A constrained Fermi-Pasta-Ulam-Tsingou problem

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Introduction

The goal is to establish a non linear stiff DAE toy model to test the behaviour of the corrected discrete gradient on a DAE. We take the well-known Fermi-Pasta-Ulam-Tsingou (FPUT) problem and propose a simple DAE version with kinematic and holonomic constraints. We then implement a simulation without simplifying the constraints.

1 The model

For symbolic computations, see https://github.com/WetzelVictor/FPUT_DAE_PHS

We consider a 1-dimensional chain of : N_m mass points and N_k springs ; $N_m = 2 * N_k$. First, we describe a cell, comprised of 2 masses and 1 spring. We then connect all the subsystems using kinematic constraints between the masses.

1.1 Sub-system

You may change the springs law in order to make the systelm non linear :

$$\mathbf{X} = [\Pi_{iL} \quad \Pi_{iR} \quad x_{ki}]^\intercal \tag{1}$$

$$\mathrm{H}(\mathbf{X}) = \frac{\Pi_{iL}^2}{2m_{iL}} + \frac{\Pi_{iR}^2}{2m_{iR}} + \frac{1}{2}x_{ki}^2 k_i \tag{2}$$

$$\theta = [m_{iL} \quad m_{iR} \quad k_i] \tag{3}$$

Hypothesis : here, $m_{iL} << m_{iR}$.

$$\begin{pmatrix} \dot{\Pi}_{iL} \\ \dot{\Pi}_{iR} \\ \dot{x}_{ki} \end{pmatrix} = \begin{bmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & -1 \\ -1 & 1 & \cdot \end{bmatrix} \cdot \begin{pmatrix} v_{m_{i,L}} \\ v_{m_{i,R}} \\ F_{ki}(x_{ki}) \end{pmatrix} \tag{4}$$

1.2 DAE-pHs

See [2] for more details :

$$\begin{array}{ll} \text{Dynamic} \\ \text{Outputs} \\ \text{Constraints} \end{array} \begin{cases} \dot{\mathbf{X}} & = [(\mathbf{J}(\mathbf{X}) - \mathbf{R}(\mathbf{X})] \nabla_{\mathbf{X}} \mathrm{H}(\mathbf{X}) + \mathbf{G}\mathbf{u} + \mathbf{B}\lambda \\ \mathbf{y} & = \mathbf{G}^\intercal \nabla_{\mathbf{X}} \mathrm{H}(\mathbf{X}) + \mathbf{G}_{yy}\mathbf{u} \\ 0 & = \mathbf{B}^\intercal \nabla_{\mathbf{X}} \mathrm{H}(\mathbf{X}) \end{cases} \tag{5}$$

where :

- $\mathbf{X}$ and $\nabla_{\mathbf{X}}\mathrm{H}(\mathbf{X})$ are vectors of N_x elements
- $\mathbf{J}(\mathbf{X})$ and $\mathbf{R}(\mathbf{X})$ are $N_x \times N_x$ matrices
- $\mathbf{u}$ and $\mathbf{y}$ are vector of N_p elements
- $\mathbf{G}$ is a $N_x \times N_p$ matrix
- λ is the vector of the N_λ Lagrange multipliers
- $\mathbf{B}$ is a $N_x \times N_\lambda$ matrix
- $\mathbf{G}_{yy}$ is a $N_p \times N_p$ matrix

1.3 Assembly

The kinematic constraints between system i and $i+1$ is :

$$0 = v_{m_{i,R}} - v_{m_{(i+1),L}} \tag{6}$$

We assume the state vector of the full system follows the following order :

$$\mathbf{X} = \begin{bmatrix} \Pi_{1L} & \Pi_{1R} & \dots & \Pi_{N_sL} & \Pi_{N_sR} & ; & x_{k1} & \dots & x_{kN_s} \end{bmatrix}^\intercal$$

The transposed constraint matrix $\mathbf{B}^\intercal$ reads :

$$\mathbf{B}^\intercal_{ij} = \begin{cases} 1 & \text{if}\, i = 2j \\ -1 & \text{if}\, i = 2j+1 \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

1.4 Variable change

We use the method also described in [1]. The left annihilator $\mathbf{B}^\perp$ of $\mathbf{B}$ is :

$$\mathbf{B}^{\perp} = \left[\begin{array}{c|c} 1 & \mathbb{0}_{1\times(N_x-1)} \\ \hline \mathbb{0}_{(N_x-N_\lambda-1)\times 1} & \begin{array}{c|c} \begin{matrix} 1 & 1 & 0 & \dots & \dots & \dots & 0 \\ 0 & 0 & 1 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \dots & \dots & \dots & 1 & 1 \end{matrix} & \mathbb{0}_{(N-1)\times(N_s)} \\ \hline \mathbb{0}_{N_s\times(2N_s-1)} & \mathbb{1}_{N_s+1} \end{array} \end{array}\right] \tag{8}$$

The variable change is :

$$\mathbf{M} = \left[\begin{array}{c} \mathbf{B}^\perp \\ \hline \mathbf{B}^\star = (\mathbf{B}^\intercal\mathbf{B})^{-1}\mathbf{B}^\intercal \end{array}\right] \tag{9}$$

where $\mathbf{B}^\star$ is the Moore-Penrose inverse of $\mathbf{B}$.

