Model Reduction of Finite Element Hamiltonian Systems With Respect to The Energy Norm

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Abstract

Here we summarize the basic concepts on how we generalize the model reduction with respect to energy norm to Hamiltonian systems.

1 Preliminaries

1.1 Finite Element Formulation

Consider the wave equation:

$$\begin{aligned} \partial_t q - p &= 0, \\ \partial_t p - \Delta q &= f, \\ q(x,0) &= q0(x), \\ p(x,0) &= p0(x). \end{aligned} \tag{1}$$

defined on the domain $\Omega \times [0,T] \subset \mathbb{R}^n \times \mathbb{R}$ We assume that the solution (q,p) to the system of differential equation (1) belongs to $H^1_{\text{per}} \times H^1_{\text{per}}$ where

$$H^1_{\text{per}} = \{u \in L^2 : \|\nabla u\| \in L^2 \text{ and } u \text{ is periodic on } \Omega\}. \tag{2}$$

We denote $(\cdot,\cdot)$ to be L^2 inner product. The solution to (1) also satisfies the weak form of finding (q,p) such that

$$
\begin{aligned}
(\partial_t q, u) - (p, u) &= 0, \\
(\partial_t p, v) + (\nabla q, \nabla v) &= 0.
\end{aligned} \tag{3}
$$

The semi-discrete mixed formulation of (4) is to find $(q_h, p_h) : [0, T] \times [0, T] \to U_h \times V_h$ such that

$$
\begin{aligned}
(\partial_t q_h, u_h) - (p_h, u_h) &= 0, \\
(\partial_t p_h, v_h) + (\nabla q_h, \nabla v_h) &= 0.
\end{aligned} \tag{4}
$$

where U_h and V_h are finite dimensional linear subspaces of H^1_{per}. Let $\{\phi_i\}_1^{\dim(U_h)}$ and $\{\psi_i\}_1^{\dim(V_h)}$ be the basis functions for U_h and V_h respectively. We define the mass matrices

$$
\begin{aligned}
M^q_{i,j} &= (\phi_j, \phi_i), \\
M^p_{i,j} &= (\psi_j, \psi_i).
\end{aligned} \tag{5}
$$

Further we define the stiffness matrices

$$
\begin{aligned}
K^q_{i,j} &= (\phi_j, \psi_i), \\
K^p_{i,j} &= (\nabla \psi_j, \nabla \phi_i).
\end{aligned} \tag{6}
$$

The semi-discrete form (4) also satisfies the system of ordinary differential equations

$$
\begin{aligned}
M^q q_t - K^q p &= 0, \\
M^p p_t + K^p q &= M^p f.
\end{aligned} \tag{7}
$$

The energy corresponding to the Hamiltonian system (1) is defined by

$$
H(q, p) = \frac{1}{2}(p, p) + \frac{1}{2}(\nabla q, \nabla q). \tag{8}
$$

The Hamiltonian defines an inner product on $(\cdot, \cdot)_H : H^1_{\text{per}} \times H^1_{\text{per}} \to \mathbb{R}$ denoted by

$$
((q_1, p_1), (q_2, p_2))_H = \frac{1}{2}(p_1, p_2) + \frac{1}{2}(\nabla q_1, \nabla q_2), \tag{9}
$$

and the corresponding energy norm $\|(q, p)\|_H = \sqrt{H(q, p)}$.

An essential feature of Hamiltonian systems is the conservation of the energy and how it evolves under numerical time-integration. For a solution

(q,p) to the Hamiltonian equation (1) we have:

$$\begin{aligned}\frac{d}{dt}\|(q,p)\|_H^2 &= \frac{1}{2}\left(\frac{d}{dt}(p,p)+\frac{d}{dt}(\nabla q,\nabla q)\right)\\ &= (\partial_t p,p)+(\nabla\partial_t q,\nabla q)\\ &= (\Delta q+f,p)+(\nabla q,\nabla q)\\ &= (f,p)-(\nabla q,\nabla q)+(\nabla q,\nabla q)\\ &= (f,p)\end{aligned} \tag{10}$$

By taking the integral over $[0,T]$ we obtain

$$H(T)=H(0)+\int_0^T (f,p)\ dt. \tag{11}$$

Now applying the Cauchy-Schwartz inequality yields,

$$\begin{aligned}H(T) &\leq H(0)+\int_0^T \|f(\cdot,t)\|_{L^2}\cdot\|p(\cdot,t)\|_{L^2}\ dt\\ &\leq H(0)+\sup_{0\leq t<T}(H)\cdot\int_0^T \|f(\cdot,t)\|_{L^2}\ dt\end{aligned} \tag{12}$$

where the last inequality is due to the fact that the energy inner product defines a norm on H^1_{per}.

