

1 SYMPLECTIC MODEL-REDUCTION WITH A WEIGHTED INNER
2 PRODUCT*

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5 **Abstract.** In the recent years, a considerable attention has been geared toward preserving
6 structures and invariants in reduced basis methods, to enhance the stability and the robustness
7 of the reduced system. In the context of Hamiltonian systems, symplectic model reduction is an
8 approach that tends to construct a reduced order system that preserve the symplectic symmetry of
9 Hamiltonian systems. However, the symplectic methods are based on the standard Euclidean inner
10 products and are not suitable for problems that are equipped with a more general inner product. In
11 this paper we generalize the symplectic model reduction method such that it can adapt to the norms
12 and the inner products most appropriate to the problem while preserving the symplectic symmetry
13 of Hamiltonian systems. To construct a reduced basis and accelerate evaluation of nonlinear terms,
14 a greedy generation of a symplectic basis is proposed. Furthermore, it is shown that the greedy
15 approach yields a norm bounded reduced basis. The accuracy and the stability of this model reduction
16 technique is illustrated through the simulations of a vibrating elastic beam and the sine-Gordon
17 equation.

18 **Key words.** Structure Preserving, Weighted MOR, Hamiltonian Systems, Greedy Reduced
19 Basis, Symplectic DEIM

20 **AMS subject classifications.** 78M34, 34C20, 35B30, 37K05, 65P10, 37J25

21 **1. Introduction.** Reduced order models have emerged as a powerful approach
22 to cope with the evermore complex new applications in engineering and science. These
23 methods, specially the reduced basis (RB) methods, substantially reduce the dimen-
24 sionality of the problem by constructing a reduced order configuration space. Explor-
25 ation of the reduced space is then possible with significant acceleration [22, 19].

26 Over the past decade, RB methods had a great success in lowering the computa-
27 tional costs of solving elliptic and parabolic differential equations [23, 24]. However,
28 model reduction of hyperbolic problems remains one of the today's challenges. These
29 problems often arise from a set of conservation laws and invariants. Such intrinsic
30 structures are lost over the course of model reduction which result in a qualitatively
31 wrong, and sometimes unstable reduced system [3].

32 Moreover, simulation of reduced models incurs solution error and estimation of
33 this error is essential in the applications of model reduction [20, 36, 16]. Finding
34 tight error bounds for the reduced system has shown to be computationally expensive
35 and often impractical. Therefore, when one is interested in a cheap surrogate for the
36 error incurred or when the conserved quantity is an output of the system, it becomes
37 imperative to preserve system structures through model order reduction.

38 Recently, constructing RB methods that can conserve intrinsic structures has
39 attracted a vast attention [2, 1, 25, 15, 7, 10, 6, 33]. Structure preservation in model
40 reduction, not only constructs a physically meaningful reduced system, but it can

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41 also enhance the robustness and stability of the reduced system. In system theory,
 42 conservation of passivity can be found in the work of [34, 18]. Energy preserving and
 43 inf-sup stable methods for finite element methods (FEM) are developed in [15, 4].
 44 Also, a conservative model reduction technique for finite-volume method is seen in
 45 [9].

46 In the context of Lagrangian and Hamiltonian systems, recent works provide a
 47 promising approach to constructing a robust and stable reduced system. Carlberg,
 48 Tuminaro, and Boggs [11] suggest that a reduced order model of a Lagrangian system
 49 should be identified by an approximated Lagrangian on a reduced order configuration
 50 space. This allows the reduced system to inherit the geometric structure of the original
 51 system. Similar approach has been adopted in the work of Maboudi Afkham and
 52 Hesthaven [2] and also in the work of Peng and Mohseni [33] for Hamiltonian systems.
 53 They construct a low-order symplectic linear vector space, i.e. a vector space equipped
 54 with a symplectic 2-form, as the reduced space. Once the symplectic reduced space is
 55 generated, a symplectic projection result in a physically meaningful reduced system.
 56 A proper time-stepping scheme can then preserve the Hamiltonian structure of the
 57 reduced system. It is shown in [2, 33] that this approach preserves the overall dynamics
 58 of the original system and helps with the stability of the reduced system. Despite the
 59 success of these method in model reduction of Hamiltonian systems, these problems
 60 are only compatible with the standard Euclidean or the L^2 inner product. Therefore,
 61 the computational structures that arise from a natural inner product of a problem
 62 will be lost over model reduction.

63 Weak formulations and inner-products defined on a Hilbert space are at the core
 64 of the error analysis of many numerical methods for solving partial differential equa-
 65 tions. Therefore, it is natural to seek for model reduction methods that consider such
 66 features. At discrete level, these features often require a Euclidean vector space to
 67 be equipped with a generalized inner product associated with a weight matrix X .
 68 Many works have been conducted to make conventional model reduction techniques
 69 compatible with such inner products [37]. However, a model reduction method that
 70 simultaneously preserves the symplectic symmetry of Hamiltonian systems is still un-
 71 known.

72 In this paper, we attempt to combine the classical model reduction method with
 73 respect to a weight matrix with the symplectic model reduction. The reduced system
 74 constructed by the new method is a generalized Hamiltonian system and the low order
 75 configuration space associated with this system is a symplectic linear vector space with
 76 a non-standard symplectic 2-form. It is demonstrated that the new method can be
 77 viewed as the natural extension to [2], therefore, it carries the structure preserving
 78 features, e.g. symplecticness and stability. We also present a greedy approach for
 79 constructing a generalized symplectic basis for the reduced system. It is well known
 80 that structured matrices are in general not norm bounded [26]. We show that the
 81 condition number of the basis generated by the greedy method is bounded by the
 82 condition number of the weight matrix X . Finally, to accelerate the evaluation of
 83 nonlinear terms in the reduced system, we present a variation of the discrete empirical
 84 interpolation method (DEIM) that preserves the symplectic structure of the reduced
 85 system.

86 What remains of this paper is organized as follows. In section 2 we cover the
 87 required background on the Hamiltonian and the generalized Hamiltonian systems.
 88 Section 3 summarizes the classical model reduction routine with respect to a weight
 89 norm and the symplectic model reduction method with respect to the standard Eu-
 90 clidean inner product. We introduce the symplectic model reduction method with

respect to a weighted inner product in section 4. Section 5 illustrates the performance of the new method through numerical simulation of the equations governing a vibrating beam and the sine-Gordon equation. We offer conclusive remarks in section 6.

2. Hamiltonian systems. In this section we discuss the basic concepts around the geometry of symplectic linear vector spaces and introduce Hamiltonian and Generalized Hamiltonian systems.

2.1. Generalized Hamiltonian systems. Let $(\mathbb{R}^{2n}, \Omega)$ be a symplectic linear vector space, with \mathbb{R}^{2n} the configuration space and $\Omega : \mathbb{R}^{2n} \times \mathbb{R}^{2n} \rightarrow \mathbb{R}$ a closed, skew-symmetric and non-degenerate 2-form on \mathbb{R}^{2n} . Given a smooth Hamiltonian function $H : \mathbb{R}^{2n} \rightarrow \mathbb{R}$, the *generalized Hamiltonian equation* of evolution reads

$$(1) \quad \begin{cases} \dot{z} = J_{2n} \nabla_z H(z), \\ z(0) = z_0. \end{cases}$$

Here $z \in \mathbb{R}^{2n}$ is the configuration coordinates and J_{2n} is a full-rank and skew-symmetric $2n \times 2n$ structure matrix such that $\Omega(x, y) = x^T J_{2n} y$, for all state vectors $x, y \in \mathbb{R}^{2n}$ [30]. Note that there always exists a coordinate transformation $\tilde{z} = T^{-1} z$, with $T \in \mathbb{R}^{2n \times 2n}$, such that J_{2n} takes the form of the *standard* symplectic structure matrix

$$(2) \quad \mathbb{J}_{2n} = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix},$$

in the new coordinate system [13]. Here 0_n and I_n are the zero matrix and the identity matrix of size $n \times n$, respectively. A central feature of Hamiltonian systems is conservation of the Hamiltonian which we summarize in the following theorem.

THEOREM 2.1. [30] *Consider the flow $\phi_t : \mathbb{R} \times \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ of the Hamiltonian system (1). Then $H \circ \phi_t = H$.*

Under a general coordinate transformation, the equations of evolution of a Hamiltonian system might not take the form (1). It turns out that only transformations which preserve the symplectic form, *symplectic transformations*, also preserve the form of a Hamiltonian system [21]. Suppose that $(\mathbb{R}^{2n}, \Omega)$ and $(\mathbb{R}^{2k}, \Lambda)$ are two symplectic linear vector spaces. A transformation $\alpha : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2k}$ is a symplectic transformation if

$$(3) \quad \Omega(x, y) = \Lambda(\alpha(x), \alpha(y)), \quad \text{for all } x, y \in \mathbb{R}^{2n}.$$

In matrix notation, i.e. when we agree upon a set of basis vectors for \mathbb{R}^{2n} and \mathbb{R}^{2k} , a linear symplectic transformation is a matrix $A \in \mathbb{R}^{2n \times 2k}$ that satisfies

$$(4) \quad A^T J_{2n} A = J_{2k}.$$

We are interested in a class of symplectic transformations that transform a symplectic structure J_{2n} into the standard symplectic structure \mathbb{J}_{2k} .

DEFINITION 2.2. *Let $J_{2n} \in \mathbb{R}^{2n \times 2n}$ be a full-rank skew-symmetric structure matrix. A matrix $A \in \mathbb{R}^{2n \times 2k}$ is J_{2n} -symplectic if*

$$(5) \quad A^T J_{2n} A = \mathbb{J}_{2k}.$$

129 Note that in the literature [30, 21], symplectic transformations are only referred to
 130 \mathbb{J}_{2n} -symplectic matrices, in contrast to Definition 2.2.

