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On the stability of POD Basis Interpolation via Grassmann Manifolds for Parametric Model Order Reduction in Hyperelasticity

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1 **On the stability of POD Basis Interpolation on**
2 **Grassmann Manifolds for Parametric Model Order**
3 **Reduction**

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32 **Abstract** Proper Orthogonal Decomposition (POD) basis interpolation on Grassmann
33 manifolds has been successfully applied to problems of parametric model order reduction
34 (pMOR). In this work we address the necessary stability conditions for the interpolation,
35 all defined from strong mathematical background. A first condition concerns the domain
36 of definition of the logarithm map. Second, we show how the stability of interpolation
37 can be lost if certain geometrical requirements are not satisfied by making a concrete
38 elucidation of the local character of linearization. To this effect, we draw special attention
39 to the Grassmannian exponential map and the optimal injectivity condition of this map,
40 related to the cut-locus of Grassmann manifolds. From this, an explicit stability condition

41 is established and can be directly used to determine the loss of injectivity in practical
42 pMOR applications. A third stability condition is formulated when increasing the number
43 p of POD modes, deduced from the principal angles of subspaces of different dimensions
44 p . Definition of this condition leads to an understanding of the non-monotonic oscillatory
45 behavior of the Reduced Order Model (ROM) error-norm with respect to the number of
46 POD modes, and on the contrary, the well-behaved monotonic decrease of the error-norm
47 in the two numerical examples presented herein. We have chosen to perform pMOR in
48 hyperelastic structures using a non-intrusive approach for inserting the interpolated spatial
49 POD ROM basis in a commercial FEM code. The accuracy is assessed by *a posteriori* error
50 norms defined using the ROM FEM solution and its high-fidelity counterpart simulation.
51 Numerical studies successfully ascertained and highlighted the implication of stability
52 conditions which are general and can be applied to a variety of other linear or nonlinear
53 problems involving parametrized ROMs generation based on POD basis interpolation on
54 Grassmann manifolds.

55 **1 Introduction**

56 In this paper we consider the notion of stability conditions of POD basis interpolation on
57 Grassmann manifolds for pMOR. This interpolation method has been used to adapt ROMs
58 to parameter changes in various engineering fields, among others, design, optimization,
59 control, uncertainty quantification, data-driven systems, etc. Here, we introduce three
60 important stability conditions that are quite essential to the interpolation method. Even
61 though we illustrate the stability conditions in hyperelastic problems, they are applicable
62 to a variety of other linear or nonlinear pMOR problems as well.

ROMs aim to decrease the computational burden of large-scale systems and solve parametrized problems by generating models with lower complexity, but accurately enough to represent the high-fidelity numerical simulations. One popular method is the Proper Orthogonal Decomposition (POD) [1, 2, 3], also known as Karhunen-Loève Decomposition (KLD) [4, 5], Singular Value Decomposition (SVD) [6] or Principal Component Analysis (PCA) [7, 8]. We need to emphasize that all these POD techniques are referred as *a posteriori* as they require some knowledge (at least partial) on the solution of the problem.

Parametric Model Order Reduction (pMOR) is a framework to generate a ROM that approximates a full-order system with high accuracy over a range of parameters. In case of solving a parametric problem using the POD, the method starts by a sampling stage during which the full-order system is solved for some rather small set of *training* points. The state variable field ‘*snapshots*’ are then compressed using the POD to generate a ROM basis that is expected to retain the most characteristic dynamics of its high-fidelity counterpart solution. Nevertheless, since the POD bases are generated for a set of training points, they are optimal only to these parameter values. Thus, a main drawback of POD is the sensitivity to parameter changes and the lack of robustness over the entire parameter space. Consequently, any ROM basis generated by the approach outlined above cannot be expected to give a good approximation away from the training point. In pMOR, the question we have to address is how to compute a good approximation of the POD basis related to a *new parameter* value. Multiple methods have been proposed for adapting POD basis to address parameter variation as thoroughly documented in related review articles [9, 10, 11].

85 In the case of nonlinear systems, even though a Galerkin projection reduces the num-
 86 ber of unknowns, the computational burden for obtaining the solution could still be high
 87 due to the prohibitive computational costs involved in the evaluation of nonlinear terms.
 88 Hence, the nonlinear Galerkin projection in principle leads to a ROM, but its evaluation
 89 may be more expensive than the evaluation of the original problem. To this effect, to
 90 make the resulting ROMs computationally efficient, POD is typically used together with
 91 a sparse sampling method, also called *hyper reduction*, such as the missing point estima-
 92 tion (MPE) [12], the empirical interpolation method (EIM) [13], the discrete empirical
 93 interpolation method (DEIM) [14], the Gappy POD method [15], and the Gauss-Newton
 94 with approximated tensors (GNAT) method [16].

95 Parametric model order reduction using *POD basis interpolation* on Grassmann man-
 96 ifolds is done initially in the field of computational fluid dynamics which was proposed for
 97 systems that are linear in state [3, 17, 18, 19]. Similar approach has been scarcely applied
 98 in hyperelasticity, like in [20], where real time simulations of hyperelastic structures have
 99 been proposed using POD basis interpolation, in combination with an asymptotic numer-
 100 ical method. Here, pMOR is used to hyperelastic structures by adapting pre-computed
 101 POD basis.

102 When addressing the question of POD basis interpolation on Grassmann manifolds,
 103 the main point is that *interpolation cannot be done in a linear space*. Indeed, any mode p
 104 POD basis performed on some snapshot matrix $\mathbf{S} \in \text{Mat}_{n, N_t}(\mathbb{R})$ give rise to a truncated
 105 matrix $\mathbf{S}_p \in \text{Mat}_{n, p}(\mathbb{R})$ (where $n = 3N_s$ and N_s, N_t respectively correspond to the num-
 106 ber of spatial points and temporal points). Now, despite the appearances, computation
 107 can not be done in the linear space $\text{Mat}_{n, p}(\mathbb{R})$ of matrices, as the matrix \mathbf{S}_p encodes a

108 p dimensional vector subspace. The goal is thus to make interpolation on the set of p
 109 dimensional subspaces of \mathbb{R}^n , which defines exactly the Grassmann manifold $\mathcal{G}(p, n)$. Such
 110 Grassmann manifold interpolation is well documented [18, 19, 3, 21, 22], and computation
 111 can be done explicitly.

112 Thus, we might have been satisfied with a simple application of the existing and now
 113 well-known formulas, using the *logarithm map* to linearize, and then the *exponential map*
 114 to return back to the manifold. Such maps are issued from the Riemannian structure
 115 of Grassmann $\mathcal{G}(p, n)$ and its associated geodesics [23]. However, applying formulae in
 116 manifolds requires the verification of certain conditions which will be addressed in this
 117 work. A first condition appears, as the logarithm map is only defined on some subset
 118 $U \subset \mathcal{G}(p, n)$ explicitly defined as a subset of non-singular matrices. So linearization can
 119 only be done once we have checked that all training points are contained in U . In fact,
 120 such a condition is usually checked, as square matrices are generically non-singular.

121 A second condition concerns the use of the exponential map, which is defined on all the
 122 vector space \mathbb{R}^d (with $d = p(n-p)$ the dimension of $\mathcal{G}(p, n)$). Nevertheless, the exponential
 123 map is not automatically stable since it is only *injective* inside a subset $V \subset \mathbb{R}^d$ deduced
 124 from the *cut-locus* [23] of the Riemannian manifold $\mathcal{G}(p, n)$. Considering all geodesics with
 125 the same starting point, such a cut-locus is in fact the set of points where such geodesics
 126 are no longer minimal, and thus the exponential map is no more injective. Without any
 127 control of such an injectivity condition, the return back of the interpolated curve *via* the
 128 exponential map can lead to some disconnected curve on the manifold, which should be
 129 avoided.

130 An explicit determination of such a cut-locus was already mentioned in [24], without
131 any proof, and a result by Kozlov [25, Theorem 12.5] make a clear understanding of such
132 a cut-locus using singular values of matrix representation of a velocity vector. We thus
133 write an explicit way to compute such a cut-locus, with clear proof. As this result is not
134 a classical one, and to be self contained, we had to develop the necessary mathematics to
135 obtain such cut-locus of the Grassmann manifold $\mathcal{G}(p, n)$, as well as the open subset V .
136 In fact, from this cut-locus and its associated subset V , it was possible to improve the
137 already known exponential injectivity condition, obtained from the *injectivity radius* of
138 Grassmann manifolds [25], and used in [3] to control computations. In most of our cases,
139 indeed, the injectivity condition issued from the cut-locus is better than the one obtained
140 from the injectivity radius.

141 Finally, a third stability condition is related to the intrinsic non-inclusion defect of
142 the interpolated subspaces of different dimensions. Indeed, a closer examination of the
143 numerical results showed that the accuracy of interpolation may not improve by increasing
144 the number of POD modes. As consequence of this new insight, it is not possible to
145 control or predict the interpolation behavior. At first glance, this fact seems inconsistent
146 with the expected improvement of the solution by increasing the number of modes. We
147 indicate that the non-connectivity of the solutions is inherited from the construction of the
148 interpolation formulae using the logarithm and the exponential maps. To prove the fact,
149 the basic tool proposed here, is the computation of the principal angles of two POD basis
150 of different mode p . By using the principal angles we can determine the geometric distance
151 between subspaces of different dimensions [26]. To this end, a new stability condition will
152 be tied with the geometric distance which measures the non-inclusion defect between these

153 subspaces. To the best of the author’s knowledge, this finding has never been reported in
154 the variety of pMOR involving POD basis interpolation on Grassmann manifolds.

155 From all this, we finally get three kinds of stability conditions, each clearly established:
156 (1) a first one about the logarithm map domain of definition, (2) a second one on the loss
157 of injectivity of the exponential map, *via* the cut-locus of Grassmann manifolds, and (3)
158 a third one about the increasing POD mode, controlled from a well-defined geometric
159 distance between subspaces of different dimensions.

160 The general framework of pMOR comprises an off-line and an on-line stage. The off-line
161 stage characterizes the potentially costly procedure of solving FEM problems associated
162 with different values of the physical or modeling parameter (training points). The on-
163 line stage consists of the POD basis interpolation on Grassmann manifolds to determine a
164 ROM basis for an unseen target parameter. Then, in this work, a non-intrusive approach is
165 introduced for the obtained spatial POD basis. Note, that this approach deviates from the
166 classical methods that relying on a Galerkin/Petrov Galerkin projection on the governing
167 equations. Instead, the ROM-FEM models are implemented by inserting the interpolated
168 spatial POD basis using linear constraint equations in Abaqus. It is evident that even by
169 constraining the degrees of freedom, the reduced model still embeds the high dimension.
170 We remark that we used a commercial code only for evaluating the stability and accuracy
171 of the adaption of POD basis via interpolation on Grassmann manifolds. This is because
172 it is not our objective to implement a method of nonlinear MOR, although it is a quite
173 challenging task to be realized in a commercial FEM code.

174 For the *mechanical part* we have chosen two low complexity problems in hyperelasticity
175 using a single parameter for pMOR to elaborate the interpolation stability primarily for

176 the clarity of exposition. We hypothesize that the stability issues addressed herein will be
177 also inherent and critical for more demanding problems. Specifically, for the pMOR, the
178 hyperelastic structures are modeled using isotropic and anisotropic constitutive laws. For
179 the anisotropic model, a subclass of transversely isotropic materials is considered where
180 the strain energy function is assumed to depend only on two invariant measures of finite
181 deformation [27,28,29,30]. At the numerical examples, we have chosen single parameters
182 associated to a) the model anisotropy defined by the fiber orientation angle, and b) the
183 material coefficients of the hyperelastic constitutive equations.

184 The paper is organized as follows. In [section 2](#) and [section 3](#), we will recall the theo-
185 retical background so to understand the way to make interpolation of POD basis using
186 the corresponding points on a Grassmann manifold. Next, in [section 4](#) we produce all ex-
187 plicit algorithms to obtain interpolation on Grassmann manifolds in which three stability
188 conditions are defined: one from the logarithm map, a second one from the exponential
189 map, and a third one from increasing the number of the POD modes. Then, [section 5](#) is
190 devoted to the mathematical proofs needed to have well-defined stability conditions. The
191 mechanical part starts with [section 6](#), which covers the basic framework of hyperelasticity
192 theory in continuum mechanics for an incompressible transverse isotropic material. In [sec-](#)
193 [tion 7](#), the interpolation performance is shown for two problems in hyperelasticity, and
194 further important computational aspects are discussed. Finally, [section 8](#) highlights the
195 main results and some important outcomes.

196 2 Problem Formulation

We consider some mechanical problem governed by a specific parameter $\lambda \in [\lambda_{min}, \lambda_{max}] \subset \mathbb{R}$ (see [section 6](#)). For each parameter λ , the solution is given by a space-time smooth field

$$(t, \mathbf{X}) \in [0; T] \times \Omega_0 \mapsto u^\lambda(\mathbf{X}, t) \in \mathbb{R}^3$$

197 where Ω_0 is a closed convex subset of \mathbb{R}^3 and $T > 0$.

198 To avoid costly computations for all values $\lambda \in [\lambda_{min}, \lambda_{max}]$, we would like to interpo-
 199 late between a finite number of FEM solutions $u_i := u^{\lambda_i}$, associated to N training points
 200 $\lambda_1, \dots, \lambda_N$. In fact, it is at the level of the POD performed on the snapshot matrices $\mathbf{S}(\lambda_i)$
 201 (defined in the next section) associated to the solutions u_i that this interpolation will be
 202 considered.

203 But one of the essential points of this POD is that it associates to each snapshot matrix
 204 $\mathbf{S}(\lambda_i)$ a certain point \mathbf{m}_i of a Grassmann manifold \mathcal{G} , and it is therefore needed at this
 205 stage to interpolate between points $\mathbf{m}_1, \dots, \mathbf{m}_N$ on \mathcal{G} . It is now proposed to detail the
 206 link between a POD reduction and the construction of a point on a Grassmann manifold.

207 3 Proper Orthogonal Decomposition and Grassmann manifolds

The POD method can be applied to curves defined in Hilbert spaces of infinite dimension. The initial idea is to determine a subspace of a given dimension p (which is the fixed number of modes of the POD), reflecting “as well as possible” this curve, as it is very well explained in [\[2, 19\]](#). In most cases, however, we do not consider the entire curve, but only a finite number of points of a Hilbert space $\mathcal{H}_{\text{spatial}} = \mathbb{R}^{N_s}$ of finite dimension N_s

(the number of space points). More precisely, any FEM solution u of our problem under consideration produces a *snapshot matrix*

$$\mathbf{S}_{jk}, \quad 1 \leq j \leq 3N_s, \quad 1 \leq k \leq N_t$$

with N_t the number of time steps. Such matrix encodes in fact N_t vectors $\mathbf{u}_k := u(\cdot, t_k) \in \mathcal{H}_{\text{spatial}}$, and we write

$$\mathbf{S} := [\mathbf{u}_1, \dots, \mathbf{u}_{N_t}]$$

Take now $\langle \cdot, \cdot \rangle$ to be the standard inner product of the Hilbert space $\mathcal{H}_{\text{spatial}}$. To any p dimensional vector subspace \mathcal{V}_p of $\mathcal{H}_{\text{spatial}}$, there is an associated orthogonal projection

$$\pi_p : \mathcal{H}_{\text{spatial}} \longrightarrow \mathcal{V}_p$$

and the POD method address the question to minimize the distance function

$$\mathcal{J}(\mathcal{V}_p) := \sum_{k=1}^{N_t} \|\mathbf{u}_k - \pi_p(\mathbf{u}_k)\|^2, \quad \|\cdot\| := \sqrt{\langle \cdot, \cdot \rangle}$$

over all p dimensional subspaces \mathcal{V}_p . It then appears that the set of all such subspaces define a *smooth compact Riemannian manifold* [31, 23]

$$\mathcal{G}(p, n) := \{\mathcal{V}_p \subset \mathcal{H}_{\text{spatial}}, \quad \dim(\mathcal{V}_p) = p\}, \quad n := 3N_s$$

208 so that any p dimensional vector subspace \mathcal{V}_p can be considered as some *point* $\mathbf{m} \in \mathcal{G}(p, n)$,

209 and the question is finally to minimize $\mathcal{J}(\mathbf{m})$ over all $\mathbf{m} \in \mathcal{G}(p, n)$.

In practice, let consider an orthonormal basis ϕ_1, \dots, ϕ_p of \mathcal{V}_p so that the matrix form of π_p is given by

$$\Phi_p \Phi_p^T, \quad \Phi_p := [\phi_1, \dots, \phi_p] \in \text{Mat}_{n,p}(\mathbb{R})$$

where $\text{Mat}_{n,p}(\mathbb{R})$ is the vector space of $n \times p$ matrices, and (right) superscript $(\cdot)^T$ denotes the transposition operation. By direct computation, the distance function \mathcal{J} is then rewritten

$$\mathcal{J}(\mathbf{m}) = \|\mathbf{S} - \Phi_p \Phi_p^T \mathbf{S}\|_{\mathbb{F}}^2$$

210 where $\|\mathbf{A}\|_{\mathbb{F}} := \sqrt{\text{tr}(\mathbf{A}\mathbf{A}^T)}$ is the Frobenius norm on $\text{Mat}_{n,p}(\mathbb{R})$.

