INSTITUTE OF COMPUTER SCIENCE

Kamiltonian Neural Networks

—— Aikaterini Papadaki ——

Goal

- Hamilton Mechanics -> *Hamiltonian Fluid Mechanics*
- HNN & ODEs -> KNN & PDEs
- Simulate the Propagation of a Wave Pulse

$$q = q(x,t)$$

Outline

1. **Introduction**
    - Hamiltonian Mechanics
    - Hamiltonian Neural Networks
2. **Proposed Model**
    - Hamiltonian PDEs
    - *Kamiltonian* Neural Networks
3. **Results**
    - Fourier Space
    - Physical Space
    - Energy Conservation

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1: Hamiltonian Mechanics

Hamiltonian System $S = (\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2N}$

$$\boxed{E_{tot} = H(\mathbf{q}, \mathbf{p})}$$

Hamilton's Equations

$$\dot{\mathbf{p}} = -\nabla_{\mathbf{q}} H(\mathbf{p}, \mathbf{q})$$

$$\dot{\mathbf{q}} = \nabla_{\mathbf{p}} H(\mathbf{p}, \mathbf{q})$$

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1: Hamiltonian Neural Networks

Hamilton's Equations

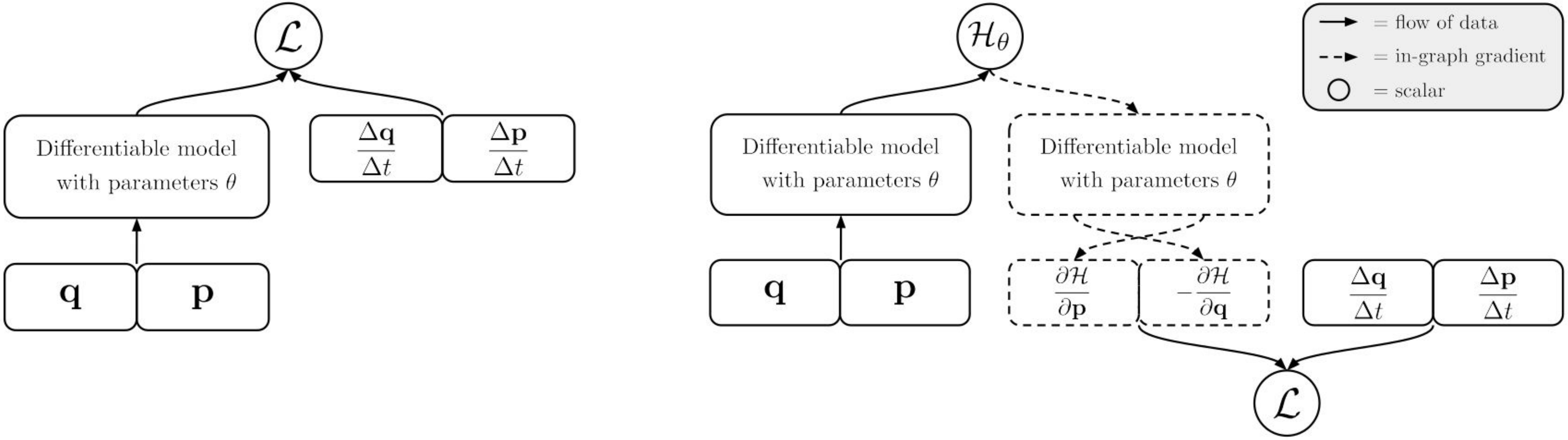
$$\dot{\mathbf{p}} = -\nabla_{\mathbf{q}} H(\mathbf{p}, \mathbf{q})$$
$$\dot{\mathbf{q}} = \nabla_{\mathbf{p}} H(\mathbf{p}, \mathbf{q})$$

Hamiltonian Neural Networks

$$\mathcal{L}_{HNN} = \left\| \frac{\partial \mathcal{H}_\theta}{\partial \mathbf{p}} - \frac{\partial \mathbf{q}}{\partial t} \right\|_2 + \left\| \frac{\partial \mathcal{H}_\theta}{\partial \mathbf{q}} + \frac{\partial \mathbf{p}}{\partial t} \right\|_2$$

Samuel Greydanus et al.,
“Hamiltonian Neural Networks”, 2019.

