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PSD-GREEDY BASIS GENERATION FOR STRUCTURE-PRESERVING MODEL ORDER REDUCTION OF HAMILTONIAN SYSTEMS*

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Abstract. Hamiltonian systems are central in the formulation of non-dissipative physical systems. They are characterized by a phase-space, a symplectic form and a Hamiltonian function. In numerical simulations of Hamiltonian systems, algorithms show improved accuracy when the symplectic structure is preserved [10]. For structure-preserving model order reduction (MOR) of Hamiltonian systems, symplectic MOR [17, 14, 11, 3, 16] can be used. It is based on a reduced-order basis that is symplectic, which requires symplectic basis generation techniques.

In our work, we discuss greedy algorithms for symplectic basis generation. We complement the procedure presented in [14] with ideas of the POD-greedy [9], which results in a new greedy symplectic basis generation technique, the PSD-greedy. Inspired by POD-greedy, we use compression techniques in the greedy iterations to enrich the basis iteratively. We prove that this algorithm computes a symplectic basis when symplectic techniques are used for compression. In the numerical experiments, we compare the discussed methods for a linear elasticity problem. The results show that improvements of up to one order of magnitude in the relative reduction error are achievable with the new basis generation technique compared to the existing greedy approach from [14].

Key words. greedy basis generation, symplectic model order reduction, structure-preservation of symplecticity, Hamiltonian systems

AMS subject classifications. 65P10, 65D15, 37M15, 34C20, 93A15

1. Introduction.

Hamiltonian systems are mathematical models designed for dynamical non-dissipative phenomena, which includes e.g. mechanical systems, like linear elasticity models [2] or truss structures [4], and wave-type and transport dominated problems [17, 14, 16]. A Hamiltonian system is characterized by a phase-space, a symplectic form and a Hamiltonian function. The dimension of the phase-space might be large, e.g. if the system stems from the discretization of a (Hamiltonian) partial differential equation. Since this dimension is directly linked to the computational power that is required to compute the solution, it might be computationally infeasible to solve the system (a) in real-time, (b) for many different parameters or (c) on small computers like e.g. smartphones. Such tasks naturally occur for (a) controller design and interactive simulations, (b) parameter studies, parameter optimization and uncertainty quantification or (c) *in situ* simulations, i.e. simulations at places which lack availability of communication structure to high-performance computing facilities. In all three cases (a) to (c), the computational demand can be decreased by computing an efficient surrogate model with model order reduction (MOR), see e.g. [1]. While classical MOR might violate the structure of the Hamiltonian system, symplectic

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MOR can be used to preserve the underlying symplectic geometry [17, 14, 11, 3, 16].

MOR requires a reduced-order basis (ROB) that is used to approximate solutions in the high-dimensional phase-space with a low number of basis vectors. The most widely used data-based basis generation techniques are based on the idea to use solutions of the high-dimensional full-order model (FOM) for different time instances and parameters as training data. These so-called snapshots are then used to compute the ROB e.g. with data-compression methods like the Proper Orthogonal Decomposition (POD), see e.g. [1]. Another approach are greedy algorithms, which are extensively used in the generation of ROBs for parametric problems, e.g. [20, 7, 9]. The ROB is built incrementally by extending the basis in several greedy iterations. Each iteration consists of two steps: (i) one or multiple snapshots which are not well approximated by the current ROB are selected. Error estimators may be used as a computationally efficient surrogate to select these snapshots, which enables a broader search. In a second step, (ii) these snapshots are used to compute an extension of the basis, which is in turn used in the next iteration. One example for a such an algorithm is the POD-greedy (also called PCA fixspace) [9]. In each greedy iteration, it uses the POD to compute an increment of the basis from a whole trajectory of snapshots. The method is standard for parametric, time-dependent problems. Also convergence statements have been derived [8].

For symplectic MOR, the classical, orthogonal basis generation techniques are not adequate since special (symplectic) ROBs are required. A greedy algorithm which generates a symplectic basis is presented in [14]. It does not use compression techniques for multiple snapshots in the greedy iteration but picks single snapshots. A symplectic Gram-Schmidt procedure [18] is used to compute a symplectic ROB. By construction, this method is limited to the generation of orthogonal, symplectic ROBs.

In our work, we propose a new greedy algorithm for symplectic basis generation, the PSD-greedy. It follows the idea of POD-greedy and uses compression techniques for trajectories of snapshots in the greedy iterations. We prove that such a technique is able to produce a symplectic ROB if a symplectic procedure is used for compression. In comparison to the previously mention approach [14], we are able to compute non-orthogonal, symplectic ROBs. Such ROBs showed superior results in [3].

In the remainder of Section 1, the required essentials of Hamiltonian systems, symplecticity and symplectic MOR are introduced. We present the new PSD-greedy algorithm in Section 2. The performance of PSD-greedy in comparison to existing symplectic basis generation techniques is analyzed in Section 3 based on a linear elasticity problem. A summery and an outlook conclude the paper in Section 4.

1.1. Hamiltonian systems and symplecticity. In the scope of this section, we restrict ourselves to autonomous, finite-dimensional, canonical Hamiltonian systems. Non-canonical systems can be redirected to the presented case with a state transformation [17]. Non-autonomous systems, i.e. systems with a time-dependent Hamiltonian function, can be reduced to the presented case if the Hamiltonian function is continuously differentiable with respect to the time variable, see e.g. [3]. We introduce the concept of a symplectic form and parametric Hamiltonian system in the following. To this end, let $\mathcal{P} \subset \mathbb{R}^p$ be the parameter domain and $\boldsymbol{\mu} \in \mathcal{P}$ be an arbitrary, but fixed, parameter vector.