Now it is classically known that minimization of \mathcal{J} is given by Eckart–Young Theorem [32,33,6,34] and can be obtained via a *singular value decomposition* of \mathbf{S} . Indeed, take this SVD to be

$$\mathbf{S} = \mathbf{U}\Sigma\mathbf{V}^T, \quad \mathbf{U} := [\phi_1, \dots, \phi_{N_t}]$$

with singular values $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{N_t}$. Then one solution of minimizing \mathcal{J} is given by

$$\mathbf{m}_0 := \text{span}(\phi_1, \dots, \phi_p)$$

which is unique whenever $\sigma_p > \sigma_{p+1}$ [2]. Let also define the *reduced model* \mathbf{S}_p of our snapshot matrix by

$$\mathbf{S}_p := \Phi_p \Phi_p^T \mathbf{S}, \quad \Phi_p := [\phi_1, \dots, \phi_p].$$

For each snapshot matrix $\mathbf{S}(\lambda_i)$ associated to training points λ_i ($i = 1, \dots, N$), we thus obtain a point

$$\mathbf{m}_i := \text{span}(\phi_1^{(i)}, \dots, \phi_p^{(i)}) \in \mathcal{G}(p, n)$$

211 once chosen a fix mode p for the POD. For a new target parameter $\tilde{\lambda}$, interpolation has
212 to be done on the Grassmann manifold $\mathcal{G}(p, n)$, which is now detailed.

213 4 ROM Adaptation Based on Interpolation on Grassmann Manifolds

214 Computation on manifold, such as the one of Lagrange interpolation, can only be done
 215 using *local coordinates*. Such local coordinates are obtained via bijective maps, which are
 216 defined, in general, on subsets U of the manifold (called the *local charts*). In the case of
 217 a Riemannian manifold, one can use the *normal coordinates* directly deduced from the
 218 geodesics of the manifold.

In our case, local charts will be given by *logarithm maps*, so we obtain smooth diffeomorphisms

$$\text{Log} : U \longrightarrow V := \text{Log}(U) \subset \mathbb{R}^d$$

219 where d is the dimension of the manifold, and the reverse operation is given by the
 220 exponential map. Nevertheless, such operation has to be well-defined, which is achieved
 221 when the exponential map is injective.

222 Such an injectivity condition was already addressed in [3], using the injectivity radius
 223 of Grassmann manifolds (see (12)). Other injectivity conditions are presented here, less
 224 restrictive than the one issued from the injectivity radius (see Remark 4.1).

225 Another instability issue is the one of increasing the number p of modes. Indeed, one
 226 should expect that the interpolation is sharpened by increasing p , which can be controlled
 227 by computing the *geometric distance* of subspaces with different dimensions, as defined
 228 in [26].

229 Let us now present in the next [subsection 4.1](#) the necessary assumptions to have a
 230 well-defined interpolation, while in [subsection 4.2](#) we produce the interpolation algorithm,
 231 taking into account all necessary stability conditions. Finally [subsection 4.3](#) focus on the
 232 explicit formulae to compare two subspaces of different dimensions.

233 *4.1 Interpolation from logarithm and exponential map: necessary assumptions*

234 Let us consider back the points N points $\{\mathbf{m}_i\}_{i=1}^N$ in the Grassmann manifold $\mathcal{G}(p, n)$,
 235 all obtained from the ROMs of the snapshot matrices (as detailed in [section 3](#)). The goal
 236 here is to obtain a *well-defined* interpolation of a spatial POD basis associated with a new
 237 target point $\tilde{\lambda}$. This is detailed in [subsection 4.2](#), and we just focus here on the main ideas
 238 issued from the seminal work in [\[18\]](#):

- 239 1. Choose a base point \mathbf{m}_0 in the family $\mathbf{m}_1, \dots, \mathbf{m}_N$, altogether with its associated
 240 logarithm map $\text{Log}_{\mathbf{m}_0}$ (from [Definition 5.9](#)).
- 241 2. Compute the velocity vectors $v_i := \text{Log}_{\mathbf{m}_0}(\mathbf{m}_i)$ all lying in a tangent plane, which is a
 242 vector space \mathbb{R}^d (with $d = p(n - p)$ the dimension of $\mathcal{G}(p, n)$).
- 243 3. Compute a new velocity vector \tilde{v} associated to a target point $\tilde{\lambda}$.
- 244 4. Obtain an interpolated point $\tilde{\mathbf{m}} := \text{Exp}_{\mathbf{m}_0}(\tilde{v}) \in \mathcal{G}(p, n)$ using the exponential map
 245 (from [\(11\)](#)) to return back to the Grassmann manifold $\mathcal{G}(p, n)$.

246 As depicted in [Figure 1](#), it is nevertheless important not to forget that the logarithm
 247 map $\text{Log}_{\mathbf{m}_0}$ is only defined on some open set $U_{\mathbf{m}_0}$, taken from [\(13\)](#) and recalled below.
 248 So a first necessary condition is that

- 249 • (C1): All points $\mathbf{m}_1, \dots, \mathbf{m}_N$ lie in $U_{\mathbf{m}_0}$.

To check such a condition, recall first that each point $\mathbf{m} \in \mathcal{G}(p, n)$ corresponds to an
 orthonormal basis stored in a $n \times p$ matrix

$$\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \text{Mat}_{n,p}(\mathbb{R}), \quad \mathbf{Y}^T \mathbf{Y} = \mathbf{I}_p.$$

250 Taking now matrices \mathbf{Y}_i corresponding to \mathbf{m}_i ($i = 0, \dots, N$), such condition translates
 251 into

252 • (C1)-matrix form: For all $i = 1, \dots, N$, the matrix $\mathbf{Y}_0^T \mathbf{Y}_i$ is non singular.

253 From this and Theorem 5.12-5.15 we deduce that the velocity vectors $v_i = \text{Log}_{\mathbf{m}_0}(\mathbf{m}_i)$ all
 254 lie in the open set $V_{\mathbf{m}_0} = \text{Log}_{\mathbf{m}_0}(U_{\mathbf{m}_0})$. Once computed the new velocity vector $\tilde{v} \in \mathbb{R}^d$,
 255 according to Theorem 5.12, a second necessary condition is then

256 • (C2): \tilde{v} is inside the open set $V_{\mathbf{m}_0}$.

257 Such a condition seems to be more intricate than the previous one, but in fact it is simply
 258 related to the singular values of a matrix. Indeed, in the case $2p \leq n$ (which will be our
 259 case), a velocity vector \tilde{v} is represented by a matrix $\tilde{\mathbf{Z}} \in \text{Mat}_{n,p}(\mathbb{R})$ such that $\tilde{\mathbf{Z}}^T \mathbf{Y}_0 = 0$
 260 (see (4)). From Lemma 5.14 and Theorem 5.15, condition (C2) simply writes

261 • (C2)-matrix form: Taking $\tilde{\theta}_1$ to be the maximum singular value of $\tilde{\mathbf{Z}}$, we have $\tilde{\theta}_1 < \pi/2$.

262 The first condition (C1) is usually trivially satisfied, and the second one (C2) can be
 263 evaluated on a range of new parameters $\tilde{\lambda}$, so to have an interval $[\tilde{\lambda}_a, \tilde{\lambda}_b]$ of well-defined
 264 interpolation. This was done on both benchmarks (see Figure 7 and 17).

Remark 4.1. In the case of the compact manifold $\mathcal{G}(p, n)$, the exponential map is defined on all the vector space \mathbb{R}^d , so it is always possible to compute a new point $\text{Exp}_{\mathbf{m}_0}(\tilde{v})$ on the Grassmann manifold, so we obtain an interpolation which can be not well-defined. In the previous work [19, 3], an injectivity condition on the exponential map was defined using the *injectivity radius* of $\mathcal{G}(p, n)$, given by (12), which translate into

$$\|\tilde{v}\| = \left(\tilde{\mathbf{Z}}^T \tilde{\mathbf{Z}} \right)^{1/2} = \left(\sum_{i=1}^p \tilde{\theta}_i^2 \right)^{1/2} < \frac{\pi}{2}$$

265 where $\tilde{\theta}_i$ are the singular values of $\tilde{\mathbf{Z}}$, leading to a weaker condition than the (C2) one
 266 (see Lemma 5.11).

267 **Remark 4.2** (Violation of stability condition (C2) from an application point of view). Let
 268 us consider the case of the north hemisphere of the $2D$ sphere of radius 1, with $\mathbf{m}_0 = N$
 269 being the North Pole. The tangent plane is simply given by \mathbb{R}^2 , and to any velocity vector
 270 $v \in \mathbb{R}^2$ corresponds a point on the north hemisphere, using the exponential map. Here,
 271 the exponential map is non injective for all $v \in \mathbb{R}^2$ with length greater than $\pi/2$. If the
 272 interpolated curve inside \mathbb{R}^2 is outside the disk of radius $\pi/2$ (see Figure 1), then the
 273 corresponding interpolated curve on the north hemisphere is disconnected.

274 4.2 Interpolation algorithm from Lagrange polynomials

275 Let us now produce the algorithm so to obtain an interpolated point $\tilde{\mathbf{m}}$ corresponding to
 276 a target parameter $\tilde{\lambda}$. Such an algorithm is directly issued from the seminal work in [18],
 277 but it is modified so to derive a stable realization of interpolation, as we have to consider
 278 conditions (C1) and (C2) from the previous subsection 4.1.

279 As detailed in section 3, the POD of mode p which was applied on snapshot matrices
 280 \mathbf{S}_i (corresponding to the parameter λ_i for $i = 1, \dots, N$) define points $\mathbf{m}_1, \dots, \mathbf{m}_N$ on the
 281 Grassmann manifold $\mathcal{G}(p, n)$, and thus matrices in $\text{Mat}_{n,p}(\mathbb{R})$ with orthonormal column
 282 vectors.

283 **Algorithm 4.3** (Interpolation on a Grassman manifold $\mathcal{G}(p, n)$).

284

285 **Input :**

- 286 • Integers p, n such that $2p \leq n$.
- 287 • Matrices $\mathbf{Y}_1, \dots, \mathbf{Y}_N$ in $\text{Mat}_{n,p}(\mathbb{R})$ such that $\mathbf{Y}_i^T \mathbf{Y}_i = \mathbf{I}_p$, respectively correspond-
- 288 ing to a given set of parameters $\lambda_1, \dots, \lambda_N$

- 289 • A target parameter $\tilde{\lambda}$

290 **Output** : A new matrix $\tilde{\mathbf{Y}}$ defining a new point $\tilde{\mathbf{m}} \in \mathcal{G}(p, n)$, corresponding to the target
291 parameter $\tilde{\lambda}$.

292 **Computations** :

1. Choose a matrix $\mathbf{Y}_0 \in \{\mathbf{Y}_1, \dots, \mathbf{Y}_N\}$ such that

$$(C1) \text{ stability : } \mathbf{Y}_0^T \mathbf{Y}_i \text{ is non singular for all } i$$

2. For each $i = 1, \dots, N$, make a thin SVD and compute an $n \times p$ matrix \mathbf{Z}_i :

$$\mathbf{Y}_i (\mathbf{Y}_0^T \mathbf{Y}_i)^{-1} - \mathbf{Y}_0 = \mathbf{U}_i \boldsymbol{\Sigma}_i \mathbf{V}_i^T$$

$$\mathbf{Z}_i := \mathbf{U}_i \arctan(\boldsymbol{\Sigma}_i) \mathbf{V}_i^T,$$

293 all issued from the logarithm map (Definition 5.9).

3. Compute an interpolated matrix and a thin SVD

$$\tilde{\mathbf{Z}} := \sum_{i=1}^N \prod_{j \neq i} \frac{\tilde{\lambda} - \lambda_j}{\lambda_i - \lambda_j} \mathbf{Z}_i = \tilde{\mathbf{U}} \tilde{\boldsymbol{\Theta}} \tilde{\mathbf{V}}$$

294 4. (C2) stability: If $\tilde{\theta}_1 > \pi/2$, with $\tilde{\theta}_1$ the largest singular value of $\tilde{\mathbf{Z}}$, then return an
295 *instability message*.

5. Otherwise return the $n \times p$ matrix

$$\tilde{\mathbf{Y}} := \mathbf{Y}_0 \tilde{\mathbf{V}} \cos \tilde{\boldsymbol{\Theta}} + \tilde{\mathbf{U}} \sin \tilde{\boldsymbol{\Theta}}$$

296 issued from the exponential map 11.

297 4.3 Instability problem due to increasing mode

As one should expect, the accuracy of the interpolation algorithm 4.3 should improve as the number p of mode increase. In fact, when considering the snapshot matrices $\mathbf{S}_1, \dots, \mathbf{S}_N$

associated to parameters $\lambda_1, \dots, \lambda_N$, a POD of mode p define subspaces $\mathcal{V}_1, \dots, \mathcal{V}_N$ of dimension p (see [section 3](#)). By construction, for another mode $p' > p$, the corresponding subspaces $\mathcal{V}'_1, \dots, \mathcal{V}'_N$ are such that

$$\mathcal{V}_i \subset \mathcal{V}'_i.$$

298 Take now a new parameter $\tilde{\lambda}$ and suppose that [algorithm 4.3](#) returns matrices $\tilde{\mathbf{Y}}$ and $\tilde{\mathbf{Y}}'$
 299 which correspond respectively to mode p and $p' > p$ interpolation. A stability condition
 300 should be

- 301 • (C3) The subspaces $\tilde{\mathcal{V}}$ and $\tilde{\mathcal{V}}'$ respectively associated to the matrices $\tilde{\mathbf{Y}}$ and $\tilde{\mathbf{Y}}'$ are
 302 such that $\tilde{\mathcal{V}} \subset \tilde{\mathcal{V}}'$.

More generally, let us consider two subspaces \mathcal{V} and \mathcal{V}' of different dimensions $p < p'$, represented by matrices $\mathbf{Y} \in \text{Mat}_{n,p}(\mathbb{R})$ and $\mathbf{Y}' \in \text{Mat}_{n,p'}(\mathbb{R})$ such that

$$\mathbf{Y}^T \mathbf{Y} = \mathbf{I}_p, \quad (\mathbf{Y}')^T \mathbf{Y}' = \mathbf{I}_{p'}.$$

303 One method to measure the non-inclusion defect between subspaces \mathcal{V} and \mathcal{V}' is to consider
 304 the *geometric distance* $\delta(\mathcal{V}, \mathcal{V}')$, issued from [\[26\]](#), and defined using *principal angles* as
 305 follows: taking singular values of $\mathbf{Y}^T \mathbf{Y}' \in \text{Mat}_{p,p'}(\mathbb{R})$ to be $\sigma_1 \geq \dots \geq \sigma_p \geq 0$, we have

$$306 \quad \delta(\mathcal{V}, \mathcal{V}') = \delta(\mathbf{Y}, \mathbf{Y}') := \left(\sum_{i=1}^{\min(p,p')} \arccos^2(\sigma_i) \right)^{1/2}. \quad (1)$$

307 We are finally able to check stability condition (C3) using the following:

- 308 1. Assume a set of POD modes $p \in \mathcal{P}_m$ and a threshold value T_V .
- 309 2. For a given integer p and a given target parameter $\tilde{\lambda}$, compute matrix $\tilde{\mathbf{Y}}$ issued from
 310 [Algorithm 4.3](#).
- 311 3. For $p' > p$ compute matrix $\tilde{\mathbf{Y}}'$ issued from the same algorithm [Algorithm 4.3](#).

312 4. As we have $\tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}} = \mathbf{I}_p$ and $(\tilde{\mathbf{Y}}')^T \tilde{\mathbf{Y}}' = \mathbf{I}_{p'}$, from Lemma 5.5, we deduce a geometric
 313 distance $\delta(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}')$ computed by (1).

314 5. Calculate the indicator ϵ for the non-inclusion between subspaces formalized as follows

$$315 \quad \epsilon = (\delta_{\max}(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}') - \delta_{\min}(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}')) / (\delta_{\min}(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}')), \quad p \in \mathcal{P}_m \quad (2)$$

316 6. If $\epsilon \geq T_V$ then return an instability message.

317 Let us now describe the utilization of the (C3) stability condition from the application
 318 point of view. Computing of the geometric distance $\delta(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}')$ leads to an understanding
 319 of the non-monotonic oscillatory behavior of the error norm due to increasing mode p .
 320 According to the numerical problems studied here, the first one (see Figure 10) clearly
 321 shows an oscillatory unstable behavior, while the second one seems stable (see Figure 20):
 322 we thus compared the two values of the indicator ϵ given by (2), for each problem, and
 323 propose $T_V = 100$ as a reference threshold.

