Reduced basis model order reduction of dissipatively perturbed constrained Hamiltonian systems

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1 Introduction

In this paper, we consider the model order reduction (MOR) of the differential algebraic equations of the form

$$\left.\begin{aligned} \dot{\boldsymbol{q}} &= \boldsymbol{\nabla}_{\boldsymbol{p}} H(\boldsymbol{q},\boldsymbol{p}), \\ \dot{\boldsymbol{p}} &= -\boldsymbol{\nabla}_{\boldsymbol{q}} H(\boldsymbol{q},\boldsymbol{p}) - \gamma \boldsymbol{p} - \boldsymbol{G}(\boldsymbol{q})^{\top}\boldsymbol{\lambda}, \\ \boldsymbol{0} &= \boldsymbol{g}(\boldsymbol{q}). \end{aligned}\right\} \tag{1}$$

why introduced? → never used → or maybe yet not included?

Here $\boldsymbol{q}(t),\ \boldsymbol{p}(t) : \mathbb{R} \to \mathbb{R}^d$ are referred to as the position and conjugate momenta, respectively, and constitute the solution of the system. The smooth function $H : \mathbb{R}^{2d} \to \mathbb{R}$ is the Hamiltonian, $\gamma > 0$ is the dissipation parameter, $\boldsymbol{g} \in \mathbb{R}^m$ are the holonomic constraints (depend only on $\boldsymbol{q}$), $\boldsymbol{G}$ is the Jacobian matrix of $\boldsymbol{g}$, i.e., $\boldsymbol{G}(\boldsymbol{q}) = \boldsymbol{g}_{\boldsymbol{q}}(\boldsymbol{q})$, and $\boldsymbol{\lambda} \in \mathbb{R}^m$ are the Lagrange multipliers. By differentiating the constraint $\boldsymbol{g}(\boldsymbol{q}) = \boldsymbol{0}$, we see that the solution of eq. (1) evolves on the manifold defined by the phase-space

key word index reduction?

$$\mathfrak{P} = \{(\boldsymbol{q},\boldsymbol{p}) \in \mathbb{R}^{2d} : \boldsymbol{g}(\boldsymbol{q}) = \boldsymbol{0},\ \boldsymbol{G}(\boldsymbol{q})\boldsymbol{\nabla}_{\boldsymbol{p}} H(\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{0}\}.$$

Here and henceforth we ~~have~~ dropped the explicit dependence of variables on t to keep the notation concise. The constraints defining $\mathfrak{P}$ are also known as the *weak invariants* of the system. Equation (1) can be thought of as a dissipative perturbation of a constrained Hamiltonian system. Constrained Hamiltonian systems find application in many areas including mechanics, chemical processes, and molecular dynamics. references?

The/A *Constrained Hamiltonian system* is an important special case of eq. (1) when $\gamma = 0$. In this special case, the Hamiltonian H and symplecticness are constants of motion of the constrained Hamiltonian system. The *Hamiltonian system* is obtained from eq. (1) when $\boldsymbol{g} = \boldsymbol{0}$, $\gamma = 0$. Structure-preserving techniques, preserving the symplecticness through MOR, have been developed in [1, 3, 6]. equiv

sounds complicated

A generalization of the Hamiltonian system is *port-Hamiltonian system*, which is the aggregate system model obtained when the core dynamics of the subsystem components are described by variational principles. MOR techniques preserving the port-Hamiltonian structure of the port-Hamiltonian systems are developed in [4].

Another relevant DAE that finds a lot of mention in the literature is the *descriptor system* linear?

so you meant pHDAE in previous paragraph?

$$\left.\begin{aligned} \boldsymbol{E}\dot{\boldsymbol{x}}(t) &= \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t), \\ \boldsymbol{y}(t) &= \boldsymbol{C}\boldsymbol{x}(t) + \boldsymbol{D}\boldsymbol{u}(t), \end{aligned}\right\}$$

where $\boldsymbol{x} \in \mathbb{R}^n$, $\boldsymbol{u} \in \mathbb{R}^m$, $\boldsymbol{y} \in \mathbb{R}^p$ are states, inputs, outputs respectively. Matrix $\boldsymbol{E} \in \mathbb{R}^{n\times n}$ is a singular matrix, and $\boldsymbol{A} \in \mathbb{R}^{n\times n}$, $\boldsymbol{B} \in \mathbb{R}^{n\times m}$, $\boldsymbol{C} \in \mathbb{R}^{p\times n}$, $\boldsymbol{D} \in \mathbb{R}^{p\times m}$. The descriptor systems have been reduced using interpolatory projection methods in [5] and using balanced truncation in [2, 7].