131 It is natural to expect a numerical integrator that solves (1) to also satisfy the
 132 conservation law expressed in Theorem 2.1. Conventional numerical time integrators,
 133 e.g. the Runge-Kutta methods, do not generally conserve the symplectic symmetry
 134 of Hamiltonian systems and often result in a wrong behavior of the solution over long
 135 time-integration. The class of time-integrators for (1) that preserve the Hamiltonian
 136 are called *Poisson integrators* [21]. To construct a general Poisson integrator, first we
 137 find a coordinate transformation $T : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$, $\tilde{z} = T^{-1}z$, such that $J_{2n} = TJ_{2n}T^T$.
 138 Then, a *symplectic integrator* can preserve the symplectic structure of the transformed
 139 system. The *Störmer-Verlet* scheme is an example of a second order symplectic time-
 140 integrator given as

$$141 \quad (6) \quad \begin{aligned} q_{m+1/2} &= q_m + \frac{\Delta t}{2} \cdot \nabla_p \tilde{H}(p_m, q_{m+1/2}), \\ p_{m+1} &= p_m - \frac{\Delta t}{2} \cdot \left(\nabla_q \tilde{H}(p_m, q_{m+1/2}) + \nabla_q \tilde{H}(p_{m+1}, q_{m+1/2}) \right), \\ q_{m+1} &= q_{m+1/2} + \frac{\Delta t}{2} \cdot \nabla_p \tilde{H}(p_{m+1}, q_{m+1/2}). \end{aligned}$$

142 Here, $\tilde{z} = (q^T, p^T)^T$, $\tilde{H}(\tilde{z}) = H(T^{-1}z)$ and the subscript m denotes the time-stepping
 143 index. Note that it is important to use a backward stable method to compute the
 144 transformation T . In this paper we use the symplectic Gaussian elimination method
 145 with a complete pivoting to compute the decomposition $J_{2n} = TJ_{2n}T^T$. However, one
 146 may use a more computationally efficient method, e.g., a Cholesky-like factorization
 147 proposed in [8] or the isotropic Arnoldi/Lanczos methods [31]. There are a few known
 148 numerical integrators that can preserve the symplectic symmetry of a generalized
 149 Hamiltonian system without requiring the computation of the transformation matrix
 150 T [21]. The implicit midpoint rule

$$151 \quad (7) \quad z_{m+1} = z_m + \Delta t \cdot J_{2n} \nabla_z H \left(\frac{z_{m+1} + z_m}{2} \right),$$

152 for (1) is an example of such integrators. For more on the construction and the
 153 applications of Poisson/symplectic integrators, we refer the reader to [21].

154 **3. Model order reduction.** In this section we summarize the fundamentals
 155 of model order reduction. We discuss the conventional approach to model order
 156 reduction with a weighted inner product. We then outline the main results presented
 157 in [2] regarding symplectic model reduction. In section 4 we shall combine the two
 158 concepts to introduce the symplectic model reduction of Hamiltonian systems with
 159 respect to a weighted inner product.

160 **3.1. Model-reduction with a weighted inner product.** Consider a dynam-
 161 ical system of the form

$$162 \quad (8) \quad \begin{cases} \dot{x}(t) = f(t, x), \\ x(0) = x_0. \end{cases}$$

163 where $x \in \mathbb{R}^m$ and $f : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ is some continuous function. In this paper we
 164 may assume that time t is the only parameter that the solution vector x depends on.
 165 Nevertheless, it is straight forward to generalize the findings of this paper to the case

166 where x also depends on a set of physical or geometrical parameters that belong to a
 167 closed and bounded subset of a Euclidean space.

168 Suppose that x lies on or very close to a low dimensional linear subspace with the
 169 basis $V = [v_1 | \dots | v_k]$, $v_i \in \mathbb{R}^m$ for $i = 1, \dots, k$. The approximated solution to (8) in
 170 this basis reads

171 (9)
$$x = Vy,$$

172 where y is the expansion coefficients of x in the basis V . Note that the method of
 173 projecting x onto the span space of V depends on the inner product and the norm
 174 defined on (8). We define the weighted inner product

175 (10)
$$[x, y]_X = x^T X y, \quad \text{for all } x, y \in \mathbb{R}^m,$$

176 for some symmetric and positive-definite matrix $X \in \mathbb{R}^{m \times m}$. We also refer to $\|\cdot\|_X$
 177 as the X -norm associated to this inner product. If we choose V to be an ortho-normal
 178 basis with respect to the X -norm ($V^T X V = I_k$), then the operator

179 (11)
$$P_{X,V}(x) = VV^T X x, \quad \text{for all } x \in \mathbb{R}^m$$

180 becomes idempotent. This means that $P_{X,V}$ is a projection operator onto the span
 181 space of V .

182 Now suppose that $\{x(t_i)\}_{i=1}^N$ is a collection of N samples of the solution to (8)
 183 at instances t_1, \dots, t_N . We would like to find V such that it minimizes the collective
 184 projection error of the samples onto the span space of V . This corresponds to the
 185 minimization problem

186 (12)
$$\begin{aligned} & \underset{V \in \mathbb{R}^{m \times k}}{\text{minimize}} \quad \sum_{i=1}^N \|x_i - P_{X,V}(x_i)\|_X, \\ & \text{subject to} \quad V^T X V = I_k. \end{aligned}$$

187 Following the derivations in [35] the above minimization is equivalent to

188 (13)
$$\begin{aligned} & \underset{V \in \mathbb{R}^{m \times k}}{\text{minimize}} \quad \|\tilde{S} - \tilde{V}\tilde{V}^T\tilde{S}\|_F, \\ & \text{subject to} \quad \tilde{V}^T\tilde{V} = I_k. \end{aligned}$$

Frobenius Norm!!
 $\|\cdot\|_F$

189 where $\tilde{V} = X^{1/2}V$, $\tilde{S} = X^{1/2}S$, S is the matrix that contains samples $\{x(t_i)\}_{i=1}^N$
 190 in its columns referred to as the *snapshot matrix*, and $X^{1/2}$ is the matrix square
 191 root of X . According to Schmidt-Mirsky-Eckart-Young theorem [29] the solution \tilde{V}
 192 to the minimization (13) is the truncated singular value decomposition (SVD) of \tilde{S} .
 193 The basis V can then be computed from $V = X^{-1/2}\tilde{V}$. The reduced system to (8)
 194 corresponding to the basis V and the projection $P_{X,V}$ then is

195 (14)
$$\begin{cases} \dot{y}(t) = V^T X f(t, Vy), \\ y(0) = V^T X x_0. \end{cases}$$

196 If k can be chosen such that $k \ll m$, then the reduced system (14) can potentially
 197 be evaluated significantly faster than the full order system (8). We refer the reader
 198 to [22, 35] for further information regarding the development and the efficiency of
 199 reduced order models.

200 It is worthwhile to note that the proper orthogonal decomposition (POD) method
 201 [22] corresponds to taking $X = I_m$. In this case, the projection $P_{I_m,V}$ constructed
 202 from the solution to (12) becomes the POD-Galerkin projection [22].

203 **3.2. Symplectic model-reduction.** Conventional model reduction methods,
 204 e.g. those introduced in subsection 3.1, do not generally preserve the conservation law
 205 expressed in Theorem 2.1. This often result in the lack of robustness in the reduced
 206 system over long time-integration. In this section we summarize the main findings of
 207 [2] regarding symplectic model order reduction of Hamiltonian systems with respect to
 208 the standard Euclidean inner product. Symplectic model reduction aims to construct
 209 a reduced system that conserves the geometric symmetry expressed in Theorem 2.1
 210 which helps with the stability of the reduced system. Consider a Hamiltonian system
 211 of the form

$$212 \quad (15) \quad \begin{cases} \dot{z}(t) = \mathbb{J}_{2n} L z(t) + \mathbb{J}_{2n} \nabla_z f(z), \\ z(0) = z_0. \end{cases}$$

213 Here $z \in \mathbb{R}^{2n}$ is the state vector, $L \in \mathbb{R}^{2n \times 2n}$ is a symmetric and positive-definite ma-
 214 trix and $f : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ is some smooth enough function. Note that the Hamiltonian
 215 for system (15) is given by $H(z) = z^T L z + f(z)$. Suppose that the solution to (15) lies
 216 on a low dimensional symplectic subspace. Let $A \in \mathbb{R}^{2n \times 2k}$ be a \mathbb{J}_{2n} -symplectic basis
 217 containing the basis vectors $A = [e_1 | \dots | e_k | f_1 | \dots | f_k]$, such that $z = Ay$ with y the
 218 expansion coefficients of z in this basis. Using the symplectic inverse $A^+ = \mathbb{J}_{2k}^T A^T \mathbb{J}_{2n}$
 219 we can construct the reduced system

$$220 \quad (16) \quad \dot{y} = A^+ \mathbb{J}_{2n} (A^+)^T A^T L A y + A^+ \mathbb{J}_{2n} (A^+)^T \nabla_y f(A y).$$

221 We refer the reader to [2] for the details of derivation. It is shown in [33] that $(A^+)^T$
 222 is also \mathbb{J}_{2n} -symplectic, therefore $A^+ \mathbb{J}_{2n} (A^+)^T = \mathbb{J}_{2k}$ and (16) reduces to

$$223 \quad (17) \quad \dot{y}(t) = \mathbb{J}_{2k} A^T L A y + \mathbb{J}_{2k} \nabla_y f(A y).$$

