A SEMI-CONTINUOUS FORMULATION FOR GOAL-ORIENTED REDUCED-ORDER MODELS

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Abstract. A semi-continuous formulation is introduced for finding bases which minimise the error in a specific output functional of a reduced-order model. The formulation is advantageous in that it can be easily applied to nonlinear problems and functionals. A general description of the approach is given, then explicit formulations are derived for the convection-diffusion and Burgers equations. Numerical results are given for both linear and non-linear functionals. These show substantial reductions in error, depending on the functional considered. Optimisation of bases for a reduced-order model based on an approximated governing equation is also described, for which large increases in accuracy are obtained.

1 Introduction

A common approach to constructing reduced-order models (ROMs) is to obtain modes using the Proper Orthogonal Decomposition (POD) of a reference dataset, and then discretise the governing equations using Galerkin projection with of a subset of these modes. Examples of such POD-ROMs include those in the fields of fluid dynamics and turbulence [1, 2, 3, 4], structural vibrations [5], biology [6], meteorology [7], and image processing. Truncated POD modes are optimal in the energy norm for the interpolation of the reference data, but the output of ROM using such modes is not necessarily optimal in the same norm. Furthermore, although a truncated set of POD modes represents the most energetic processes within the reference data, these might not the processes of interest. This can be the case, for example, when considering problems in acoustics, where the perturbations of interest are much smaller in energy than the main flow. Bui-Thanh et al. [8] addressed these issues by developing a Goal-Oriented model-constrained optimisation procedure for identifying truncated bases. In this approach, the truncated set of modes is optimised for the representation of a given output functional with the ROM imposed as a constraint. This was demonstrated to provide significant increases in accuracy.

The approach in [8] presented the construction of ROMs from large linear time-invariant (LTI) systems, e.g. $M\dot{u} + Ku = F$, where $u(t) \in \mathbb{R}^N$ is the system state and $\dot{u}(t)$ is the derivative of u(t) with respect to time. In this case $M \in \mathbb{R}^{N \times N}$ and $K \in \mathbb{R}^{N \times N}$ are matrixes with the spatial dimensions of the reference data, while the vector $F \in \mathbb{R}^N$ defines the input to the system. As the formulation is expressed in terms of an algebraic system, we refer to it as a Fully-Discrete Formulation (FDF) for Goal-Oriented ROMs. Depending on the origin of the reference dataset, however, the definition of M and K is not always clear. When the reference dataset comes from a numerical simulation, they might be constructed from the numerical method employed. When the dataset comes from experiments, no obvious method for constructing them exists. The precise definition of M and K also affects the efficiency of the optimisation process, but in a way which is difficult to anticipate. A further issue is the treatment of the boundary conditions. For the ROM it might be useful to use alternate formulations for boundary conditions (such as weak Dirichlet BCs) which can be difficult to implement through the derivation of M, K and F. Finally, the procedure to extend the FDF to nonlinear PDEs and functionals is not entirely clear.

In this paper, we describe an alternative to the FDF, a semi-Continuous Formulation (SCF). In this approach, the ROM and the optimisation technique are defined in a continuous setting, but the reference dataset remains discrete. This clarifies the treatment of nonlinear PDEs and functionals, and avoids the need to define arbitrary M, K matrices. After a brief introduction to the construction of POD ROM, the basic approach of the SCF is described in section 2. Then the performance of the SCF is demonstrated using three examples. The first is a simple linear model problem that considers both linear and nonlinear functionals. The second is a nonlinear model problem. The last is a problem that considers governing equations which only approximate the dynamics of the reference dataset.

2 Reduced-Order Models with Discrete Basis Functions

Consider the general PDE

$$\mathcal{L}(u) = f \tag{1}$$

$$u(0) = u_0 \tag{2}$$

subject to appropriate boundary conditions, for which a goal functional, g, is defined

$$g = g(u) \tag{3}$$

A ROM of (1) can be derived by assuming representing the state u(t) using a linear combination of m basis functions,