→ see related work in mail

The research on MOR of DAEs so far has mainly focused on the reduced basis MOR of the port-Hamiltonian systems and on interpolatory and balanced truncation MOR of the descriptor systems. In this paper, we take a reduced-basis approach to MOR of the nonlinear DAE (1). Out (r) objective is twofold:

- To reduce eq. (1) using the reduced basis method such that the conformal symplecticness of the equation is preserved through MOR
- To accelerate the simulation of the reduced order model (ROM) using a nonlinearity reduction technique, such as DEIM, by structure-preserving hyper-reduction of the conservative and constraining forces in eq. (1) reference, name symplectic DEIM?

In the end, we conduct numerical experiments on the ROM using a conformal symplectic numerical method to solve it.

2 MOR of eq. (1)

We begin by addressing our first objective – structure-preserving reduction (SPR) of eq. (1) using a reduced basis method. To this end, let us consider the following generalization of eq. (1).

no initial value?

$$\left.\begin{aligned} \dot{\boldsymbol{z}} &= \boldsymbol{J}\nabla_z \tilde{H}(\boldsymbol{z}) - \gamma \boldsymbol{z}, \\ \boldsymbol{0} &= \boldsymbol{g}(\boldsymbol{q}). \end{aligned}\right\} \tag{2}$$

cref? eqref?

Here $\boldsymbol{z}(t) : \mathbb{R} \to \mathbb{R}^{2d}$ is the solution of the system, and the structure matrix $\boldsymbol{J}$ is skew-symmetric and non-singular. The smooth function $\tilde{H} = H + \boldsymbol{g}^\top \boldsymbol{\lambda}$ is the augmented Hamiltonian, $\gamma > 0$ is the dissipation parameter, and $\boldsymbol{g} \in \mathbb{R}^m$ are the constraints. The separable system (1) can be deduced from eq. (2) replacing γ by $\gamma/2$, $H(\boldsymbol{z})$ by $H(\boldsymbol{q}, \boldsymbol{p}) + \frac{\gamma}{2}\boldsymbol{z}$, and the structure matrix $\boldsymbol{J}$ ~~by~~ with

scalar scalar vector

some typo here?

→ see next page

$$J = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{I} \\ -\boldsymbol{I} & \boldsymbol{0} \end{bmatrix}.$$

The system (2) is *conformal symplectic* since

$$d\boldsymbol{z} \wedge \boldsymbol{J}^{-1} d\boldsymbol{z} = -2\gamma d\boldsymbol{z} \wedge \boldsymbol{J}^{-1} d\boldsymbol{z},$$

not sure about hat product, but these looks like $\gamma = -\frac{1}{2}$? is there a typo?

where $d\boldsymbol{z}$ is the solution of the variational equation associated with (2). We refer to eq. (2) as *constrained perturbed Hamiltonian system* (CPHS).

Let us assume that we ~~have~~ obtained the projection bases $\boldsymbol{V}_r$, $\boldsymbol{W}_r$ such that

$$\boldsymbol{z}(t) \approx \boldsymbol{V}_r \boldsymbol{z}_r(t), \ \nabla_z \tilde{H}(\boldsymbol{z}(t)) \approx \boldsymbol{W}_r \boldsymbol{f}_r(t),$$