1.5 New variables

Denoting $\mathbf{Z} = \mathbf{MX}$ the new states, we have :

$$\mathbf{Z} = \left[\begin{array}{c} \Pi_{L1} \\ \Pi_{12} \\ \vdots \\ \Pi_{(N_s-1)N_s} \\ \Pi_{RN_s} \\ x_{k1} \\ \vdots \\ x_{kN_s} \\ \hline \Delta\Pi_{12} \\ \vdots \\ \Delta\Pi_{(N_s-1)N_s} \end{array}\right] = \left[\begin{array}{c} \Pi_{L1} \\ \Pi_{R1} + \Pi_{L2} \\ \vdots \\ \Pi_{R(N_s-1)} + \Pi_{LN_s} \\ \Pi_{RN_s} \\ x_{k1} \\ \vdots \\ x_{kN_s} \\ \hline \frac{\Pi_{R1}-\Pi_{L2}}{2} \\ \vdots \\ \frac{\Pi_{R(N_s-1)}-\Pi_{LN_s}}{2} \end{array}\right]$$

1.6 Hamiltonian

We assume springs are linear for now, to simplify notations. Therefore the Hamiltonian can be expressed in its quadratic form :

$$\mathrm{H}(\mathbf{X}) = \frac{1}{2}\mathbf{X}^\intercal \mathbf{Q} \mathbf{X}$$

$$\text{with} \quad \mathbb{Q} = \mathrm{diag}\left(m_{1L}^{-1} \quad m_{1R}^{-1} \quad \dots \quad m_{N_sL}^{-1} \quad m_{N_sR}^{-1} \quad ; x_{k1} \quad \dots \quad x_{kN_s}\right)$$

With the variable change, the Hamiltonian reads :

$$\mathrm{H}(\mathbf{X} = \mathbf{M}^{-1}\mathbf{Z}) = \frac{1}{2}\mathbf{Z}^\intercal \underbrace{\mathbf{M}_i^{-\intercal}\mathbb{Q}^{(1)}\mathbf{M}_i^{-1}}_{\mathbb{Q}^{(2)}} \mathbf{Z}$$

1.7 Constraints

Let us split $\mathbf{Z}$ into :

- $\mathbf{Z}_1$ the unconstrained states, which dynamic is determined by on ODE
- $\mathbf{Z}_2$ the constrained states, which value is computed by solving an algebraic system (variables $\Delta_{i(i+1)} \forall i \in [1, N_s - 1]$)

After applying the variable change to the system, the N_λ constraints are given by :

$$0 = \frac{\partial \mathrm{H}(\mathbf{Z})}{\partial \left(\mathbf{Z}_2\right) i}$$

For each $\mathbf{Z}_{2i}$, the constraint is :

$$0 = \Delta\Pi_{i(i+1)} \left(\frac{1}{m_{Ri}} + \frac{1}{m_{L(i+1)}}\right) + \Pi_{i(i+1)} \left(\frac{1}{2m_{Ri}} - \frac{1}{m_{2L(i+1)}}\right) \tag{10}$$

1.8 Matrix formulation

Let us divide $\mathbb{Q}^{(2)}$ accordingly to $\mathbf{Z}$, the constraints system is :

$$\begin{aligned} &\text{find} \quad \mathbf{Z}_2 \quad \text{such as} \\ &[\mathbb{Q}^{(2)}]_{12}\mathbf{Z}_1 + [\mathbb{Q}^{(2)}]_{22}\mathbf{Z}_2 = 0 \\ \text{where} \quad \mathbb{Q} = &\begin{bmatrix} [\mathbb{Q}^{(2)}]_{11} & [\mathbb{Q}^{(2)}]_{12} \\ [\mathbb{Q}^{(2)}]_{12} & [\mathbb{Q}^{(2)}]_{22} \end{bmatrix} \end{aligned}$$

Références

[1] Flavio Cardoso Ribeiro. “Port-hamiltonian Modeling and Control of a Fluid-structure System : Application to Sloshing Phenomena in a Moving Container Coupled to a Flexible Structure.” Thèse de doct. Institut Supérieur de l’Aéronautique et de l’Espace, déc. 2016. URL : https://depozit.isae.fr/theses/2016/2016_Cardoso_Ribeiro_Flavio_Luiz_D.pdf.

[2] A. J. van der Schaft. “Port-Hamiltonian Differential-Algebraic Systems”. In : *Surveys in Differential-Algebraic Equations I*. Sous la dir. d’Achim Ilchmann et Timo Reis. Berlin, Heidelberg : Springer Berlin Heidelberg, 2013, p. 173-226. ISBN : 978-3-642-34928-7. DOI : 10.1007/978-3-642-34928-7_5. URL : https://doi.org/10.1007/978-3-642-34928-7_5.