$$\hat{u} = \sum_{j=1}^{m} \alpha_j \phi_j \tag{4}$$

where $\hat{u}(t)$ is the approximation of u. Assuming the basis functions (ϕ_j) are defined at discrete points, a projection matrix $\Phi \in \mathbb{R}^{N \times m}$ can then be defined which contains as columns ϕ_j , i.e. $\Phi = [\phi_1, \phi_2, \cdots, \phi_m]$. A vector $\alpha(t) \in \mathbb{R}^m$ contains the corresponding modal amplitudes. The ROM and goal functional \hat{g} are then expressed as

$$\int_{\Omega} \phi_i (\mathcal{L}(\hat{u}) - f) d\Omega = 0$$
(5)

$$\int_{\Omega} \phi_i (\hat{u}_0 - u_0) d\Omega = 0 \tag{6}$$

$$\hat{g} = g(\hat{u}) \tag{7}$$

where $i = 1, 2, \dots, m$.

2.1 Proper Orthogonal Decomposition

For a collection of snapshots, $u(t_j)$, $j = 1, \dots, N_t$, where $u(t_j) \in \mathbb{R}^N$ is the solution of governing equation (1) at time t_j , a reference dataset matrix $U \in \mathbb{R}^{N \times N_t}$ can be defined as $U = [u(t_1), u(t_2), \dots, u(t_{N_t})] = [u_1, u_2, \dots, u_{N_t}]$. The POD modes can be derived by a Singular Value Decomposition of U or Eigenvalue Decomposition of U^2 .

The POD basis functions can also be found by seeking an orthonormal set, Φ , where $\phi_i^T \phi_j = 1$ (i = j) and $\phi_i^T \phi_j = 0$ $(i \neq j)$, that solves the problem

$$\Phi = arg_{\Phi}minE(\Phi) \tag{8}$$

The error measure $E(\Phi)$ between the reference data and their representation in the reduced space is defined in L^2 -norm sense

$$E(\Phi) = \sum_{n=1}^{N_t} \| u_n - \tilde{u}_n \|^2$$
(9)

where $\tilde{u}_n = \sum_{i=1}^m (u_n^T \phi_i) \phi_i$ and $|| u_n ||^2 = u_n^T u_n$.

The POD is an optimal basis in the sense that it minimises the error given by (9). Note that this optimality applies only to the representation of a known u_n in the reduced space, \tilde{u} , not the solution of the ROM, \hat{u} , i.e. $\tilde{u} \neq \hat{u}$. It means that the error expression yields no information regarding the accuracy of the ROM's solution and whether \hat{u} is a good approximation of u. The POD modes thus are not necessarily optimal for other goal functionals, for example a local gradient of the ROM's solution.

2.2 The Semi-Continuous Formulation

The SCF leads to an optimisation problem that finds an orthonormal basis Φ which minimises the difference between the goal functional g over $[0, t_f]$ in the full space and reduced space, subject to satisfying a ROM constructed using the underlying governing equations. The problem of determining Φ can be written as

$$\arg_{\Phi,\alpha} \min \mathcal{G} = \frac{1}{2} \int_0^{t_f} \int_\Omega (g - \hat{g})^2 d\Omega dt + \frac{\beta}{2} \int_\Omega \sum_{i,j=1}^m \left(\delta_{ij} - \phi_i \phi_j\right)^2 d\Omega \tag{10}$$

subject to
$$\int_{\Omega} \phi_k(\mathcal{L}(\hat{u}) - f) d\Omega = 0, \ k = 1, 2, \cdots, m \quad (\text{ROM})$$
(11)

$$\int_{\Omega} \phi_k(\hat{u}_0 - u_0) d\Omega = 0, \ k = 1, 2, \cdots, m \quad \text{(Initial Condition)} \tag{12}$$

$$\hat{g} = g(\hat{u}) \tag{13}$$

where \mathcal{G} is the objective functional. This approach focuses on the reduction of the error for a particular g rather than the state u. Note that the formulation (10)-(13) is continuous with the exception of the ϕ_k and g, which are discrete. The second term in (10) is a regularisation term that penalises the derivation of Φ from an orthonormal set, with β as a regularisation parameter.