A Hamiltonian system is described by the triplet $(\mathbb{V}, \omega, \mathcal{H})$ consisting of (a) a finite-dimensional vector space $\mathbb{V}$, the so-called phase-space, (b) a symplectic form $\omega : \mathbb{V} \times \mathbb{V} \to \mathbb{R}$ and (c) a Hamiltonian function $\mathcal{H} : \mathbb{V} \times \mathcal{P} \to \mathbb{R}$, which is at least one times continuously differentiable in the first argument. It can be shown that the phase-space is necessarily even-dimensional and thus, isomorphic to $\mathbb{R}^{2N}$, which is why we restrict to $\mathbb{V} = \mathbb{R}^{2N}$ in the following [5]. A symplectic form is a skew-symmetric and non-degenerate bilinear form. In the canonical case, the symplectic form can be expressed in terms of the Poisson matrix $\mathbb{J}_{2N}$ with

$$\omega_{2N}(\boldsymbol{v},\ \boldsymbol{w}) = \boldsymbol{v}^{\mathsf{T}}\mathbb{J}_{2N}\boldsymbol{w}, \qquad \mathbb{J}_{2N} = \begin{bmatrix} \boldsymbol{0}_N & \boldsymbol{I}_N \\ -\boldsymbol{I}_N & \boldsymbol{0}_N \end{bmatrix}, \qquad \begin{aligned} \mathbb{J}_{2N}^{\mathsf{T}}\mathbb{J}_{2N} &= \boldsymbol{I}_{2N} \\ \mathbb{J}_{2N}^{\mathsf{T}} &= -\mathbb{J}_{2N}, \end{aligned} \tag{1.1}$$

where $\boldsymbol{0}_N \in \mathbb{R}^{N\times N}$ is the matrix with all zeros and $\boldsymbol{I}_N \in \mathbb{R}^{N\times N}$ the identity matrix.

A continuously differentiable map $\boldsymbol{g} : \mathbb{R}^{2m} \supset \Omega \to \mathbb{R}^{2N}$ with $m \leq N$ is called symplectic (with respect to ω_{2N} and ω_{2m} on Ω), if

$$\left(D_{\boldsymbol{x}}\boldsymbol{g}(\boldsymbol{x})\right)^{\mathsf{T}}\mathbb{J}_{2N}D_{\boldsymbol{x}}\boldsymbol{g}(\boldsymbol{x}) = \mathbb{J}_{2m} \qquad \text{for all } \boldsymbol{x} \in \Omega, \tag{1.2}$$

where $D_{\boldsymbol{x}}\boldsymbol{g}(\boldsymbol{x}) \in \mathbb{R}^{2N\times 2m}$ is the Jacobian defined on Ω. For linear maps $\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$, $\boldsymbol{A} \in \mathbb{R}^{2N\times 2m}$, we call the coefficient matrix $D_{\boldsymbol{x}}\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{A}$ a symplectic matrix, if it fulfills (1.2).

For every symplectic matrix $\boldsymbol{A} \in \mathbb{R}^{2N\times 2m}$, there exists its symplectic inverse

$$\boldsymbol{A}^{+} := \mathbb{J}_{2m}^{\mathsf{T}}\boldsymbol{A}^{\mathsf{T}}\mathbb{J}_{2N} \quad \text{such that} \quad \boldsymbol{A}^{+}\boldsymbol{A} = \mathbb{J}_{2m}^{\mathsf{T}}\boldsymbol{A}^{\mathsf{T}}\mathbb{J}_{2N}\boldsymbol{A} \overset{(1.2)}{=} \mathbb{J}_{2m}^{\mathsf{T}}\mathbb{J}_{2m} \overset{(1.1)}{=} \boldsymbol{I}_{2m}. \tag{1.3}$$

A solution of the parametric Hamiltonian system for a fixed parameter $\boldsymbol{\mu} \in \mathcal{P}$ is a curve $\boldsymbol{x}(\bullet, \boldsymbol{\mu}) : I_t \to \mathbb{R}^{2N}$, $I_t = [t_0, t_{\text{end}}]$, in the phase-space which is a solution to the initial value problem for $t \in I_t$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x}(t,\boldsymbol{\mu}) = \mathbb{J}_{2N}\nabla_{\boldsymbol{x}}\mathcal{H}(\boldsymbol{x}(t,\boldsymbol{\mu}),\boldsymbol{\mu}), \qquad \boldsymbol{x}(t_0,\boldsymbol{\mu}) = \boldsymbol{x}_0(\boldsymbol{\mu}) \tag{1.4}$$

known as Hamilton's equation with initial datum $(t_0, \boldsymbol{x}_0(\boldsymbol{\mu}))$, $\boldsymbol{x}_0(\boldsymbol{\mu}) \in \mathbb{R}^{2N}$.

An important property of Hamiltonian systems is that the solution preserves the Hamiltonian function over time, i.e. $\mathcal{H}(\boldsymbol{x}(t,\boldsymbol{\mu}),\boldsymbol{\mu}) = \mathcal{H}(\boldsymbol{x}_0(\boldsymbol{\mu}),\boldsymbol{\mu})$ for all $t \in I_t$. Furthermore, the flow of the system is a symplectic map (1.2), see e.g. [10].

