

Last Class ...

Example: Mass-Spring-Damper, Real World System

Reliable Physical Theory

$$\mathcal{R}(\mathbf{u}, \tau; \mathbf{r}) = \mathbf{0}$$

$$m\ddot{x} + c\dot{x} + kx = 0$$

$$\mathbf{u} = \begin{bmatrix} x \\ \dot{x} \end{bmatrix} \quad \tau = \begin{bmatrix} c \\ k \end{bmatrix} \quad \mathbf{r} = \begin{bmatrix} m \\ x(0) \\ \dot{x}(0) \end{bmatrix}$$

$$\tau = (\mathbf{u}, \mathbf{v}, \mathbf{s}, \theta)$$

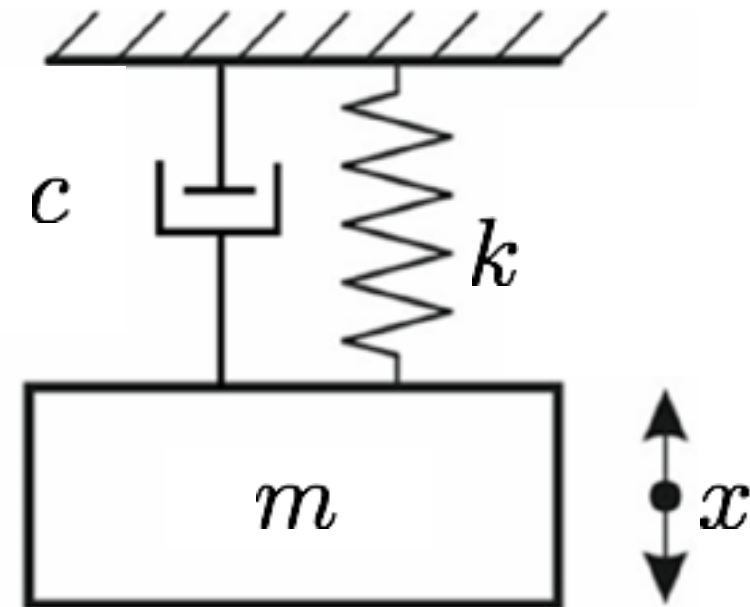
$$k = \text{const}$$

$$c(T) = \exp\left(\frac{T_0}{T} - 1\right)$$

$$\dot{T} = c(T)\dot{x}^2 - \frac{T - T_0}{t_T}$$

$$\mathbf{v} = T \quad \mathbf{s} = \begin{bmatrix} T_0 \\ t_T \end{bmatrix} \quad \theta = k$$

Real World Embedded Model



$$\mathbf{y} = x$$
$$\mathbf{q} = \max(\dot{x})$$

Bayesian Machine Learning Approach to the Quantification of Uncertainties on Ab Initio Potential Energy Surfaces [2]

[2] S. Venturi, R. L. Jaffe, and M. Panesi, “Bayesian Machine Learning Approach to the Quantification of Uncertainties on Ab Initio Potential Energy Surfaces”, The Journal of Physical Chemistry A, Special Virtual Issue “Machine Learning in Physical Chemistry”, Vol. 124, No. 25 (2020)