The result is a constrained minimisation problem, for which we can use Lagrange multipliers, i.e. $\lambda(t) \in \mathbb{R}^m$ and $\mu \in \mathbb{R}^m$, also known as adjoint state variables, to construct Lagrangian functional \mathscr{L} . To simplify the expression of \mathscr{L} , one can define

$$E = (g - \hat{g})^2 \qquad G_1 = \sum_{i,j=1}^m (\delta_{ij} - \phi_i \phi_j)^2 G_2^k = \phi_k(\mathcal{L}(\hat{u}) - f) \qquad G_3^k = \phi_k(\hat{u}_o - u_o)$$

The Lagrangian functional can then be written as

$$\mathscr{L} = \int_{\Omega} \left(\frac{1}{2} \int_0^{t_f} E dt + \frac{\beta}{2} G_1 + \sum_{k=1}^m \int_0^{t_f} \lambda_k G_2^k dt + \sum_{k=1}^M \mu_k G_3^K \right) d\Omega \tag{14}$$

The optimality conditions can be derived by taking variations of the Lagrangian functional with respect to λ_k , μ_k , α_q and ϕ_q . Setting the first variation of the Lagrangian functional with respect to λ_k and μ_k to zero, arguing that the variation of λ_k is arbitrary in $[0, t_f]$, simply recovers the ROM (11) and initial condition (12). Setting the first variation of the Lagrangian functional with respect to α_q to zero, and arguing that the variation of α_q is arbitrary in $[0, t_f]$, yields the adjoint equation, final condition for λ and definition of μ

$$\int_{\Omega} \left[\frac{1}{2} \frac{\partial E}{\partial \alpha_q} + \sum_{k=1}^m \lambda_k \frac{\partial G_2^k}{\partial \alpha_q} - \frac{d}{dt} \left(\sum_{k=1}^m \lambda_k \frac{\partial G_2^k}{\partial \dot{\alpha}_q} \right) \right] d\Omega = 0$$
(15)

$$\lambda_q(t_f) = 0 \tag{16}$$

$$\mu_q = \lambda_q(0) \tag{17}$$

Taking the first derivative of the Lagrangian functional with respect to ϕ_q , arguing that the variation of ϕ_q is arbitrary in the interval Ω and that it is zero at the boundary of Ω $(\partial \Omega)$, yields the gradient expression

$$\delta \mathscr{L}_{\phi_q} = \int_0^{t_f} \left[\frac{1}{2} \frac{\partial E}{\partial \phi_q} + \sum_{k=1}^m \lambda_k \frac{\partial G_2^k}{\partial \phi_q} - \frac{d}{dx} \left(\sum_{k=1}^m \lambda_k \frac{\partial G_2^k}{\partial \phi_{qx}} \right) \right] dt + \frac{\beta}{2} \sum_{k=1}^m \frac{\partial G_1^k}{\partial \phi_q} + \sum_{i=1}^m \mu_k \frac{\partial G_3^k}{\partial \phi_q} = 0$$

$$(18)$$

We solve this unconstrained minimisation problem using a trust-region inexact-Newton conjugate-gradient method [8, 9]. The gradient required by Newton's method can be computed efficiently by an adjoint method, by first solving the ROM (11) with initial condition (12) to get $\alpha(t)$, then solving the adjoint equations (15)-(17) to get $\lambda(t)$ and μ , finally computing the gradient (18) by known Φ , α , λ and μ . In the conjugate-gradient algorithm the Hessian matrix (H) is needed. H always appears in the form Hd, however, so to avoid calculating H we treat Hd (Hessian-vector product) as a group, so that Hdis defined as

$$Hd = \frac{\delta \mathcal{L}_{\Phi}(\Phi + \epsilon d) - \delta \mathcal{L}_{\Phi}(\Phi)}{\epsilon}$$
(19)

where ϵ represents a small increment of d. The Hessian-vector product is then approximated by the directional derivative of the gradient with respect to the search direction [10].

As optimisation problem is not necessarily convex, the choice of initial guess is important. In [8] two strategies are proposed: (1) the initial guess is a set of POD modes; (2) the initial guess for the case of m basis functions is chosen to be the solution of the optimisation problem for m - 1 basis functions plus an arbitrary mth function. In the following numerical tests, we always use a set of POD modes as an initial guess.

3 Linear PDE example

We first consider the one-dimensional linear convection-diffusion equation. The initialboundary value problem is given by

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} - k\frac{\partial^2 u}{\partial x^2} = f \tag{20}$$

$$u_0 = \sin(2\pi x) \tag{21}$$

$$u(0,t) = 0 (22)$$

$$u(1,t) = 0$$
 (23)

with a = 2, k = 0.1, f = 1.