(t)

respectively, for some $\boldsymbol{f}_r \in \mathbb{R}^r$. Assuming $\boldsymbol{V}_r^\top \boldsymbol{W}_r = \boldsymbol{I}$, it follows that

$$\begin{aligned} \boxed{\nabla_z \tilde{H}(\boldsymbol{V}_r \boldsymbol{z}_r) \approx \nabla_z \tilde{H}(\boldsymbol{z})} & \\ &\approx \boldsymbol{W}_r \boldsymbol{f}_r(t) \\ &= \boldsymbol{W}_r \boldsymbol{V}_r^\top \boldsymbol{W}_r \boldsymbol{f}_r(t) \\ &\approx \boldsymbol{W}_r \boldsymbol{V}_r^\top \nabla_z \tilde{H}(\boldsymbol{V}_r \boldsymbol{z}_r) \\ &= \boldsymbol{W}_r \nabla_{\boldsymbol{z}_r} \tilde{H}_r(\boldsymbol{z}_r), \end{aligned}$$

$\nabla_z \tilde{H}$ continuous ok ✓

where $\tilde{H}_r(\boldsymbol{z}_r) = \tilde{H}(\boldsymbol{V}_r \boldsymbol{z}_r)$.

Substituting $\boldsymbol{z}(t) \approx \boldsymbol{V}_r \boldsymbol{z}_r(t)$, $\nabla_z \tilde{H}(\boldsymbol{V}_r \boldsymbol{z}_r) \approx \boldsymbol{W}_r \nabla_{\boldsymbol{z}_r} \tilde{H}_r(\boldsymbol{z}_r)$ in eq. (2), plus: multiply with $W_r^\top$ from left one gets the reduced system

\dot{z}_r

centralizes the dot

$$\left.\begin{aligned} \dot{\boldsymbol{z}}_r &= \boldsymbol{J}_r \nabla_{\boldsymbol{z}_r} \tilde{H}_r(\boldsymbol{z}_r) - \gamma \boldsymbol{z}_r, \\ \boldsymbol{0} &= \boldsymbol{g}(\boldsymbol{q}_r), \end{aligned}\right\} \tag{3}$$

where $\boldsymbol{J}_r = \boldsymbol{W}_r^\top \boldsymbol{J} \boldsymbol{W}_r$ is skew-symmetric, and $\boldsymbol{q}_r$ denotes the first half of the vector $\boldsymbol{V}_r \boldsymbol{z}_r$. The reduced system (3) is again conformal symplectic because the Jacobian $\partial_{\boldsymbol{z}_r \boldsymbol{z}_r} \tilde{H}_r$ is symmetric.

We further reduce the nonlinearities in eq. (3) with the discrete empirical interpolation method (DEIM). To this end, let us assume that the Hamiltonian H can be expressed as

rather: non-quadratic?

$$H = \frac{1}{2}\boldsymbol{z}^\top \boldsymbol{Q} \boldsymbol{z} + h(\boldsymbol{z})$$

sizes of U_l, U_l, E?

(t)

with $\boldsymbol{Q}$ being a positive-definite matrix and h being the nonlinear part of H. Let us define $\tilde{h} = h + \boldsymbol{g}^\top \boldsymbol{\lambda}$, and assume that $\nabla_{\boldsymbol{z}} \tilde{h}(\boldsymbol{z}) \approx \boldsymbol{U}_l \boldsymbol{k}_l(t)$ and that $\boldsymbol{V}_r^\top \boldsymbol{Q} \boldsymbol{V}_r = \boldsymbol{I}$, $\boldsymbol{U}_l^\top \boldsymbol{Q} \boldsymbol{U}_l = \boldsymbol{I}$. Let us further assume the DEIM projection basis $\mathbb{P} = \boldsymbol{U}_l(\boldsymbol{E}^\top \boldsymbol{U}_l)^{-1} \boldsymbol{E}^\top$ for the hyper-reduction of $\tilde{h}$. Then the hyper-reduced system reads

$E = ?$

why invertible?