1.2 Energy Preservation in Semi-Discrete mixed Formulation

Let $U_h \in U$ and $V_h \in V$ be finite dimensional proper subspaces of U and V respectively. Furthermore, suppose that $\pi_u : U \to U_h$ and $p_v : V \to V_h$ be the L^2 projection operators. By adding and subtracting $(\pi_U q, u_h)$ and $(\pi_V p, v_h)$ to the semi-discrete mixed formulation (4) we obtain

$$\begin{aligned}(\dot{q},u_h)+(\pi_U\dot{q},u_h)-(\pi_U\dot{q},u_h)-(p,u_h)+(\pi_V p,u_h)-(\pi_V p,u_h)&=0\\ (\dot{p},v_h)+(\pi_V\dot{p},v_h)-(\pi_V\dot{p},vh)+(\nabla q,\nabla v_h)+(\nabla\pi_U q,\nabla v_h)-(\nabla\pi_U q,\nabla v_h)&=(f,v_h)\end{aligned} \tag{13}$$

Having in mind that $q-\pi_U q$ and $p-\pi_V p$ are orthogonal to U_h and V_h, respectively, we can omit many terms from above to obtain

$$\begin{aligned}(\pi_U\dot{q},u_h)-(\pi_V p,u_h)&=(\pi_U\dot{q}-\dot{q},u_h)\\ (\pi_V\dot{p},v_h)+(\nabla\pi_U q,\nabla v_h)&=(\pi_V\dot{p}-\dot{p},v_h)+(f,v_h)\end{aligned} \tag{14}$$

Now if we add the original weak form (4) to the above we retrieve

$$\begin{aligned}(\pi_U \dot{q} - \dot{q}_h, u_h) - (\pi_V p - p_h, u_h) &= (\pi_U \dot{q} - \dot{q}, u_h) \\ (\pi_V \dot{p} - \dot{p}_h, v_h) + (\nabla \pi_U q - \nabla q_h, \nabla v_h) &= (\pi_V \dot{p} - \dot{p}, v_h)\end{aligned} \tag{15}$$

We define new variables $\theta = \pi_U q - q_h \in U_h$, $\rho = \pi_V p - p_h \in V_h$, $\mu = \pi_U q - q$ and $\xi = \pi_V p - p$. Then equation (15) turns into

$$\begin{aligned}(\dot{\theta}, u_h) - (\rho, u_h) &= (\dot{\mu}, u_h) \\ (\dot{\rho}, v_h) + (\nabla \theta, \nabla v_h) &= (\dot{\xi}, v_h)\end{aligned} \tag{16}$$

To bound this we use the energy norm

$$\begin{aligned}\frac{d}{dt} H(\theta,\rho)^2 = \frac{d}{dt}\|(\theta,\rho)\|^2 &= (\dot{\rho}, \rho) + (\nabla \dot{\theta}, \nabla \theta) \\ &= (\dot{\xi}, \rho) - (\nabla \theta, \nabla \rho) - (\rho, \Delta \theta) - (\dot{\mu}, \Delta \theta) \\ &= (\dot{\xi}, \rho) + (\nabla \dot{\mu}, \nabla \theta) \\ &= (\dot{\xi}, \rho) + (\dot{\mu}, \theta)_{\nabla}\end{aligned} \tag{17}$$

where $(\cdot,\cdot)_{\nabla} = (\nabla \cdot, \nabla \cdot)$. Finally by applying the Cauchy inequality we obtain

$$\begin{aligned}H^2(\theta,\rho)^2(T) &\leq \int_0^T \|\dot{\xi}\|\|\rho\| + \|\dot{\mu}\|_{\nabla}\|\theta\|_{\nabla}\ dt \\ &\leq \sqrt{2}\int_0^T \underbrace{(\|\rho\| + \|\theta\|_{\nabla})}_{H(\theta,\rho)}(\|\dot{\xi}\| + \|\dot{\mu}\|_{\nabla})\ dt \\ &\leq \sqrt{2}\cdot \sup_{0\leq t<T} H(\theta,\rho)\int_0^T \|\dot{\xi}\| + \|\dot{\mu}\|_{\nabla}\ dt\end{aligned} \tag{18}$$

