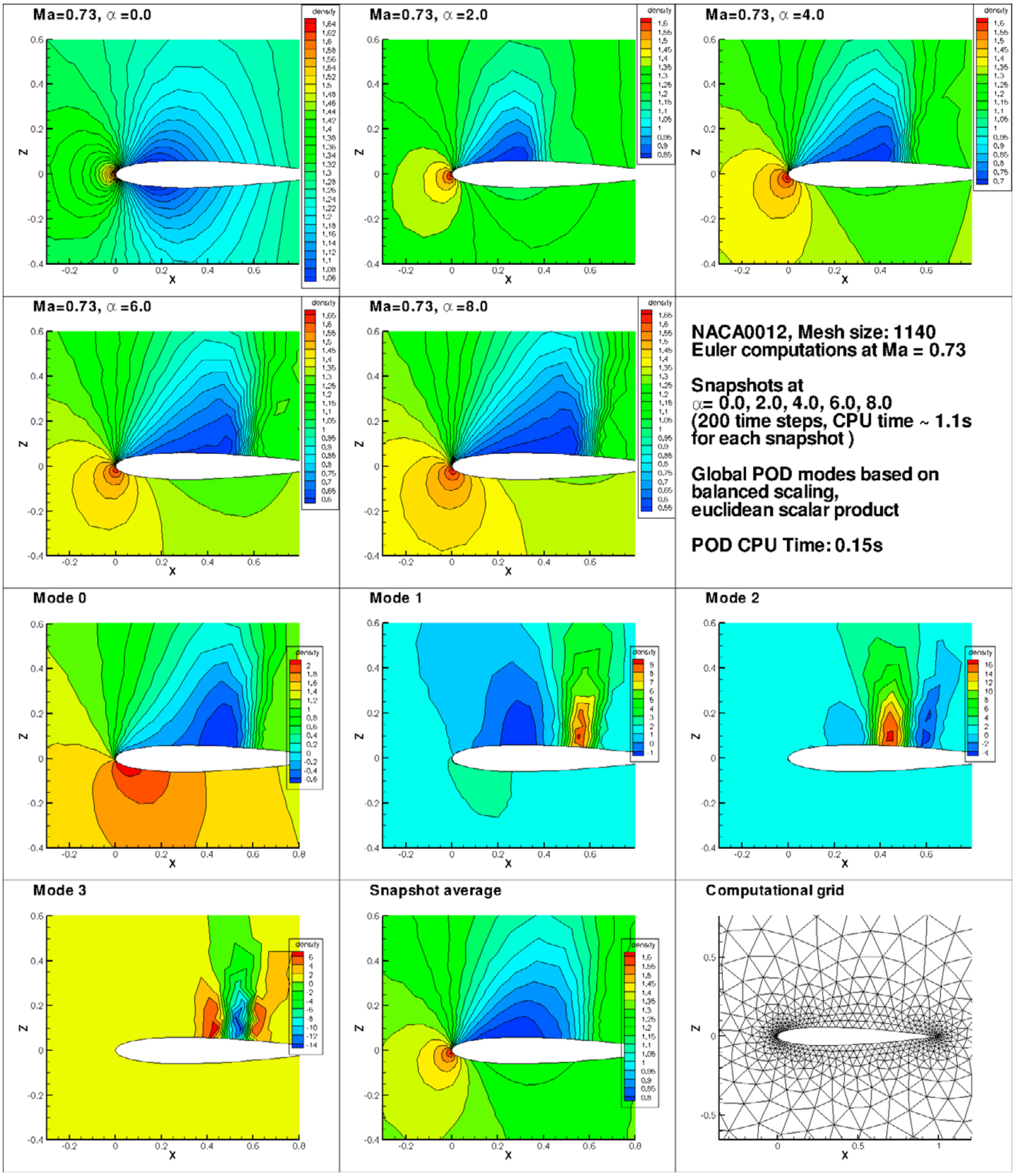

Figure 3: Snapshot set and POD modes used for building the ROM at Mach 0.73. Density fields. Lower right: Computational mesh.