1: Hamiltonian Neural Networks



(a) Baseline NN (b) Hamiltonian NN

Samuel Greydanus et al.,
“Hamiltonian Neural Networks”, 2019.

1: Hamiltonian Neural Networks

1. Ideal Mass-Spring

$$\mathcal{H} = \frac{1}{2}kq^2 + \frac{p^2}{2m}$$

2. Ideal Pendulum

$$\mathcal{H} = 2mgl(1 - \cos q) + \frac{l^2 p^2}{2m}$$

3. Two-Body problem

$$\mathcal{H} = \frac{|\mathbf{p}_{\mathrm{CM}}|^2}{m_1 + m_2} + \frac{|\mathbf{p_1}|^2 + |\mathbf{p_2}|^2}{2\mu} + g\frac{m_1 m_2}{|\mathbf{q_1} - \mathbf{q_2}|^2}$$

3 Layers

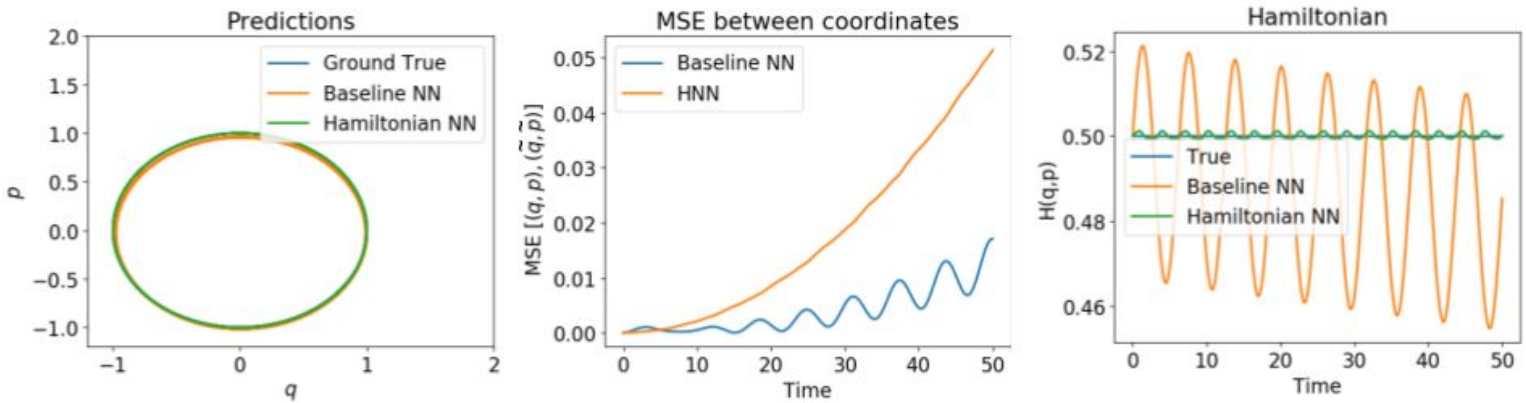
Fully Connected NN

- Baseline
- Hamiltonian

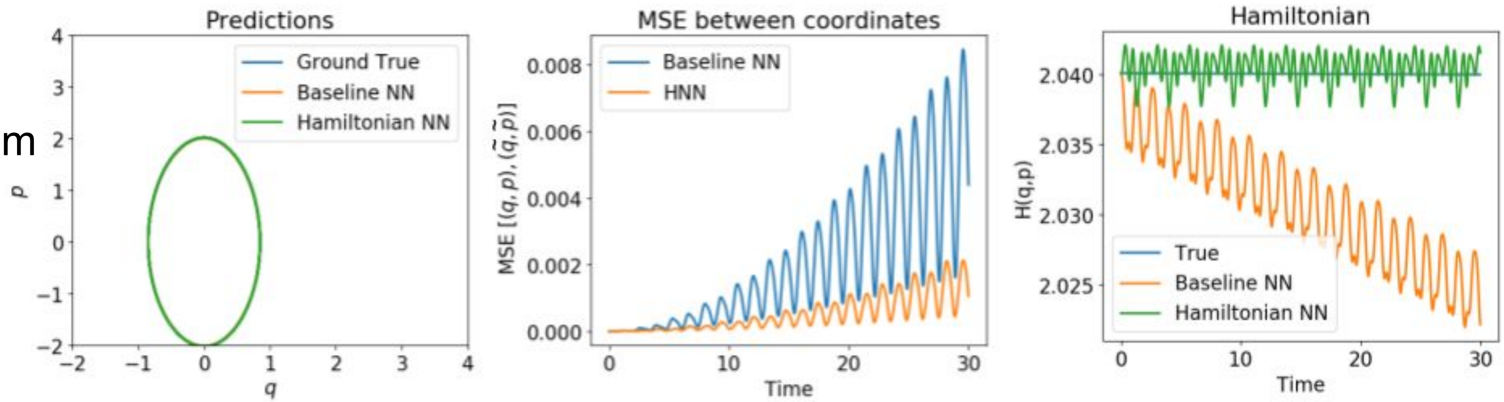
Samuel Greydanus et al.,
“Hamiltonian Neural Networks”, 2019.