1.2. Symplectic model order reduction. Symplectic MOR follows the idea of general projection-based MOR techniques to approximate the solution in a low-dimensional subspace

$$\operatorname{colspan}(\boldsymbol{V}) = \mathcal{V} \subset \mathbb{R}^{2N}, \qquad \dim(\mathcal{V}) = 2n \ll 2N, \qquad \boldsymbol{V} \in \mathbb{R}^{2N\times 2n}.$$

In contrary to classical MOR, (a) this subspace is required to be a symplectic (and thus even-dimensional) subspace and (b) a symplectic projection is used instead of an orthogonal projection [17]. This choice ensures that the symplectic structure is preserved and the reduced system can be expressed by a Hamiltonian system of reduced-order $2n$ with the reduced Hamiltonian $\mathcal{H}_{\mathrm{r}} : \mathbb{R}^{2n} \times \mathcal{P} \to \mathbb{R}$, $(\boldsymbol{x}_{\mathrm{r}}, \boldsymbol{\mu}) \mapsto \mathcal{H}(\boldsymbol{V}\boldsymbol{x}_{\mathrm{r}}, \boldsymbol{\mu})$. The symplectic subspace can be computed with symplectic basis generation techniques. In the following, we describe three of such methods which are relevant for our new algorithm.

In [17], the Proper Symplectic Decomposition (PSD) was proposed. It follows the idea of the method of snapshots [19], which collects solution vectors $\boldsymbol{x}_{i,j}^{\mathrm{s}} := \boldsymbol{x}(t_i, \boldsymbol{\mu}_j)$ (so-called snapshots) of the FOM for different time instances t_i and parameter vectors $\boldsymbol{\mu}_j \in \mathcal{P}$ for $i = 1, \ldots, n_t$ and $j = 1, \ldots, n_{\boldsymbol{\mu}}$, which we denote in the following, by reindexing, as $\boldsymbol{x}_i^{\mathrm{s}}$ for $i = 1, \ldots, n_{\mathrm{s}} := n_t n_{\boldsymbol{\mu}}$. The PSD chooses the basis to minimize the symplectic projection error of all snapshots

$$\underset{\boldsymbol{V} \in \mathbb{R}^{2N \times 2n}}{\text{minimize}} \sum_{i=1}^{n_{\mathrm{s}}} \left\| \left(\boldsymbol{I}_{2N} - \boldsymbol{V}\boldsymbol{V}^{+} \right) \boldsymbol{x}_i^{\mathrm{s}} \right\|_2^2 \qquad \text{subject to } \boldsymbol{V}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{V} = \mathbb{J}_{2n}, \tag{1.5}$$

where the constraint ensures that $\boldsymbol{V}$ is a symplectic matrix and thus, that the symplectic inverse $\boldsymbol{V}^{+}$ exists. Due to strong non-convexity, no general solution could be derived so far. The authors of [17] derived several approaches to obtain an ROB in the set of orthogonal, symplectic bases, which is a subset of the set of symplectic bases.

A greedy algorithm is presented in [14]. It computes an orthogonal, symplectic ROB. Each iteration $1 \leq j \leq n_{\mathrm{s}}$ consists of two steps: (i) the snapshot $\boldsymbol{x}_{i_j}^{\mathrm{s}}$ with maximum symplectic projection error is selected to extend the ROB of the previous iteration. Then, (ii) a symplectic Gram-Schmidt procedure, see e.g. [18], is used to compute a symplectic ROB, which spans the symplectic subspace of the previous iteration united with the symplectic space spanned by $\boldsymbol{x}_{i_j}^{\mathrm{s}}$ and $\mathbb{J}_{2N}^{\mathsf{T}} \boldsymbol{x}_{i_j}^{\mathrm{s}}$.

More general bases are discussed in our work [3] with a technique that is able to compute non-orthogonal, symplectic ROBs. It is based upon the SVD-like decomposition [21, 22] of the snapshot matrix $\boldsymbol{X}_{\mathrm{s}} := [\boldsymbol{x}_1^{\mathrm{s}}, \ldots, \boldsymbol{x}_{n_{\mathrm{s}}}^{\mathrm{s}}] \in \mathbb{R}^{2N \times n_{\mathrm{s}}}$ that stacks the snapshots as columns. By removing the restriction of the ROB to be orthogonal, this method showed in the numerical experiments to require less basis vectors compared to the previously introduced orthogonal, symplectic basis generation methods.

2. Main results.

We introduce PSD-greedy in analogy to POD-greedy. In contrast to POD-greedy, we use symplectic instead of orthogonal techniques to compress trajectories in each iteration of the greedy algorithm. The advantage of this concept in comparison to the existing symplectic greedy approach [14] is twofold: (i) if, in a next step, error estimators are used to select the snapshots for enrichment, compressing a whole time series instead of selecting single snapshots of maximum projection error over all time steps alleviates known stagnation issues [7, 9] of greedy basis generation. On the other hand, (ii) we are able to use non-orthogonal basis generation techniques by which we expect similar improvements for the parametric case as observed in [3].

Following the idea of general greedy algorithms, our procedure operates iteratively and extends the ROB from iteration $i - 1$ to i by adding basis vectors to the ROB, which is reflected by adding the new vectors as columns to the matrix representation $\boldsymbol{V}_i$ of the ROB. For symplectic ROBs, this requires a special treatment in order to preserve the symplecticity, which is discussed in the following lemma. For the ease of notation, if we introduce a symplectic matrix $\boldsymbol{V} \in \mathbb{R}^{2N \times 2m}$ in the following, then the submatrices $\boldsymbol{E}_{\boldsymbol{V}}, \boldsymbol{F}_{\boldsymbol{V}} \in \mathbb{R}^{2N \times m}$ denote the first and the last m columns of $\boldsymbol{V}$ such that $\boldsymbol{V} = [\boldsymbol{E}_{\boldsymbol{V}}, \boldsymbol{F}_{\boldsymbol{V}}]$. Symplecticity of $\boldsymbol{V}$ is, by insertion in (1.2), equivalent to the following conditions on $\boldsymbol{E}_{\boldsymbol{V}}$ and $\boldsymbol{F}_{\boldsymbol{V}}$:

$$\boldsymbol{E}_{\boldsymbol{V}}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{E}_{\boldsymbol{V}} = \boldsymbol{F}_{\boldsymbol{V}}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{F}_{\boldsymbol{V}} = \boldsymbol{0}_m \qquad \text{and} \qquad \boldsymbol{E}_{\boldsymbol{V}}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{F}_{\boldsymbol{V}} = \boldsymbol{I}_m. \tag{2.1}$$