Here we used the fact that $H(\theta,\rho)(0) = 0$. And now by a theorem in [Symplectic-mixed finite element approximation of linear acoustic wave equations, Robert C. Kirby Thinh Tri Kieu] we get

$$H^2(\theta,\rho)(T) \leq \sqrt{2}\int_0^T \|\dot{\xi}\| + \|\dot{\mu}\|_{\nabla}\ dt \tag{19}$$

By assuming regularity on $\dot{\xi}$ and $\dot{\mu}$ and with theory of interpolation we can achieve several error estimations on the Finite Element solution.

1.3 Error Estimation in the Energy Norm

We define the error in the energy/Hamiltonian norm as

$$\epsilon(t) = \|(q - q_h, p - p_h)\|_H \tag{20}$$

Using the triangle inequality, we obtain

$$\sup \epsilon(t) \leq \sup \underbrace{\|(\mu, \xi)\|_H}_{I} + \sup \underbrace{\|(\theta, \rho)\|_H}_{II} \tag{21}$$

For part I we can directly apply error estimation in the theory of interpolation, under regularity assumptions on q and p. Also for part II we can apply the error estimate obtain in (19).

2 Model Reduction With Respect to the Energy Inner Product

The energy norm appears naturally in the error analysis of the finite element methods. Suppose that $a(\cdot,\cdot)$ is the bilinear form corresponding to the variational formulation

$$a(u, v) = L(v), \quad u, v \in V \tag{22}$$

Where V is some appropriate Hilbert space. The finite element discretization of equation (22) is

$$a(u_h, v_v) = L(v_h), \quad u_h, v_h \in V_h \subset V \tag{23}$$

The energy inner product associated to (24) is defined as

$$(u_h, v_h)_a = a(u_h, v_h), \tag{24}$$

which implies the energy norm $\|\cdot\|_a$. In vector notation we have

$$(u_h, v_h)_a = \bar{u}^T X \bar{v} = u, \tag{25}$$

where $\bar{u}$ and $\bar{v}$ are expansion coefficients of u_h and v_h in the finite element basis, and X is a positive definite matrix, usually taken to be the stiffness matrix. Note that we can rewrite an energy norm in terms of the 2-norm as $\|\bar{u}\|_a = \|X^{1/2}u\|_2$.

The energy inner product induces a projection. Energy projection of function u_h onto e reads

$$(u_h, e)_a \cdot e = \bar{u}_h^T X \bar{e} \cdot \bar{e} = \bar{e}\bar{e}^T X u_h. \tag{26}$$

Therefore the matrix $\bar{e}\bar{e}^T X$ is the energy projection operator in the matrix notation. Now suppose that $W = [w_1, \dots, w_k]$ is an expansion coefficients of a basis with respect to some finite element basis. Then the energy projection of a function s onto the span space of W would be $WW^T Xs$. It is often desirable to find a basis W that minimizes the energy projection error of a set of functions $\{s_1, \dots, s_N\}$. We have

$$\begin{aligned} \min \sum_{i=1}^{N} \|s_i - WW^T X s_i\|_a &= \min \sum_{i=1}^{N} \|X^{1/2} s_i - X^{1/2} WW^T X s_i\|_2 \\ &= \min \sum_{i=1}^{N} \|\tilde{s}_i - \tilde{W}\tilde{W}^T \tilde{s}_i\|_2 \\ &= \min \|\tilde{S} - \tilde{W}\tilde{W}^T \tilde{S}\|_2. \end{aligned} \tag{27}$$

Where $\tilde{W} = X^{1/2}W$ and $\tilde{s}_i = X^{1/2}s_i$ and $\tilde{S}$ is the matrix containing $\tilde{s}_i$. The Smidth-Mirskey theorem implies that the solution to the above minimization is the truncated singular value decomposition of the matrix $\tilde{S}$.