1: Simple Physics Tasks

Mass Spring

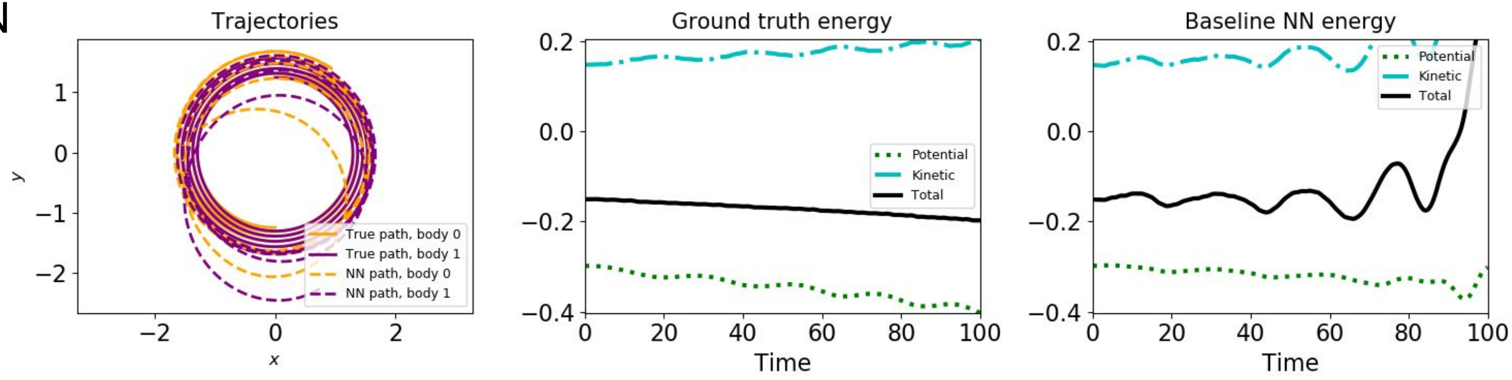


Ideal Pendulum

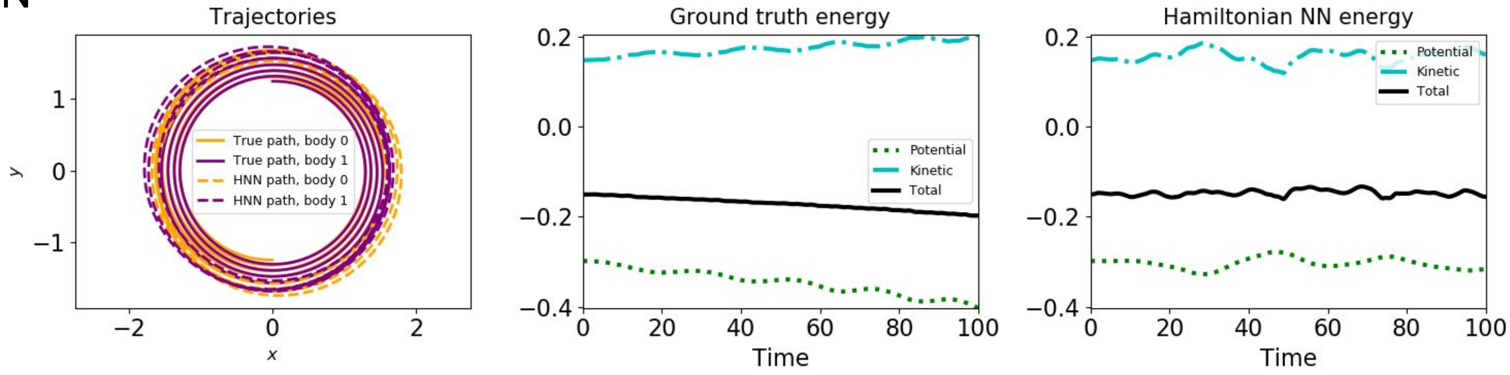


1: 2-Body Problem

Baseline NN



Hamiltonian NN



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2:Hamiltonian PDEs

Linear Wave Equation $q_{tt} = \partial_x \sigma'(q_x)$

Hamiltonian Functional

$$q_t = p$$
$$p_t = \partial_x \sigma'(q_x)$$

$$H(q,p) = \int_0^A \left[\frac{1}{2}p^2 + \sigma(q_x)\right] dx$$

Symplectic Discretization

$$q_i = i\,\Delta x, \quad i = 0, 1, \ldots, N$$
$$t_j = j\,\Delta t, \quad j = 0, 1, \ldots, M$$

$$H(q,p) = \sum_{i=1}^{N} \left[\frac{1}{2}|p_i|^2 + \frac{1}{2}|q_{x_i}|^2\right]$$

2:Hamiltonian PDEs

$$H(q,p) \qquad (q_i, p_i),\ i = 0, 1, \ldots, N$$

Discrete Fourier Transform

$$H(\hat{q},\hat{p}) \qquad (\hat{q}_k, \hat{p}_k),\ k = 0, 1, \ldots, L$$

Kamiltonian Functional

$$H(\hat{q},\hat{p}) = K$$

$$K = \sum_{k=0}^{L} \left[\frac{1}{2L} |\hat{p}_k|^2 + \frac{1}{2L} \left(\frac{2\pi i k}{L} \right)^2 |\hat{q}_k|^2 \right]$$

2:Hamiltonian PDEs

Kamiltonian Functional

$$H(\hat{q}, \hat{p}) = K$$

$$K = \sum_{k=0}^{L} \left[\frac{1}{2L} |\hat{p}_k|^2 + \frac{1}{2L} \left(\frac{2\pi i k}{L} \right)^2 |\hat{q}_k|^2 \right]$$