224 This system is a Hamiltonian system with the Hamiltonian $\tilde{H}(y) = y^T A^T L A y + f(A y)$.
 225 To reduce the complexity of evaluating the nonlinear term in (17), we may apply
 226 the discrete empirical interpolation method (DEIM) [5, 12]. Assuming that $\nabla_z f(z)$
 227 lies on a low dimensional subspace with a basis U the DEIM approximation reads

$$228 \quad (18) \quad \nabla_z f(z) \approx U (\mathcal{P}^T U)^{-1} \mathcal{P}^T \nabla_z f(z).$$

229 Here \mathcal{P} is the interpolating index matrix [12]. For a general choice of U the approxi-
 230 mation in (18) destroys the Hamiltonian structure in (17). It is shown in [2] that by
 231 taking $U = (A^+)^T$ we can recover the Hamiltonian structure in (17). Therefore, the
 232 reduced system to (15) becomes

$$233 \quad (19) \quad \begin{cases} \dot{y}(t) = \mathbb{J}_{2k} A^T L A y + \mathbb{J}_{2k} (\mathcal{P}^T (A^+)^T)^{-1} \mathcal{P}^T \nabla_z f(A y), \\ y(0) = A^+ z_0. \end{cases}$$

234 Note that the Hamiltonian formulation of (19) allows us to integrate it using a sym-
 235 plectic integrator. This conserves the symmetry expressed in Theorem 2.1 at the level
 236 of the reduced system. It is also shown in [2, 33] that the stability of the critical points
 237 of (15) is preserved in the reduced system and the difference of the Hamiltonians of
 238 the two system (15) and (19) is constant. Therefore, the overall behavior (19) is close
 239 to the full order Hamiltonian system (15). In the next subsection we discuss methods
 240 for generating a \mathbb{J}_{2n} -symplectic basis A .

241 **3.3. Greedy generation of a \mathbb{J}_{2n} -symplectic basis.** Suppose that S is the
 242 snapshot matrix containing the time instances $\{z(t_i)\}_{i=1}^N$ of the solution to (15). We
 243 would like to find the \mathbb{J}_{2n} -symplectic basis A such that the collective symplectic pro-
 244 jection error of samples in S onto the span space of A is minimized.

245 (20)
$$\begin{aligned} & \underset{A \in \mathbb{R}^{n \times k}}{\text{minimize}} \quad \|S - P_{I,A}^{\text{symp}}(S)\|_2, \\ & \text{subject to} \quad A^T \mathbb{J}_{2n} A = I_{2k}. \end{aligned}$$

246 Here $P_{I,A}^{\text{symp}} = AA^+$ is the symplectic projection operator with respect to the standard
 247 Euclidean inner production onto the span space of A . Note that $P_{I,A}^{\text{symp}} \circ P_{I,A}^{\text{symp}} =$
 248 $P_{I,A}^{\text{symp}}$ [33, 2].

249 Direct approaches to solve (20) are often inefficient. Some SVD-type solutions to
 250 (20) are proposed by [33]. However, these solutions are only suited for the standard
 251 Euclidean inner product and cannot be generalized to be compatible with a weighted
 252 inner product.

253 The greedy generation of a \mathbb{J}_{2n} -symplectic basis aims to find a near optimal so-
 254 lution to (20) in an iterative procedure. This method enhances the overall accuracy
 255 of the basis by adding the best possible basis vectors at each iteration. Suppose that
 256 $A_{2k} = [e_1 | \dots | e_k | f_1 | \dots | f_k]$ is a \mathbb{J}_{2n} -symplectic basis. We may assume that A_{2k} is also
 257 an ortho-normal basis [2]. The first step of the greedy methods is to find the snapshot
 258 $z(t^{k+1})$, that is worst approximated by the basis A_{2k} .

259 (21)
$$t^{k+1} := \underset{t}{\operatorname{argmax}} \|z(t) - P_{I,A}^{\text{symp}}(z(t))\|_2.$$

260 If e_{k+1} is the vector obtained by \mathbb{J}_{2n} -orthogonalizing $z(t^{k+1})$ with respect to A_{2k} [2],
 261 then the enriched basis A_{2k+2} reads

262 (22)
$$A_{2k+2} = [e_1 | \dots | e_k | e_{k+1} | f_1 | \dots | f_k | \mathbb{J}_{2n}^T e_{k+1}].$$

263 It is easily checked that A_{2k+2} is \mathbb{J}_{2n} -symplectic and ortho-normal. We point out that
 264 the choice of orthogonalization routine generally depends on the application. In this
 265 paper we use the symplectic Gram-Schmidt (GS) process as the orthogonalization
 266 routine. However the isotropic Arnoldi method or the isotropic Lanczos method [31]
 267 are among backward stable alternatives.

268 Evaluation of the projection error is impractical for parameter-dependent prob-
 269 lems. The loss in the Hamiltonian function can be used as a cheap surrogate to the
 270 projection error.

271 (23)
$$\omega^{k+1} = \underset{\omega \in \Omega}{\operatorname{argmax}} |H(z(\omega)) - H(P_{I,A}^{\text{symp}}(z(\omega)))|.$$

272 Here $\Omega \subset \mathbb{R}^d$ is a closed and bounded set of parameters that the original Hamiltonian
 273 system depends on. It is shown in [2] that the loss in the Hamiltonian is constant in
 274 time. Therefore, ω^{k+1} can be identified prior to time integration.

275 We summarized the greedy algorithm for generating a \mathbb{J}_{2n} -symplectic basis in
 276 Algorithm 1. The first loop constructs a \mathbb{J}_{2n} -symplectic for the Hamiltonian system
 277 (15), and the second loop adds the nonlinear snapshots to the symplectic inverse of
 278 the basis. We refer the reader to [2] for more detail on the generation and properties
 279 of a symplectic basis. In section 4 we will show how this algorithm can be generalized
 280 to support any weighted inner product.

Algorithm 1 The greedy algorithm for generation of a \mathbb{J}_{2n} -symplectic basis**Input:** Tolerated projection error δ , initial condition z_0

1. $t^1 \leftarrow t = 0$
2. $e_1 \leftarrow z_0$
3. $A \leftarrow [e_1 | \mathbb{J}_{2n}^T e_1]$
4. $k \leftarrow 1$
5. **while** $\|z(t) - P_{I,A}^{\text{symp}}(z(t))\|_2 > \delta$ for all $t \in [0, T]$
6. $t^{k+1} := \underset{t \in [0, T]}{\text{argmax}} \|z(t) - P_{I,A}^{\text{symp}}(z(t))\|_2$
7. \mathbb{J}_{2n} -orthogonalize $z(t^{k+1})$ to obtain e_{k+1}
8. $A \leftarrow [e_1 | \dots | e_{k+1} | \mathbb{J}_{2n}^T e_1 | \dots | \mathbb{J}_{2n}^T e_{k+1}]$
9. $k \leftarrow k + 1$
10. **end while**
11. compute $(A^+)^T = [e'_1 | \dots | e'_k | \mathbb{J}_{2n}^T e'_1 | \dots | \mathbb{J}_{2n}^T e'_k]$
12. **while** $\|\nabla f(z(t)) - P_{I,(A^+)^T}^{\text{symp}}(\nabla f(z(t)))\|_2 > \delta$ for all $t \in [0, T]$
13. $t^{k+1} := \underset{t \in [0, T]}{\text{argmax}} \|\nabla f(z(t)) - P_{I,(A^+)^T}^{\text{symp}}(\nabla f(z(t)))\|_2$
14. \mathbb{J}_{2n} -orthogonalize $\nabla f(z(t^{k+1}))$ to obtain e'_{k+1}
15. $(A^+)^T \leftarrow [e'_1 | \dots | e'_{k+1} | \mathbb{J}_{2n}^T e'_1 | \dots | \mathbb{J}_{2n}^T e'_{k+1}]$
16. $k \leftarrow k + 1$
17. **end while**
18. $A \leftarrow \left((A^+)^T \right)^+$

Output: \mathbb{J}_{2n} -symplectic basis A .

281 **4. Symplectic model-reduction with a weighted inner product.** In this
 282 section we will combine the concept of model reduction with a weighted inner product
 283 in subsection 3.1 with the symplectic model reduction discussed in subsection 3.2. We
 284 will discuss how the new method can be viewed as a natural extension to the original
 285 symplectic method. Finally, we generalize the greedy method for the symplectic basis
 286 generation, and the symplectic model reduction of nonlinear terms to be compatible
 287 with any weighted inner product.

288 **4.1. Generalization of the symplectic projection.** As discussed in subsection
 289 3.1, proper error analysis of methods for solving partial differential equations
 290 often require using a weighted inner product. This is particularly important when
 291 dealing with Hamiltonian systems, where the system energy can induce a norm that
 292 is fundamental to the dynamics of the system.

293 Consider a Hamiltonian system of the form (15) together with the weighted inner
 294 product defined in (10) with $m = 2n$. Also suppose that the solution z to (15) lies on
 295 a $2k$ dimensional symplectic subspace with the basis A . We would like to construct a
 296 projection operator that minimizes the projection error with respect to the X -norm
 297 while preserving the symplectic dynamics of (15) in the projected space. Consider
 298 the operator $P : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ defined as

$$299 \quad (24) \quad P = A \mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X.$$

300 It is easy to show that P is idempotent if and only if

$$301 \quad (25) \quad \mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X A = I_{2k}.$$

(Q: What about the next?