324 5 Riemannian geometry of Grassmann Manifolds

325 The purpose of this section is to recall the main results about Grassmann manifolds, as
 326 well as new ones about the *cut-locus* and injectivity condition for the exponential map.
 327 As far as we know, the normal coordinates are classically defined using the exponential
 328 map restricted on an open disk deduced from the injectivity radius [25,3]. In fact, it will
 329 be possible to go beyond such an injectivity radius, using an open set deduced from the
 330 *cut-locus* of the Grassmann manifold, all this being detailed in subsection 5.4.

331 Note that some results recalled here are classical, either given in their matrix forms [22,
 332 18,21,19,3,41], or given in a more abstract one [42,25], but it was necessary to write

333 them back for our proofs to be clearly established. All details about general differential
 334 Riemannian geometry can be found in [43, 31, 23].

From now on, let us consider two integers p, n such that $p \leq n$ and take $\mathcal{G}(p, n)$ to be the Grassmann manifold of p dimensional subspaces of \mathbb{R}^n . A first way to obtain a point $\mathbf{m} \in \mathcal{G}(p, n)$ is to consider a basis $\mathbf{y}_1, \dots, \mathbf{y}_p$ of the associated subspace

$$\mathbf{m} = \text{Vect}(\mathbf{y}_1, \dots, \mathbf{y}_p).$$

Without loss of generality, we can assume the case of *orthonormal basis*, so \mathbf{m} can be represented by a matrix

$$\mathbf{Y} := [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \text{Mat}_{n,p}(\mathbb{R}), \quad \mathbf{Y}^T \mathbf{Y} = \mathbf{I}_p.$$

Such matrix \mathbf{Y} is not unique, as any matrix in the set

$$\{\mathbf{Y}\mathbf{P}, \quad \mathbf{P} \in \text{O}(p)\}, \quad \text{O}(p) := \{\mathbf{P} \in \text{Mat}_{p,p}(\mathbb{R}), \quad \mathbf{P}^T \mathbf{P} = \mathbf{I}_p\},$$

335 can represent the same point \mathbf{m} .

From this, the Grassmann manifold $\mathcal{G}(p, n)$ is obtained as a *quotient space* [43, Chapter 21] of the (compact) space of p ordered orthonormal vectors of \mathbb{R}^n . More specifically [44, Appendix C.2], first define the compact Stiefel manifold $\mathcal{St}^c(p, n)$ to be the set of p orthonormal vectors $\{\mathbf{y}_1, \dots, \mathbf{y}_p\}$ of \mathbb{R}^n . Taking any basis of \mathbb{R}^n , such a set can be represented by a rank p matrix

$$\mathbf{Y} := [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \text{Mat}_{n,p}(\mathbb{R}), \quad \mathbf{Y}^T \mathbf{Y} = \mathbf{I}_p.$$

336 This led to define a *fiber bundle* [45, 46], which is also a *submersion* [43]:

$$337 \quad \pi : \mathbf{Y} \in \mathcal{St}^c(p, n) \mapsto \pi(\mathbf{Y}) = \mathbf{m} := \{\mathbf{Y}\mathbf{P}, \quad \mathbf{P} \in \text{O}(p)\} \in \mathcal{G}(p, n) \quad (3)$$

338 Informally speaking, it means that any point \mathbf{m} of the Grassmann manifold $\mathcal{G}(p, n)$ can
 339 be represented by any point \mathbf{Y} of the *fiber* $\pi^{-1}(\mathbf{m})$ (Figure 2).

340 5.1 The Grassmann Manifold and its Riemannian metric

341 From the submersion π given by (3), the Grassmann manifold $\mathcal{G}(p, n)$ can inherit the
 342 geometry of the Stiefel manifold $\mathcal{St}^c(p, n)$ and its Riemannian structure [23].

First, the Stiefel manifold $\mathcal{St}^c(p, n) \subset \text{Mat}_{n,p}(\mathbb{R})$, is naturally endowed with an inner product given by

$$\langle \mathbf{Z}_1, \mathbf{Z}_2 \rangle := \text{tr}(\mathbf{Z}_1^T \mathbf{Z}_2), \quad \mathbf{Z}_1, \mathbf{Z}_2 \in \text{Mat}_{n,p}(\mathbb{R}).$$

343 Now, we need to attach, to each $\mathbf{m} \in \mathcal{G}(p, n)$ a *tangent space* $T_{\mathbf{m}}\mathcal{G}(p, n)$, which is a vector
 344 space isomorphic to $\mathbb{R}^{p \times (n-p)}$, equipped with a scalar product (depending smoothly on
 345 \mathbf{m}), so that $\mathcal{G}(p, n)$ becomes a Riemannian manifold.

346 In fact, there is no canonical way to get a representation of a velocity vector $v \in$
 347 $T_{\mathbf{m}}\mathcal{G}(p, n)$, as it depends on the choice of a matrix $\mathbf{Y} \in \mathcal{St}^c(p, n)$ defining \mathbf{m} (see Figure 2):
 348 for any $\mathbf{Y} \in \pi^{-1}(\mathbf{m})$, we define indeed its associated *horizontal space* by:

$$349 \quad \text{Hor}_{\mathbf{Y}} := \{\mathbf{Z} \in \text{Mat}_{n,p}(\mathbb{R}), \quad \mathbf{Z}^T \mathbf{Y} = \mathbf{0}\}. \quad (4)$$

350 Finally:

1. The tangent space $T_{\mathbf{m}}\mathcal{G}(p, n)$ is isomorphic to any $\text{Hor}_{\mathbf{Y}}$ with \mathbf{Y} such that $\pi(\mathbf{Y}) = \mathbf{m}$.

An isomorphism is given by

$$d\pi_{\mathbf{Y}|_{\text{Hor}_{\mathbf{Y}}}} : \text{Hor}_{\mathbf{Y}} \longmapsto T_{\mathbf{m}}\mathcal{G}(p, n).$$

351 2. For any $v \in T_{\mathbf{m}}\mathcal{G}(p, n)$, the unique $\mathbf{Z} \in \text{Hor}_{\mathbf{Y}}$ such that

$$352 \quad d\pi_{\mathbf{Y}} \cdot \mathbf{Z} = v \quad (5)$$

353 is called a *horizontal lift* of v .

3. For any $\mathbf{P} \in O(p)$, then \mathbf{ZP} is another horizontal lift of v (but belonging to the vector space $\text{Hor}_{\mathbf{YP}}$) and

$$d\pi_{\mathbf{YP}} \cdot (\mathbf{ZP}) = v.$$

The Riemannian metric on the Grassmannian $\mathcal{G}(p, n)$ is then defined by

$$\langle v_1, v_2 \rangle_{\mathbf{m}} := \langle \mathbf{Z}_1, \mathbf{Z}_2 \rangle_{\mathbf{Y}},$$

354 with $\pi(\mathbf{Y}) = \mathbf{m}$ and \mathbf{Z}_1 (resp. \mathbf{Z}_2) a horizontal lift of v_1 (resp. v_2) in $\text{Hor}_{\mathbf{Y}}$.

355 For the proofs of the following subsections, an interesting geometric approach, due to
356 Zhou [47], is given by:

Lemma 5.1. *Let $\mathbf{m} \in \mathcal{G}(p, n)$ and $v \in T_{\mathbf{m}}\mathcal{G}(p, n)$, with $2p \leq n$. Then, there exists an orthonormal basis $\mathbf{y}_1, \dots, \mathbf{y}_n$ of \mathbb{R}^n such that*

$$\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \pi^{-1}(\mathbf{m}), \quad \mathbf{Z} = [\theta_1 \mathbf{y}_{p+1}, \dots, \theta_p \mathbf{y}_{2p}] \in \text{Hor}_{\mathbf{Y}},$$

$$\theta_1 \geq \dots \geq \theta_p \geq 0.$$

Proof Let us consider any $\mathbf{Y} \in \pi^{-1}(\mathbf{m})$ and a horizontal lift \mathbf{Z} of v such that $\mathbf{Z}^T \mathbf{Y} = \mathbf{0}$.

We define a thin singular value decomposition of \mathbf{Z} , so we can find orthonormal vectors $\mathbf{u}_1, \dots, \mathbf{u}_p$ in \mathbb{R}^n and $\mathbf{v}_1, \dots, \mathbf{v}_p$ in \mathbb{R}^p such that

$$\mathbf{Z} = \sum \theta_i \mathbf{u}_i \mathbf{v}_i^T, \quad \theta_1 \geq \dots \geq \theta_p \geq 0.$$

From the condition $\mathbf{Z}^T \mathbf{Y} = \mathbf{0}$ we thus deduce that $\mathbf{y}_1, \dots, \mathbf{y}_p, \mathbf{u}_1, \dots, \mathbf{u}_p$ is a family of orthonormal vectors. Taking now the matrix $\mathbf{P} := [\mathbf{v}_1, \dots, \mathbf{v}_p] \in O(p)$ and $\mathbf{Y}' := \mathbf{Y}\mathbf{P} \in \pi^{-1}(\mathbf{m})$, we obtain

$$\mathbf{Z}' := [\theta_1 \mathbf{y}_{p+1}, \dots, \theta_p \mathbf{y}_{2p}] \in \text{Hor}_{\mathbf{Y}\mathbf{P}}, \quad \mathbf{y}_{p+i} := \mathbf{u}_i,$$

357 so we can conclude.

Remark 5.2. In the case when $2p > n$, that is $p > n - p$, then we can only write a horizontal lift as

$$\mathbf{Z} = [\theta_1 \mathbf{y}_{p+1}, \dots, \theta_{n-p} \mathbf{y}_n, \underbrace{\mathbf{0}, \dots, \mathbf{0}}_{2p-n \text{ times}}], \quad \theta_1 \geq \dots \geq \theta_{n-p} \geq 0.$$

358 *5.2 Geodesics and distance on Grassmann manifolds*

359 The Grassmann manifold $\mathcal{G}(p, n)$ being equipped with a Riemannian metric, it is possible
360 to define the length of any curve $c : [0; 1] \rightarrow \mathcal{G}(p, n)$:

$$361 \quad L(c) = \int_0^1 \langle \dot{c}(t), \dot{c}(t) \rangle_{c(t)} dt \quad (6)$$

362 and so the associated *Riemannian distance*

$$363 \quad d_r(\mathbf{m}, \mathbf{m}') := \inf\{L(c), \quad c(0) = \mathbf{m}, c(1) = \mathbf{m}'\}. \quad (7)$$

364 To obtain an explicit computation of such a distance, one can use the *geodesics* obtained
365 from the Riemannian metric and its associated *Levi-Civita connection* [23, 43] (see also [45,
366 III.6]). First recall that for Grassmann manifold, geodesics are obtained explicitly [42, 22]:

367 **Theorem 5.3.** Let $\mathbf{m} \in \mathcal{G}(p, n)$ and $v \in T_{\mathbf{m}}\mathcal{G}(p, n)$ with horizontal lift given by $\mathbf{Z} \in \text{Hor}_{\mathbf{Y}}$,
 368 where $\pi(\mathbf{Y}) = \mathbf{m}$ and $\mathbf{Y}^T \mathbf{Y} = \mathbf{I}_p$. Let $\mathbf{Z} = \mathbf{U}\Theta\mathbf{V}^T$ be a thin singular value decomposition
 369 of \mathbf{Z} . Then

$$370 \quad \alpha_v : t \in \mathbb{R} \mapsto \pi(\mathbf{Y}\mathbf{V} \cos(t\Theta) + \mathbf{U} \sin(t\Theta)) \in \mathcal{G}(p, n) \quad (8)$$

371 is the unique maximal geodesic such that $\alpha_v(0) = \mathbf{m}$ and $\dot{\alpha}_v(0) = v$, maximality meaning
 372 here that such curve is defined on all \mathbb{R} .

Remark 5.4. There is another approach proposed in [47] which produces a more intrinsic formula for the geodesics. Indeed, let us consider $2p \leq n$ and take back the result from Lemma 5.1. Then one horizontal lift of v can write

$$\mathbf{Z} = [\theta_1 \mathbf{y}_{p+1}, \dots, \theta_p \mathbf{y}_{2p}], \quad \theta_1 \geq \dots \geq \theta_p \geq 0.$$

where $\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \pi^{-1}(\mathbf{m})$ and $\mathbf{y}_1, \dots, \mathbf{y}_{2p}$ is an orthonormal family. The unique geodesic obtained from velocity vector v is then defined by $\pi(\mathbf{Y}(t))$, with

$$\mathbf{Y}(t) = [\cos(\theta_1 t) \mathbf{y}_1 + \sin(\theta_1 t) \mathbf{y}_{p+1}, \dots, \cos(\theta_p t) \mathbf{y}_p + \sin(\theta_p t) \mathbf{y}_{2p}].$$

We observe that the norm of the velocity vector is given by

$$\|v\| = \sqrt{\sum \theta_i^2}.$$

373 In fact, all matrices given by (8) are lying in $\mathcal{St}^c(p, n)$:

Lemma 5.5. Let $\mathbf{m} \in \mathcal{G}(p, n)$ and $v \in T_{\mathbf{m}}\mathcal{G}(p, n)$. Take $\mathbf{Y} \in \pi^{-1}(\mathbf{m})$ and $\mathbf{Z} \in \text{Hor}_{\mathbf{Y}}$ like in statement of Theorem 5.3. Then for any $t \in \mathbb{R}$ we have

$$\mathbf{Y}(t) := \mathbf{Y}\mathbf{V} \cos(t\Theta) + \mathbf{U} \sin(t\Theta) \in \mathcal{St}^c(p, n), \text{ meaning that } \mathbf{Y}(t)^T \mathbf{Y}(t) = \mathbf{I}_p.$$

Proof By direct computation we have:

$$\begin{aligned}\mathbf{Y}(t)^T \mathbf{Y}(t) &= \cos^2(t\boldsymbol{\Theta}) + \sin^2(t\boldsymbol{\Theta}) + \mathbf{X} + \mathbf{X}^T, \quad \mathbf{X} := \sin(t\boldsymbol{\Theta})\mathbf{U}^T \mathbf{Y} \mathbf{V} \cos(t\boldsymbol{\Theta}) \\ &= \mathbf{I}_p + \mathbf{X} + \mathbf{X}^T.\end{aligned}$$

As we have $\mathbf{Z} = \mathbf{U}\boldsymbol{\Theta}\mathbf{V}^T$ and $\mathbf{Z}^T \mathbf{Y} = 0$ we deduce that

$$\mathbf{V}\boldsymbol{\Theta}\mathbf{U}^T \mathbf{Y} = 0, \quad \mathbf{V} \in O(p) \implies \boldsymbol{\Theta}\mathbf{U}^T \mathbf{Y} = 0.$$

374 and thus $\sin(t\boldsymbol{\Theta})\mathbf{U}^T \mathbf{Y} = 0$ for all t , which concludes the proof.