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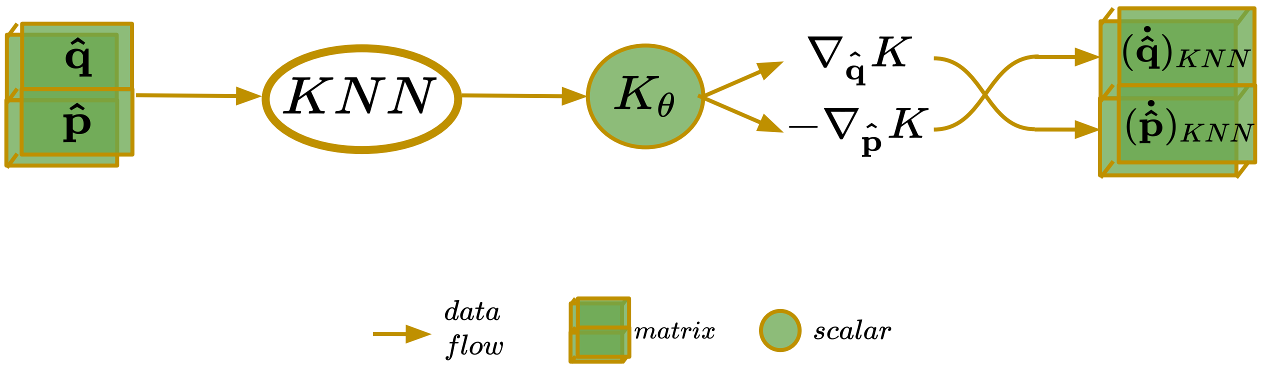
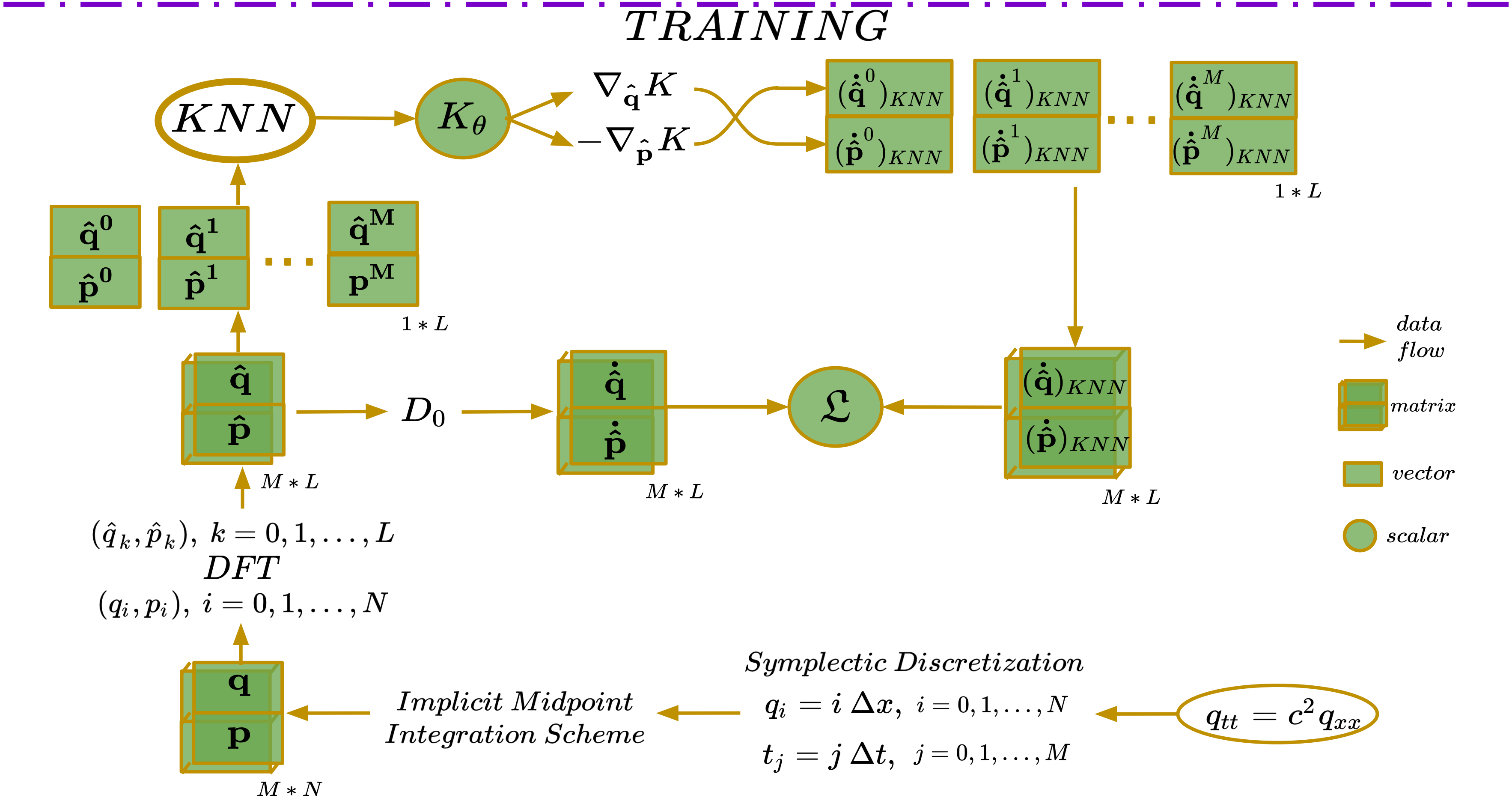
2:Kamiltonian Neural Networks