(Q: more general \mathbb{J}_{2n} ?)

This means that P is a projection operator onto the span space of A . Suppose that S is the snapshot matrix containing the time samples $\{z(t_i)\}_{i=1}^N$ of the solution to (15). We like to find the basis A that minimizes the projection error of the samples in S with respect to P .

$$\begin{aligned} \text{minimize}_{A \in \mathbb{R}^{2n \times 2k}} & \|S - P(S)\|_X, \\ \text{subject to } & \mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X A = I_{2k}. \end{aligned}$$

by (24) we have

$$\begin{aligned} \sum_i \|S - P(S)\|_X^2 &= \|S - A \mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X S\|_X^2 \\ &= \|X^{1/2} S - X^{1/2} A \mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X S\|_2^2 \\ &= \|\tilde{S} - \tilde{A} \tilde{A}^+ \tilde{S}\|_2. \end{aligned}$$

Here $\tilde{S} = X^{1/2} S$, $\tilde{A} = X^{1/2} A$ and $\tilde{A}^+ = \mathbb{J}_{2k}^T \tilde{A}^T J_{2n}$ is the symplectic inverse of \tilde{A} with respect to the skew-symmetric matrix $J_{2n} = X^{1/2} \mathbb{J}_{2n} X^{1/2}$. Note that the symplectic inverse in (27) is a generalization of the symplectic inverse introduced in subsection 3.2. Therefore, we may use the same notation (the superscript +) for both. We summarized the properties of this generalization in Theorem 4.1. With the introduced notations, the condition (25) turns into $\tilde{A}^+ \tilde{A} = I_{2k}$ which is equivalent to $\tilde{A}^T J_{2n} \tilde{A} = \mathbb{J}_{2k}$. In other words, this condition implies that \tilde{A} has to be a J_{2n} -symplectic matrix. Finally we can rewrite the minimization (26) as

$$\begin{aligned} \text{minimize}_{A \in \mathbb{R}^{2n \times 2k}} & \|\tilde{S} - P_{X, \tilde{A}}^{\text{symp}}(\tilde{S})\|_2, \\ \text{subject to } & \tilde{A}^T J_{2n} \tilde{A} = \mathbb{J}_{2k}. \end{aligned}$$

where $P_{X, \tilde{A}}^{\text{symp}} = \tilde{A} \tilde{A}^+$ is the symplectic projection with respect to the X -norm onto the span of \tilde{A} . At the first glance, the minimization (28) might look similar to (20). However, since \tilde{A} is J_{2n} -symplectic, and the projection operator depends on X , we need to seek for alternative approaches to find a near optimal solution to (28).

Similar to (20), direct approaches to solving (28) are impractical. Furthermore, there are no SVD-type methods known to the authors, that solve (28). However, the greedy generation of the symplectic basis can be generalized to generate a near optimal basis \tilde{A} . The generalized greedy method is discussed in subsection 4.2.

Now suppose that a basis A that solves (28) is in hand such that $z = Ay$ with $y \in \mathbb{R}^{2k}$, the expansion coefficients of z in the basis of A . Using (25) we may write the reduced system to (15) as

$$(29) \quad \dot{y} = \mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X \mathbb{J}_{2n} L A y + \mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X \mathbb{J}_{2n} \nabla_z f(z).$$

Since $\nabla_z H(z) = Lz + \nabla_z f(z)$, we may use the chain rule to write

$$(30) \quad \nabla_z H(z) = (\mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X)^T \nabla_y H(Ay).$$

Finally the reduced system (29) simplifies to

$$(31) \quad \begin{cases} \dot{y}(t) = J_{2k} A^T L A y + J_{2k} \nabla_y f(Ay), \\ y(0) = \tilde{A}^+ X^{1/2} z_0. \end{cases}$$

Q: Why is this correct generalized symplecticness condition?

Wrong in matrix form, as $\|\cdot\|_2$ is not sum of columnwise 2-norms
Write as sum over snapshots or use Frobenius norm instead of 2-norm

$A = X^{1/2} \tilde{A}$ with \tilde{A}
Solving (28)

$$z \approx \tilde{A} = Ay$$

Q: How does X enter,
 $A^T \mathbb{J}_{2n}$? ?? Argument
under please check

! Make sure no $X^{1/2}$ or $X^{-1/2}$
is required!!!
in computations

Emphasize this, as this
is different to the
"straightforward state form".

why not
"inverse"? use consistent notation.

1
2

334 where $J_{2k} = \tilde{A}^+ J_{2n} (\tilde{A}^+)^T$ is a skew-symmetric matrix. The system (31) is a general-
 335 ized Hamiltonian system with the Hamiltonian defined as $\tilde{H}(y) = y^T A^T L A y + f(A y)$.
 336 Therefore, a Poisson integrator can preserve the symplectic symmetry associated with
 337 (31).

338 We close this section by summarizing the properties of the symplectic inverse in
 339 the form of the following theorem.

340 **THEOREM 4.1.** Let $A \in \mathbb{R}^{2n \times 2k}$ be a J_{2n} -symplectic basis where $J_{2n} \in \mathbb{R}^{2n}$ is a
 341 full rank and skew-symmetric matrix. Furthermore, suppose that $A^+ = J_{2k}^T A^T J_{2n}$ is
 342 the symplectic pseudo-inverse. Then the following holds:

- 343 1. $A^+ A = I_{2k}$.
- 344 2. $(A^+)^T$ is J_{2n}^{-1} -symplectic.
- 345 3. $\left((A^+)^T \right)^T = A$.
- 346 4. Let $J_{2n} = X^{1/2} J_{2n} X^{1/2}$. Then A is ortho-normal with respect to the X -norm,
 347 if and only if $(A^+)^T$ is ortho-normal with respect to the X^{-1} -norm.

348 *Proof.* it is straight forward to show all statements using the definition of a sym-
 349 plectic basis. \square

350 **4.2. Greedy generation of a J_{2n} -symplectic basis.** In this section we modify
 351 the greedy algorithm introduced in subsection 3.8 to construct a J_{2n} -symplectic basis.
 352 Ortho-normalization is an essential step in most greedy approaches to basis generation
 353 [22, 35]. Here, we summarize a variation of the Gram-Schmidt orthogonalization
 354 process, known as the *symplectic Gram-Schmidt* process.

355 Suppose that Ω is a symplectic form defined on \mathbb{R}^{2n} such that $\Omega(x, y) = x^T J_{2n} y$,
 356 for all $x, y \in \mathbb{R}^{2n}$ and some full rank and skew-symmetric matrix $J_{2n} = X^{1/2} J_{2n} X^{1/2}$.
 357 We would like to build a basis of size $2k + 2$ in an iterative manner. We start with
 358 some initial vector, e.g. $e_1 = z_0$. It is known that a symplectic basis is even di-
 359 mensional [30]. We may take $T e_1$, where $T = X^{-1/2} J_{2n}^T X^{1/2}$ is a candidate for the
 360 second basis vector. It is easily checked that $\tilde{A}_2 = [e_1 | T e_1]$ is J_{2n} -symplectic and
 361 consequently, \tilde{A}_2 is the first basis generated by the greedy approach. Next, suppose
 362 that $\tilde{A}_{2k} = [e_1 | \dots | e_k | T e_1 | \dots | T e_k]$ is generated in k -th step of the greedy method
 363 and $z \notin \text{span}(\tilde{A}_{2k})$ is provided. We aim to J_{2n} -orthogonalize z with respect to the
 364 basis \tilde{A}_{2k} . This means we should find coefficients $\alpha_i, \beta_i \in \mathbb{R}$, for $i = 1, \dots, k$ such that

$$(32) \quad \Omega \left(z + \sum_{i=1}^k \alpha_i e_i + \sum_{i=1}^k \beta_i T e_i, \sum_{i=1}^k \bar{\alpha}_i e_i + \sum_{i=1}^k \bar{\beta}_i T e_i \right) = 0,$$

366 for all possible $\bar{\alpha}_i, \bar{\beta}_i \in \mathbb{R}$, $i = 1, \dots, k$. It is easily checked that this problem has the
 367 unique solution

$$(33) \quad \alpha_i = -\Omega(z, T e_i), \quad \beta_i = \Omega(z, e_i).$$

369 If we take $\tilde{z} = z - \sum_{i=1}^k \Omega(z, T e_i) e_i + \sum_{i=1}^k \Omega(z, e_i) T e_i$, then the next candidate pair
 370 of basis vectors are $e_{k+1} = \tilde{z}/\|\tilde{z}\|_X$ and $T e_{k+1}$. Finally, the basis generated at the
 371 ($k + 1$)th step of the greedy method is given by

$$(34) \quad \tilde{A}_{2k+2} = [e_1 | \dots | e_k | e_{k+1} | T e_1 | \dots | T e_k | T e_{k+1}].$$

373 It is checked easily that \tilde{A}_{2k+2} is J_{2n} -symplectic. We point out that the symplectic
 374 Gram-Schmidt orthogonalization process is chosen due to its simplicity. However, in

to emphasize that A is not a structured matrix.
 A is not necessarily symplectic

Why \tilde{A}
 instead of A ?
 A would seem
 natural, as
 previously
 $\tilde{A} = X^{1/2} A$
 hence:
 A J_{2n} -symp.
 $\Leftrightarrow \tilde{A}$ J_{2n} -symp.

additional
 formulae for even in
 more compact matrix-
 vector form
 not sure
 if possible

or using symplectic
 projection?