3.1 SCF for convection-diffusion

To define a ROM using the SCF, we first insert (20) in the reduced space into (14) to get the Lagrangian functional

$$\mathscr{L}(\Phi, \alpha, \lambda, \mu) = \frac{1}{2} \int_{0}^{t_{f}} \int_{0}^{1} (g - \hat{g})^{2} dx dt + \frac{\beta}{2} \sum_{i,j=1}^{m} \left(\delta_{ij} - \int_{0}^{1} \phi_{i} \phi_{j} dx \right)^{2} + \int_{0}^{t_{f}} \sum_{i=1}^{m} \lambda_{i} \int_{0}^{1} \phi_{i} (\hat{u} + a\hat{u}_{x} - k\hat{u}_{xx} - f) dx dt + \sum_{i=1}^{m} \mu_{i} \int_{0}^{1} \phi_{i} (\hat{u}_{0} - u_{0}) dx$$

$$(24)$$

As in Section 2, the ROM and initial condition are

$$\sum_{j=1}^{m} \dot{\alpha}_{j} \int_{0}^{1} \phi_{i} \phi_{j} d + a \sum_{j=1}^{m} \alpha_{j} \int_{0}^{1} \phi_{i} \phi_{jx} dx - k \sum_{j=1}^{m} \alpha_{j} \int_{0}^{1} \phi_{i} \phi_{jxx} dx$$
$$= \int_{0}^{1} \phi_{i} f dx \tag{25}$$

$$\sum_{j=1}^{m} \alpha_0 \int_0^1 \phi_i \phi_j dx = \int_0^1 \phi_i u_0 dx$$
(26)

Noting $\Phi|_0^1 = 0$ and integrating by parts, the adjoint equations are

$$-\sum_{i=1}^{m} \dot{\lambda}_{i} \int_{0}^{1} \phi_{q} \phi_{i} dx - a \sum_{i=1}^{m} \lambda_{i} \int_{0}^{1} \phi_{q} \phi_{ix} dx + k \sum_{i=1}^{m} \lambda_{i} \int_{0}^{1} \phi_{qx} \phi_{ix} dx$$
$$= \int_{0}^{1} [(g - \hat{g})\hat{g}' \phi_{q}] dx \tag{27}$$

$$\lambda_i(t_f) = 0, \tag{28}$$

$$\mu_i = \lambda_i(0) \tag{29}$$

While the gradient is

$$\delta \mathscr{L}_{\phi_q} = \int_0^{t_f} \left(\hat{g} - g \right) \hat{g}' \alpha_q dt + 2\beta \sum_{j=1}^m \phi_j \left(\int_0^1 \phi_q \phi_j dx - \delta_{qj} \right) + \int_0^{t_f} \left\{ \left(\lambda_q \sum_{j=1}^m \dot{\alpha}_j \phi_j + \dot{\alpha}_q \sum_{i=1}^m \lambda_i \phi_i \right) + a \left(\lambda_q \sum_{j=1}^m \alpha_j \phi_{jx} - \alpha_q \sum_{i=1}^m \lambda_i \phi_{ix} \right) - k \left(\lambda_q \sum_{j=1}^m \alpha_j \phi_{jxx} + \alpha_q \sum_{i=1}^m \lambda_i \phi_{ixx} \right) - \lambda_q f \right\} dt + \left[\mu_q \sum_{j=1}^m \alpha_j(0) \phi_j + \alpha_q(0) \sum_{i=1}^m \mu_i \phi_i - \mu_q u_0 \right]$$
(30)

Note that before calculating the gradient we have reduced the second derivative of ϕ_j to the first derivative through integration by parts.