375 As a consequence of Hopf-Rinow Theorem [23, Theorem 2.103], any two points of the
376 Grassmann manifold can be joined by a length minimizing geodesic. An explicit expression
377 of such a geodesic is given also in [25]):

378 **Theorem 5.6.** *Let $\mathbf{m}, \mathbf{m}' \in \mathcal{G}(p, n)$ be any two points on the Grassmann manifold $\mathcal{G}(p, n)$.*

379 *Then, for $2p \leq n$:*

(1) *There exists an orthonormal family $\mathbf{y}_1, \dots, \mathbf{y}_n$ of \mathbb{R}^n such that*

$$\begin{aligned}\mathbf{Y}' &= [\cos(\theta_1)\mathbf{y}_1 + \sin(\theta_1)\mathbf{y}_{p+1}, \dots, \cos(\theta_p)\mathbf{y}_p + \sin(\theta_p)\mathbf{y}_{2p}] \in \pi^{-1}(\mathbf{m}'), \\ \mathbf{Y} &= [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \pi^{-1}(\mathbf{m}),\end{aligned}$$

380 *with $\theta_i \in [0, \pi/2]$ are the Jordan's principal angles between \mathbf{Y} and \mathbf{Y}' , meaning that*

381 *$\theta_i = \arccos(\sigma_{p-i+1})$, where $0 \leq \sigma_p \leq \dots \leq \sigma_1$ are the singular values of $\mathbf{Y}^T \mathbf{Y}'$.*

(2) *A length minimizing geodesic from \mathbf{m} to \mathbf{m}' is given by $t \in [0, 1] \mapsto \pi(\mathbf{Y}(t))$ with*

$$\mathbf{Y}(t) := [\cos(t\theta_1)\mathbf{y}_1 + \sin(t\theta_1)\mathbf{y}_{p+1}, \dots, \cos(t\theta_p)\mathbf{y}_p + \sin(t\theta_p)\mathbf{y}_{2p}].$$

382 *Furthermore, such length minimizing geodesic is unique if and only if $\theta_1 < \pi/2$.*

In the case $2p > n$, the same result holds using

$$\mathbf{Y}' = [\cos(\theta_1)\mathbf{y}_1 + \sin(\theta_1)\mathbf{y}_{p+1}, \dots, \cos(\theta_{n-p})\mathbf{y}_{n-p} + \sin(\theta_{n-p})\mathbf{y}_{n-p}, \\ \mathbf{y}_{n-p+1}, \dots, \mathbf{y}_p] \in \pi^{-1}(\mathbf{m}).$$

Proof Take any $\mathbf{Y} \in \pi^{-1}(\mathbf{m})$ and $\mathbf{Y}' \in \pi^{-1}(\mathbf{m}')$. Let now consider a *reordered* SVD of the square matrix $\mathbf{Y}^T \mathbf{Y}'$:

$$\mathbf{Y}^T \mathbf{Y}' = \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^T, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_p & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_1 \end{pmatrix}, \quad \mathbf{U}, \mathbf{V} \in \mathbf{O}(p),$$

with singular values $0 \leq \sigma_p \leq \dots \leq \sigma_1$. Define

$$\widehat{\mathbf{Y}} := \mathbf{Y} \mathbf{U} \in \pi^{-1}(\mathbf{m}), \quad \widehat{\mathbf{Y}}' := \mathbf{Y}' \mathbf{V} \in \pi^{-1}(\mathbf{m}')$$

and write

$$\widehat{\mathbf{Y}} = [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \text{Mat}_{n,p}(\mathbb{R}), \quad \widehat{\mathbf{Y}}' = [\mathbf{x}_1, \dots, \mathbf{x}_p] \in \text{Mat}_{n,p}(\mathbb{R})$$

so we can deduce from $\widehat{\mathbf{Y}}^T \widehat{\mathbf{Y}}' = \boldsymbol{\Sigma}$ the inner products

$$\langle \mathbf{y}_i, \mathbf{x}_j \rangle = \sigma_{p-i+1} \delta_{ij}, \quad \sigma_{p-i+1} \in [0, 1].$$

Using a direct induction on i , we obtain a family of orthonormal vectors $\mathbf{y}_{p+1}, \dots, \mathbf{y}_{2p}$ such that

$$\mathbf{x}_i = \cos(\theta_i)\mathbf{y}_i + \sin(\theta_i)\mathbf{y}_{p+i}, \quad \theta_i := \arccos(\sigma_{p-i+1}), \quad \langle \mathbf{y}_i, \mathbf{y}_{p+j} \rangle = 0$$

383 which conclude the proof of (1).

Now, from Remark 5.4, any other geodesic from \mathbf{m} to \mathbf{m}' reads $t \mapsto \pi(\mathbf{Y}(t))$ with

$$\mathbf{Y}(t) = [\cos(\alpha_1 t)\mathbf{y}_1 + \sin(\alpha_1 t)\mathbf{y}_{p+1}, \dots, \cos(\alpha_p t)\mathbf{y}_p + \sin(\alpha_p t)\mathbf{y}_{2p}], \quad \pi(\mathbf{Y}(1)) = \mathbf{m}'$$

so that $\cos(\alpha_i) = \cos(\theta_i)$ and $\alpha_i = \theta_i + k_i\pi$, with $k_i \in \mathbb{Z}$. We deduce that the length of this geodesic is given by

$$\left(\sum_{i=1}^p (\theta_i + k_i\pi)^2 \right)^{1/2}.$$

As $(\theta + k\pi)^2 \geq \theta^2$ for all $k \in \mathbb{Z}$ and $\theta \in [0, \pi/2]$, we deduce length minimization for $k_i = 0$.

Non unicity can only occur if and only if there is non-zero $k_i \in \mathbb{Z}$ such that $\theta_i + k_i\pi = -\theta_i$, so that

$$k_i = \frac{-2\theta_i}{\pi} \in \mathbb{Z} - \{0\}$$

384 which translate into $\theta_i = \theta_{i-1} = \dots = \theta_1 = \pi/2$, which conclude the proof.

385 As a consequence of Theorem 5.6, for any two points \mathbf{m} and \mathbf{m}' of $\mathcal{G}(p, n)$ the Rie-
386 mannian distance is given by

$$387 \quad d_r(\mathbf{m}, \mathbf{m}') = \left(\sum_{i=1}^p \theta_i^2 \right)^{1/2} \quad (9)$$

388 with θ_i the Jordan's principal angles as defined in the statement of the theorem. Finally,
389 the *diameter* of $\mathcal{G}(p, n)$ (the maximum distance between two points) is given by

$$390 \quad \text{diam} = \sqrt{r} \frac{\pi}{2}, \quad r = \min(p, n - p). \quad (10)$$

391 5.3 Exponential and logarithm map on Grassmann manifolds

392 By exploiting geodesics of a Riemannian manifold, it is possible to establish local maps
393 using *normal coordinates* [23] defined from the exponential map.

394 In the case of Grassmann manifolds, the exponential map is obtained from the exact
395 formulation of the geodesics (see Theorem 5.3).

396 **Definition 5.7** (Exponential map). For any point $\mathbf{m} \in \mathcal{G}(p, n)$, let consider the tangent
 397 plane $T_{\mathbf{m}}\mathcal{G}(p, n) \simeq \mathbb{R}^d$, with $d = p(n - p)$ the dimension of $\mathcal{G}(p, n)$. Then the exponential
 398 map is defined by

$$399 \quad \text{Exp}_{\mathbf{m}} : v \in T_{\mathbf{m}}\mathcal{G}(p, n) \mapsto \pi(\mathbf{Y}\mathbf{V} \cos \Theta + \mathbf{U} \sin \Theta) \in \mathcal{G}(p, n) \quad (11)$$

400 where $\mathbf{Y} \in \pi^{-1}(\mathbf{m})$ and $\mathbf{Z} = \mathbf{U}\Theta\mathbf{V}^T$ is a thin SVD of a horizontal lift $\mathbf{Z} \in \text{Hor}_{\mathbf{Y}}$ of v .

401 Such a map is only a diffeomorphism *locally*, meaning that there exists some open
 402 set $W \subset T_{\mathbf{m}}\mathcal{G}(p, n)$ containing 0 such that $(\text{Exp}_{\mathbf{m}})|_W$ is a diffeomorphism, which thus
 403 makes it possible to define local coordinates on W . A first way to do so is to consider the
 404 *injectivity radius* and thus the open disk:

$$405 \quad D_{\mathbf{m}} := \{v \in T_{\mathbf{m}}\mathcal{G}(p, n), \quad \|v\| < \pi/2\}, \quad (12)$$

where $\pi/2$ is the injectivity radius of Grassmann manifolds [25]. We obtain here a local
 map

$$(\text{Exp}_{\mathbf{m}})|_{D_{\mathbf{m}}} : D_{\mathbf{m}} \longrightarrow \text{Exp}_{\mathbf{m}}(D_{\mathbf{m}}).$$

406 It turns out that in our case, it is possible to go beyond this injectivity radius. To do so,
 407 a logarithm map is directly define at each point of the Grassmann manifold.

408 First, for any point $\mathbf{m} \in \mathcal{G}(p, n)$, let us define the open set

$$409 \quad U_{\mathbf{m}} := \{\mathbf{m}' \in \mathcal{G}(p, n), \quad \mathbf{Y}^T \mathbf{Y}' \text{ is invertible}, \quad \pi(\mathbf{Y}) = \mathbf{m}, \quad \pi(\mathbf{Y}') = \mathbf{m}'\}. \quad (13)$$

410 A more geometric insight of such an open set is given by a lemma directly deduced from
 411 Jordan's principal angles (see Theorem 5.6):

412 **Lemma 5.8.** *For any $\mathbf{m}, \mathbf{m}' \in \mathcal{G}(p, n)$, take $0 \leq \theta_p \leq \dots \leq \theta_1 \leq \pi/2$ to be their*
 413 *corresponding Jordan's principal angles. Then $\mathbf{m}' \in U_{\mathbf{m}}$ if and only if $\theta_1 < \pi/2$.*

414 From now on, let us suppose that $2p \leq n$, while the case $2p > n$ is straightforward.

Following Theorem 5.6, we can find an orthonormal family $\mathbf{y}_1, \dots, \mathbf{y}_n$ of \mathbb{R}^n such that

$$\mathbf{Y}' = [\cos(\theta_1)\mathbf{y}_1 + \sin(\theta_1)\mathbf{y}_{p+1}, \dots, \cos(\theta_p)\mathbf{y}_p + \sin(\theta_p)\mathbf{y}_{2p}] \in \pi^{-1}(\mathbf{m}'), \quad (14)$$

$$\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \pi^{-1}(\mathbf{m}),$$

415 and then $\mathbf{Y}^T \mathbf{Y}' = \cos \boldsymbol{\Theta}$. The classical definition of the logarithm map [3] makes use of a
416 thin SVD of

$$417 \quad \mathbf{Y}' (\mathbf{Y}^T \mathbf{Y}')^{-1} - \mathbf{Y} = [\tan(\theta_1)\mathbf{y}_{p+1}, \dots, \tan(\theta_p)\mathbf{y}_{2p}] \quad (15)$$

418 where singular values are well-defined (as a consequence of Lemma 5.8). From all this, it
419 is possible to have the following definition, using the arctan function:

Definition 5.9 (Logarithm map in Grassmann manifolds). For any $\mathbf{m} \in \mathcal{G}(p, n)$, take the open set $U_{\mathbf{m}}$ defined by (13). Then the logarithm map at \mathbf{m} is given by

$$\text{Log}_{\mathbf{m}} : \mathbf{m}' \in U_{\mathbf{m}} \mapsto \text{Log}_{\mathbf{m}}(\mathbf{m}') \in T_{\mathbf{m}}\mathcal{G}(p, n)$$

where an horizontal lift \mathbf{Z} of $\text{Log}_{\mathbf{m}}(\mathbf{m}')$ is defined using a thin SVD

$$\mathbf{Y}' (\mathbf{Y}^T \mathbf{Y}')^{-1} - \mathbf{Y} = \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^T, \quad \mathbf{Y}' \in \pi^{-1}(\mathbf{m}'),$$

so that

$$\mathbf{Z} := \mathbf{U} \arctan(\boldsymbol{\Sigma}) \mathbf{V}^T.$$

As a direct consequence of (14) and (15), the horizontal lift \mathbf{Z} of $v = \text{Log}_{\mathbf{m}}(\mathbf{m}')$ encodes the Jordan's principal angles between \mathbf{m} and \mathbf{m}' , as we can write in the orthonormal basis $\mathbf{y}_1, \dots, \mathbf{y}_n$ of \mathbb{R}^n :

$$\mathbf{Z} = [\theta_1 \mathbf{y}_{p+1}, \dots, \theta_p \mathbf{y}_{2p}].$$

420 From Remark 5.4, we deduce that we have $\text{Exp}_{\mathbf{m}}(v) = \mathbf{m}'$, leading to:

Lemma 5.10. *For any $\mathbf{m} \in \mathcal{G}(p, n)$, the map $\text{Log}_{\mathbf{m}}$ is a diffeomorphism from $U_{\mathbf{m}}$ onto $\text{Log}_{\mathbf{m}}(U_{\mathbf{m}})$, with inverse map given by the exponential map at \mathbf{m} :*

$$\text{Exp}_{\mathbf{m}} \circ \text{Log}_{\mathbf{m}} = \text{id}_{U_{\mathbf{m}}}.$$

421 As a conclusion of this subsection, we obtain here normal coordinates on all the open
 422 set $U_{\mathbf{m}}$, which is in fact an improvement compared to the open set deduced from the
 423 injectivity radius disk, thanks to the lemma:

Lemma 5.11. *For any $\mathbf{m} \in \mathcal{G}(p, n)$ and n, p such that $\min(p, n - p) \geq 2$, the open set $U_{\mathbf{m}}$ given by (13) strictly contains $\text{Exp}_{\mathbf{m}}(D_{\mathbf{m}})$, with $D_{\mathbf{m}}$ given by (12):*

$$\text{Exp}_{\mathbf{m}}(D_{\mathbf{m}}) \subsetneq U_{\mathbf{m}}.$$

Proof The inclusion follows from Theorem 5.15 as any $v \in D_{\mathbf{m}}$ is such that

$$\|v\| < \frac{\pi}{2}.$$

To obtain a strict inclusion we follow Remark 5.4 in the case $2p \leq n$. Let us consider an orthonormal basis $\mathbf{y}_1, \dots, \mathbf{y}_n$ and v with horizontal lift given by

$$\mathbf{Z} = [\theta_1 \mathbf{y}_{p+1}, \dots, \theta_p \mathbf{y}_{2p}].$$

Then we can find $\theta_1, \dots, \theta_p$ such that

$$\|v\| = \left(\sum \theta_i^2 \right)^{1/2} \geq \pi/2 \text{ and } \theta_1 < \pi/2$$

using for instance

$$\theta_i := \alpha < \frac{\pi}{2} \text{ with } \frac{\pi}{2} \leq \sqrt{p}\alpha.$$

424 *5.4 Cut-locus and exponential map injectivity on Grassmann manifolds*

425 In this final subsection, it is proposed to establish the link between the open set $U_{\mathbf{m}}$
 426 defined by (13) and the cut-locus of Grassmann manifolds. Such a notion of cut-locus is
 427 particularly related to the loss of injectivity of the exponential map. As far as we know,
 428 such a result about the cut-locus was suggested in [24], but without any clear proof nor
 429 statement.

Let us take back here the geodesic $t \in \mathbb{R} \mapsto \alpha_v(t)$ from (8), with non-zero initial velocity $v \in T_{\mathbf{m}}\mathcal{G}(p, n)$. Define now

$$I_v := \{t \in \mathbb{R}, \quad (\alpha_v)|_{[0,t]} \text{ is length minimal}\} = [0, \rho(v)],$$

430 where $\rho(v)$ is some bounded real number (see [23, Section 2.C.7]). A first result is given
 431 by [23, Theorem 3.77]:

432 **Theorem 5.12.** *Let $\mathbf{m} \in \mathcal{G}(p, n)$ and*

$$433 \quad V_{\mathbf{m}} := \{v \in T_{\mathbf{m}}\mathcal{G}(p, n), \quad \rho(v) > 1\} \cup \{0\}. \quad (16)$$

Then $V_{\mathbf{m}}$ is an open neighborhood of $0 \in T_{\mathbf{m}}\mathcal{G}(p, n)$ and the map

$$(\text{Exp}_{\mathbf{m}})|_{V_{\mathbf{m}}} : V_{\mathbf{m}} \longrightarrow \text{Exp}_{\mathbf{m}}(V_{\mathbf{m}})$$

434 *is a diffeomorphism.*

435 The image of the boundary $\partial V_{\mathbf{m}}$ then define the cut-locus:

Definition 5.13 (Cut-locus). For any point $\mathbf{m} \in \mathcal{G}(p, n)$, the cut-locus of \mathbf{m} is given by

$$\text{Cut}(\mathbf{m}) := \{\text{Exp}_{\mathbf{m}}(\rho(v)v), \quad \|v\| = 1\}.$$

436 In the specific case of Grassmann manifolds, there is a way to explicitly obtain the
 437 bound $\rho(v)$, while the main ideas are directly taken from [25, Theorem 12.5]:

Lemma 5.14. *Let $\mathbf{m} \in \mathcal{G}(p, n)$ and $v \in T_{\mathbf{m}}\mathcal{G}(p, n)$, with horizontal lift given by some $\mathbf{Z} \in \text{Mat}_{n,p}(\mathbb{R})$. Then we have*

$$\rho(v) = \frac{\pi}{2\theta_1},$$

438 where θ_1 is the maximal singular value of \mathbf{Z} and thus, taking back the open set $V_{\mathbf{m}}$ defined
 439 by (16) we have

$$440 \quad V_{\mathbf{m}} = \left\{ v \in T_{\mathbf{m}}\mathcal{G}(p, n), \quad \theta_1 < \frac{\pi}{2} \right\} \cup \{0\}. \quad (17)$$

Proof From Lemma 5.1, we can consider an orthonormal basis $\mathbf{y}_1, \dots, \mathbf{y}_n$ of \mathbb{R}^n such that $\mathbf{Y} \in \pi^{-1}(\mathbf{m})$ and a horizontal lift \mathbf{Z} of v are given by (for $2p \leq n$):

$$\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_p], \quad \mathbf{Z} = [\theta_1 \mathbf{y}_{p+1}, \dots, \theta_p \mathbf{y}_{2p}],$$

441 where $0 \leq \theta_p \leq \dots \leq \theta_1$ are the singular values of any horizontal lift of v .