$$\left.\begin{aligned} \dot{\hat{\boldsymbol{z}}}_r &= \boldsymbol{J}_r \nabla_{\hat{\boldsymbol{z}}_r} \hat{H}_r(\hat{\boldsymbol{z}}_r) - \gamma \hat{\boldsymbol{z}}_r \\ \boldsymbol{0} &= \boldsymbol{g}(\hat{\boldsymbol{q}}_r). \end{aligned}\right\} \tag{4}$$

scalar matrix scalar

Here $\hat{H} = \frac{1}{2}\boldsymbol{z}^\top \boldsymbol{Q} \boldsymbol{z} + \mathbb{P}\tilde{h}(\mathbb{P}^\top \boldsymbol{z})$, and $\nabla_{\hat{\boldsymbol{z}}_r} \hat{H}_r(\hat{\boldsymbol{z}}_r) = \boldsymbol{z}_r + \boldsymbol{V}_r^\top \mathbb{P} \nabla_{\boldsymbol{z}} \tilde{h}(\mathbb{P}^\top \boldsymbol{V}_r \hat{\boldsymbol{z}}_r)$. The hyper-reduced system (4) is also conformal symplectic because the Jacobian of $\hat{H}_r$ is symmetric. Indeed

$$\partial_{\hat{\boldsymbol{z}}_r^2} \hat{H}_r(\hat{\boldsymbol{z}}_r) = \boldsymbol{I} + \boldsymbol{V}_r^\top \mathbb{P} \partial_{\boldsymbol{z}^2} \tilde{h}(\mathbb{P}^\top \boldsymbol{V}_r \hat{\boldsymbol{z}}_r) \mathbb{P}^\top \boldsymbol{V}_r.$$

isn't that clear from $\hat{H}_r$ scalar-valued + C^2? (due to Lemma of Schwarz?) i.e. maybe not necessary to write out the derivative?

matrix with DEIM indices

$\hat{H}_r(z_r) = \hat{H}(V_r z_r)$

How is (2) a generalization of (1)?

$$\left.\begin{aligned} \dot{\boldsymbol{z}} &= \boldsymbol{J}\nabla_z \tilde{H}(\boldsymbol{z}) - \tilde{\gamma}\boldsymbol{z}, \\ \mathbf{0} &= \boldsymbol{g}(\boldsymbol{q}). \end{aligned}\right\} \qquad (2)$$

$$\left.\begin{aligned} \dot{\boldsymbol{q}} &= \boldsymbol{\nabla}_{\boldsymbol{p}} H(\boldsymbol{q},\boldsymbol{p}), \\ \dot{\boldsymbol{p}} &= -\boldsymbol{\nabla}_{\boldsymbol{q}} H(\boldsymbol{q},\boldsymbol{p}) - \gamma\boldsymbol{p} - \boldsymbol{G}(\boldsymbol{q})^\top \boldsymbol{\lambda}, \\ \mathbf{0} &= \boldsymbol{g}(\boldsymbol{q}). \end{aligned}\right\} \qquad (1)$$

$$\tilde{H}(z) = H(z) + g(q)^T \lambda + \gamma/4 \; z^T \begin{bmatrix} & I \\ I & \end{bmatrix} z$$

$$\tilde{\gamma} = \gamma/2$$

$$\nabla_z \tilde{H}(z) = \nabla_z H(z) + \begin{bmatrix} g(q)^T \lambda \\ 0 \end{bmatrix} - \gamma/2 \; \overbrace{\begin{bmatrix} & I \\ I & \end{bmatrix} z}^{= \begin{bmatrix} p \\ q \end{bmatrix}}$$

$$\begin{bmatrix} & I \\ -I & \end{bmatrix} \nabla_z \hat{H}(z) + \tilde{\gamma} z = \begin{bmatrix} \nabla_p H(z) - \gamma/2 \; q + \gamma/2 \; q \\ -\left(\nabla_q H(z) + g(q)^T \lambda - \gamma/2 \; p\right) + \gamma/2 \; p \end{bmatrix} \checkmark$$

→ maybe that is wrong in the numerics yet?

not sure how much novelty is in this method compared to Cecilia DEIM / DEIM in [4]

