

I

Dynamics

$$\boldsymbol{\nu} = \mathbf{K}^{-1} \boldsymbol{\Psi}$$

II

Tensor DDP

AD tools twice: $\frac{\partial^2 \boldsymbol{\nu}}{\partial^2 \mathbf{q}}$ $\mathcal{O}(n^3)$

Tensor contraction: $\boldsymbol{\gamma}^\top \frac{\partial^2 \boldsymbol{\nu}}{\partial^2 \mathbf{q}}$ $\mathcal{O}(n^3)$

III

mRNEAc DDP

$$\boldsymbol{\gamma}^\top \frac{\partial^2 \boldsymbol{\nu}}{\partial^2 \mathbf{q}} = \mathsf{T}_1 + \mathsf{T}_2 + \mathsf{T}_2^\top$$

$$\mathsf{T}_1 = \frac{\partial}{\partial \mathbf{q}} \left[\frac{\partial}{\partial \mathbf{q}} \text{mRNEAc}(\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}, \mathbf{a}_g, \boldsymbol{\lambda}, \boldsymbol{\mu}, \boldsymbol{\pi}) \right] \quad \mathcal{O}(n^2)$$

$$\mathsf{T}_2 = \frac{\partial}{\partial \mathbf{q}} \text{mRNEAc} \left(\mathbf{q}, 0, \frac{\partial \ddot{\mathbf{q}}}{\partial \mathbf{q}}, 0, \frac{\partial \boldsymbol{\lambda}}{\partial \mathbf{q}}, \boldsymbol{\mu}, \boldsymbol{\pi} \right) \quad \mathcal{O}(n^2)$$

$$\text{where } \begin{bmatrix} \boldsymbol{\mu} \\ \boldsymbol{\pi} \end{bmatrix} = -\mathbf{K}^{-1} \boldsymbol{\gamma}$$