Q: Why is $T e_{k+1}$ lin. indep. of

$\{e_1, \dots, e_{k+1}, T e_1, \dots, T e_k\}$

problems where there is a need for a large basis, this process might be impractical. In such cases, one may use a backward stable routine, e.g. the isotropic Arnoldi method or the isotropic Lanczos method [31].

It is well known that symplectic bases, in general, are not norm bounded [27]. The following theorem guarantees that the greedy method for generating a J_{2n} -symplectic basis yields a bounded basis.

THEOREM 4.2. *The basis generated by the greedy method for constructing a J_{2n} -symplectic basis is ortho-normal with respect to the X -norm.*

Proof. Let $\tilde{A}_{2k} = [e_1 | \dots, e_k | Te_1 | \dots | Te_k]$ be the J_{2n} -symplectic basis generated at the k th step of the greedy method. Using the fact that \tilde{A}_{2k} is J_{2n} -symplectic, one can check that

$$(35) \quad [e_i, e_j]_X = [Te_i, Te_j]_X = \Omega(e_i, Te_j) = \delta_{i,j}, \quad i, j = 1, \dots, k,$$

and

$$(36) \quad [e_i, Te_j]_X = \Omega(e_i, e_j) = 0 \quad i, j = 1, \dots, k,$$

where $\delta_{i,j}$ is the Kronecker delta function. This shows that $\tilde{A}_{2k}^T X \tilde{A}_{2k} = I_{2k}$, i.e., \tilde{A}_{2k} is an ortho-normal basis with respect to the X -norm. \square

We point out that if we take $X = I_{2n}$, then the greedy process generates a J_{2n} -symplectic basis. As the matter of fact, with this choice, the greedy method discussed above becomes identical to the greedy process discussed in ~~subsection 3.3~~, since $T = X^{-1/2} J_{2n}^T X^{1/2} = J_{2n}^T$.

For identifying the best vectors to be added to a set of basis vectors, we may use similar error functions to those introduced in ~~subsection 3.3~~. The projection error can be used to identify the snapshot that is worst approximated by a given basis \tilde{A}_{2k} :

$$(37) \quad z^{k+1} := \operatorname{argmax}_{z \in \mathbb{R}^{2n}} \|X^{1/2} z - P_{X, \tilde{A}_{2k}}^{\text{symp}}(X^{1/2} z)\|_2.$$

Or alternatively we can use the loss in the Hamiltonian function in (23) for parameter dependent problems. We summarized the greedy method for generating a J_{2n} -symplectic matrix in Algorithm 2.

It is shown in [2] that under natural assumptions on the solution manifold of (15), the original greedy method for symplectic basis generation converges exponentially fast. We expect similar convergence rate for the generalized greedy method, since the X -norm is topologically equivalent to the standard Euclidean norm [17], for a full rank matrix X .

4.3. Efficient evaluation of nonlinear terms. Evaluating the nonlinear term in (31) still contains a computational complexity proportional to the size of the full order system (15). To overcome this inefficiency, we may take a similar approach to subsection 3.2. The DEIM approximation of the nonlinear term in (31) yields

$$(38) \quad \dot{y} = J_{2k} A^T L A y + \tilde{A}^+ X^{1/2} J_{2n} U (\mathcal{P}^T U)^{-1} \mathcal{P}^T \nabla_z f(z).$$

Here U is a basis for the nonlinear snapshots $\{\nabla_z f(z(t_i))\}_{i=1}^N$, and \mathcal{P} is the interpolating index matrix [12]. As discussed in ~~subsection 3.2~~, for a general choice of U , the reduced system (31) does not take a Hamiltonian form. Applying the chain rule on (38) gives

$$(39) \quad \dot{y} = J_{2k} A^T L A y + \tilde{A}^+ X^{1/2} J_{2n} U (\mathcal{P}^T U)^{-1} \mathcal{P}^T X^{1/2} (\tilde{A}^+)^T \nabla_y f(Ay).$$

Q:
 So equivalent in greedy
 as orthogonal,
& normal \Rightarrow \mathbb{C}_{k+1}

good!

constructed from

chain rule gives $\nabla_y f(Ay) = \tilde{A}^+ \nabla_z f(z)$

why is this equal? Please give
 1 or 2 more steps of the
 derivation

Algorithm 2 The greedy algorithm for generation of a J_{2n} -symplectic basis

Input: Tolerated projection error δ , initial condition z_0 , the snapshots $\{\tilde{z}(t_i)\}_{i=1}^N = \{X^{1/2}z(t_i)\}_{i=1}^N$, full rank matrix $X = X^T > 0$

1. $T \leftarrow X^{-1/2}J_{2n}^TX^{1/2}$
2. $t^1 \leftarrow t = 0$
3. $e_1 \leftarrow X^{1/2}z_0$
4. $\tilde{A} \leftarrow [e_1 | Te_1]$
5. $k \leftarrow 1$
6. **while** $\|\tilde{z}(t) - P_{X, \tilde{A}}^{\text{symp}}(\tilde{z}(t))\|_2 > \delta$ for all $t \in [0, T]$
7. $t^{k+1} := \underset{t \in [0, T]}{\text{argmax}} \|\tilde{z}(t) - P_{X, \tilde{A}}^{\text{symp}}(\tilde{z}(t))\|_2$
8. J_{2n} -orthogonalize $\tilde{z}(t^{k+1})$ to obtain e_{k+1}
9. $\tilde{A} \leftarrow [e_1 | \dots | e_{k+1} | Te_1 | \dots | Te_{k+1}]$
10. $k \leftarrow k + 1$
11. **end while**
12. $A \leftarrow X^{-1/2}\tilde{A}$

Output: J_{2n} -symplectic basis \tilde{A} and the reduced basis A

without $X^{1/2}, \tilde{X}^{-1/2}$

(Q: So A is not
symplectic?)

no

417 Now if we require $U = X^{1/2}(\tilde{A}^+)^T$ then the complex expression in (39) reduces to

418 (40)
$$\dot{y} = J_{2k}A^T L A y + J_{2k}\nabla_y f(Ay),$$

419 and hence we recover the Hamiltonian structure. This gives rise to the reduced system

420 (41)
$$\begin{cases} \dot{y}(t) = J_{2k}A^T L A y + J_{2k}(\mathcal{P}^T X^{1/2}(\tilde{A}^+)^T)^{-1} \mathcal{P}^T \nabla_z f(z), \\ y(0) = \tilde{A}^+ X^{1/2} z_0. \end{cases}$$

421 We now discuss how to ensure $X^{1/2}(\tilde{A}^+)^T$ to be a basis for the nonlinear snapshots. Note that if $z \in \text{span}(X^{1/2}(\tilde{A}^+)^T)$ then $X^{-1/2}z \in \text{span}((\tilde{A}^+)^T)$. Therefore, 422 it is sufficient to require $(\tilde{A}^+)^T$ to be a basis for $\{X^{-1/2}\nabla_z f(z(t_i))\}_{i=1}^N$. Theorem 4.1 423 indicates that $(\tilde{A}^+)^T$ is a J_{2n}^{-1} -symplectic basis and that the transformation between 424 \tilde{A} and $(\tilde{A}^+)^T$ does not affect the symplectic feature of the bases. Consequently, from 425 426 A we may compute $(\tilde{A}^+)^T$ and enrich it with snapshots $\{X^{-1/2}\nabla_z f(z(t_i))\}_{i=1}^N$. Once 427 $(\tilde{A}^+)^T$ represents the nonlinear term with the desired accuracy, we may compute 428 $\tilde{A} = \left((\tilde{A}^+)^T \right)^T$ to obtain the reduced basis for (41). Note that Theorem 4.1 429 implies that $(\tilde{A}^+)^T$ is ortho-normal with respect to the X^{-1} -norm. This affects the 430 ortho-normalization process. We summarized the process of generating a basis for the 431 nonlinear terms in Algorithm 3.

432 **4.4. Offline/online decomposition.** Model order reduction becomes particularly useful for parameter dependent problems or in multi-query settings. For the 433 purpose of most efficient computation, it is important to delineate high dimensional 434 ($\mathcal{O}(n)$) computations from low dimensional ($\mathcal{O}(k)$) ones in the implementation phase. 435 Time intensive high dimensional quantities are computed only once for a given problem 436 in the offline phase and cheaper low dimensional computations can be performed 437 in the online phase. This segregation or compartmentalization of quantities, according 438 to their computational cost, is referred to as the offline/online decomposition. 439

440 More precisely, one can decompose the computations into following stages:

$\mathcal{O}(k^d)$ for $1 \leq d \leq N$

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$\mathcal{O}(n^d)$

Algorithm 3 Generation of a basis for nonlinear terms

Input: Tolerated projection error δ , J_{2n} -symplectic basis \tilde{A} of size $2k$, the snapshots $\{\tilde{z}(t_i)\}_{i=1}^N = \{X^{-1/2}\nabla_z f(z(t_i))\}_{i=1}^N$, full rank matrix $X = X^T > 0$

1. $T \leftarrow X^{1/2} J_{2n}^T X^{-1/2}$
2. compute $(\tilde{A}^+)^T$
3. **while** $\|\tilde{z}(t) - P_{X^{-1}, (\tilde{A}^+)^T}^{\text{symp}}(\tilde{z}(t))\|_2 > \delta$ for all $t \in [0, T]$
4. $t^{k+1} := \underset{t \in [0, T]}{\operatorname{argmax}} \|\tilde{z}(t) - P_{X^{-1}, (\tilde{A}^+)^T}^{\text{symp}}(\tilde{z}(t))\|_2$
5. J_{2n}^{-1} -orthogonalize $\tilde{z}(t^{k+1})$ to obtain e_{k+1}
6. $(\tilde{A}^+)^T \leftarrow [e_1 | \dots | e_{k+1} | Te_1 | \dots | Te_{k+1}]$
7. $k \leftarrow k + 1$
8. **end while**
9. $\tilde{A} \leftarrow \left((\tilde{A}^+)^T \right)^T$

Output: J_{2n} -symplectic basis \tilde{A}

441 *Offline stage*: Quantities in this stage are computed only once and then used in
442 the online stage.