This implies that the Jacobian $\partial_{\hat{\boldsymbol{z}}_r^2}\hat{H}_r(\hat{\boldsymbol{z}}_r)$ is symmetric and, therefore,

$$\begin{aligned}\frac{1}{2}d\dot{\hat{\boldsymbol{z}}}_r \wedge \boldsymbol{J}_r^{-1}d\hat{\boldsymbol{z}}_r &= d\hat{\boldsymbol{z}}_r \wedge \partial_{\hat{\boldsymbol{z}}_r^2}\hat{H}_r(\hat{\boldsymbol{z}}_r) - \gamma d\hat{\boldsymbol{z}}_r \wedge \boldsymbol{J}_r^{-1}d\hat{\boldsymbol{z}}_r \\ &= -\gamma d\hat{\boldsymbol{z}}_r \wedge \boldsymbol{J}_r^{-1}d\hat{\boldsymbol{z}}_r\end{aligned}$$

where $d\hat{\boldsymbol{z}}_r$ is the solution of the variational equation associated with eq. (4). Equation (4) can now be solved with a conformal symplectic integrator to obtain the hyper-reduced solution $\hat{\boldsymbol{z}}_r$.

We summarize the process of obtaining eq. (4) in Table 1 (c.f. Algorithm 5 of[4]).

rather use Algorithm environment

Table 1: POD-DEIM structure-preserving reduction of CPHS (2).

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1. Select a positive-definite $\boldsymbol{Q}$ such that
$$H = \frac{1}{2}\boldsymbol{z}^\top \boldsymbol{Q}\boldsymbol{z} + h(\boldsymbol{z}).$$
2. Generate the solutions $\boldsymbol{z}(t)$ and construct the snapshot matrices
$$\begin{aligned}\mathbb{Z} &= [\boldsymbol{z}(t_0), \boldsymbol{z}(t_1), \ldots, \boldsymbol{z}(t_N)] \\ \mathbb{F} &= [\nabla_z\tilde{H}(\boldsymbol{z}(t_0)), \nabla_z\tilde{H}(\boldsymbol{z}(t_1)), \ldots, \nabla_z\tilde{H}(\boldsymbol{z}(t_N))] \\ \mathbb{K} &= [\nabla_z\tilde{h}(\boldsymbol{z}(t_0)), \nabla_z\tilde{h}(\boldsymbol{z}(t_1)), \ldots, \nabla_z\tilde{h}(\boldsymbol{z}(t_N))]\end{aligned}$$
3. Truncate the SVD of $\mathbb{Z}$, $\mathbb{F}$, $\mathbb{K}$ to obtain the POD bases $\boldsymbol{V}_r$, $\boldsymbol{W}_r$, and $\boldsymbol{U}_l$, respectively, such that
$$\boldsymbol{z}(t) \approx \boldsymbol{V}_r\boldsymbol{z}_r(t),\ \nabla_z\tilde{H}(\boldsymbol{z}) \approx \boldsymbol{W}_r\boldsymbol{f}_r(t),\ \nabla_z\tilde{h}(\boldsymbol{z}) \approx \boldsymbol{U}_l\boldsymbol{k}_l(t).$$
Ensure that the bases satisfy $\boldsymbol{W}_r^\top\boldsymbol{V}_r = \boldsymbol{I}$, $\boldsymbol{V}_r^\top\boldsymbol{Q}\boldsymbol{V}_r = \boldsymbol{I}$, and $\boldsymbol{U}_l^\top\boldsymbol{Q}\boldsymbol{U}_l = \boldsymbol{I}$.
4. Construct the DEIM projection $\mathbb{P} = \boldsymbol{U}_l(\boldsymbol{E}^\top\boldsymbol{U}_l)^{-1}\boldsymbol{E}^\top$.
5. The POD-DEIM reduced system reads as eq. (4).

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3 Numerical results

what is the motivation behind this equation?

In this section, we consider eq. (1) with

non-fat q?

rather use $H(q,p)$ as before

$$H(t) = \frac{1}{2}\|\boldsymbol{p}(t)\|^2 - \sum_{i=1}^{d}\cos(\boldsymbol{q}_i(t)),\ d = 3, \gamma = 0.1,\ \boldsymbol{g}(\boldsymbol{q}) = \sum_{i=1}^{d}(\alpha_i q_i^2) - 1,\ \|\boldsymbol{\alpha}\| = 1. \quad (5)$$

is α given or a variable?

We will reduce and simulate eq. (5) in structure-preserving manner.

isn't that very low-dimensional?
maybe good as dummy example?

Work in progress ..

References

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