EFFECTS OF DISCRETIZATION ON REDUCIBILITY FOR PDE MODELS WITH VARIABLE GEOMETRY: A PRELIMINARY STUDY

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Abstract. When modelling boundary value problems numerically, the choice of discretization is of great importance. While the effect of the discretization on the approximation accuracy has been studied extensively, little has been said about model order reduction aspects. In this study, we explore how this choice can affect the reducibility of geometrically parameterized models. In particular, the focus is on comparing the performance of isogeometric and conventional finite element methods. To this end, we use a hybrid Krylov-POD procedure to reduce isogeometric and finite element models of two test cases involving linear dynamics. The results of this preliminary investigation indicate that isogeometric methods may lead to models that are more amenable to reduction.

1 Introduction

The numerical solution of moderately complex partial differential equations (PDEs) is a task that most modern computer systems can manage without much trouble. However, when studying parameterized PDEs, hardware capacity may quickly be surpassed since the computational effort required for simulating a single instantiated model is already quite substantial. The problem becomes all the more pronounced in multi-query situations, where the parameter space needs to be sampled in hundreds or thousands of points. These situations often arise in practical parameter studies, for instance in the context of design optimization, control, or uncertainty quantification.

The problem of cost can be addressed through the use of surrogate models. Such models act as a substitute for the high-fidelity (also called truth) model and are meant to reduce computational load while preserving an acceptable level of accuracy. Surrogate modelling is a vast field encompassing both black-box (data-driven) and invasive methodologies. An important class consists of parametric model order reduction (PMOR) techniques [1], which rely on a dimension-reducing system projection. These techniques are particularly effective since they explicitly use the available information on the model structure.

In case the geometry is considered variable, the domain discretization will also be affected as the parameter varies. Since PMOR operates directly on the discrete matrices, reduction characteristics implicitly depend on the discretization. It is intuitively clear that, for PMOR techniques to be effective, the physical significance of each discrete variable should remain relatively constant. At the very least mesh topology should be preserved. The fact that topology preservation is necessary has been recognized by several authors [2, 3, 4], but to the best of our knowledge little to no attention has been devoted to the less obvious questions of how to best reshape the computational mesh and which function spaces to choose.

The tight integration between geometric and analytic models offered by isogeometric (IG) methods [5] suggests that a combination of isogeometric analysis (IGA) and PMOR could be highly effective when used to reduce problems with parameterized geometry. IG models automatically provide continuous mesh changes as the geometry is varied. The resulting link between the degrees of freedom (DOF) for different parametric instances might be exploited to construct reduction bases that are valid across larger regions of the parameter space. In the past, IGA has been combined with PMOR techniques [6, 7], but no explicit comparison to conventional methods is provided.

Presently, we aim to investigate how the choice of discretization may affect the reducibility of the resulting (geometrically) parametrized models. In particular, IGA is compared to conventional finite element analysis (FEA). The further structure of the paper is as follows: In Sections 2 and 3, we give an overview of the methodology and its supporting theory. This is followed by an application to two case studies in Section 4. The main conclusions are formulated in the final part.

2 Full order model description: discretization of PDE models

The focus in the present work is on linear, dynamic and continuous systems, as encountered for example in structural dynamics and (vibro-)acoustics. In an abstract sense, the stationary behaviour of such systems can usually be described by an elliptic boundary value problem. As a model problem, let us consider the inhomogeneous Helmholtz equation with Dirichlet boundary conditions (BC). The problem is to find a solution u on a domain Ω with boundary Γ such that

$$(\nabla^2 + k^2)u = -f \quad \text{on } \Omega,$$

$$u = 0 \quad \text{on } \Gamma,$$
 (1)

where ∇^2 represents the harmonic operator, k is the wavenumber and f is a distributed forcing field. Physically, the oscillating field u might represent e.g. a pressure. The weak formulation, obtained using standard techniques [8], may be written in terms of a continuous bilinear form a and a continuous linear functional l:

$$a(u,v) = l(v) \quad \forall v \in H_0^1, \tag{2}$$

where H_0^1 is the Hilbert space of functions that satisfy the Dirichlet BC and whose values and first derivatives are (Lebesgue) square integrable. As long as k^2 does not equal an eigenvalue of the Helmholtz operator, a will be weakly coercive and the existence of a unique solution is guaranteed by the Nečas Theorem [8].