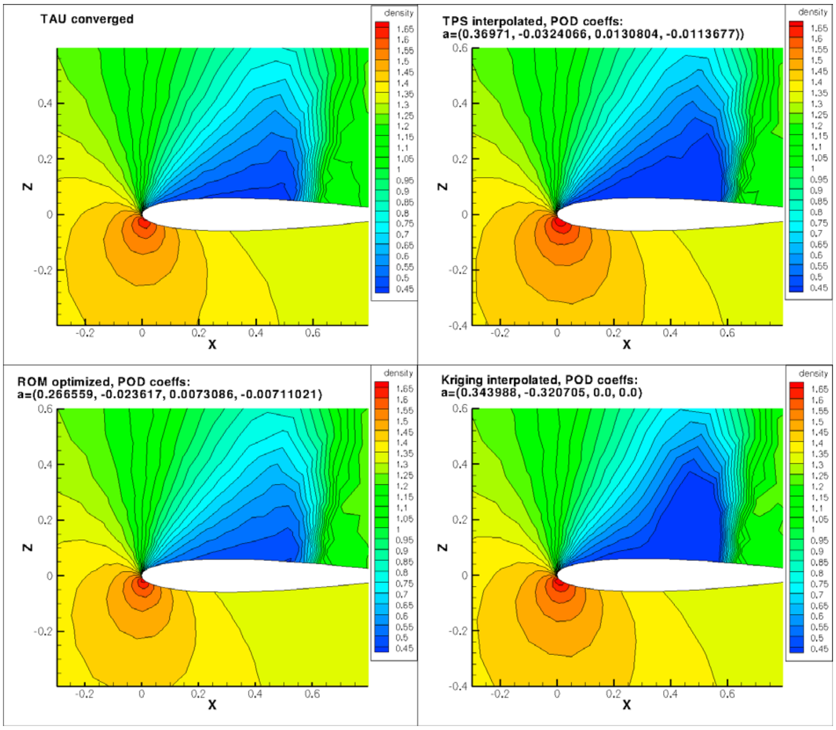

Figure 4: Comparison of the flow approximations via TPS extrapolation, Kriging extrapolation and POD-based ROM with converged reference TAU CFD solution. Transonic case: Mach 0.73, angle of attack $\alpha = 11.0°$.

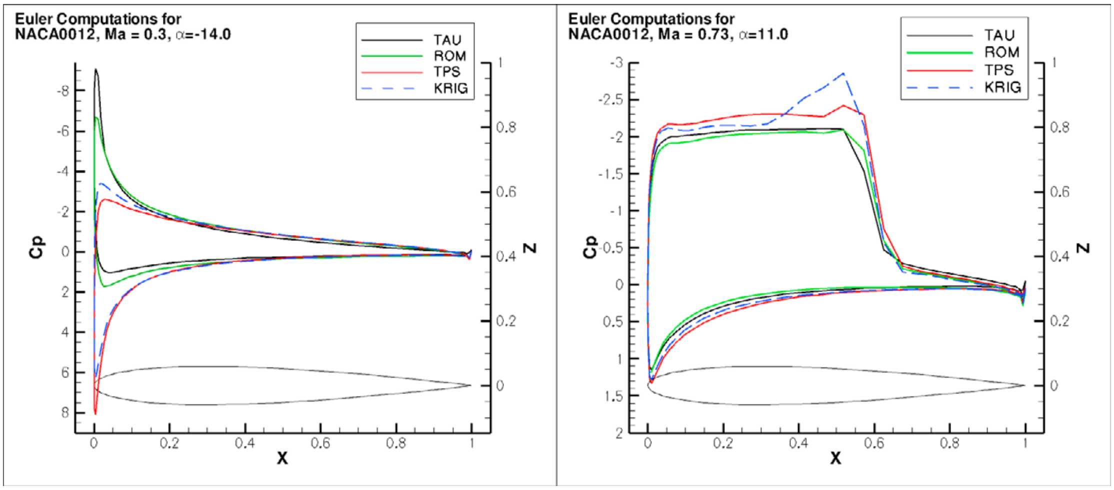

Figure 5: Comparison of the surface pressure distributions approximated via TPS extrapolation, Kriging extrapolation and POD-based ROM with converged reference TAU CFD solution. Left side: subsonic, Mach 0.3, angle of attack $\alpha = -14.0°$. Right side: transonic, Mach 0.73, angle of attack $\alpha = 11.0°$.

From a mathematical point of view, the problem order has been reduced by the factor $2,280$ in the first and by the factor $1,140$ in the second case.
Approximate flow solutions were computed at extrapolatory conditions, where the flow is difficult to predict using snapshot-based methods. Results of a POD-based interpolation approach using Kriging or TPS estimators and of the ROM were compared. While the ROM comes at a higher computational cost than the interpolation-based methods, the corresponding approximate flow solutions were significant closer to the CFD solution, considered as the exact reference, than those obtained via the interpolation methods. The shock present in the transonic case was best captured by the ROM.
Since the computational grid associated with the NACA0012 airfoil is of relatively small size, all computations were performed very fast and the total computational expenses are assumed to be dominated by computational overhead. Hence, CPU time effort is not the appropriate measure for judging these preliminary results, but the absolute number of residual evaluations. In this regard, acceleration by a factor of 17 in the subsonic case, resp. of 15 in the transonic case was obtained by using the ROM compared to the full-order TAU solution. Note that the difference in the acceleration factors is caused by the different number of residual evaluations required to obtain the reference CFD solution (229 resp. 201), whereas the ROM converged in both the subsonic and transonic case after the same number of 13 iterations.
The data transformation described in section 2.2 rendered an application of the POD-subspace restricted least-squares method to the above test cases possible in the first place.
Future work will address applying the method to large industrial 3D test cases and the Navier-Stokes equations, as well as a comparison of the global POD method to variable-by-variable POD. The latter approach results in a gain of information, but comes at a higher number of optimization parameters.

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