In the case of a linear PDE, the SCF can be written in a LTI form, allowing a direct contrast with the FDF. To do so we first define the integrals in space for SCF using the trapezoidal rule:

$$\int_0^1 f(x)g(x)dx \approx \sum_{i=1}^{N-1} \bar{f}_i \bar{g}_i h$$

where \bar{f}_i and \bar{g}_i represent the average values of f and g on each interval, i.e. $\bar{f} = \frac{f_i + f_{i+1}}{2}$, and h is the length of the subinterval of integration. The integration can be written in matrix form: $\int_0^1 f(x)g(x)dx \approx \bar{\mathbf{f}}^T \Delta \bar{\mathbf{g}}$, by defining $\mathbf{f} = [\bar{f}_1 \cdots \bar{f}_{N-1}]^T$, $\mathbf{g} = [\bar{g}_1 \cdots \bar{g}_{N-1}]^T$, and Δ as a matrix containing only h on the diagonal. This allows the ROM and the adjoint equation to be expressed as:

$$\mathcal{M}\dot{\alpha} + \mathcal{K}\alpha = \mathbf{b} \qquad (ROM) \tag{31}$$

$$-\mathcal{M}^T \dot{\lambda} + \mathcal{K}_{\lambda} \lambda = \mathbf{b}_{\lambda} \qquad \text{(Adjoint Equation)} \tag{32}$$

where $\mathcal{M} = \bar{\Phi}^T \Delta \bar{\Phi}$, $\mathcal{K} = \underline{a}(\bar{\Phi}^T \Delta \bar{\Phi}') - k(\bar{\Phi}^T \Delta \bar{\Phi}'')$, $b = \bar{\Phi}^T \Delta f$, $\mathcal{K}_{\lambda} = -a(\bar{\Phi}^T \Delta \bar{\Phi}') + k(\bar{\Phi}'^T \Delta \bar{\Phi}')$ and $b_{\lambda} = \bar{\Phi}^T \Delta (g - \hat{g})\hat{g}'$. Here the matrices \mathcal{M} , \mathcal{K} and \mathcal{K}_{λ} are directly associated with the process of integration and differentiation required, allowing their influence on the results to be anticipated. In FDF, one might construct M, K using an arbitrary discretisation method for the governing equations, but the impact of the discretisation choices on the final results is less clear. The gradient can be written in matrix form as:

$$\delta\mathscr{L}_{\Phi} = \int_{0}^{t_{f}} (\hat{g} - g) \hat{g}' \alpha^{T} dt + 2\beta \Phi (\bar{\Phi}^{T} \Delta \bar{\Phi} - I) + \int_{0}^{t_{f}} \left[\Phi (\lambda \dot{\alpha}^{T} + \dot{\alpha} \lambda^{T}) + (-a\Phi' - k\Phi'')\lambda \alpha^{T} + (a\Phi' + k\Phi'')\alpha \lambda^{T} - f\lambda^{T} \right] dt + \Phi (\mu \alpha_{0}^{T} + \alpha_{0} \mu^{T}) - u_{0} \mu^{T}$$

$$(33)$$

Note that the definition of goal functional g in SCF remains general, i.e. not limited in linear functions of u.

3.2 Comparison with a POD-ROM

When the goal functional is set to be the solution over the entire domain, i.e. g = u, the SCF seeks to minimise the same error norm as POD interpolation. In this case, however, the error is in terms of the solution \hat{u} of the the ROM. Typical results are shown in Fig. 1. The optimal modes perform slightly better than POD modes, due to the enforcement of the model constraint.

Other goal functionals, however, illustrate the benefit of the goal-oriented approach. In Fig. 2, SCF results are shown for a goal functional of g = u only in the region $0 \le x \le 0.5$. The optimal modes provide a clear improvement over the POD modes. For small m, the error is reduced by one order of magnitude.



Another function of interest might be $g = u_x|_{x=0}$, which is calculated here in the discrete context by: $u_x|_{x=0} = \frac{u|_{x=h} - u|_{x=0}}{h}$, where h is the spatial step of the reference data. From Fig. 3, we can see the optimal modes give a substantial improvement upon the POD modes.

Finally a nonlinear goal functional, $g = u^2$ for u in the region $0 \le x \le 1$ and $0 \le t \le 0.249$. In this case optimal modes are modestly better than POD modes (Fig. 4), as could be anticipated by the result for g = u.