To obtain numerical approximations, a suitable problem discretization needs to be introduced. In the present paper, two 'paradigms' are studied: (conventional) FEA and IGA. For both methods, the most common approach to constructing discrete approximations is a Galerkin projection, where the search spaces for the functions uand v are taken to be identical, finite-dimensional subspaces of H_0^1 . Let the functions ϕ^i , $i = 1 \dots N$ consitute a basis of this space, then the elements of the (dynamic) stiffness matrix and force vector are given by

$$K_{dyn}^{ij} = a(\phi^j, \phi^i), \quad f^i = l(\phi^i). \tag{3}$$

The discrete problem is now a linear system, which can be concisely represented using matrix notation:

$$\boldsymbol{K}_{dyn}\boldsymbol{u} = \boldsymbol{f}.$$
 (4)

It is common to make the dependence on the dynamic parameter k explicit, writing

$$(\boldsymbol{K} - k^2 \boldsymbol{M}) \boldsymbol{u} = \boldsymbol{f}.$$
 (5)

Not only the solution field, but also the domain itself has to be discretized in order to accomodate more complex geometries. In an abstract sense, the geometry is approximated by the image of a (set of) parent domain(s) $\tilde{\Omega}$ after a geometric transformation:

$$\Omega \approx \bigcup_{i=1}^{n_{el}} T_i(\tilde{\Omega}_i),\tag{6}$$

where n_{el} is the number of parent domains. Usually, the transformations T_i are chosen to lie in the same subspace as u on the subdomain $T_i(\tilde{\Omega}_i)$: this is the isoparametric concept.

Although variations to this pattern exist – e.g. collocation of the strong form [9] or sub- and superparametric approaches [10] – the basic strategy described above is often used in practice and provides a common ground between IGA and FEM. In this case both paradigms turn out to be very similar on a conceptual level, even though the emphasis is often placed on their differences. The remainder of this section provides a more detailed picture of each method's specifics.

Finite element discretization An important choice in developing the problem discretization – and setting apart FEA and IGA – is the choice of the discrete function space. By the isoparametric concept, both the unknown field and the domain geometry are approximated within this space. The classical FEA relies on (low-order) polynomial functions, which are applied in a piecewise manner: the entire problem domain is subdivided into elements with simple shapes that can be represented with tensor-product polynomials. In most cases, the geometry can only be approximately represented, which inevitably leads to errors. This error is not necessarily made smaller by refinement since this operation may be based on the coarse approximation rather than the original geometry.

While the approach can be applied to arbitrary geometries, it is not always an easy task. Meshing must be done carefully since it has a strong impact on the approximation accuracy. Furthermore, design variability is often not taken into account in (automatic) meshing procedures. Because the definition of the geometry is separated from analysis, even small design modifications cause the mesh to be rebuilt from the ground up. Besides the obvious cost penalty, projection-based reduction methods cannot be applied as even for geometrically similar meshes, the DOF numbering may be different. Related problems are encountered in fluid-structure-interaction, shape optimization and nonlinear mechanics. To address such issues, mesh morphing techniques have been developed; see [11] for an overview of the various methods. Many of these techniques still entail solving a considerably difficult subproblem, and caution always remains necessary to prevent low-quality meshes.

Isogeometric discretization The isogeometric method treats the selection of shape functions in reverse, taking the (spline) functions defining the geometry and adapting the analysis accordingly. The driving factor for this paradigm switch is twofold. First of all, the description (6) of the domain Ω is exact even at the coarsest refinement level, thus avoiding errors due to approximate geometry descriptions. Be-

sides this important advantage, the meshing step can be entirely eliminated since the discretization of the domain comes along with the geometry. Hence a computational 'mesh' is obtained at no added cost.

In computer graphics applications, non-uniform rational B-splines (NURBS) are standard in representing freeform objects, since they allow intuitive modelling and are able to represent conic sections exactly [12]. A NURBS curve $\mathbf{R}(\xi)$ is defined by a knot vector $[\xi_1 \dots \xi_k], \ 0 \leq \xi_1 \leq \dots \leq \xi_k$, a polynomial order l, and a set of control points and weights $\mathbf{P}_i \in \mathbb{R}^D, \ w_i \in \mathbb{R}, \ i = 1 \dots k - l - 1$:

$$\mathbf{R}(\xi) = \frac{\sum_{i=1}^{k-l-1} N_i^l(\xi) w_i \mathbf{P}_i}{\sum_{j=1}^{k-l-1} N_j^l(\xi) w_j},\tag{7}$$

where $N_i^l(\xi)$ are the B-spline basis functions derived from the knot vector. An important property of NURBS curves is that they have continuity C^{l-m} across knots of multiplicity m. For non-repeated knots and elevated polynomial orders, high smoothness is attained which can be exploited for solving higher-order problems. Because knot duplication and order elevation do not commute, refinement in isogeometric analysis can be done in different ways. IGA is even able to offer a continuity-increasing refinement procedure called k-refinement [5].