Now, from Theorem 5.6 the geodesic $\alpha(t) = \pi(\mathbf{Y}(t))$ with

$$\mathbf{Y}(t) = [\cos(\theta_1 t) \mathbf{y}_1 + \sin(\theta_1 t) \mathbf{y}_{p+1}, \dots, \cos(\theta_p t) \mathbf{y}_p + \sin(\theta_p t) \mathbf{y}_{2p}]$$

442 is minimal for all $t \leq \pi/(2\theta_1)$, and is not unique anymore for $t = \pi/(2\theta_1)$. From [23,
 443 Corollary 2.111], α is no longer minimal on $[0, \pi/(2\theta_1) + \varepsilon]$ for all $\varepsilon > 0$, so we can conclude
 444 (the proof being the same for $2p > n$). The last equation (17) is straightforward.

445 Our main result is now:

Theorem 5.15. *For any $\mathbf{m} \in \mathcal{G}(p, n)$ we have*

$$\text{Exp}_{\mathbf{m}}(V_{\mathbf{m}}) = U_{\mathbf{m}}$$

with $U_{\mathbf{m}}$ and $V_{\mathbf{m}}$ respectively defined by (13) and (16). Furthermore, the cut-locus at \mathbf{m} is given by:

$$\text{Cut}(\mathbf{m}) = \{\mathbf{m}', \quad \mathbf{Y}^T \mathbf{Y}' \text{ is singular}, \quad \pi(\mathbf{Y}) = \mathbf{m}, \quad \pi(\mathbf{Y}') = \mathbf{m}'\}.$$

Proof Taking back Lemma 5.14 recall that

$$V_{\mathbf{m}} = \left\{ v \in T_{\mathbf{m}}\mathcal{G}(p, n), \quad \theta_1 < \frac{\pi}{2} \right\} \cup \{0\}$$

where θ_1 is the maximal singular value of any horizontal lift $\mathbf{Z} \in \text{Mat}_{n,p}(\mathbb{R})$ of v . Take now any $v \in V_{\mathbf{m}}$ and define an orthonormal basis $\mathbf{y}_1, \dots, \mathbf{y}_n$ of \mathbb{R}^n like in Lemma 5.1, so that for $2p \leq n$

$$\text{Exp}_{\mathbf{m}}(v) = \pi([\cos(\theta_1)\mathbf{y}_1 + \sin(\theta_1)\mathbf{y}_{p+1}, \dots, \cos(\theta_p)\mathbf{y}_p + \sin(\theta_p)\mathbf{y}_{2p}]), \quad \theta_1 < \pi/2.$$

446 From Lemma 5.8 we deduce that $\text{Exp}_{\mathbf{m}}(v) \in U_{\mathbf{m}}$ and thus $\text{Exp}_{\mathbf{m}}(V_{\mathbf{m}}) \subset U_{\mathbf{m}}$.

447 The converse is a direct consequence of Theorem 5.6 and Lemma 5.8, all proof being
448 the same for $2p > n$. Finally, the statement for $\text{Cut}(\mathbf{m})$ follows in the same way, so we
449 can conclude.

450 6 Application to Hyperelasticity

451 6.1 Kinematics of Continuum Mechanics Framework

452 Let $\Omega_0 \subset R^3$ and $\Omega \subset R^3$ represent the reference and the current configurations of a body,
453 parameterized in \mathbf{X} and in \mathbf{x} , respectively. The non-linear deformation map $\varphi : \Omega_0 \rightarrow \Omega$ at
454 time t , transforms the referential (material) position \mathbf{X} into the related current (spacial)
455 position $\mathbf{x} = \varphi(\mathbf{X}, t)$. The deformation gradient \mathbf{F} is defined by

$$456 \quad \mathbf{F} := \nabla\varphi(\mathbf{X}) = \frac{\partial\varphi(\mathbf{X})}{\partial\mathbf{X}} = \frac{\partial\mathbf{x}}{\partial\mathbf{X}} \quad (18)$$

457 with the Jacobian $J(\mathbf{X}) = \det(\mathbf{F}) > 0$ (volume ratio). The right and left Cauchy-Green
 458 tensors are defined as $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ and $\mathbf{B} = \mathbf{F}\mathbf{F}^T$, respectively.

459 The three principal invariants of \mathbf{C} which are identical to those of \mathbf{B} are defined as

$$460 \quad I_1 = \text{tr}(\mathbf{C}), \quad I_2 = \frac{1}{2}[(\text{tr}(\mathbf{C}))^2 - \text{tr}(\mathbf{C}^2)], \quad I_3 = \det(\mathbf{C}). \quad (19)$$

461 6.2 Incompressible Transverse Isotropic Material

462 A material with one family of fibers is considered where the stress at a material point
 463 depends not only on the deformation gradient \mathbf{F} but also on the fiber direction. The fibers
 464 are modeled by a *flow* [23] obtained from some unit vector field \mathbf{a}_0 on Ω_0 . The direction
 465 of a fiber at point $\mathbf{X} \in \Omega_0$ is thus obtained by the unit vector $\mathbf{a}_0(\mathbf{X})$, $|\mathbf{a}_0| = 1$.

Note that the unit vector field \mathbf{a}_0 induces a unit vector field \mathbf{a} on current configuration Ω defined by

$$\mathbf{F}(\mathbf{X})\mathbf{a}_0(\mathbf{X}) = \alpha\mathbf{a}(\mathbf{x})$$

466 where the length changes of the fibers along its direction \mathbf{a}_0 is determined by the stretch
 467 α as the ratio between the current and the reference configuration.

Consequently, since $|\mathbf{a}| = 1$, we can define the square of the stretch α following the symmetries of the deformation gradient

$$\alpha^2 = \mathbf{a}_0\mathbf{F}^T\mathbf{F}\mathbf{a}_0 = \mathbf{a}_0\mathbf{C}\mathbf{a}_0.$$

468 *6.3 Linearization of the principle of internal virtual work in the spatial description*

469 The linearization of the internal virtual work in the spatial description reads (see Section
470 8.4 in [35])

$$471 \quad D_{\Delta \mathbf{u}} \delta W_{int}(\mathbf{u}, \delta \mathbf{u}) = \int_{\Omega} (\text{grad} \delta \mathbf{u} : \mathbb{c} : \text{grad} \Delta \mathbf{u} + \text{grad} \delta \mathbf{u} : \text{grad} \Delta \mathbf{u} \boldsymbol{\sigma}) dv \quad (20)$$

472 or in index notation (with Einstein convention on repeated indices),

$$473 \quad D_{\Delta \mathbf{u}} \delta W_{int}(\mathbf{u}, \delta \mathbf{u}) = \int_{\Omega} \frac{\partial \delta u_a}{\partial x_b} (\delta_{ac} \sigma_{bd} + \mathbb{c}_{abcd}) \frac{\partial \Delta u_c}{\partial x_d} dv \quad (21)$$

474 where the term $\delta_{ac} \sigma_{bd} + \mathbb{c}_{abcd}$ is the effective elasticity tensor in the spatial description.

475 The term $\delta_{ac} \sigma_{bd}$ corresponds to the geometrical stress contribution to linearization (initial

476 stress contribution at every increment) whereas \mathbb{c}_{abcd} represents the material contribution

477 to linearization. The elasticity tensor \mathbb{c}_{abcd} in the spatial description is derived from the

478 push-forward of the linearized second Piola-Kirchhoff stress tensor which yields the lin-

479 earized Kirchhoff stress tensor $\Delta \boldsymbol{\tau}$ from relation

$$480 \quad \Delta \boldsymbol{\tau} = J \mathbb{c} : \text{grad} \Delta \mathbf{u} \quad (22)$$

481 Replacing the direction $\Delta \mathbf{u}$ of the directional derivative with the velocity vector \mathbf{v} , $\Delta \boldsymbol{\tau}$

482 and $\text{grad} \Delta \mathbf{u}$ result in the Lie time derivative $\mathcal{L}_v(\boldsymbol{\tau})$ of $\boldsymbol{\tau}$ and the spatial velocity gradient

483 $\mathbf{l} = \dot{\mathbf{F}} \mathbf{F}^{-1}$, respectively. Again, using the minor symmetries of \mathbb{c} , the following relation can

484 be written

$$485 \quad \mathcal{L}_v(\boldsymbol{\tau}) = \text{Oldr}(\boldsymbol{\tau}) = \dot{\boldsymbol{\tau}} - \mathbf{l} \boldsymbol{\tau} - \boldsymbol{\tau} \mathbf{l}^T = J \mathbb{c} : \mathbf{d} \quad (23)$$

486 where $\text{Oldr}(\boldsymbol{\tau})$ denotes the objective Oldroyd stress rate (convected rate) of the con-
 487 travariant Kirchhoff stress tensor $\boldsymbol{\tau}$ and $\mathbf{d} = \text{sym}(\mathbf{l})$ (symmetric part of \mathbf{l}) the rate of the
 488 deformation tensor. At this point we have to recall that for structural elements (shells,
 489 membranes, beams, trusses) Abaqus/Standard uses the elasticity tensor related to the
 490 Green-Naghdi objective rate. The detailed constitutive model used here is given in [27].

491 7 Numerical Investigations

492 The objective of this section is to assess the stability issues of POD basis interpolation on
 493 Grassmann manifolds by using two examples of hyperelastic structures.

494 7.1 Abaqus implementation of POD-ROM approximations

495 To implement a ROM for FEM analysis, a non-intrusive approach is utilized to insert the
 496 interpolated spatial POD basis into a commercial code. Specifically, a ROM is constructed
 497 using the multi-point constraint equations in Abaqus [36]. A linear multi-point constraint
 498 requires that a linear combination of nodal variables is equal to zero:

$$499 \quad A_1 u_i^P + A_2 u_j^Q + \dots + A_N u_k^R = 0 \quad (24)$$

500 where u_i^P is the nodal variable at node P , degree of freedom i and $A_i, (i = 1, \dots, N)$
 501 are coefficients that define the relative motion of the nodes. In Abaqus/Standard the
 502 first nodal variable specified (u_i^P corresponding to A_1) will be eliminated to impose the
 503 constraint. In addition, the coefficient A_1 should not be set to zero. For the construction
 504 of a ROM, p reference points are created corresponding to the total number of POD

505 modes. These reference points are used to define the constraint equations for introducing
 506 the spatial POD modes and to assign the extra degrees of freedom corresponding to the
 507 unknown ‘temporal’ variables. Thus, the interpolated spatial basis $\tilde{\Phi}_p := [\tilde{\phi}_1, \dots, \tilde{\phi}_p] \in$
 508 $\text{Mat}_{n,p}(\mathbb{R})$ representing the subspace $\tilde{\mathbf{m}} := \text{span}(\tilde{\phi}_1, \dots, \tilde{\phi}_p)$ on $\mathcal{G}(p, n)$ is imposed to the
 509 linear constraint equations as follows:

$$510 \quad u(x_l, t, \tilde{\lambda}) - \sum_{h=1}^p \tilde{\phi}_h(x_l) \psi_h(t) = 0 \quad (25)$$

511 where $x_l, (l = 1, \dots, N_s)$ is related to the nodal point positions, $\tilde{\phi}_h(x_l)$ represent the
 512 associated spatial POD h -mode for x_l , and $\psi_h(t)$ is the ‘temporal’ variable assigned to
 513 the reference point h that has to be determined. Note also that the system of equations
 514 defined in (25) has to be generated for each degree of freedom.

515 **Remark 7.1.** In fact this is not a standard POD-Galerkin approach since we are not
 516 projecting the linearized system of equations onto the interpolated spatial POD basis.
 517 But it serves us to assess the stability and accuracy of the ROM FEM model which is
 518 constructed by the interpolated POD basis. We mention again that generating an efficient
 519 ROM model is not the objective of this work.

520 7.2 Inflation of a spherical balloon

521 The first pMOR example concerns the inflation of a spherical balloon considering the
 522 material anisotropy defined by the fiber orientation angle as a parameter. The sphere has
 523 an initial radius of $R = 10$, thickness $h = 0.5$ and is loaded by an internal hydrostatic
 524 pressure of $P = 40$ (no units). The FEM analysis is performed on an octant S_0 of the
 525 sphere using plane symmetry boundary conditions, as depicted in Figure 3, where three

526 radial points $A(R, 0, 0)$, $B(0, R, 0)$ and $C(0, 0, R)$ are defined on each axis, respectively.
 527 Three-node shell elements (S3R) are used for the mesh [36]. A total number of 514 elements
 528 are generated with 228 nodes. The hyperelastic constitutive behavior is implemented in
 529 Abaqus/Standard with a user-defined subroutine (UMAT) [36].

530 **Remark 7.2.** The fiber orientation has to be defined on each point $M \in S_0$ using an
 531 orthonormal basis of the tangent plane $T_M S_0$, which has to be specified.

532 The choice made in Abaqus is to consider first an outward normal $\mathbf{n}(M)$ to this tangent
 533 plane and then a first vector $\mathbf{E}_1(M)$ as the orthogonal projection (normalized) of $\mathbf{e}_1 :=$
 534 $(1, 0, 0)$ onto $T_M S_0$. The second unit vector is the cross product $\mathbf{E}_2(M) := \mathbf{n}(M) \wedge \mathbf{E}_1(M)$.

535 *Explicit fiber orientations on the sphere octant*

Now, let us make an explicit definition of the fiber orientations, with parameter some
 angle θ using the local basis $\mathbf{E}_1(M), \mathbf{E}_2(M)$ on the tangent plane $T_M S_0$ as explained in
 Remark 7.2. More specifically, take

$$M = (\cos(u) \sin(v), \sin(u) \sin(v), \cos(v)) \in S_0, \quad (u, v) \in \left] 0; \frac{\pi}{2} \right[\times \left] 0; \frac{\pi}{2} \right[$$

and then define

$$\mathbf{E}_1(M) := \frac{\mathbf{X}^h}{\|\mathbf{X}^h\|}, \quad \mathbf{X}^h := \begin{pmatrix} 1 - \cos^2(u) \sin^2(v) \\ -\sin(u) \cos(u) \sin^2(v) \\ -\cos(u) \sin(v) \cos(v) \end{pmatrix},$$

$$\mathbf{E}_2(M) := \mathbf{n}(M) \wedge \mathbf{E}_1(M).$$

536 Note here that the vector \mathbf{X}^h corresponds to the orthogonal projection of the vector
 537 $(1, 0, 0)$ onto the tangent plane $T_M S_0$.

Finally, the unit vector defining the fiber orientation is given by (see Figure 4 for some examples).

$$\mathbf{a}_0(\theta) := \cos(\theta)\mathbf{E}_1(M) + \sin(\theta)\mathbf{E}_2(M)$$

538 *Model of strain energy function*

For a homogeneous transversely isotropic non-linear material, let consider a free energy function that depends only on two invariants (I_1, I_4)

$$\Psi = \Psi(I_1(\mathbf{C}), I_4(\mathbf{C}, \mathbf{a}_0))$$

539 where $I_1 = \text{tr}(\mathbf{C})$, while

$$540 \quad I_4 = \mathbf{a}_0 \mathbf{C} \mathbf{a}_0, \quad (26)$$

is the invariant related to anisotropy. Since we assume incompressibility of the isotropic matrix material, i.e., $I_3 = 1$, the free energy is enhanced by an indeterminate Lagrange multiplier p which is identified as a reaction pressure

$$\Psi = \Psi[I_1(\mathbf{C}), I_4(\mathbf{C}, \mathbf{a}_0)] + p(I_3 - 1).$$

541 The specific model used here is developed for membranous or thin shell-like sheets
542 considering a plane stress state throughout the sheet [27]. Following the method proposed
543 in [37,38], the strain energy function is defined as

$$544 \quad \Psi(I_1, I_4) := c_0(\exp(Q) - 1), \quad Q := c_1(I_1 - 3)^2 + c_2(I_4 - 1)^2 \quad (27)$$

545 where $c_i, i = 0, 1, 2$ are material parameters defined as: $c_0 = 86.1$, $c_1 = 0.0059$ and
546 $c_2 = 0.031$ (dimensionless).

547 **Remark 7.3.** This model introduces an inherent constitutive coupling between the isotropic
 548 and anisotropic material response. In order to avoid non-physical behavior of soft tissues,
 549 the related strain-energy function must be polyconvex [39]. It can be shown that poly-
 550 convexity of a (continuous) strain-energy function implies that the corresponding acoustic
 551 tensor is elliptic for all deformations, which means from the physical point of view that
 552 only real wave speeds occur; then the material is said to be stable. In (27), the anisotropic
 553 term $c_2(I_4 - 1)^2$ is activated only when $I_4 \geq 1$ (the actual fiber stretches are greater than
 554 unity).

555 Moreover, as discussed in [40], the constitutive description based on (27) is limited
 556 to deformations in which the in-plane strains are positive or tensile, and is not able
 557 to incorporate the behavior of the structure in compression. Due to the membrane-like
 558 geometry, it is unlikely to support compressive strains without buckling. This limitation
 559 extends to the issue of bending stiffness, which is neglected in this model.