2.1 Symplectic Model Reduction With Respect to an Energy Inner Product

To fit the energy norm into the symplectic framework, we need to modify the energy projections operator. Suppose that A contains the basis vectors (the expansion coefficients of a set of functions in a FEM basis) in its column space. For now We assume this basis is even dimensional. We define the sympelctic projection onto the span of A with respect to the energy weight X as

$$P(s) = AA^{\times} Xs, \tag{28}$$

Where J is the standard symplectic matrix and $A^{\times}$ is defined as

$$A^{\times} = J^T A^T X J \tag{29}$$

Note that if we ensure
$$A^{\times} X A = I, \tag{30}$$
with I the identity matrix, then we see that the operator $AJ^T A^T XJX$ becomes idempotent since

$$\begin{aligned}(AJ^T A^T XJX)^2 &= A(J^T A^T XJ)XAJ^T A^T XJX \\ &= A(A^{\times} XA)J^T A^T XJX \\ &= AJ^T A^T XJX.\end{aligned} \tag{31}$$

This means that $AJ^T A^T XJX$ is a projection operator onto the span space of A. Now if we require the energy norm of the projection of a snapshot matrix S onto the span of A to be minimized with respect to an energy norm we would have

$$\min \|S - AJ^T A^T XJXS\|_a = \min \|X^{1/2} S - X^{1/2} AJ^T A^T XJXS\|_2. \tag{32}$$

We define $\tilde{S} = X^{1/2} S$, $\tilde{A} = X^{1/2} A$ and the skew-symmetric matrix $\tilde{J} = X^{1/2} J X^{1/2}$. Then equation (31) turns into

$$\min \|\tilde{S} - \tilde{A} J^T \tilde{A}^T \tilde{J} \tilde{S}\|_2. \tag{33}$$

Finally if we define the pseudo inverse $\tilde{A}^{+} = J^T A^T X^{1/2} \tilde{J}$ then minimization (31) is equivalent to
$$\min \|\tilde{S} - \tilde{A}\tilde{A}^{+}\tilde{S}\|_2. \tag{34}$$
Note that condition (30) is equivalent to

$$\tilde{A}^{+}\tilde{A} = I, \tag{35}$$

which is satisfied when
$$\tilde{A}^T \tilde{J} \tilde{A} = J. \tag{36}$$
The later condition holds when $\tilde{A}$ is a Poisson transformation. Therefore the minimization (32) is now rewritten as

$$\begin{aligned}&\min \|\tilde{S} - \tilde{A}\tilde{A}^{+}\tilde{S}\|_2, \\ &\text{subject to } \tilde{A}^T \tilde{J} \tilde{A} = J.\end{aligned} \tag{37}$$

2.2 Model Reduction with a Symplectic and Energy Projected Basis

Suppose that the FEM discretization of a linear Hamiltonian system takes the form

$$\dot{x} = JLx, \tag{38}$$

where x is the expansion coefficients of the FEM basis functions and L is some linear positive definite matrix square. Let A be the basis to a reduced subspace such that $x \approx Ay$ where y is the expansion coefficients of x in the basis of A. This implies

$$A\dot{y} = JLAy. \tag{39}$$

Multiplying both sides with $A^{\times}X$ yields

$$\dot{y} = A^{\times}XJLAy, \tag{40}$$

due to condition (30). Having in mind that $Lx = \nabla_x H(x)$ for some Hamiltonian function H, we recover

$$\nabla_x H(x) = \nabla_x H(Ay) = (A^{\times}X)^T \nabla_y H(Ay). \tag{41}$$

This implies that

$$\dot{y} = A^{\times}XJ(A^{\times}X)^T A^T LAy = A^{\times}XJX(A^{\times})^T A^T LAy, \tag{42}$$

which can be simplified to the system

$$\dot{y} = \tilde{A}^{+}\tilde{J}(\tilde{A}^{+})^T A^T LAy. \tag{43}$$

This is a Poisson system since $\tilde{A}^{+}\tilde{J}(\tilde{A}^{+})^T$ is skew-symmetric. A Poisson integrator can therefore preserve the Hamiltonian along integral curves.