- 443 1. Generate the weighted snapshots $\{X^{1/2}z(t_i)\}_{i=1}^N$ and the weighted snapshots
444 of the nonlinear term $\{X^{-1/2}.\nabla_z f(z(t_i))\}_{i=1}^N$
- 445 2. Generate a J_{2n} -symplectic basis for the solution snapshots and the snapshots
446 of the nonlinear terms according Algorithms 2 and 3, respectively.
- 447 3. Assemble the reduced order model (19).

448 *Online stage*: Reduced model (19) is simulated for multiple parameter sets and
449 desired output is extracted in this stage.

450 We use this decomposition to perform experiments in the next section.

451 **5. Numerical results.** In this section we discuss the performance of the sym-
452 lectic model reduction with a weighted inner product. In subsection 5.1 we apply
453 this model reduction method to the equations of a vibrating elastic beam. We ex-
454 amine the evaluation of nonlinear terms in the model reduction of the sine-Gordon
455 equation, in section 5.1.

456 **5.1. The elastic beam equation.** Consider the equations governing small de-
457 formations of a clamped elastic body $\Gamma \subset \mathbb{R}^3$ as

$$(42) \quad \begin{cases} u_{tt}(t, x) = \nabla \cdot \sigma + f, & x \in \Gamma, \\ u(0, x) = \vec{0}, & x \in \Gamma, \\ \sigma \cdot n = T, & x \in \partial\Gamma_T, \\ u(t, x) = \vec{0}, & x \in \partial\Gamma \setminus \partial\Gamma_T, \end{cases}$$

459 and

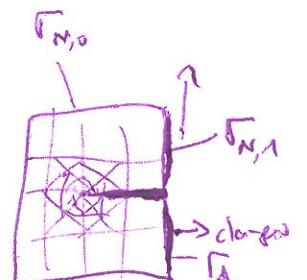
$$(43) \quad \sigma = \lambda(\nabla \cdot u)I + \mu(\nabla u + (\nabla u)^T).$$

461 Here u is the displacement vector field defined on Γ , subscript t denotes derivative
462 with respect to time, σ is the stress tensor, f is the body force per unit volume, λ
463 and μ are Lamé's elasticity parameters for material in Γ , I is the identity tensor, n

$\Gamma \rightarrow \mathbb{R}^3$ $\Gamma \rightarrow \mathbb{R}^{3 \times 3}$ the

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1
? 5.2
Plot.
aviod !!
or make clear that
approach is limited
to small problems...
1



block with cracks
& highly refined
mesh around origin

→ X largely differing
entraes.

misleading, as typically $\|\nabla u\|_2 := \sqrt{\langle \nabla u, \nabla u \rangle}$, but here you mean Euclidean 2-norm.
simply write $\nabla u \in (\mathbb{L}^2(\Gamma))^3$

464 is the outward unit normal vector at the boundary and $T : \partial\Gamma_T \rightarrow \mathbb{R}^3$ is the traction
465 at the boundary $\partial\Gamma_T$ [28].

466 We define a vector valued function space where we seek for the solution to (42)
467 as $V = \{u \in L^2(\Gamma) : (\|\nabla u\|_2 \in L^2) \text{ and } u = \vec{0} \text{ on } \partial\Gamma_T\}$, equipped with the standard
468 L^2 inner product $(\cdot, \cdot) : V \times V \rightarrow \mathbb{R}$. To formulate the weak formulation of (42), we
469 multiply it with the vector valued test function $v \in V$ and integrate over Γ

$$(44) \quad \int_{\Gamma} u_{tt} \cdot v \, dx = \int_{\Gamma} (\nabla \cdot \sigma) \cdot v \, dx + \int_{\Gamma} f \cdot v \, dx.$$

471 We may integrate the first term on the right hand side by parts to obtain

$$(45) \quad \int_{\Gamma} u_{tt} \cdot v \, dx = - \int_{\Gamma} \sigma : \nabla v \, dx + \int_{\partial\Gamma_T} (\sigma \cdot n) \cdot v \, ds + \int_{\Gamma} f \cdot v \, dx,$$

473 where $\sigma : \nabla v$ is the tensor inner product. Note that the skew-symmetric part of ∇v
474 vanishes over the product $\sigma : \nabla v$, since σ is symmetric. By prescribing the boundary
475 conditions to (45) we recover

$$(46) \quad \int_{\Gamma} u_{tt} \cdot v \, dx = - \int_{\Gamma} \sigma : \text{Sym}(\nabla v) \, dx + \int_{\partial\Gamma_T} T \cdot v \, ds + \int_{\Gamma} f \cdot v \, dx,$$

477 with $\text{Sym}(\nabla v) = (\nabla v + (\nabla v)^T)/2$. The variational form associated to (42) then reads

$$(47) \quad (u_{tt}, v) = -a(u, v) + L(v), \quad u, v \in V,$$

479 where

$$(48) \quad \begin{aligned} a(u, v) &= \int_{\Gamma} \sigma : \text{Sym}(\nabla v) \, dx, \\ L(v) &= \int_{\partial\Gamma_T} T \cdot v \, ds + \int_{\Gamma} f \cdot v \, dx. \end{aligned}$$

481 To obtain the FEM discretization of (47), we discretize the domain Γ into a triangulated
482 mesh, which discretizes the domain into a set of disjoint tetrahedrons. Furthermore,
483 we define vector valued piece-wise linear basis functions $\{\phi_i\}_{i=1}^{N_h}$, referred to as
484 the hat functions, and define the FEM space V_h as an approximation of V over these
485 set of basis functions. Projecting (47) onto V_h gives us the discretized weak form

$$(49) \quad ((u_h)_{tt}, v_h) = -a(u_h, v_h) + L(v_h), \quad u_h, v_h \in V_h.$$

487 Any particular function u_h can be expressed as $u_h = \sum_{i=1}^{N_h} q_i \phi_i$, where q_i , $i = 1, \dots, N_h$, are the expansion coefficients. Therefore, by choosing test functions $v_h = \phi_i$, $i = 1, \dots, N_h$, we obtain the ordinary differential equation

$$(50) \quad M \ddot{q} = -K q + g_q.$$

491 where $q = (q_1, \dots, q_{N_h})^T$, $M \in \mathbb{R}^{N_h \times N_h}$ is given as $M_{i,j} = (\phi_i, \phi_j)$, $K \in \mathbb{R}^{N_h \times N_h}$
492 is given as $K_{i,j} = a(\phi_i, \phi_j)$ and $g_q = (L(v_1), \dots, L(v_{N_h}))^T$. We now introduce the
493 canonical coordinate $p = M \dot{q}$ to recover the Hamiltonian system

$$(51) \quad \dot{z} = \mathbb{J}_{2N_h} L z + g_{qp}, \quad \text{the stiffness matrix}$$

the mass matrix

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a(ϕ_j, ϕ_i) ? typically in FEM order of arguments changes.

495 where

496 (52)
$$z = \begin{pmatrix} q \\ p \end{pmatrix}, \quad L = \begin{pmatrix} K & 0 \\ 0 & M^{-1} \end{pmatrix}, \quad g_{qp} = \begin{pmatrix} 0 \\ g_p \end{pmatrix},$$

497 together with the Hamiltonian function $H(z) = z^T L z + z^T \mathbb{J}_{2N_h}^T g_{qp}$. An appropriate
 498 FEM setup leads to a symmetric and positive-definite matrix L . Therefore, it seems
 499 natural to take $X = L$, the energy matrix associated to (51). System parameters are
 500 summarized in the table below. For further information regarding the problem set
 501 up, we refer the reader to [28].

good!

The

Domain shape	box: $l_x = 1, l_y = 0.2, l_z = 0.2$
No. mesh points	$n_x = 10, n_y = 4, n_z = 4$
Time discretization size	$\Delta t = 0.01$
Gravitational force	$g = (0, 0, -0.4)^T$
Traction	$T = \vec{0}$
Lamé parameters	$\lambda = 1.25, \mu = 1.0$
Degrees of freedom	$2N_h = 1650$

502 step
 503 We used the Störmer-Verlet scheme (6) to integrate (51) in time and generate the
 504 time snapshots. Projection operators $P_{X,V}$, $P_{I,A}^{\text{symp}}$ and $P_{X,\tilde{A}}^{\text{symp}}$ are then constructed
 505 according to subsections 3.1 to 3.3, respectively. After computing the transformation
 506 $J_{2k} = T \mathbb{J}_{2k} T^T$, the reduced systems resulted from $P_{I,A}^{\text{symp}}$ and $P_{X,\tilde{A}}^{\text{symp}}$ are integrated
 507 in time using the Störmer-Verlet scheme. The reduced system yielded by $P_{X,V}$ is
 508 integrated using a second order implicit Runge-Kutta method. Note that the Störmer-
 509 Verlet scheme is not used since the canonical form of a Hamiltonian system is destroyed
 510 when applying $P_{X,V}$.

511 Figure 1(a) shows the decay of the singular values of the time snapshots S and
 512 $X^{1/2}S$ respectively. We notice that the decay of the two matrices are different and as
 513 the matter of fact the decay saturates for $X^{1/2}S$.