560 *Snapshot matrices and error norms*

561 In what follows, the training points corresponding to the fiber orientation angle θ
 562 will be denoted with parameter λ for convenience with the previous sections. FEM sim-
 563 ulations are performed in Abaqus/Standard for the arbitrary chosen points $\lambda_i \in \mathcal{A}_s =$
 564 $\{0, 45, 50, 60, 85, 90\}$. It is easy to see that the spherical balloon changes from a pumpkin
 565 (Figure 5(a)) to rugby shaped (Figure 5(d)) for $\lambda = 0$ and $\lambda = 90$, respectively. Ob-
 566 serve also in Figure 4 that the fiber orientation on the sphere is far from being trivial for
 567 $\theta \in]0; 90[$.

568 The target point for interpolation is set to $\tilde{\lambda} = 75$. Thus, it is natural to constraint the
 569 training set to $\mathcal{A}_t = \{50, 60, 85, 90\}$ (see Figure 5 for some FEM results). We note that

570 the target point $\tilde{\lambda} = 75$ represents a worst case scenario for assessing the interpolation
 571 accuracy since it is spaced nearly at the maximum distance between the adjacent training
 572 points $\lambda = 60$ and $\lambda = 85$. Additionally, another reason for this choice is the remarkable
 573 shape transition of the spherical balloon inflation in this range of fibration angles as can
 574 been seen from Figure 5(b) and Figure 5(c), respectively. Hence, this selection gives an
 575 upper bound of the interpolation accuracy over the considered parametric range.

576 For each simulation, a sequence of uniform time snapshots is extracted from the model
 577 database. From the discretization of the space-time fields (displacement/rotation), the
 578 snapshot matrices $\mathbf{S}(\lambda_i)$ of size $(n = 1728) \times (N_t = 1000)$ are formed. The eigenvalue
 579 spectrum of the matrices $\mathbf{S}(\lambda_i)$ corresponding to training points $\lambda_i \in A_t$ is shown in a
 580 log-log scale in Figure 6. The condition number of the matrices is of the order of $1.0e + 10$.
 581 Notice that the distance between the first and the second eigenvalue is of two orders of
 582 magnitude.

583 To quantify the interpolation accuracy, the relative L_2 -error norm (in time) for a
 584 given target point $\tilde{\lambda}$ is evaluated with respect to the high-fidelity FEM solution. Using
 585 the interpolated and the high-fidelity FEM snapshot matrices $\tilde{\mathbf{S}}$ and \mathbf{S}^{FEM} , respectively,
 586 the following error measure is defined at each time snapshot

$$587 \quad e_{L_2}(\tilde{\mathbf{S}}) = \frac{\|\tilde{\mathbf{u}}_i - \mathbf{u}_i^{\text{FEM}}\|_{L_2}}{\|\mathbf{u}_i^{\text{FEM}}\|_{L_2}}, \quad i = 1, \dots, N_t \quad (28)$$

588 In addition, the relative Frobenius error norm represents a global error measure which
 589 considers the error in the full time interval of the time steps

$$590 \quad e_F(\tilde{\mathbf{S}}) = \|\tilde{\mathbf{S}} - \mathbf{S}^{\text{FEM}}\|_F / \|\mathbf{S}^{\text{FEM}}\|_F \quad (29)$$

591 Using the linear constraint equations defined in (25), p reference points (for each POD
 592 mode) are created to assign the spatial POD basis representing the interpolated subspace
 593 $\tilde{\mathbf{m}} \in \mathcal{G}(p, n)$ and the unknown temporal variables. Thus, the total number of equations of
 594 the ROM-FEM model is $6 \times p$ while the total number of equations of the corresponding
 595 high-fidelity FEM model is $288 \times 6 = 1728$.

596 *Stability conditions (C1) and (C2)*

597 First we need to know if the interpolation is (C1) and (C2) stable.

598 **Stability (C1).** All points $\mathbf{m}_1, \dots, \mathbf{m}_N \in \mathcal{G}(p, n)$ lie in $U_{\mathbf{m}_0}$, given by (13). We need
 599 to check that for all $i = 1, \dots, N$, the matrix $\mathbf{Y}_0^T \mathbf{Y}_i$ is non singular. (C1) condition is
 600 satisfied for all $i = 1, \dots, N$ and $p = 1, 2, 5, 10, 20$ POD modes considered.

601

602 **Stability (C2).** We need to know if all velocity vectors $\tilde{v}(\lambda)$ belong to the subset $V_{\mathbf{m}_0}$
 603 given by (17), for the parametric range $\lambda \in [\lambda_1, \lambda_N]$. Thus, we have to check that the first
 604 (maximum) singular value θ_1 of a horizontal lift $\tilde{\mathbf{Z}}(\lambda)$ of the velocity vector $\tilde{v}(\lambda)$ is such
 605 that $\theta_1 < \pi/2$, for all $\lambda \in [\lambda_1, \lambda_N]$. We proceed by uniformly sampling 401 points over the
 606 parametric range $[50; 90]$. Figure 7 shows the maximum eigenvalue θ_1 of the horizontal lift
 607 $\tilde{\mathbf{Z}}(\lambda)$ for all samples using $\mathbf{m}_0(\lambda = 85)$ as a reference point on the Grassmann manifold.
 608 These curves provide all important information for the (C2) stability of interpolation
 609 by detecting the exact intervals of the loss of injectivity of the exponential mapping for
 610 various POD modes $p = 1, 2, 5, 10, 20$. Observe the loss of injectivity in a specific interval
 611 of the parameter range for modes $p = 10, 20$. A remarkable result is the loss of injectivity
 612 inside the parameter range and not at the boundaries where the exponential map becomes
 613 again injective. Note also that by increasing the dimension p , the curves shift more rapidly

614 closer to $\pi/2$. Moreover, Figure 7 reveals that interpolation is (C2) stable for the target
 615 point $\tilde{\lambda} = 75$ for all POD modes p .

616 *Interpolation accuracy and stability condition (C3)*

617 Figure 8 and Figure 9 show the relative L_2 -error norm $e_{L_2}(\tilde{\mathbf{S}})$ and the Frobenius
 618 error norm $e_F(\tilde{\mathbf{S}})$ for the target point $\tilde{\lambda}$ of the ROM-FEM solution constructed from the
 619 interpolated p dimensional spatial modes. Additionally, Table 1 shows the Grassmannian
 620 dimension for the different number of POD modes.

Table 1: Dimension of the Grassmann manifold $\mathcal{G}(p, n)$

Number of modes	$p = 1$	$p = 2$	$p = 5$	$p = 10$	$p = 20$
Dimension: $p(n - p)$	1727	3452	8615	17180	34160

621 **Stability (C3).** We need to check if the interpolated subspaces $\tilde{\mathcal{V}}$ and $\tilde{\mathcal{V}}'$ respectively
 622 associated to matrices $\tilde{\mathbf{Y}}$ and $\tilde{\mathbf{Y}}'$ corresponding to modes p and $p' > p$ interpolation, are
 623 such that $\tilde{\mathcal{V}} \subset \tilde{\mathcal{V}}'$. Before examining if the interpolation is (C3) stable, first notice from
 624 Figure 8 and Figure 9 which display the relative error norms (28) and (29), respectively,
 625 that the error is minimum for $p = 2$ POD modes and increases by introducing additional
 626 modes which at first glance contradicts the expected improvement of the solution by
 627 increasing the number of modes. In this case, the non-monotonic error behavior and the
 628 random oscillations follows from the non-inclusion defect between subspaces \mathcal{V} and \mathcal{V}'
 629 obtained by using different number of POD modes. To prove that fact, we compute the
 630 geometric distance $\delta(\mathcal{V}, \mathcal{V}')$ using the principal angles defined in (1). We assume a set of
 631 POD modes $p \in \mathcal{P}_m = \{1, 2, 5, 10, 20\}$ and a threshold value $T_V = 100$. Figure 10 lists

632 the distances of the obtained POD basis of various dimensions $p \in \mathcal{P}_m$ in a symmetric
 633 table form. Observe that i) $\delta(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}') \neq 0$ for all $p \neq p'$ and ii) $\delta(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}')$ increase rapidly for
 634 $p > 2$. Thus, this table explains why the relative error norms (Figure 8 and Figure 9) have
 635 a minimum at $p = 2$ modes. Since the relative error ϵ given by (2) is $\epsilon = 554.03 > T_V$, we
 636 can conclude that the interpolation is not (C3) stable. The results make clear and prove
 637 the non-inclusion defect of different subspaces which in turn give rise to the oscillatory
 638 behavior of the error norms as described above.

639 Moreover, the interpolation accuracy is assessed using the relative displacement error
 640 $e_{\mathbf{u}} = \|\tilde{\mathbf{u}}(t) - \mathbf{u}^{FEM}(t)\|_{L_2} / \|\mathbf{u}^{FEM}(t)\|_{L_2}$ at the nodal points computed for $p = 1, 2, 5$ and
 641 10 POD modes. Figure 11 and Figure 12 present the local error at the increment state
 642 $t = 0.002$ and at the final increment state $t = 1$ displayed at the position vector $\mathbf{x}^{FEM}(t)$
 643 of the high-fidelity FEM model, respectively. In general, different patterns of the spatial
 644 error distribution can be observed with respect to the number of POD modes. In the
 645 majority of cases, the maximum error is located at the boundary points of the octant S_0
 646 of the initially spherical balloon where plane symmetries are imposed and at points of
 647 maximum displacement. Again, observe that the error is not decreasing by using more
 648 POD modes as Figure 12 shows.

649 Finally, Figure 13 shows the time-displacement histories for the radial points A, B
 650 and C on the initially spherical balloon for the ROM-FEM model compared against its
 651 high-fidelity counterpart solution using POD mode $p = 1$. It can be observed that the
 652 interpolated ROM-FEM solution delivers good accuracy and is accurate enough to predict
 653 the anisotropic balloon inflation at the target parameter.

654 *7.3 Structure with multiple components*

655 For the second example, the stability of pMOR is investigated for a hyperelastic structure
 656 considering the material stiffness as a parameter. The model consists of two basic compo-
 657 nents: a plane shell section which is connected with six truss elements (non-symmetrically)
 658 (see Figure 14). The plane section has dimensions 20×20 (mm), a constant thickness of
 659 0.5 mm and is meshed with rectangular shells (S4). The hyperelastic model defined in (27)
 660 (UMAT) is assigned to the plane section in which the fiber orientations are aligned with the
 661 x-axis. The following parameters are used: $c_0 = 0.0520$ (kPa), $c_1 = 4.63$ and $c_2 = 22.6$. The
 662 truss elements are of type T3D2 with a cross-section area of 1 mm^2 . For these elements,
 663 an isotropic incompressible hyperelastic material model is implemented into Abaqus/-
 664 Standard subroutine UHYPER [36]. The material model is derived from the following
 665 strain-energy function

$$666 \quad U = \alpha_1(\exp[\alpha_2(I_1 - 3)] - 1) \quad (30)$$

667 where α_1 and α_2 are material parameters defined as: $\alpha_1 = 0.0565$ kPa and α_2 is
 668 used for the parametric analysis. At the boundary of the plane section ($x = 0$) and at
 669 the foundations of the truss elements all degrees of freedom are set to zero. A constant
 670 hydrostatic pressure of 120 mmHg is applied at the bottom side of the plane section.

671 *Snapshot matrices for pMOR*

672 The FEM simulations are performed using Abaqus/Standard (Implicit). For the expo-
 673 nential parameter α_2 , the following set of training points are chosen where for convenience
 674 with the previous sections we changed the notation to $\lambda \in \{5, 10, 15, 20, 25, 30\}$. Figure 15

675 shows the second Piola-Kirchhoff stress-stretch curves for the corresponding parameter
 676 values which reveals a wide spectrum of stress values. For each parametric simulation, a
 677 sequence of snapshots uniformly distributed over time using an increment of $\Delta t = 0.001$
 678 is extracted for all nodes of the plane structure from the model database. The space-time
 679 snapshot matrices $\mathbf{S}(\lambda_i) \in \mathbb{R}^{n \times N_t}$ of size $(n = 726) \times (N_t = 1000)$ are associated to nodal
 680 displacement and rotational fields. The following training points $\lambda_i \in A_t = \{15, 20, 25, 30\}$
 681 are arbitrary chosen for estimating the target point $\tilde{\lambda} = 17.5$. After construction of the set
 682 of low-dimensional POD basis for the training points λ_i , a POD basis for the target point
 683 $\tilde{\lambda}$ is interpolated on a Grassmann manifold using Lagrange interpolation. Then, the inter-
 684 polated POD spatial basis is introduced in Abaqus using the linear constraint equations
 685 (Section 7.1) to construct a ROM for FEM analysis associated to the target parameter
 686 point. For each ROM FEM model of p POD modes, the same number of reference points
 687 are created to assign the interpolated spatial POD modes and the unknown ‘temporal’
 688 variables that need to be determined.

689 The eigenvalue spectrum of snapshot matrices \mathbf{S}_i corresponding to training points
 690 $\lambda_i \in A_t$ is shown in a log-log scale in Figure 16. It is evident that the distance between the
 691 first three eigenvalues is of one order of magnitude each. In our experiments we perform
 692 interpolation using $p = 1, 2, 5, 10, 20$ POD modes since they capture the most important
 693 characteristics of the system.

694 *Stability conditions (C1) and (C2)*

695 First we need to know if the interpolation is well-defined by evaluating the (C1) and
 696 (C2) stability conditions.

697 **Stability (C1).** This condition requires that all points $\mathbf{m}_1, \dots, \mathbf{m}_N \in \mathcal{G}(p, n)$ lie in
 698 $U_{\mathbf{m}_0}$ given by (13). Thus, we need to check if the matrix $\mathbf{Y}_0^T \mathbf{Y}_i$ is non-singular for all
 699 $i = 1, \dots, N$. Since this condition is satisfied for all $i = 1, \dots, N$ and $p = 1, 2, 5, 10, 20$
 700 POD modes considered in this example, the interpolation is (C1) stable.

701 **Stability (C2).** We need to know if all velocity vectors $\tilde{v}(\lambda)$ belong to the subset
 702 $V_{\mathbf{m}_0}$ given by (17), for the parametric range $\lambda \in [\lambda_1, \lambda_N]$. Thus we have to check that the
 703 first (largest) singular value θ_1 of an horizontal lift $\tilde{\mathbf{Z}}(\lambda)$ of the velocity vector $\tilde{v}(\lambda)$ is such
 704 that $\theta_1 < \pi/2$, for all $\lambda \in [\lambda_1, \lambda_N]$. We proceed by uniformly sampling 151 points over the
 705 parametric range [15; 30]. Figure 17 shows the largest eigenvalue θ_1 of the horizontal lift
 706 $\tilde{\mathbf{Z}}(\lambda)$ for all samples using $\mathbf{m}_0(\lambda = 15)$ as a reference point on the Grassmann manifold.
 707 From these curves we are able to assess the (C2) stability of interpolation by detecting the
 708 exact intervals of the loss of injectivity of the exponential map over the parametric range
 709 for different number of POD modes p . It is clear that for $p \leq 10$ the interpolation is stable
 710 over the entire parametric range. Observe the loss of injectivity in a specific interval of
 711 parameter λ for $p = 20$ modes. Again, as in the previous example, note that by increasing
 712 the dimension p , the curves progressively tend to shift closer to $\pi/2$. Moreover, Figure 17
 713 reveals that interpolation is (C2) stable for the target point $\tilde{\lambda} = 17.5$ for all POD modes
 714 p .

715 *Interpolation accuracy and stability condition (C3)*

716 The accuracy of interpolation is assessed by comparing the relative L_2 -error norm
 717 $e_{L_2}(\tilde{\mathbf{S}})$ and the relative Frobenius error norm $e_F(\tilde{\mathbf{S}})$ defined by the ROM FEM model and
 718 its high-fidelity solution against the number of POD modes p , as shown in Figure 18 and

719 Figure 19, respectively. Additionally, Table 2 illustrates the Grassmannian dimension for
 720 the corresponding number of POD modes p .

721 **Stability (C3).** We need to check if the interpolated subspaces $\tilde{\mathcal{V}}$ and $\tilde{\mathcal{V}}'$ respectively
 722 associated to matrices $\tilde{\mathbf{Y}}$ and $\tilde{\mathbf{Y}}'$ correspond to mode p and $p' > p$ interpolation, are
 723 such that $\tilde{\mathcal{V}} \subset \tilde{\mathcal{V}}'$. Before performing this stability test, observe the monotonic decrease of
 724 the relative error norms (28) and (29) by increasing mode p , as depicted in Figure 18 and
 725 Figure 19, respectively. We are now ready to see how the geometric distance $\delta(\mathcal{V}, \mathcal{V}')$ using
 726 the principal angles defined in (1) relates to the error norm behavior. Again, we assume
 727 a set of POD modes $p \in \mathcal{P}_m = \{1, 2, 5, 10, 20\}$ and a threshold value $T_V = 100$. To this
 728 end, we compute the distances $\delta(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}')$ of the interpolated POD basis on Grassmann
 729 manifolds $\mathcal{G}(p, n)$ of various dimensions $p \in \mathcal{P}_m$, plotted in a symmetric table form, as
 730 Figure 20 shows. Again, the results prove the non-connectivity of different subspaces of
 731 various dimensions p . What is remarkable to observe in this case, is that the geometric
 732 distance $\delta(\tilde{\mathbf{Y}}, \tilde{\mathbf{Y}}') \approx 0$ for all $p \neq p'$. Moreover, the indicator ϵ given by (2) is here
 733 $\epsilon = 73.60 < T_V$, which is sufficiently small to assure a (C3) stable interpolation.

