Last Class ...

Example: Mass-Spring-Damper, Real World System

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

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

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

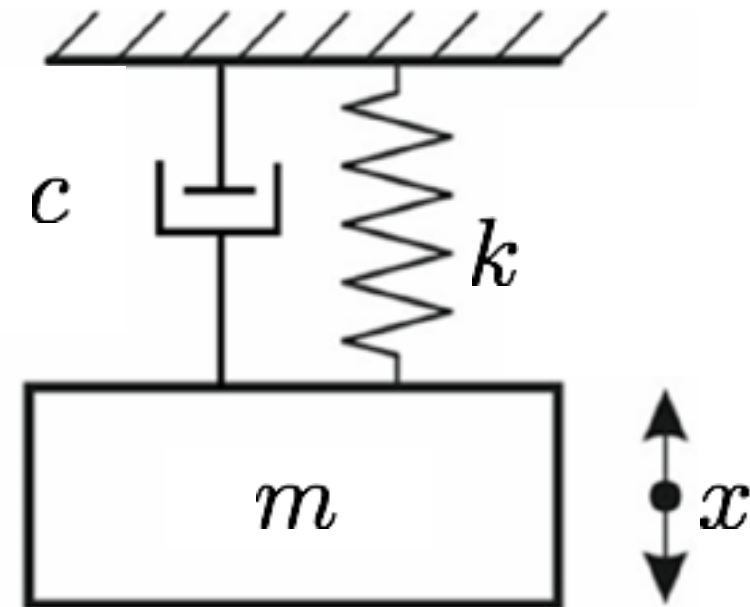$$\tau = (\mathbf{u}, \mathbf{v}, \mathbf{s}, \theta)$$

$$k = \text{const}$$

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

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

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

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

A Bayesian Neural Network Approach to the Quantification of Uncertainties
on Ab Initio Potential Energy Surfaces