LEMMA 2.1. *If $\boldsymbol{V} \in \mathbb{R}^{2N \times 2m_{\boldsymbol{V}}}$ and $\boldsymbol{W} \in \mathbb{R}^{2N \times 2m_{\boldsymbol{W}}}$ are symplectic matrices, then the matrix stacking the $2m_{\boldsymbol{U}} := 2m_{\boldsymbol{V}} + 2m_{\boldsymbol{W}}$ columns of $\boldsymbol{V}$ and $\boldsymbol{W}$ with*

$$\boldsymbol{U} := [\boldsymbol{E}_{\boldsymbol{U}}, \boldsymbol{F}_{\boldsymbol{U}}] \in \mathbb{R}^{2N \times 2m_{\boldsymbol{U}}}, \quad \boldsymbol{E}_{\boldsymbol{U}} := [\boldsymbol{E}_{\boldsymbol{V}}, \boldsymbol{E}_{\boldsymbol{W}}], \quad \boldsymbol{F}_{\boldsymbol{U}} := [\boldsymbol{F}_{\boldsymbol{V}}, \boldsymbol{F}_{\boldsymbol{W}}] \tag{2.2}$$

is a symplectic matrix if and only if $\boldsymbol{W}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{V} = \boldsymbol{0}_{2m_{\boldsymbol{W}} \times 2m_{\boldsymbol{V}}}$.

Proof. The symplecticity of $\boldsymbol{U}$ is expressed with (2.1) in terms of the three conditions on $\boldsymbol{E_U}$ and $\boldsymbol{F_U}$. Firstly, it holds

$$\boldsymbol{E}_{\boldsymbol{U}}^{\mathsf{T}} \mathbb{J}_{2n} \boldsymbol{E}_{\boldsymbol{U}} = \begin{bmatrix} \boldsymbol{E}_{\boldsymbol{V}}^{\mathsf{T}} \\ \boldsymbol{E}_{\boldsymbol{W}}^{\mathsf{T}} \end{bmatrix} \mathbb{J}_{2n} \begin{bmatrix} \boldsymbol{E}_{\boldsymbol{V}} & \boldsymbol{E}_{\boldsymbol{W}} \end{bmatrix} = \mathbf{0}_{m_{\boldsymbol{U}}},$$

which is equivalent to $\boldsymbol{E}_{\boldsymbol{W}}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{E}_{\boldsymbol{V}} = \mathbf{0}_{m_{\boldsymbol{W}} \times m_{\boldsymbol{V}}}$ by using the symplecticity of $\boldsymbol{V}$ and $\boldsymbol{W}$. Analogously, the two conditions, $\boldsymbol{F}_{\boldsymbol{U}}^{\mathsf{T}} \mathbb{J}_{2n} \boldsymbol{F}_{\boldsymbol{U}} = \mathbf{0}_{m_{\boldsymbol{U}}}$ and $\boldsymbol{E}_{\boldsymbol{U}}^{\mathsf{T}} \mathbb{J}_{2n} \boldsymbol{F}_{\boldsymbol{U}} = \boldsymbol{I}_{m_{\boldsymbol{U}}}$, are equivalent to

$$\boldsymbol{F}_{\boldsymbol{W}}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{F}_{\boldsymbol{V}} = \boldsymbol{F}_{\boldsymbol{W}}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{E}_{\boldsymbol{V}} = \boldsymbol{E}_{\boldsymbol{W}}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{F}_{\boldsymbol{V}} = \mathbf{0}_{m_{\boldsymbol{W}} \times m_{\boldsymbol{V}}}.$$

The four derived conditions on $\boldsymbol{E_V}, \boldsymbol{F_V}, \boldsymbol{E_W}$ and $\boldsymbol{F_W}$ are in turn equivalent to the single condition $\boldsymbol{W}^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{V} = \mathbf{0}_{2m_{\boldsymbol{W}} \times 2m_{\boldsymbol{V}}}$. □

Note that under the assumptions of Lemma 2.1, the result $\boldsymbol{U}$ is guaranteed to be a symplectic matrix. From (1.2), it follows that $\boldsymbol{U}$ is of full column rank and the linearly independent columns form a basis of colspan $(\boldsymbol{U})$.

The new symplectic basis generation technique, the PSD-greedy, is presented in Algorithm 1. The algorithm computes a symplectic basis represented by $\boldsymbol{V}_{i_{\max}}$ with $i_{\max}$ greedy iterations. The user inputs a finite parameter set $M \subset \mathcal{P}$, an error tolerance $r_{\text{tol}} > 0$ and a snapshot generation algorithm $\boldsymbol{X}_{\text{s}} : M \to \mathbb{R}^{2N \times n_{\text{s}}(\boldsymbol{\mu})}$, where the number of snapshots $n_{\text{s}}(\boldsymbol{\mu})$ might vary with $\boldsymbol{\mu}$.