514 Figure 1(b) shows the conservation of the Hamiltonian for all the methods men-
 515 tioned above. It is observed that the symplectic methods do preserve the Hamiltonian
 516 and system energy. However, the Hamiltonian blows up for the reduced system con-
 517 structed by the projection $P_{X,V}$. It is also noticeable that as the basis V gets larger,
 518 the Hamiltonian blows up faster.

519 Figure 1(c) shows the L^2 error between the projected systems and the full order
 520 system. We notice that the reduced system obtained by the non-symplectic method is
 521 unstable. It is known that classical reduced basis methods generally become exceedingly
 522 unstable as the reduced basis is enriched. This can also be observed here where the
 523 reduced system constructed by $P_{X,V}$ is more unstable as k increases. On the other
 524 hand, symplectic methods yield a stable reduced system. As the matter of fact, even
 525 as the system constructed by the projection $P_{X,\tilde{A}}^{\text{symp}}$ is not based on the L^2 projection,
 526 the error remains bounded with respect to the L^2 norm.

527 Figure 1(d) also indicates that the classical model reduction method based on
 528 the projection $P_{X,V}$ does not necessarily yield a stable reduced system. However, the
 529 symplectic methods provide a stable reduced system under long time-integration. We
 530 observe that the original symplectic also provide an accurate solution with respect to
 531 the X -norm. Nevertheless, the relation between the two norms in general depends on
 532 the problem set up and the initial and the boundary conditions [14].

- $\partial\Gamma$ traction domain?
- what force f ?
- plausibility of #dofs?

(word missing)
 non structure-preserving may

comment:
 then change of
 int. & ext. b. does not allow to
 conclude the reason
 on int. & ext. b.
 from exp.)

too general, there
 are also nicely
 stable solvers.

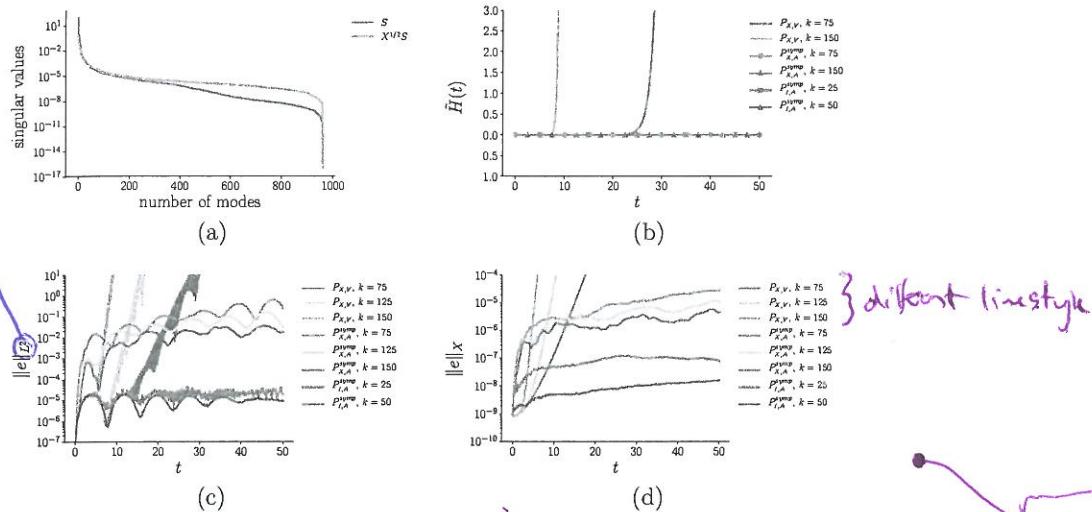


FIG. 1. Numerical results related to the beam equation. (a) the decay of the singular values. (b) conservation of the Hamiltonian. (c) error with respect to the L^2 norm. (d) error with respect to the X -norm.

5.2. The sine-Gordon equation. The sine-Gordon equation arise in differential geometry and quantum physics [32]. This equation is a nonlinear generalization of the linear wave equation, given as

$$536 \quad (53) \quad \begin{cases} u_t(t, x) = v, & x \in \Gamma, \\ v_t(t, x) = u_{xx} - \sin(u), \\ u(t, 0) = 0, \\ u(t, L) = 2\pi. \end{cases}$$

537 Here, $x \in \Gamma$ is an one dimensional box of length L , $u, v : \Gamma \rightarrow \mathbb{R}$ are scalar functions.
 538 The Hamiltonian associated to (53) is

$$539 \quad (54) \quad H(q, p) = \int_{\Gamma} \frac{1}{2} v^2 + \frac{1}{2} u_x^2 + 1 - \cos(u) \, dx.$$

One can check that $u_t = \delta H / \delta v$ and $v_t = -\delta H / \delta u$. The sine-Gordon equation admits the soliton solution

$$u(t, x) = 4 \arctan \left(\exp \left(\pm \frac{x - x_0 - ct}{\sqrt{1 - c^2}} \right) \right),$$

where the plus and minus signs are known as the *kink* and the *anti-kink* solutions, respectively. Here $|c| < 1$ is the wave speed. We discretize the box into n equi-distant grid point $x_i = i\Delta x$, $i = 1, \dots, n$. Furthermore, we use standard finite-differences schemes to discretize (53) to obtain

$$547 \quad (56) \qquad \dot{z} = \mathbb{J}_{2n} L z + \mathbb{J}_{2n} g(z) + \mathbb{J}_{2n} c_b.$$

Q: Where is wave speed appearing
in (53)?

or $n+1$?
is

548 Here $z = (q^T, p^T)^T$, $q(t) = (u(t, x_1), \dots, u(t, x_N))^T$, $p(t) = (v(t, x_1), \dots, v(t, x_N))^T$,
 549 c_b is the term corresponding to the boundary conditions and

550 (57)
$$L = \begin{pmatrix} D_x^T D_x & 0_N \\ 0_N & I_n \end{pmatrix}, \quad g(z) = \begin{pmatrix} \sin(q) \\ \vec{0} \end{pmatrix},$$

551 where D_x is the standard matrix differentiation operator. We may take $X = L$ as the
 552 weight matrix associated to (56). The discrete Hamiltonian, then takes the form

553 (58)
$$H_{\Delta x} = \Delta x \cdot \frac{1}{2} \|p\|^2 + \Delta x \cdot \|D_x q\|^2 + \sum_{i=1}^n \Delta x \cdot (1 - \cos(q_i)).$$

554 The system parameters can be found in the table below.

555 *skip*

Domain length	box: $L = 50$
No. grid points	$n = 500$
Time discretization size	$\Delta t = 0.01$
Wave speed	$c = 0.2$

556 The midpoint scheme (7) is used to integrate (53) in time and generate the snapshot
 557 matrix S . Similar to the previous subsection, projection operators $P_{X,V}$, $P_{I,A}^{\text{symp}}$
 558 and $P_{X,\tilde{A}}^{\text{symp}}$ are used to construct a reduced system. To accelerate the evaluation of the
 559 nonlinear term, the symplectic methods discussed in subsections 3.1 and 3.2 are cou-
 560 pled with the projection operators $P_{I,A}^{\text{symp}}$ and $P_{X,A}^{\text{symp}}$, respectively. Furthermore, the
 561 DEIM approximation is used for efficient evaluation of the reduced system obtained by
 562 the projection $P_{X,V}$. The midpoint rule is also used to integrate the reduced systems
 563 in time. Figure 2 shows the numerical results corresponding to reduced model without
 564 treating the nonlinear terms, while the results corresponding to the accelerated
 565 evaluation of the nonlinear term are presented in Figure 3.

566 Figure 2(a) shows the decay of the singular values of matrices S and $X^{1/2}S$.
 567 Similar to the previous section, we observe a saturation in the decay of the singular
 568 values of $X^{1/2}S$ compared to the singular values of S . This indicates that reduced
 569 bases, based on a weighted inner product, should be chosen to be larger to provide
 570 similar accuracy as those which are based on the L^2 inner product.

571 Figure 2(b) displays the error in the Hamiltonian. It is observed that the sym-
 572 plectic approaches conserve the Hamiltonian. However, the classical approaches do
 573 not necessarily conserve the Hamiltonian. We point out using the projection operator
 574 $P_{X,V}$ helped with the boundedness of the Hamiltonian. The contrary is observed when
 575 we apply the POD with respect to the L^2 inner-product, i.e. applying the projection
 576 operator $P_{I,V}$. This can be seen in the results presented in [33], where the unbounded-
 577 ness of the Hamiltonian is observed when $P_{I,V}$ is applied to the sine-Gordon equation.
 578 Nevertheless, only the symplectic model reduction routines consistently preserve the
 579 Hamiltonian.