734 Finally, Figure 21 shows a comparison of the predicted time histories of selected nodal
 735 total displacements for the ROM FEM model using $p = 20$ POD modes against the
 736 high-fidelity FEM solution. It is evident that all nodal time-histories are nearly identical.

Table 2: Dimension of the Grassmann manifold $\mathcal{G}(p, n)$

Number of modes	$p = 1$	$p = 2$	$p = 5$	$p = 10$	$p = 20$
Dimension: $p(n - p)$	725	1448	3605	7160	14120

737 **8 Conclusions**

738 Effective mathematical definitions for necessary stability conditions of POD basis inter-
739 polation on Grassmann manifolds for pMOR are given. Special attention has been paid
740 on the definition of local maps on Grassmann manifolds considering the logarithm and
741 exponential maps. In this context, the notion of cut–locus is introduced since it optimally
742 captures the loss of injectivity of the exponential map. The formulae for the Grassmannian
743 cut–locus to establish a stable interpolation is mathematically proved. Another intrinsic
744 condition is defined by computing the geometric distance of the interpolated POD basis of
745 different POD mode. This condition explained oscillations of the error norm with increas-
746 ing mode, and on the contrary, solutions with monotonic behavior. The pMOR benchmark
747 examples in hyperelasticity revealed important aspects of interpolation stability.

748 **9 Acknowledgements**

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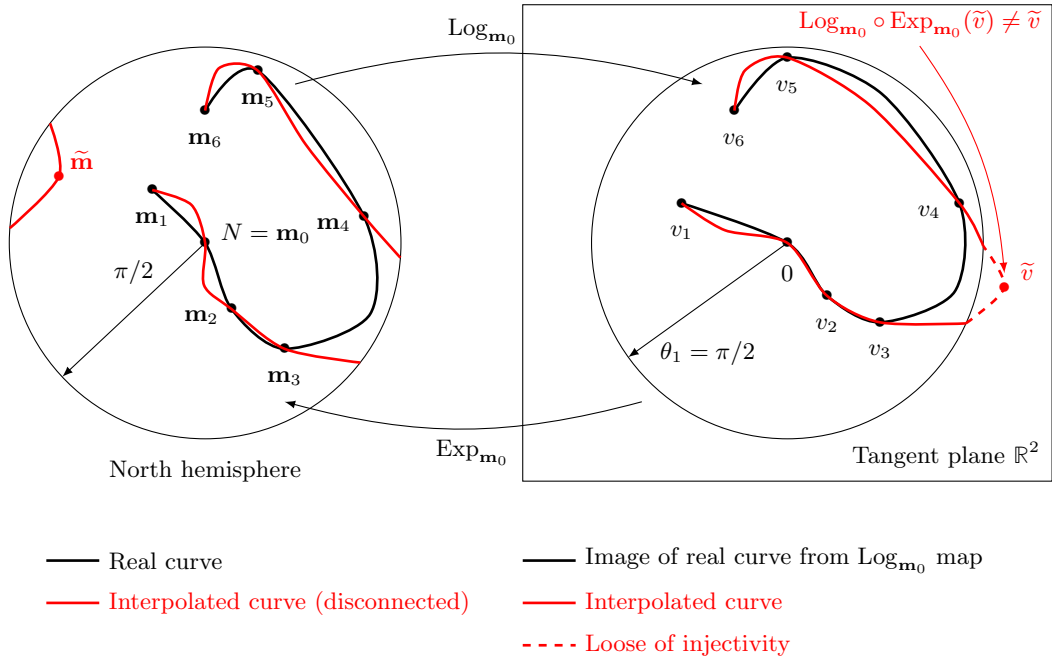


Fig. 1: Loss of injectivity of the exponential map

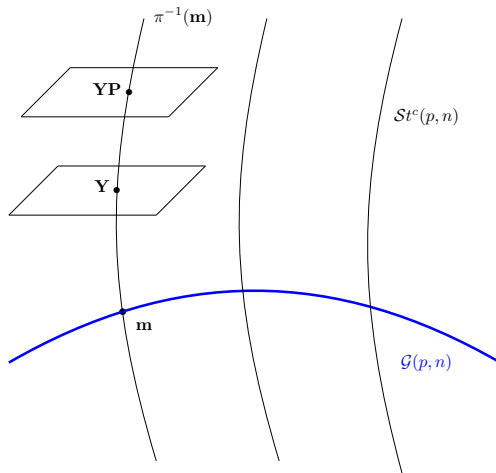


Fig. 2: Schematic of a fiber bundle.

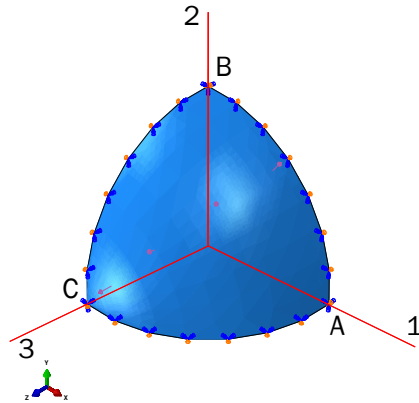


Fig. 3: Geometry of an octant S_0 of a spherical balloon made of transversely isotropic hyperelastic material. Three radial points A, B and C are defined on axis 1,2 and 3, respectively; plane symmetry boundary conditions are used.

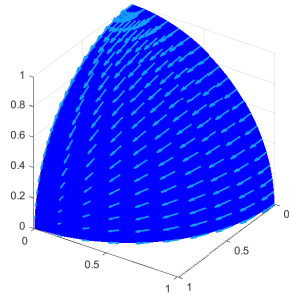
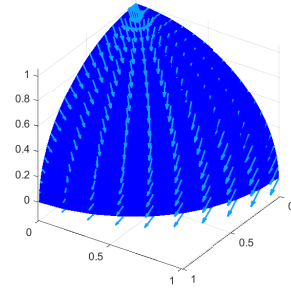
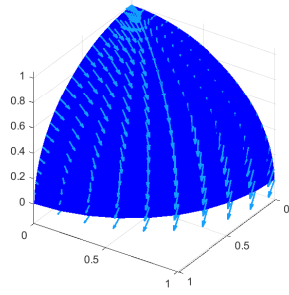
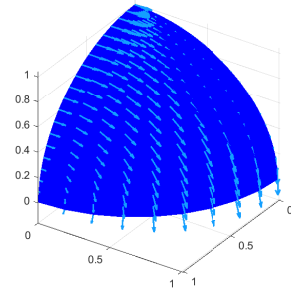
(a) Fibers orientation with $\theta = 0$ degree(b) Fibers orientation with $\theta = 45$ degree(c) Fibers orientation with $\theta = 60$ degree(d) Fibers orientation with $\theta = 90$ degree

Fig. 4: Different fibers on the sphere.

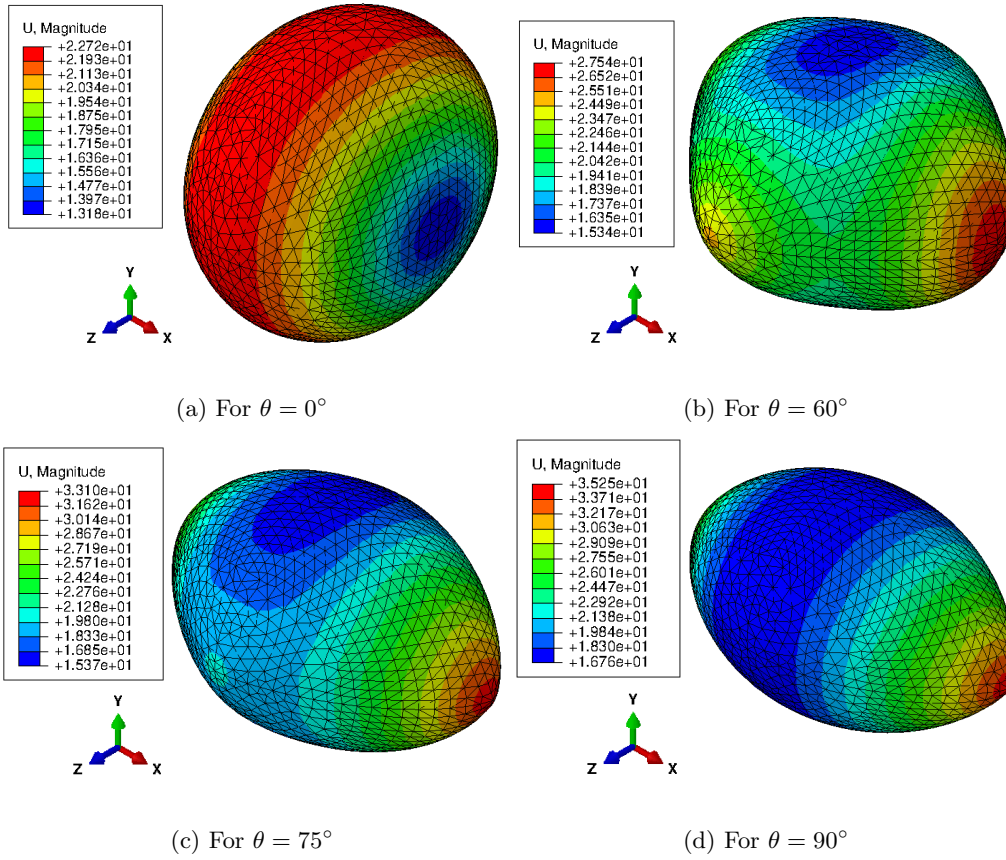


Fig. 5: Inflation modes of the benchmark anisotropic spherical balloon after reconstruction of the complete balloon using the plane symmetries conditions at the boundaries of the octant S_0 .

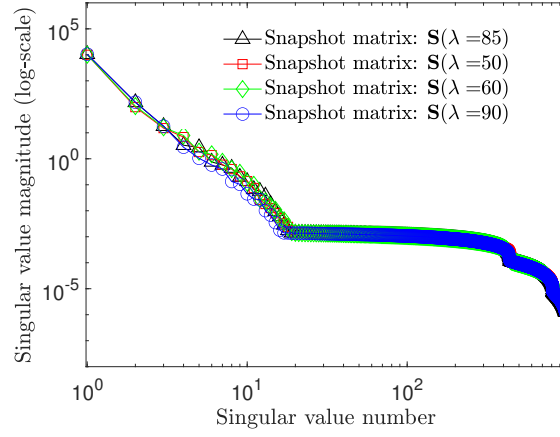


Fig. 6: The eigenvalue spectrum of snapshot matrices \mathbf{S}_i corresponding to training points $\lambda_i = 50, 60, 85, 90$.

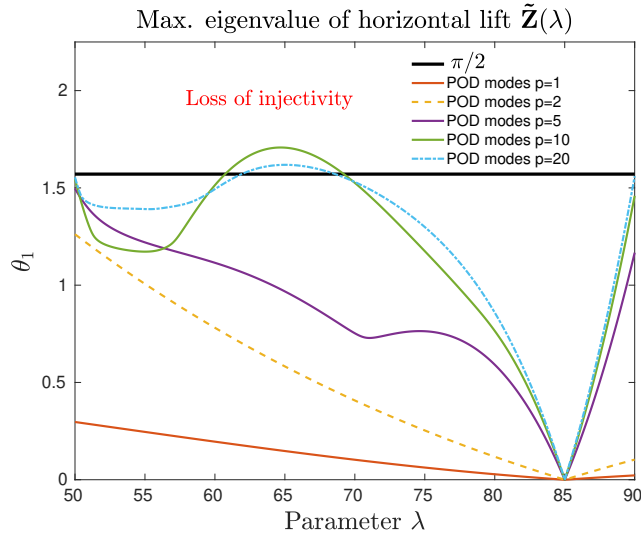


Fig. 7: Stability (C2); Computation of the maximum eigenvalue θ_1 of the horizontal lift $\tilde{\mathbf{Z}}(\lambda)$ over the parametric range $\lambda \in [50; 90]$. Observe the loss of injectivity in a specific interval in the parametric range for POD modes $p = 10, 20$. Reference point on Grassmann manifold $\mathbf{m}_0(\lambda = 85)$.

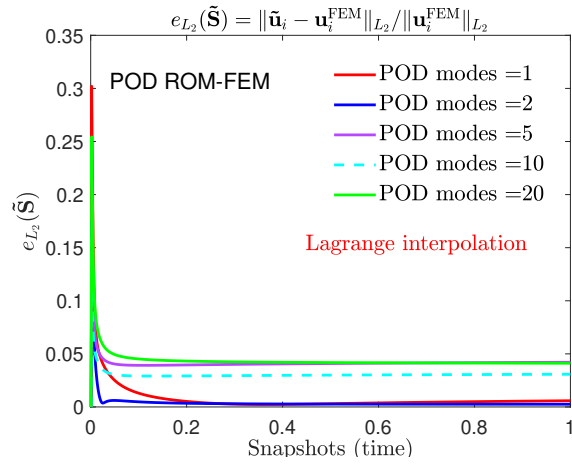


Fig. 8: Relative L_2 -error norm $e_{L_2}(\tilde{\mathbf{S}})$ against the number of POD vectors for the POD ROM-FEM; target point: $\tilde{\mathbf{m}}(\lambda = 75)$.

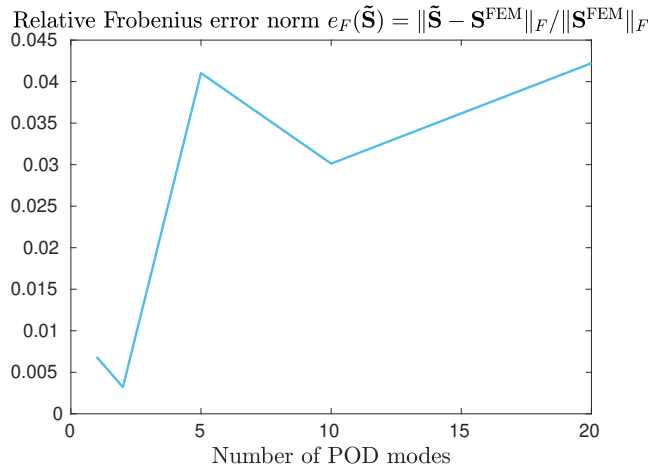


Fig. 9: Relative Frobenius error norm against the number of POD vectors for the POD ROM-FEM; target point: $\tilde{\mathbf{m}}(\lambda = 75)$.

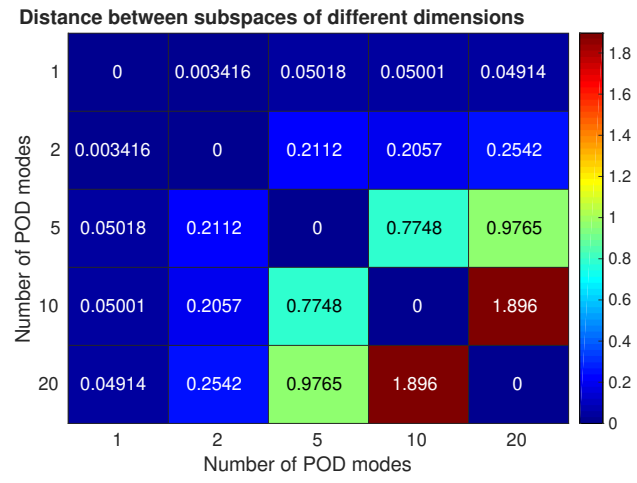


Fig. 10: Stability (C3); Geometric distance $\delta(\mathbf{Y}, \mathbf{Y}')$ between interpolated subspaces of different dimensions.