We use different submodules in the algorithm: The algorithm is formulated in terms of a modular symplectic basis generation technique `PSD` $(\bullet)$ that is used to compute an extension of the basis from the residual $\boldsymbol{R}_i$. The requirements on this procedure are discussed in Lemma 2.2. The function $\Delta(\bullet, \bullet)$ computes an error indicator with respect to the basis given in the first argument for the parameter vector given in the second argument. Examples are the symplectic projection error (1.5) or the true reduction error as introduced later in Equation (3.2). Furthermore, error estimators might be used to lower the computational cost of this operation, which enables a broader search. The *extend*$(\bullet, \bullet)$ function is supposed to extend the matrix in the first argument by the matrix given in the second argument in the fashion of Equation (2.2).

In the first iteration of the algorithm, the ROB $\boldsymbol{V}_0$ is empty. When computing the error in lines 3 and 5 and the residual in line 6 for $\boldsymbol{V}_0$, all terms linked to $\boldsymbol{V}_0$ are neglected, i.e. set to zero.

We do not restrict how many basis vectors are added in each iteration. The simplest choice is to add a fixed number $\Delta n_1 = \cdots = \Delta n_{i_{\max}}$, $\Delta n_i := n_i - n_{i-1}$, of basis vectors in each iteration. More adaptivity is obtained if the module `PSD` $(\bullet)$ chooses the number of basis vectors in each iteration based on the given residual.

Algorithm 1: PSD-greedy algorithm based on a symplectic basis generation technique PSD $(\bullet)$ that is supposed to fulfill the assumptions of Lemma 2.2.

Input: finite parameter set $M \subset \mathcal{P}$, error tolerance $r_{\text{tol}} > 0$, snapshot-generation algorithm $\boldsymbol{X}_{\text{s}} : M \to \mathbb{R}^{2N \times n_{\text{s}}}$

Output: symplectic basis $\boldsymbol{V}_{i_{\max}} \in \mathbb{R}^{2N \times 2n_{i_{\max}}}$, number of iterations $i_{\max}$

$\boldsymbol{E}_0 \leftarrow [\ ]$, $\boldsymbol{F}_0 \leftarrow [\ ]$, $\boldsymbol{V}_0 \leftarrow [\boldsymbol{E}_0, \boldsymbol{F}_0]$ ▷ start with empty basis

$i \leftarrow 0$

while $\exists \boldsymbol{\mu} \in M : \Delta(\boldsymbol{V}_i,\ \boldsymbol{\mu}) > r_{tol}$ **do**

  $i \leftarrow i + 1$

  $\boldsymbol{\mu}_i \leftarrow \text{argmax}_{\boldsymbol{\mu} \in M} \Delta(\boldsymbol{V}_i,\ \boldsymbol{\mu})$

  $\boldsymbol{R}_i \leftarrow (\boldsymbol{I}_{2N} - \boldsymbol{V}_{i-1}\boldsymbol{V}_{i-1}^{+})\boldsymbol{X}_{\text{s}}(\boldsymbol{\mu}_i)$ ▷ compute residual w.r.t. previous basis

  $\boldsymbol{V}_i^{\text{ext}} \leftarrow \texttt{PSD}(\boldsymbol{R}_i)$ ▷ compute extension

  $\boldsymbol{V}_i \leftarrow \texttt{extend}(\boldsymbol{V}_{i-1},\ \boldsymbol{V}_i^{\text{ext}})$ ▷ extend basis 'symplectically', see Eq. (2.2)

end

$i_{\max} \leftarrow i$

LEMMA 2.2. *Consider $\boldsymbol{R} \in \mathbb{R}^{2N \times n_{\boldsymbol{R}}}$. We assume that $\mathit{PSD}(\boldsymbol{R})$ returns a ROB represented by $\boldsymbol{V}^{ext} \in \mathbb{R}^{2N \times 2m_{\boldsymbol{V}^{ext}}}$ for an arbitrary $m_{\boldsymbol{V}^{ext}} \leq N$ which fulfills*

1. *$\boldsymbol{V}^{ext}$ is a symplectic matrix and*
2. colspan $(\boldsymbol{V}^{ext})$ *is a subspace of* colspan $(\boldsymbol{R})$.

Let $\boldsymbol{X} \in \mathbb{R}^{2N \times n_{\boldsymbol{X}}}$, $n_{\boldsymbol{X}} \in \mathbb{N}$. For every symplectic matrix $\boldsymbol{W} \in \mathbb{R}^{2N \times 2m_{\boldsymbol{W}}}$, the extended matrix $\boldsymbol{U} := \mathit{extend}(\boldsymbol{W},\ \boldsymbol{V}^{ext})$ is a symplectic matrix if $\boldsymbol{V}^{ext} = \mathit{PSD}(\boldsymbol{R})$ with $\boldsymbol{R} = (\boldsymbol{I}_{2N} - \boldsymbol{W}\boldsymbol{W}^{+})\boldsymbol{X}$.

Proof. With Lemma 2.1, it is sufficient to show $\boldsymbol{W}^{\mathsf{T}}\mathbb{J}_{2N}\boldsymbol{V}^{\text{ext}} = \boldsymbol{0}_{2m_{\boldsymbol{W}} \times 2m_{\boldsymbol{V}^{\text{ext}}}}$ since $\boldsymbol{W}$ and $\boldsymbol{V}^{\text{ext}}$ are symplectic matrices by assumption. Due to assumption (2) on $\boldsymbol{V}^{\text{ext}}$, there exists a matrix $\boldsymbol{C} \in \mathbb{R}^{n_{\boldsymbol{X}} \times 2m_{\boldsymbol{V}^{\text{ext}}}}$ such that we can express $\boldsymbol{V}^{\text{ext}} = \boldsymbol{R}\boldsymbol{C}$. With the identity