580 Figure 2(c) exhibits the L^2 error between the solution of the projected systems
 581 and the original system. The behavior of the solution is investigated for $k = 100$,
 582 $k = 125$ and $k = 150$. We observe that all systems that are projected with respect
 583 to the X -norm are bounded. As the results in [33] suggest, the Euclidean inner-
 584 product does not necessarily yield a bounded reduced system. Moreover, we notice
 585 that the symplectic projection $P_{X,\tilde{A}}^{\text{symp}}$ result in a substantially more accurate reduced
 586 system compared to the reduced system yielded from $P_{X,V}$. This is because the

Euclidean, not L^2

use other symbol

Euclidean, not L^2

*add comment:
 interpret differently,
 this means that
 an assumed standard
 a basis obtained by
 a standard basis
 is non-weighted POD
 with respect to energy
 it may be highly
 relative energy that is
 cut off may be
 inaccurate
 may be highly inaccurate
 in terms of the
 true physical energy
 inner product.*

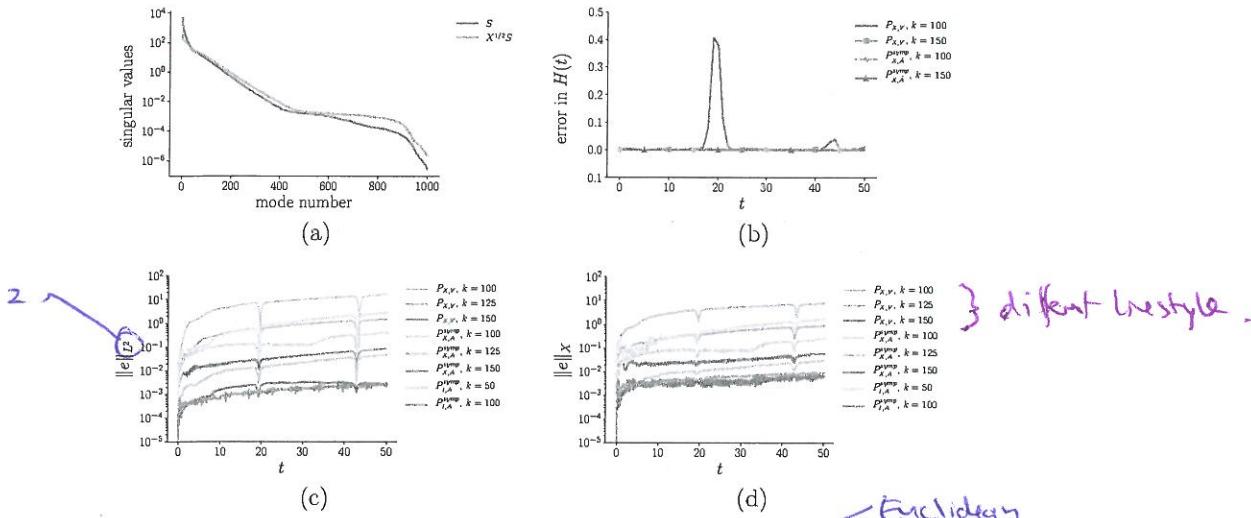


FIG. 2. Numerical results related to the sine-Gordon equation. (a) the decay of the singular values. (b) error in the Hamiltonian. (c) error with respect to the L^2 norm. (d) error with respect to the X -norm.

overall behavior of the original system due to the symplectic structure is translated correctly to the reduced system constructed with the symplectic projection. Whereas for systems constructed by the classical method, the Hamiltonian structure is lost.

The error with respect to the X -norm between the solution of the original system and the projected systems are presented in Figure 2(d). We see that the behavior of the X -norm error is similar to the L^2 norm, however the growth of the error is slower for methods based on a weighted inner product. Note that the connection between the error in the L^2 -norm and the X -norm is problem dependent. It is also observed that symplectic methods are substantially more accurate.

Figure 3 shows the performance of the different model reduction methods, when an efficient method is adopted in evaluating the nonlinear term in (56). This figure compares the symplectic approaches against non-symplectic methods. For all simulations, the size of the reduced basis for (56) is kept as $k = 100$. The size of the basis of the nonlinear term is then chosen as $k_n = 75$ and $k_n = 100$. For symplectic methods, a basis for the nonlinear term is constructed according to Algorithm 3, whereas for non-symplectic methods, the DEIM is applied. Note that for symplectic methods, the basis for the nonlinear term is added to the symplectic basis A . This means that the size of the reduced system is larger compared to the classical approach.

Figure 3(a) and Figure 3(b) show the error with respect to the L^2 -norm and the X -norm between the solution of the projected systems compared to the solution of the original system, respectively. We observe that all solutions are bounded and the behavior of the error in the L^2 -norm and the X -norm is similar. We observe that enriching the DEIM basis does not increase the overall accuracy of the system projected using $P_{X,V}$ (orange lines). Furthermore, applying the DEIM to a symplectic reduced system (green lines) also destroys the symplectic nature of the reduced system, as suggested in subsection 4.3. Therefore, it is essential to adopt a symplectic approach to reduce the complexity of evaluating the nonlinear terms. We observe that

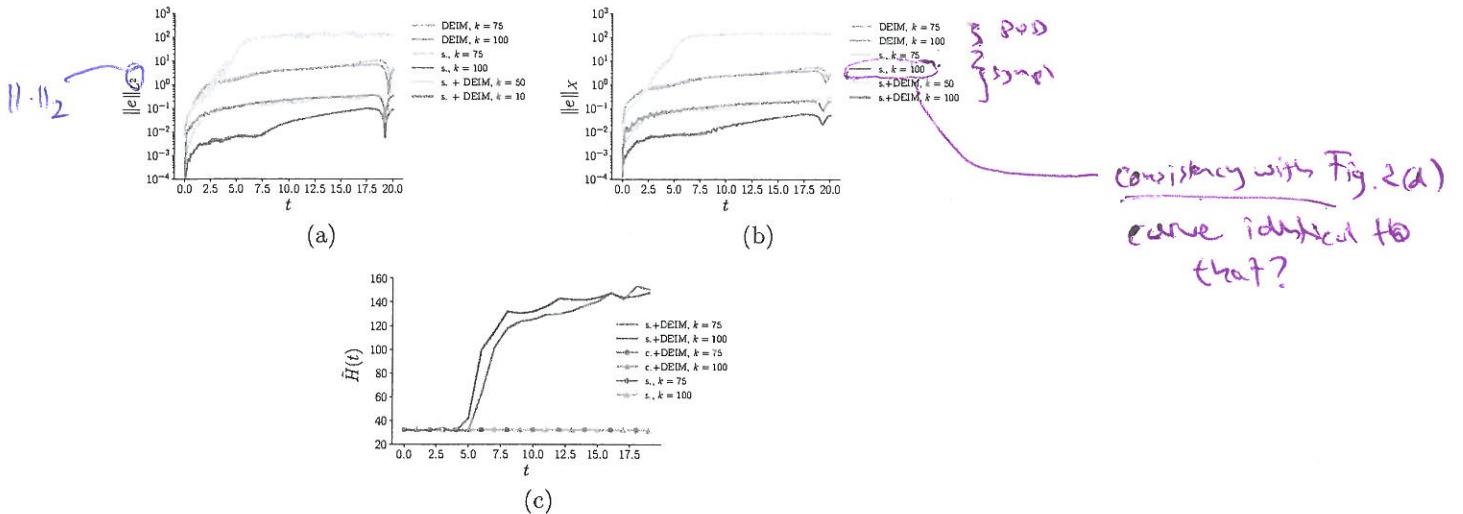


FIG. 3. Numerical results related to the sine-Gordon equation with efficient evaluation of the nonlinear terms. Here, “c.+DEIM” indicates classical model reduction with the DEIM, “s.+DEIM” indicates symplectic model reduction with the DEIM and “s.” indicates symplectic model reduction with symplectic treatment of the nonlinear term. (a) error with respect to the L^2 norm. (b) error with respect to the X -norm. (c) error in the Hamiltonian.

the symplectic method presented in subsection 4.3 provides not only an accurate approximation of the nonlinear term, but also preserves the symplectic structure of the reduced system. Moreover, enriching such a basis consistently increases the accuracy of the solution, as suggested in Figure 3(a) and Figure 3(b).

Figure 3(b) shows the conservation of the Hamiltonian for different methods. It is again seen that applying the DEIM to a symplectic reduced system destroys the Hamiltonian structure, therefore the Hamiltonian is not preserved.

6. Conclusion. In this paper we present a model reduction routine that combines the classic model reduction method with respect to a weighted inner product with the symplectic model reduction. This allows the reduced system to be defined with respect to the norms and inner-products, natural to the problem. Furthermore, the symplectic nature of the reduced system will preserve the Hamiltonian structure of the original system, which results in robustness and enhanced stability in the reduced system.

We demonstrate that including the weighted inner-product in the symplectic model reduction can be viewed as a natural extension of the symplectic method. Therefore, the stability preserving properties of the symplectic method generalize naturally to the new method.

Numerical results suggest the classic model reduction methods with respect to an weighted inner product can help with the boundedness of the system. However, only the symplectic treatment can consistently increase the accuracy of the reduced system. This is consistent with the fact the symplectic methods preserve the Hamiltonian structure.

We also exhibit that to accelerate the evaluation of the nonlinear terms, adopting a symplastic approach is essential. This allows an accurate reduced system that is

(Conclusion sounds repetitive)

639 consistently enhanced when the basis for the nonlinear term is enriched.

640 Hence, the symplectic model-reduction with respect to a weighted inner product
 641 can provide an accurate and robust reduced system that carry the norms and inner
 642 products most appropriate to the problem.

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 647 of this paper.

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- 763

Q: In standard MOR, when having a weighted inner prod. $\langle \cdot, \cdot \rangle_X$,
 then POD, etc. is equivalently performed by state transf $\tilde{z} := X^{1/2} z$
 and then solving this sysn for \tilde{z} and POD wrt Euclidean inner prod.
 Is this also valid here, i.e. does procedure give same result as
state-transformed system? If yes (hopefully) then the only reason why
 not simply state-transf + Euclidean-symp.-MOR is the avoidance of $X^{1/2}$
 in the procedure. So your method must be formulated without $X^{1/2}$ to
 give a benefit! Please give a "Remark X.Y ((Avoidance of $X^{1/2}$))" at
 the end.

If no (strange) please check possible adjustment to obtain this equivalence.