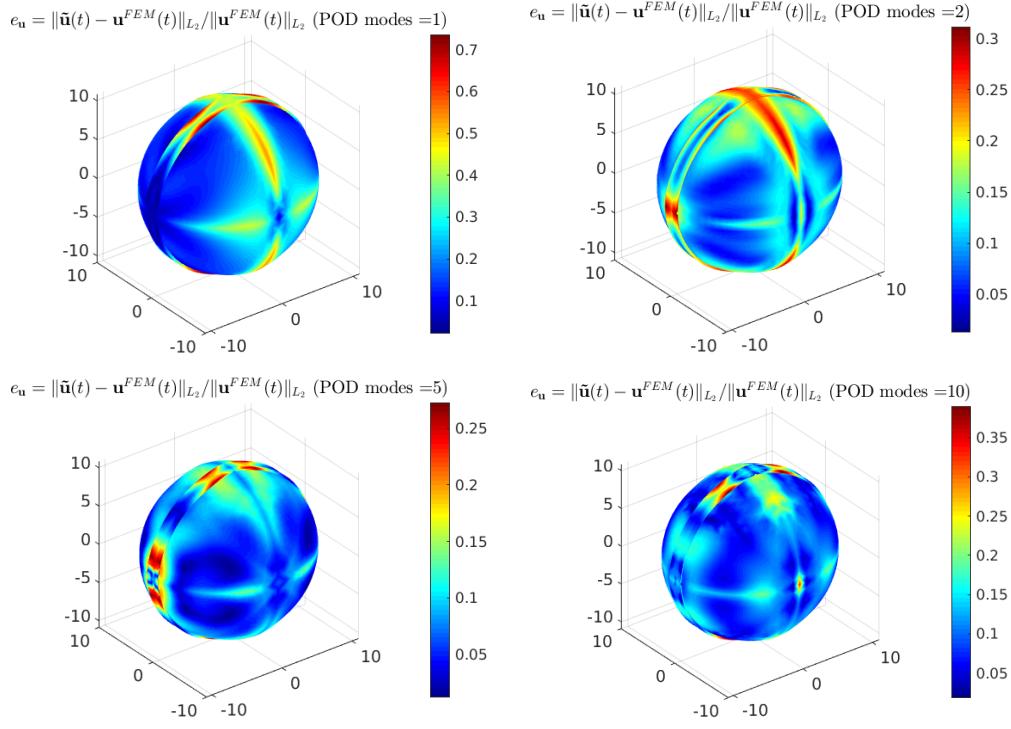


Fig. 11: Relative displacement error $e_{\mathbf{u}} = \|\tilde{\mathbf{u}}(t) - \mathbf{u}^{FEM}(t)\|_{L_2} / \|\mathbf{u}^{FEM}(t)\|_{L_2}$ at the nodal points at state $t = 0.002$ for POD modes $p = \{1, 2, 5, 10\}$ displayed at the position vector $\mathbf{x}^{FEM}(t)$ of the high-fidelity FEM model; target point: $\tilde{\mathbf{m}}(\lambda = 75)$.

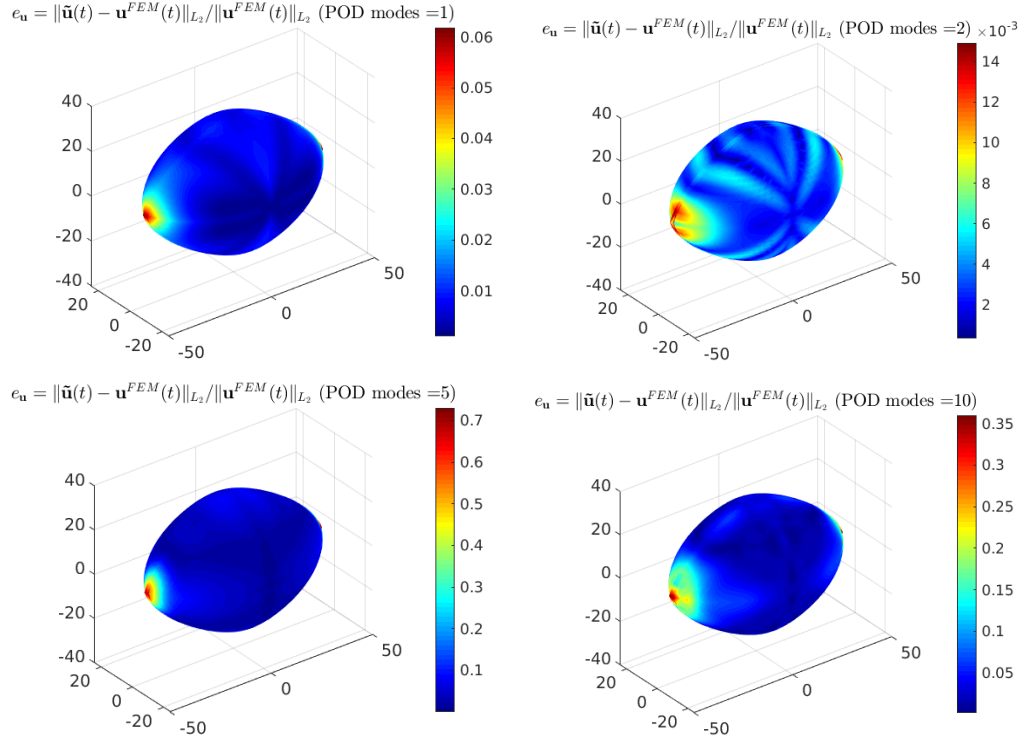


Fig. 12: Relative displacement error $e_{\mathbf{u}} = \|\tilde{\mathbf{u}}(t) - \mathbf{u}^{FEM}(t)\|_{L_2} / \|\mathbf{u}^{FEM}(t)\|_{L_2}$ at the nodal points at state $t = 1$ for POD modes $p = \{1, 2, 5, 10\}$ displayed at the position vector $\mathbf{x}^{FEM}(t)$ of the high-fidelity FEM model; target point: $\tilde{\mathbf{m}}(\lambda = 75)$.

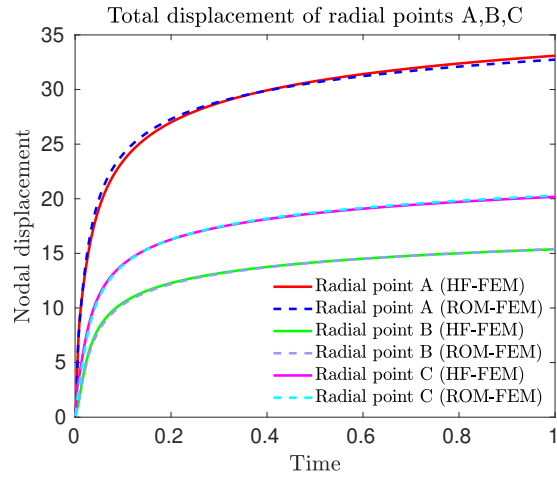


Fig. 13: POD ROM-FEM model using Lagrange interpolation; comparison of the displacement of radial points A,B and C against the high-fidelity FEM solution; training points: $\mathbf{m}_0(\lambda = 85)$ (reference point); $\mathbf{m}_1(\lambda = 50)$; $\mathbf{m}_2(\lambda = 60)$; $\mathbf{m}_3(\lambda = 90)$; target point: $\tilde{\mathbf{m}}(\lambda = 75)$; POD modes $p = 1$.

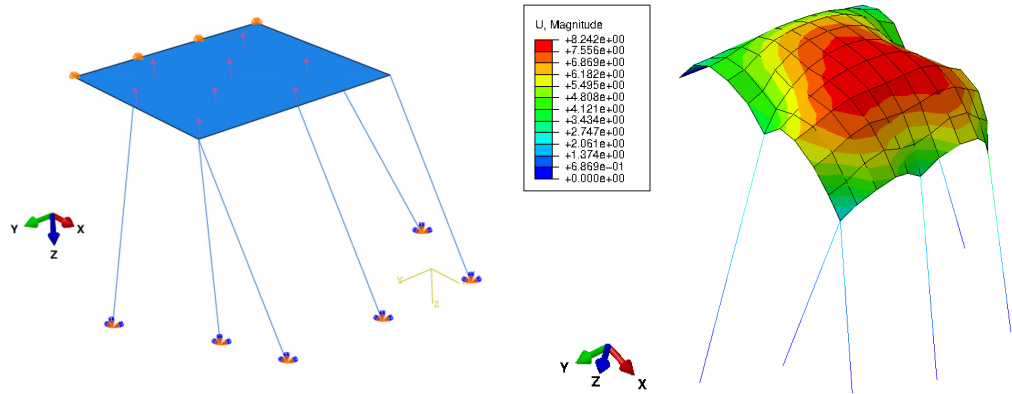


Fig. 14: Geometry, boundary conditions and total displacement of the structural multi-component model subjected to hydrostatic pressure, comprised of an anisotropic hyperelastic plane shell section which is non-symmetrically supported by a set of hyperelastic truss elements.

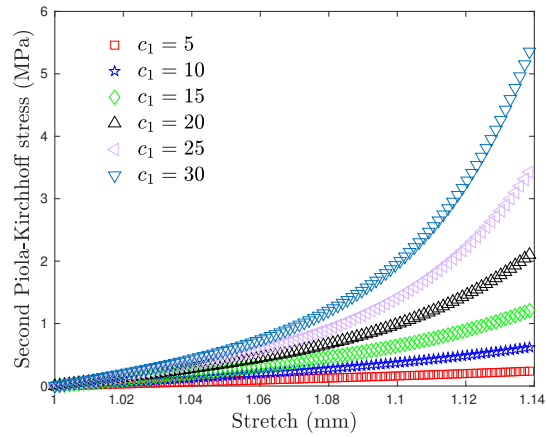


Fig. 15: Second Piola-Kirchhoff stress vs stretch for the examined parameter range.

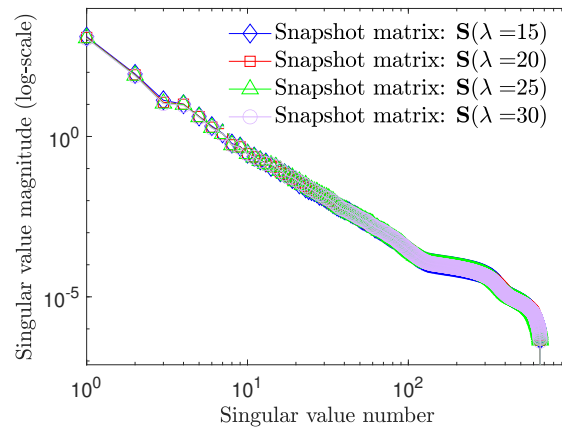


Fig. 16: The eigenvalue spectrum of snapshot matrices \mathbf{S}_i corresponding to training points

$\lambda_i \in A_t = \{15, 20, 25, 30\}$.

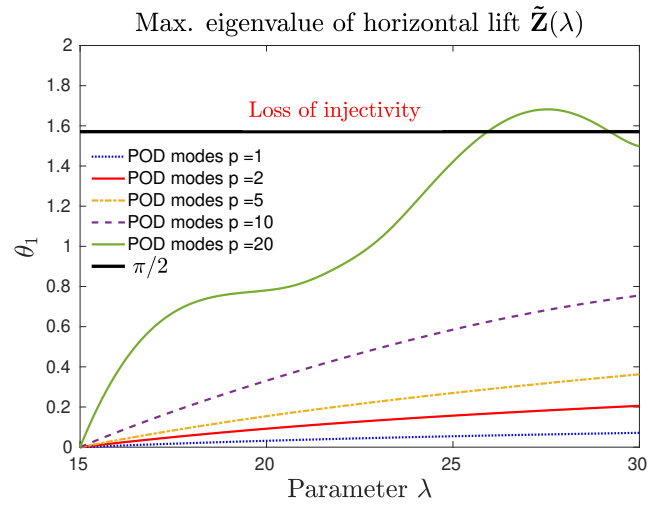


Fig. 17: Stability (C2); Computation of the maximum eigenvalue θ_1 of the horizontal lift $\tilde{\mathbf{Z}}(\lambda)$ over the parametric range $[15; 30]$. Observe the loss of injectivity in a specific interval of parameters for POD modes $p = 20$. Reference point on Grassmann manifold $\mathbf{m}_0(\lambda = 15)$.

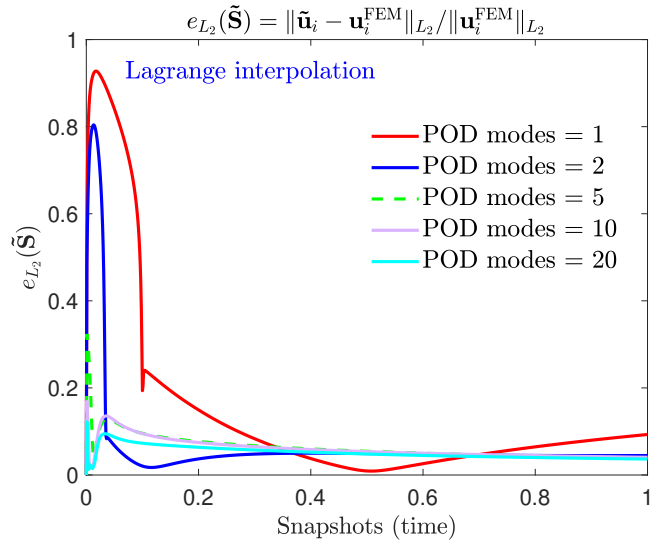


Fig. 18: POD ROM-FEM; relative L_2 -error norm $e_{L_2}(\tilde{\mathbf{S}})$ against the number of POD vectors; target point: $\tilde{\mathbf{m}}(\lambda = 17.5)$.

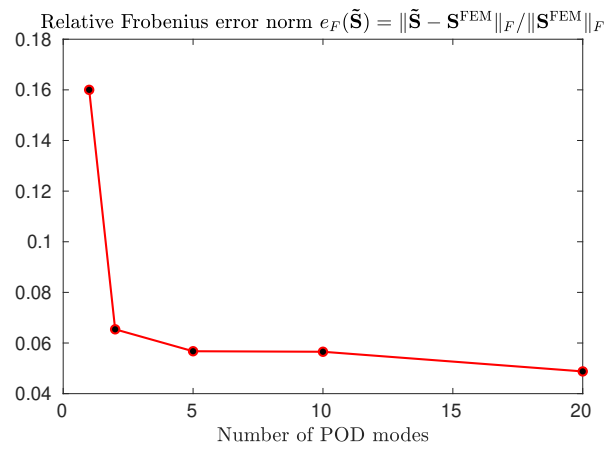


Fig. 19: Relative Frobenius error norm against the number of POD vectors for the POD ROM-FEM; target point: $\tilde{\mathbf{m}}(\lambda = 17.5)$.

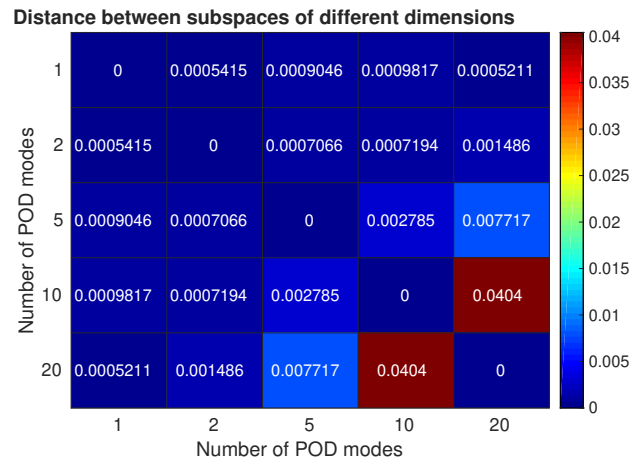


Fig. 20: Stability (C3); Geometric distance $\delta(\mathbf{Y}, \mathbf{Y}')$ between interpolated subspaces of different dimensions p .

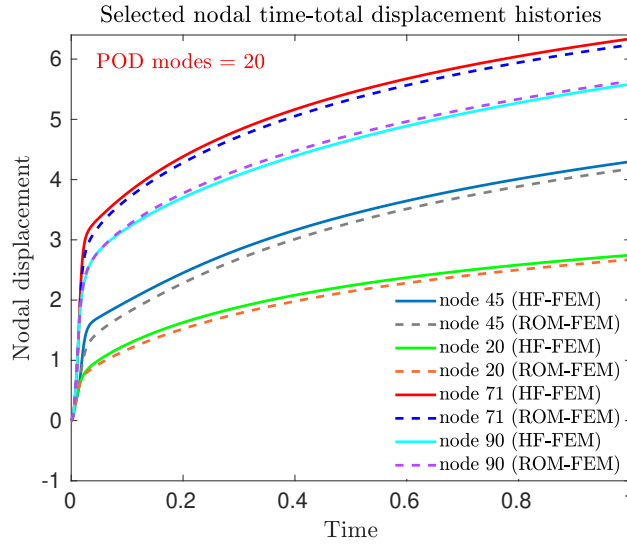


Fig. 21: POD ROM-FEM; comparison of selected nodal time-displacement histories against the high-fidelity FEM solution; training points: $\mathbf{m}_0(\lambda = 15)$; $\mathbf{m}_1(\lambda = 20)$; $\mathbf{m}_2(\lambda = 25)$; $\mathbf{m}_3(\lambda = 30)$; target point: $\tilde{\mathbf{m}}(\lambda = 17.5)$; POD modes = 20.

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