$$\boldsymbol{W}^{\mathsf{T}}\mathbb{J}_{2N}\boldsymbol{W}\boldsymbol{W}^{+} \overset{(1.3)}{=} \boldsymbol{W}^{\mathsf{T}}\mathbb{J}_{2N}\boldsymbol{W}\mathbb{J}_{2m_{\boldsymbol{W}}}^{\mathsf{T}}\boldsymbol{W}^{\mathsf{T}}\mathbb{J}_{2N} \overset{(1.2)}{=} \mathbb{J}_{2m_{\boldsymbol{W}}}\mathbb{J}_{2m_{\boldsymbol{W}}}^{\mathsf{T}}\boldsymbol{W}^{\mathsf{T}}\mathbb{J}_{2N} \overset{(1.1)}{=} \boldsymbol{W}^{\mathsf{T}}\mathbb{J}_{2N},$$

it indeed holds

$$\boldsymbol{W}^{\mathsf{T}}\mathbb{J}_{2N}\boldsymbol{V}^{\text{ext}} = \boldsymbol{W}^{\mathsf{T}}\mathbb{J}_{2N}(\boldsymbol{I}_{2n} - \boldsymbol{W}\boldsymbol{W}^{+})\boldsymbol{X}\boldsymbol{C} = \boldsymbol{0}_{2m_{\boldsymbol{W}} \times 2m_{\boldsymbol{V}^{\text{ext}}}}.$$

□

The symplecticity of all matrices $\boldsymbol{V}_i$ in Algorithm 1 follows from Lemma 2.2 with induction over the iteration index i. The induction basis holds since for $i = 1$ the ROB $\boldsymbol{V}_1 = \boldsymbol{V}_1^{\text{ext}}$ is symplectic by assumption 1 of Lemma 2.2.

3. Numerical experiments. As numerical example, we inspect a linear elasticity problem parametrized by the Lamé parameters and a parameter for external forces collected in the parameter vector $\boldsymbol{\mu} := [\lambda_{\text{L}}, \mu_{\text{L}}, F_{\max}] \subset \mathbb{R}^3_{>0}$ for a three-dimensional domain $\Omega \subset \mathbb{R}^3$. The governing Hamiltonian PDE with the Hamiltonian function

$$\mathcal{H}_{\text{PDE}}(\boldsymbol{u}, \boldsymbol{w}; \boldsymbol{\mu}) = \frac{1}{2}\int_{\Omega} \varrho^{-1}\left\|\boldsymbol{w}\right\|_2^2 + \langle \boldsymbol{\sigma}(\boldsymbol{u}; \boldsymbol{\mu}),\ \boldsymbol{\varepsilon}(\boldsymbol{u})\rangle_{\text{F}}\, \mathrm{d}\boldsymbol{\xi}, \qquad \varrho \in \mathbb{R}_{>0} \text{ fixed},$$

is solved for the unknown displacement and momentum $\boldsymbol{u}, \boldsymbol{w} : I_t \times \Omega \to \mathbb{R}^3$ for appropriate boundary conditions, where

$$\boldsymbol{\sigma}(\boldsymbol{u}; \boldsymbol{\mu}) = \lambda_{\text{L}}\, \text{trace}\,(\boldsymbol{\varepsilon}(\boldsymbol{u}))\, \boldsymbol{I}_3 + 2\mu_{\text{L}}\boldsymbol{\varepsilon}(\boldsymbol{u}) \in \mathbb{R}^{3\times 3}, \quad \boldsymbol{\varepsilon}(\boldsymbol{u}) = \frac{1}{2}\left(\nabla_{\boldsymbol{\xi}}\boldsymbol{u} + (\nabla_{\boldsymbol{\xi}}\boldsymbol{u})^{\mathsf{T}}\right) \in \mathbb{R}^{3\times 3}$$

are the stress and the strain tensor and $\langle \bullet, \bullet \rangle_{\mathrm{F}}$ is the Frobenius inner-product, i.e. the summed element-wise products. The domain Ω imitates a simple fusiform muscle (see Figure 3.1). An external load is applied in axial direction on the right boundary. The parameter domain $\mathcal{P}$ is based on the parameters given in [12] with

$$\lambda_{\mathrm{L}} \in [6\text{e}4,\ 1.2\text{e}5]\ \mathrm{N/m^2}, \quad \mu_{\mathrm{L}} \in [6\text{e}3,\ 1.22\text{e}4]\ \mathrm{N/m^2}, \quad F_{\max} \in [0.49,\ 5.89]\ \mathrm{N}$$

and a fixed density $\rho = 1059.7\ \mathrm{kg/m^3}$. The time interval is $I_t := [0, 0.5]s$. Although the mechanics are too simple to build a realistic muscle model, we investigate how well the Hamiltonian formulation and symplectic MOR are potentially suited for the reduction of the mechanical part of three-dimensional muscle models.

We use the Finite Element Method [6] with 1920 first-order Lagrangian elements to discretize the equations, which results in a (time-dependent) Hamiltonian system (1.4) with the quadratic Hamiltonian function

$$\mathcal{H}(\boldsymbol{x}, t, \boldsymbol{\mu}) = \frac{1}{2}\boldsymbol{x}^{\mathsf{T}}\boldsymbol{H}\boldsymbol{x} + \boldsymbol{x}^{\mathsf{T}}\begin{bmatrix} -\boldsymbol{f}(t,\boldsymbol{\mu}) \\ \mathbf{0}_{N\times 1} \end{bmatrix}, \qquad \boldsymbol{H}(\boldsymbol{\mu}) := \begin{bmatrix} \boldsymbol{K}(\boldsymbol{\mu}) & \mathbf{0}_N \\ \mathbf{0}_N & \boldsymbol{M}^{-1}(\boldsymbol{\mu}) \end{bmatrix}, \tag{3.1}$$

where $\boldsymbol{K}(\boldsymbol{\mu}), \boldsymbol{M}(\boldsymbol{\mu}) \in \mathbb{R}^{N\times N}$ are the stiffness and the mass matrix and $\boldsymbol{f}(t,\boldsymbol{\mu}) \in \mathbb{R}^N$ is the vector of external forces with $N = 15,066$.