Surfaces and volumes (commonly called patches) are constructed by taking the tensor product of two, respectively three NURBS curves. The shape and parameterization are determined by a control net, comparable to a structured mesh in FEM. This structure is somewhat limiting in the sense that only topologically simple geometries can be represented, but this is only a sidenote in the context of the present study. On the contrary, the provision of a mesh that naturally adapts to changing geometry can be considered beneficial with respect to the central hypothesis of this work: as the mesh changes in a continuous fashion, the essential meaning of the DOF is preserved quite well, which is supposed to lead to better reducibility. Moreover, and unlike FEM, isogeometric methods are robust to poor-quality parameterizations [13]. This freedom might be exploited to achieve better reduction performance.

3 Parametric model order reduction through projection

A semi-discretized, Laplace-transformed, second-order dynamic system – both for FEM and IGA – can be represented in matrix form as

$$\left(s^2 \boldsymbol{M} + s \boldsymbol{C} + \boldsymbol{K}\right) \boldsymbol{u} = \boldsymbol{f},\tag{8}$$

where M is the mass matrix, C is the damping matrix and K is the static stiffness matrix, while the Laplace variable s now takes on the role of the dynamic parameter.

Note how (5) is a generic, although simplified, example of such a system; more complex PDE models may be discretized and transformed to the form (8) in a similar way.

The reduction of systems like (8) is the topic of 'ordinary' MOR, which encompasses techniques developed in the fields of structural dynamics, numerical mathematics and control [14]. The common idea is to decrease the effective number of DOF from N to n by applying a projection transformation, i.e.

$$\boldsymbol{W}^{T}\left(s^{2}\boldsymbol{M}+s\boldsymbol{C}+\boldsymbol{K}\right)\boldsymbol{V}\underline{\boldsymbol{u}}=\boldsymbol{W}^{T}\boldsymbol{f},$$
(9)

with $\mathbf{V}, \mathbf{W} \in \mathbb{R}^{N \times n}$ and $n \ll N$. The projection is one-sided if $\mathbf{V} = \mathbf{W}$ and twosided otherwise. For simplicity, we assume the former here, but this choice may also be motivated by the need for stability preservation [15]. In order to construct the projection matrix, we apply the Krylov subspace technique for second-order systems described in [16].

The models considered here have a more general, implicit, parametric dependence. Hence a PMOR technique with greater applicability is necessary. In the present work we choose to adopt a hybrid scheme similar to [17]. We make use of the local reduction bases built with the Krylov method: a global reduction space, valid for the entire parametric domain, is found as the union of local spaces for several parametric instances. Suppose a set of n_s local reduction spaces has been given as the column span of matrices $V_i \in \mathbb{R}^{N \times n_l}$. Their union is given by the range of the concatenated matrix $[V_1 \ V_2 \ \dots \ V_{n_s}]$. However, the columns of this matrix may no longer be linearly independent, let alone mutually orthogonal. Using a singular value decomposition (SVD), the rank is revealed and the dominant directions can be identified. We have

$$[\boldsymbol{V}_1 \ \boldsymbol{V}_2 \ \dots \ \boldsymbol{V}_{n_s}] = \boldsymbol{R} \boldsymbol{\Sigma} \boldsymbol{L}^T, \tag{10}$$

where $\Sigma \in \mathbb{R}^{N \times (n_l n_s)}$ contains the singular values σ_i on the diagonal and $R \in \mathbb{R}^{N \times N}$, $L \in \mathbb{R}^{n_l n_s \times n_l n_s}$ are orthonormal matrices. It can be shown that the SVD provides an optimal decomposition of the snapshot matrix [18]: most information about the snapshots is contained within the first columns of R. Moreover, the relative information content of the *i*-th left singular vector is proportional to σ_i^2 and the information lost in the truncation is proportional to $\sum_{i=r+1}^{n_l n_s} \sigma_i^2$ if *r* columns are kept.

It is further noted that, by virtue of this last property, the singular value decomposition is a useful tool for assessing the problem's intrinsic amenability to reduction. In [8], the following reducibility test is proposed: first collect several high-fidelity snapshots into a matrix, next calculate its SVD and then consider the singular values. If the values show rapid decay, then the information contained within the snapshots can be represented using a low number of singular vectors. Provided a representative number of samples are taken, this implies that solutions reside in a low-dimensional subspace. If the reduction technique described here is used, this test can be carried out without large cost penalties since the snapshots are calculated anyway.