Figure 3: Comparison error $(g = u|_{x=h})$ Figure 4: Comparison error $(g = u^2)$

4 Nonlinear PDE example

Now we consider the one-dimensional Burgers equation as the governing equation:

$$u_t + uu_x - \frac{1}{Re}u_{xx} = f \tag{34}$$

$$u_0 = \sin(2\pi x) \tag{35}$$

with homogeneous Dirichlet boundary conditions and where Re = 10, f = 1. As in Section 2, after integrating by parts the ROM becomes $(\Phi|_0^1 = 0)$:

$$\sum_{j=1}^{m} \dot{\alpha}_j \int_0^1 \phi_i \phi_j dx - \frac{1}{2} \int_0^1 \phi_{ix} (\sum_{j=1}^{m} \alpha_j \phi_j)^2 dx + \frac{1}{Re} \sum_{j=1}^{m} \alpha_j \int_0^1 \phi_{ix} \phi_{jx} dx = \int_0^1 \phi_i f dx \quad (36)$$

Table 1 compares the specific expressions of the convection term (au_x and uu_x respectively) in the adjoint equation and the gradient for previous and this examples.

Table 1: Different expressions for convection-diffusion and Burgers example

	Convection-diffusion	Burgers
Adjoint equation	$-a\sum_{i=1}^m \lambda_i \int_0^1 \phi_q \phi_{ix} dx$	$-\sum_{i=1}^{m} \lambda_i \int_0^1 \phi_q \phi_{ix} \bigg(\sum_{j=1}^{m} \alpha_j \phi_j \bigg) dx$
Gradient	$a\lambda_q \left(\sum_{j=1}^m \alpha_j \phi_{jx}\right) - a\alpha_q \left(\sum_{j=1}^m \alpha_i \phi_{ix}\right)$	$\left(\sum_{j=1}^{m} \alpha_{j} \phi_{j}\right) \lambda_{q} \left(\sum_{j=1}^{m} \alpha_{j} \phi_{jx}\right) - \left(\sum_{j=1}^{m} \alpha_{j} \phi_{jy}\right) \alpha_{q} \left(\sum_{j=1}^{m} \alpha_{i} \phi_{ix}\right)\right)$

Fig. 5(a) shows the results for g = u ($0 \le x \le 1$). The reduction in the error is not more than 5%, so in this case the model constraint does not add substantially to the accuracy of the ROM. When g = u ($0 \le x \le 0.5$), the optimal modes are much better than POD modes (Fig. 5(b)).



Figure 5: Comparison the error

Fig. 6 shows results for the nonlinear goal functional $g = u^2$, for u in the region $0 \le x \le 1$ and $0 \le t \le 0.499$. In this case there is a modest improvement, in spite of the lack of improvement for the g = u case.



Figure 6: Comparison the error when $g = u^2$

5 An Approximate PDE example

In this section we use the SCF to find optimal modes when the governing equation used for the ROM is a PDE that only approximates dynamics of the known dataset. Specifically, we consider the approximation of solutions of the Burgers equation using the convection-diffusion equation. For the latter $k = \frac{1}{Re}$, f has the same value as that in Burgers equation used to generate the reference data, and a equals \bar{u} , where

$$\bar{\bar{u}} = \frac{1}{N} \frac{1}{N_t} \sum_{j=1}^N \sum_{i=1}^{N_t} u_{ij}$$
(37)

Fig. 7 shows results for g = u for which the SCF modes are substantially more accurate. In this case the effect of the model constraint is large, allowing the SCF modes to partially compensate for the inaccuracy of the PDE approximation.



Figure 7: The error versus number of modes for approximated PDE when g = u

6 Conclusions

In this paper a semi-continuous formulation (SCF) for determining Goal-Oriented ROMs is presented. In contrast with a fully-discrete formulation, the SCF does not rely on priori specification of discretisation matrices, the choice of which is not obvious when using experimental data as reference data, and whose effects on the results of the procedure are difficult to anticipate. The SCF separates the approximations used for the ROM and the processing of the discrete reference data, which avoids the specification of discretisation matrices and clarifies the treatment of nonlinear PDEs and goal functionals.

Results from linear and non linear model problems confirm that the benefits of using a goal-oriented approach can be substantial, particularly when only part of the domain is of interest. In all cases improvements over POD-ROMs where observed, but for goal functionals close to that minimised by POD interpolation, the benefits were significant only when the governing equation used to derive the ROM roughly approximated the dynamics of the reference data.

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