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

Babak Maboudi Afkham
Department of Mathematids
EPFL

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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:

$$\partial_t q - p = 0,$$

$$\partial_t p - \Delta q = f,$$

$$q(x, 0) = q0(x),$$

$$p(x, 0) = p0(x).$$
(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

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

$$(\partial_t q, u) - (p, u) = 0,$$

$$(\partial_t p, v) + (\nabla q, \nabla v) = 0.$$
(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

$$(\partial_t q_h, u_h) - (p_h, u_h) = 0,$$

$$(\partial_t p_h, v_h) + (\nabla q_h, \nabla v_h) = 0.$$
(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

$$M_{i,j}^{q} = (\phi_{j}, \phi_{i}),$$

 $M_{i,j}^{p} = (\psi_{j}, \psi_{i}).$ (5)

Further we define the stiffness matrices

$$K_{i,j}^{q} = (\phi_j, \psi_i),$$

$$K_{i,j}^{p} = (\nabla \psi_j, \nabla \phi_i).$$
(6)

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

$$M^q q_t - K^q p = 0,$$

$$M^p p_t + K^p q = M^p f.$$
(7)

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

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

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

$$\frac{d}{dt} \| (q, p) \|_H^2 = \frac{1}{2} \left(\frac{d}{dt} (p, p) + \frac{d}{dt} (\nabla q, \nabla q) \right)$$

$$= (\partial_t p, p) + (\nabla \partial_t q, \nabla q)$$

$$= (\Delta q + f, p) + (\nabla q, \nabla q)$$

$$= (f, p) - (\nabla q, \nabla q) + (\nabla q, \nabla q)$$

$$= (f, p)$$
(10)

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

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

Now applying the Cauchy-Schwartz inequality yields,

$$H(T) \leq H(0) + \int_{0}^{T} \|f(\cdot,t)\|_{L^{2}} \cdot \|p(\cdot,t)\|_{L^{2}} dt$$

$$\leq H(0) + \sup_{0 \leq t < T} (H) \cdot \int_{0}^{T} \|f(\cdot,t)\|_{L^{2}} dt$$
(12)

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

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

$$(\dot{q}, u_h) + (\pi_U \dot{q}, u_h) - (\pi_U \dot{q}, u_h) - (p, u_h) + (\pi_V p, u_h) - (\pi_V p, u_h) = 0$$

$$(\dot{p}, v_h) + (\pi_V \dot{p}, v_h) - (\pi_V \dot{p}, v_h) + (\nabla q, \nabla v_h) + (\nabla \pi_U q, \nabla v_h) - (\nabla \pi_U q, \nabla v_h) = (f, v_h)$$
(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

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

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

$$(\pi_U \dot{q} - \dot{q}_h, u_h) - (\pi_V p - p_h, u_h) = (\pi_U \dot{q} - \dot{q}, u_h) (\pi_V \dot{p} - \dot{p}_h, v_h) + (\nabla \pi_U q - \nabla q_h, \nabla v_h) = (\pi_V \dot{p} - \dot{p}, v_h)$$
(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

$$(\dot{\theta}, u_h) - (\rho, u_h) = (\dot{\mu}, u_h)$$

$$(\dot{\rho}, v_h) + (\nabla \theta, \nabla v_h) = (\dot{\xi}, v_h)$$
(16)

To bound this we use the energy norm

$$\frac{d}{dt}H(\theta,\rho)^{2} = \frac{d}{dt}\|(\theta,\rho)\|^{2} = (\dot{\rho},\rho) + (\nabla\dot{\theta},\nabla\theta)$$

$$= (\dot{\xi},\rho) - (\nabla\theta,\nabla\rho) - (\rho,\Delta\theta) - (\dot{\mu},\Delta\theta)$$

$$= (\dot{\xi},\rho) + (\nabla\dot{\mu},\nabla\theta)$$

$$= (\dot{\xi},\rho) + (\dot{\mu},\theta)_{\nabla}$$
(17)

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

$$H^{2}(\theta,\rho)^{2}(T) \leq \int_{0}^{T} \|\dot{\xi}\| \|\rho\| + \|\dot{\mu}\|_{\nabla} \|\theta\|_{\nabla} dt$$

$$\leq \sqrt{2} \int_{0}^{T} \underbrace{(\|\rho\| + \|\theta\|_{\nabla})}_{H(\theta,\rho)} (\|\dot{\xi}\| + \|\dot{\mu}\|_{\nabla}) dt$$

$$\leq \sqrt{2} \cdot \sup_{0 \leq t \leq T} H(\theta,\rho) \int_{0}^{T} \|\dot{\xi}\| + \|\dot{\mu}\|_{\nabla} dt$$
(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

$$H^{2}(\theta,\rho)(T) \leq \sqrt{2} \int_{0}^{T} \|\dot{\xi}\| + \|\dot{\mu}\|_{\nabla} dt$$
 (19)

By assuming regularity on ξ 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

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

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 (23) 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

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

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 $\bar{e}\bar{e}^TX$ 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^TXs . 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

$$\min \sum_{i=1}^{N} \|s_{i} - WW^{T}Xs_{i}\|_{a} = \min \sum_{i=1}^{N} \|X^{1/2}s_{i} - X^{1/2}WW^{T}Xs_{i}\|_{2}$$

$$= \min \sum_{i=1}^{N} \|\tilde{s}_{i} - \tilde{W}\tilde{W}^{T}\tilde{s}_{i}\|_{2}$$

$$= \min \|\tilde{S} - \tilde{W}\tilde{W}^{T}\tilde{S}\|_{2}.$$
(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 projection operator. Suppose that A contains a set of 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 a symplectic 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

$$A^{\times}XA = I, (30)$$

with I the identity matrix, then we see that the operator AJ^TA^TXJX becomes idempotent since

$$(AJ^{T}A^{T}XJX)^{2} = A\underbrace{J^{T}A^{T}XJ}_{A^{\times}}XAJ^{T}A^{T}XJX$$

$$= A\underbrace{A^{\times}XA}_{I}J^{T}A^{T}XJX$$

$$= AJ^{T}A^{T}XJX.$$
(31)

This means that AJ^TA^TXJX 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

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

We define $\tilde{S}=X^{1/2}S,\ \tilde{A}=X^{1/2}A$ and the skew-symmetric matrix $\tilde{J}=X^{1/2}JX^{1/2}$. 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 $\tilde{A}^+ = J^T A^T X^{1/2} \tilde{J} = J^T \tilde{A}^T \tilde{J}$ then the 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

$$\min \|\tilde{S} - \tilde{A}\tilde{A}^{+}\tilde{S}\|_{2},
\text{subject to } \tilde{A}^{T}\tilde{J}\tilde{A} = J.$$
(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 square matrix. 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

$$\dot{y} = A^{\times} X J L A y,\tag{40}$$

due to the 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

$$\dot{y} = A^{\times} X J (A^{\times} X)^T A^T L A y = A^{\times} X J X (A^{\times})^T A^T L A y, \tag{42}$$

which can be simplified to the system

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

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.