The Hamiltonian system is discretized equidistantly in time with $n_t = 1000$ time steps with the implicit midpoint rule [10]. This method is a symplectic time integration scheme and preserves quadratic invariants like the quadratic Hamiltonian (3.1). The use of a symplectic integrator in combination with symplectic MOR is imperative to preserve the symplectic structure throughout the whole simulation pipeline, which enables preservation of the system energy or stability [17, 14].

The experiments are conducted in the MOR framework pyMOR [15]. The special architecture of this open-source software makes use of highly abstract interfaces which allows a seamless integration with external PDE solver libraries. In our experiments, we used the bindings to the Finite Element software package FEnics [13].

We present two experiments which investigate (a) the training and (b) how well the trained models generalize to parameter vectors that are not included in the training set. We use the $L_2(I_t, \mathbb{R}^{2N})$ norm with an $\boldsymbol{H}_{\mathrm{fix}}$-weighted norm in space

$$\|\boldsymbol{x}(t)\|^2_{L_2,\boldsymbol{H}_{\mathrm{fix}}} := \int_{I_t} \|\boldsymbol{x}(t)\|^2_{\boldsymbol{H}_{\mathrm{fix}}}\,\mathrm{d}t, \qquad \|\boldsymbol{x}(t)\|^2_{\boldsymbol{H}_{\mathrm{fix}}} := (\boldsymbol{x}(t))^{\mathsf{T}}\,\boldsymbol{H}_{\mathrm{fix}}\boldsymbol{x}(t),$$

where the integral over time is approximated with the composite trapezoidal rule and $\boldsymbol{H}_{\mathrm{fix}} := \boldsymbol{H}(\boldsymbol{\mu}_{\mathrm{fix}})$ is a weighting matrix for a fixed parameter vector $\boldsymbol{\mu}_{\mathrm{fix}} \in \mathcal{P}$ such that

$$\lambda_{\mathrm{L}} = 80\,690\ \mathrm{N/m^2}, \quad \mu_{\mathrm{L}} = 8\,966\ \mathrm{N/m^2}, \quad F_{\max} \approx 3.83\ \mathrm{N}.$$

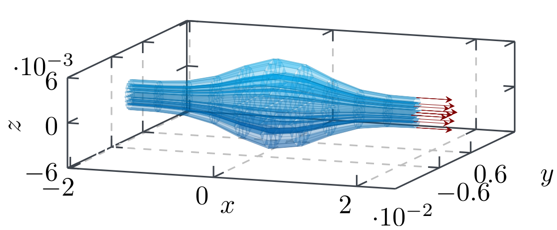

FIG. 3.1. *Discretized Fusiform-muscle-shaped domain Ω in blue and boundary traction (Neumann values) as dark red arrows.*

TABLE 3.1
Greedy MOR techniques used in the experiments. Classified by orthogonality and symplecticity.

Greedy MOR technique	abbreviation	ortho.	sympl.	ref.
POD-greedy with $\boldsymbol{H}_{\text{fix}}$ as inner product matrix	POD_G	✓	✗	[9]
Based on symplectic Gram–Schmidt	sGS_G	✓	✓	[14]
PSD-greedy with `PSD`(•) submodule:				
PSD Complex SVD	PSD_G cSVD	✓	✓	[17]
PSD SVD-like decomposition	PSD_G SVD-like	✗	✓	[3]

The bases are compared with the absolute and the relative reduction error

$$e_{\text{abs},i}(\boldsymbol{\mu}) := \left\| \boldsymbol{x}(t,\boldsymbol{\mu}) - \boldsymbol{V}_i \boldsymbol{x}_{\text{r},i}(t,\boldsymbol{\mu}) \right\|_{L_2,\boldsymbol{H}_{\text{fix}}}, \quad e_{\text{rel},i}(\boldsymbol{\mu}) := \frac{e_{\text{abs},i}(\boldsymbol{\mu})}{\left\| \boldsymbol{x}(t,\boldsymbol{\mu}) \right\|_{L_2,\boldsymbol{H}_{\text{fix}}}}, \tag{3.2}$$

where $\boldsymbol{x}(t,\boldsymbol{\mu}) \in \mathbb{R}^{2N}$ is the solution of the FOM and $\boldsymbol{V}_i \in \mathbb{R}^{2N\times 2n_i}$, $\boldsymbol{x}_{\text{r},i}(t,\boldsymbol{\mu}) \in \mathbb{R}^{2n_i}$ are the ROB and the solution of the reduced model of the ith greedy iteration.

In both experiments, we investigate four different greedy basis generation techniques (see Table 3.1). These include the POD-greedy (POD_G) with $\boldsymbol{H}_{\text{fix}}$ as inner product matrix, two PSD-greedy (PSD_G cSVD and PSD_G SVD-like) and the existing symplectic greedy approach (sGS_G). The subindex $(\bullet)_\text{G}$ indicates that all of them are greedy methods. The two `PSD`(•) submodules investigated for the PSD-greedy, PSD complex SVD and PSD SVD-like decomposition, are chosen based on our observations in [3]. Both methods fulfill the assumptions of Lemma 2.2. The PSD complex SVD computes a minimizer of the symplectic projection error (1.5) in the set of orthogonal, symplectic ROBs and is, thus, chosen to investigate the performance of PSD-greedy with orthogonal, symplectic compression techniques. The PSD SVD-like decomposition is the only basis generation technique that computes a non-orthogonal, symplectic ROB. It is used to examine the behavior of PSD-greedy with non-orthogonal, symplectic compression techniques.