4 Validation of reduced order model accuracy

4.1 Curved beam

As a first example, consider a simply supported beam subject to a harmonic transverse point load (see Figure 1). The beam curvature radius R is taken as the variable geometric parameter. Two discretizations are constructed following the finite element and isogeometric paradigms. The FE model is built using the commercial software package NX Nastran. The beam is equally divided into a total of 60 linear elements of the type CBAR [19], leading to a model with 183 DOF. For the IG discretization, an in-house code based on Euler-Bernoulli theory is used. As the original geometry is decribed with a quadratic NURBS curve, order-two shape functions are used and the model is h-refined until 182 DOF are obtained.

The frequency-domain reduction bases are found using the Krylov algorithm with 6 order-two expansion points equally spread over the 0-500 Hz frequency interval. These local bases are constructed at five parametric configurations, corresponding to radii of 0.15, 0.1875, 0.375 and 0.75 meters as well as the straight beam. After the SVD, 18 global vectors are retained. This basis is used to reduce models with an unsampled radius of 0.25 m. The frequency response function (FRF) errors of the reduced order models relative to truth models are plotted in on the left in Figure 2. It is remarkable that the IG approach leads to errors that are far below those of the FE approach, when each is compared to its original full order representation. The SVD-based reducibility test described in Section 3 also indicates that the discrete solution manifold is of lower dimension in case the IG description is used. A set of snapshots is generated for the 6-by-6 grid of frequencies and radii used before. In Figure 2 (right), the relative magnitudes of the singular values of the snapshot matrix are shown; the IG case displays a markedly stronger decay and the values are already significantly lower at the 18-th singular value.

4.2 Acoustic cavity

Secondly, a 2-dimensional interior acoustic problem is treated. We examine a hard-walled air-filled resonant cavity, shaped like a square with curved sides (Figure 3). A monopole source located at the top right corner excites a pressure response associated to a standing wave pattern. The pressure at a certain interior point –



Figure 1: Problem definition of the curved beam.

whose location varies along with the geometry – is taken as an output. The variable parameter defines the inwards or outwards curvature of the sides. The 2D-acoustics module of the COMSOL software package is used in creating the FE discretizations, where a mapped mesh is provided by an internal morphing function. An in-house extension of the GeoPDEs toolbox [20, 21] generates the IG model matrices of the exact, h-refined geometry. Both models finally encompass 10201 pressure DOF, corresponding to a 100-by-100 square grid of linear elements.

In this case, the parametric domain is sampled at four locations, with curvature radii R equal to $\pm\sqrt{2}/10$ and $\pm\sqrt{2}/5$ meters. At every point a local basis is derived from 6 expansion points of order 5 at frequencies between 50 Hz and 550 Hz. The total of 120 basis vectors is reduced to 100 by truncation of the SVD. The FRF errors occuring when reducing a model representing an ordinary square are then calculated. As in the previous example, Figure 4 shows that a reduced FE model performs slightly but consistently worse than a reduced IG model with the same number of DOF, at least in the relevant frequency range. The snapshots' singular values also attribute higher importance to the later components and show that the difference in reducibility is smaller than in the beam case.

5 Conclusion

Even though it is clear that the domain discretization of geometrically parameterized PDE models can have a profound impact on the effectiveness of PMOR methods, the existing literature on the topic is scarce. While this observation applies to conventional FE approaches, the relatively new IG methods deserve specific attention. Because of their strong connection between the design and analysis models, as well as their robustness to mesh distortions, improved reduction performance may be ex-



Figure 2: Reducibility for the curved beam. (Left) Reduction errors on the FRF (in %). (Right) Relative magnitude of the singular values.

pected. Our work provides some numerical experiments testing this hypothesis. The focus is on linear dynamic models emerging from oscillating, continuous systems.

After briefly touching the theoretical background and motivations for the investigation, a combined Krylov-POD reduction method and a reducibility test are described. These tools are applied to two test problems, comprising a dynamically loaded beam and an acoustic cavity. The reduced IG model provides a slight to moderate accuracy gain over the reduced FE model, providing some evidence to support the hypothesis. A full validation will require more tests and is the topic of future research. Importantly, theoretical insights are needed to better understand which effects come into play.

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Value
343 ms^{-1}
$1.225 \ \rm kgm^{-3}$
$1 m^{3-1} s^{-2}$
$2\mathrm{m}$
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Figure 3: Problem definition of the acoustic cavity.

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Figure 4: Reducibility for the acoustic cavity. (Left) Reduction errors on the FRF (in %). (Right) Relative magnitude of the singular values.

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