As training set $M \subset \mathcal{P}$, a $4\times4\times4$ Cartesian grid is used. Each iteration $2\Delta n_i = 2$ vectors are added. The termination condition is set to leave the greedy algorithm after $i_{\max} = 30$ greedy iterations, which results in a ROB of dimension $2n_{i_{\max}} = 60$.

The results of the training experiment are presented in Figure 3.2 with the maximum absolute reduction error (3.2) over all 64 training parameter vectors $\boldsymbol{\mu} \in M$. We observe that POD_G is not able to reduce the problem without introducing big errors whereas all symplectic methods show a decreasing error. The decline is mostly monotonic which means that the incrementally extended reduced models do improve the reduction error in every iteration. We observe a stagnation of PSD_G cSVD for $i > 10$ with a maximal absolute error of 10^{-3}. The other two symplectic methods, sGS_G and PSD_G SVD-like, are able to further decrease the error. The PSD_G SVD-like outperforms the other methods for all $i > 1$, which is underlined by an improvement of one order of magnitude for $i \in \{6, 7\}$. This matches the observations of our work in [3]. In line with those results, the superiority is assumed to stem from removing the requirement of orthogonality of the ROB, which poses less constraints on the basis generation and leaves more leeway for the ROB to adapt to the data more precisely with less basis vectors.

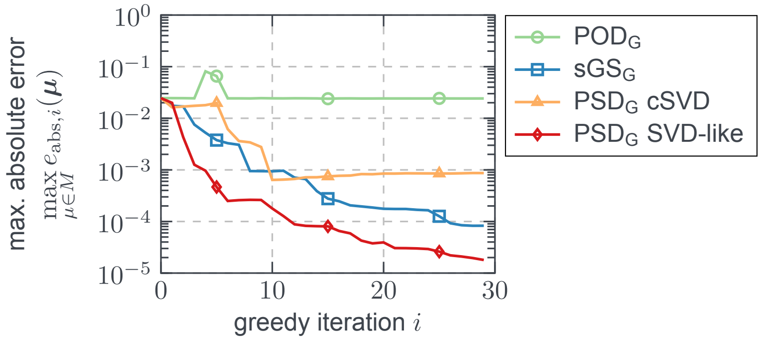

FIG. 3.2. *Maximum absolute reduction error over* 64 *parameter vectors for training.*

In the second experiment, we consider 100 random parameter vectors $\boldsymbol{\mu} \in \mathcal{P} \setminus M$ that were not used in training. The results are presented in Figure 3.3 in terms of the relative reduction error (3.2) of 15 ROBs $\boldsymbol{V}_i$ with ROB size $2n_i$. Boxplots are used to visualize the statistics of the relative error (3.2) for the 100 random parameter vectors, where the whiskers indicate the minimum and maximum relative error. The observations of the training transfer directly to the test results. This means that the symplectic methods do not only perform well on the training parameter vectors but are able to generalize to random parameter vectors in the parameter domain. Except for $\mathrm{PSD_G}$ cSVD, the decline of the mean value of the relative error is in most of the cases monotonic. The superiority of the non-orthogonal $\mathrm{PSD_G}$ SVD-like basis generation technique also transfers from the training to the test experiment. With ROB sizes $2n_i \geq 12$, the median of the relative error of $\mathrm{PSD_G}$ SVD-like is always below 1% relative error which occurs for $\mathrm{sGS_G}$ with $2n_i \geq 32$. This means, the new $\mathrm{PSD_G}$ SVD-like is able to reduce the ROB size by a factor of 2.6 compared to $\mathrm{sGS_G}$ while achieving the same relative error.

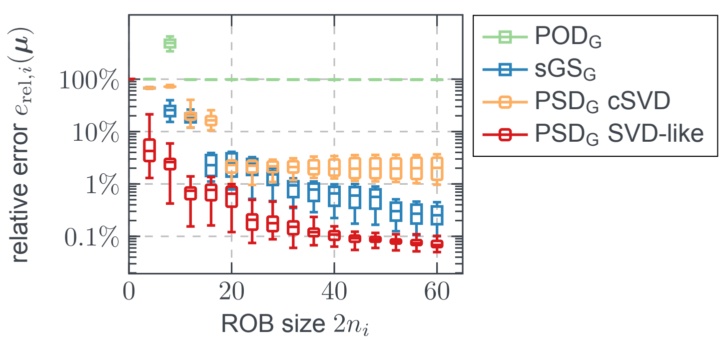

FIG. 3.3. *Statistics of the relative error over* 100 *random test parameter vectors.*

4. Summary and outlook. We presented a new greedy algorithm, PSD-greedy, to compute a symplectic ROB, which is relevant for structure-preserving MOR of parametric Hamiltonian systems. It adopts the idea of POD-greedy to use compression methods in each greedy iteration to enrich the reduced-order basis. We proved that it is sufficient to use symplectic methods for compression in order to compute a symplectic basis. The numerical experiments showed that improvements of up to one order of magnitude in the relative reduction error are achievable with the new basis generation technique compared to the existing greedy approach.

Further work should analyze the convergence rates of symplectic greedy algorithms. This is not straightforward since convergence results for greedy algorithms available in the literature rely on the orthogonality of the ROB [9, 14], which is not required by our algorithm. Furthermore, error estimators should be used in a next step to avoid the expensive evaluation of the full-order model during greedy iterations in order to find the parameter with maximum error.

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