Kamiltonian Neural Network

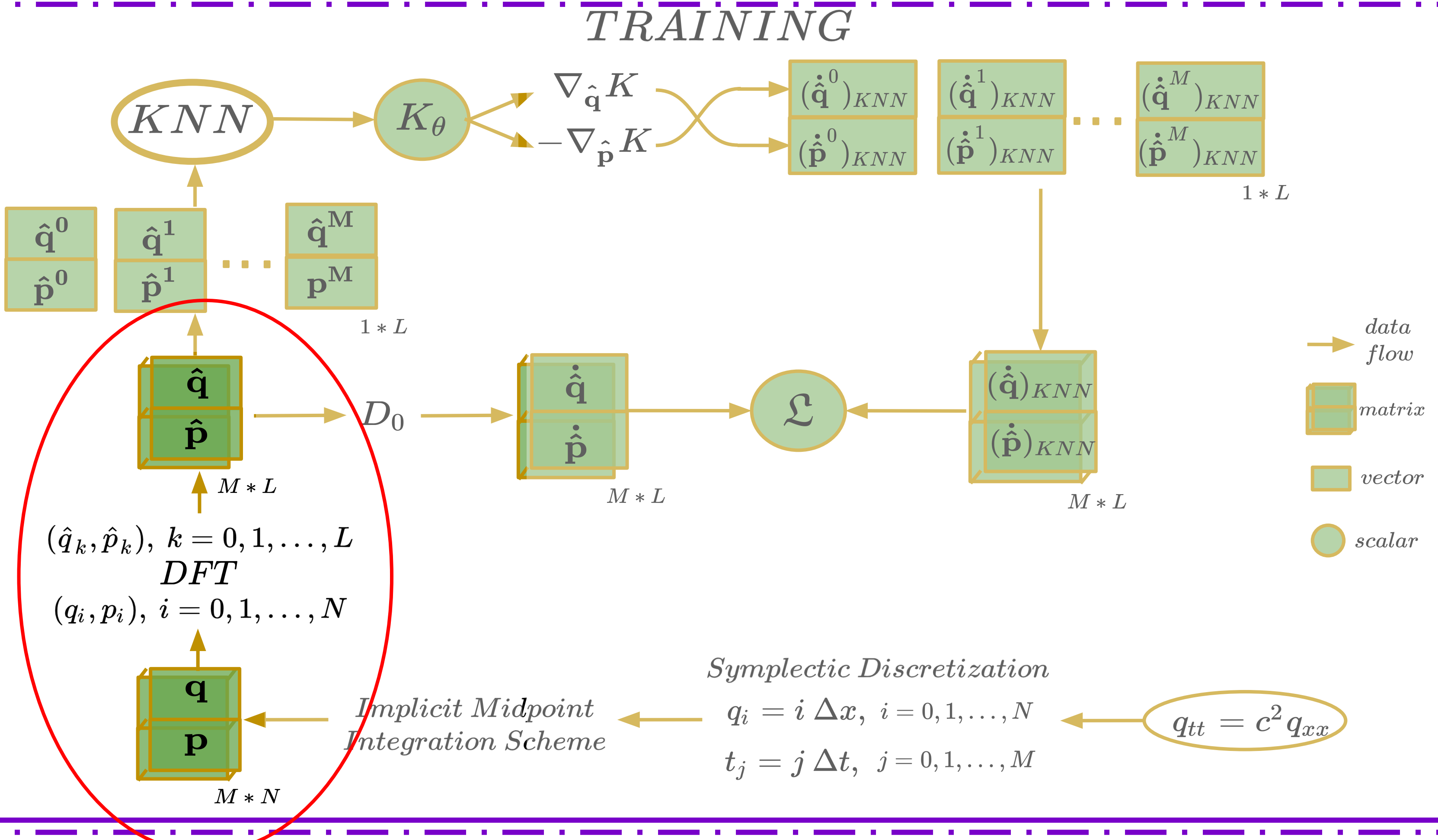


* KNN -> Fourier Space -> Independent of Discretization

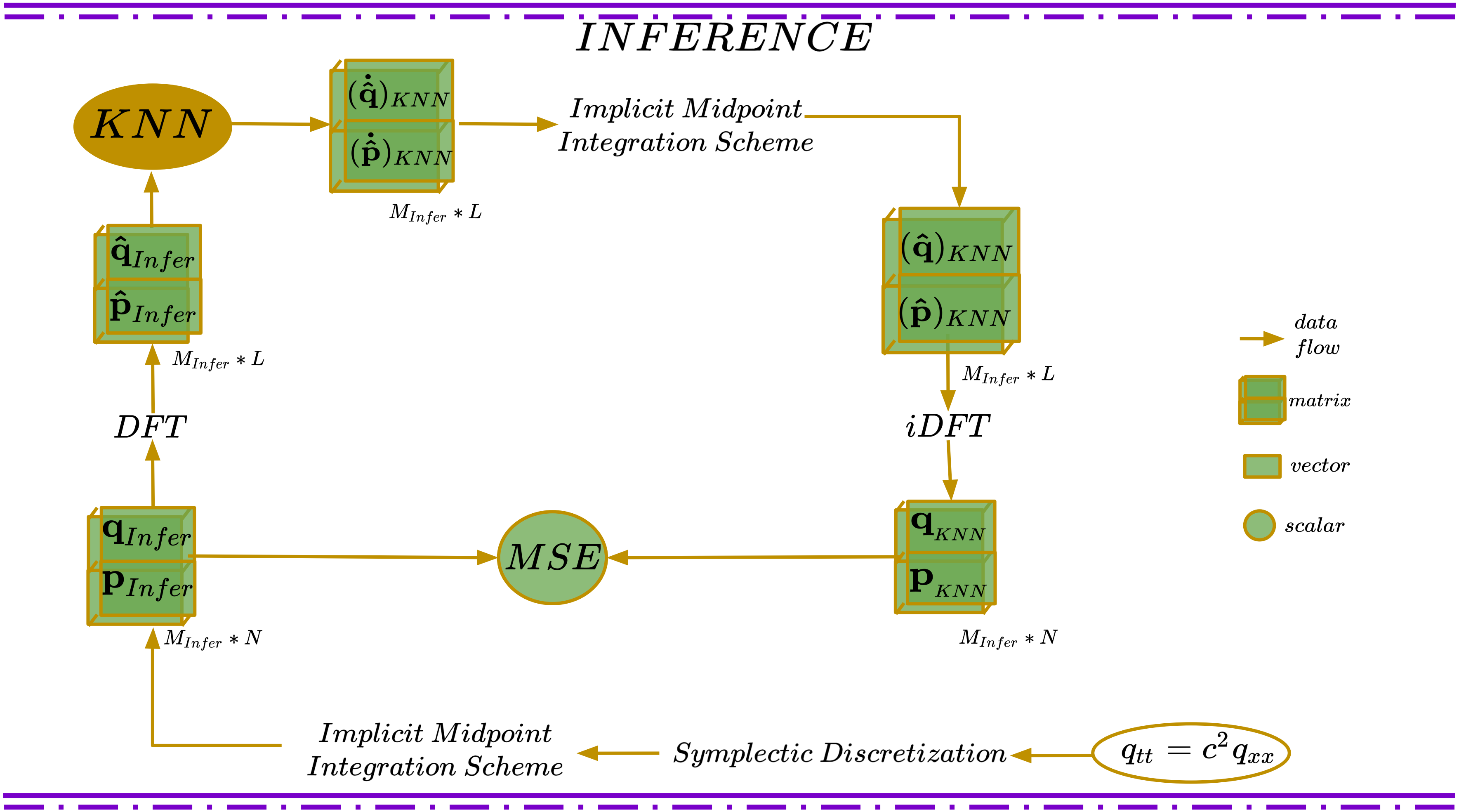
2:Kamiltonian Neural Networks



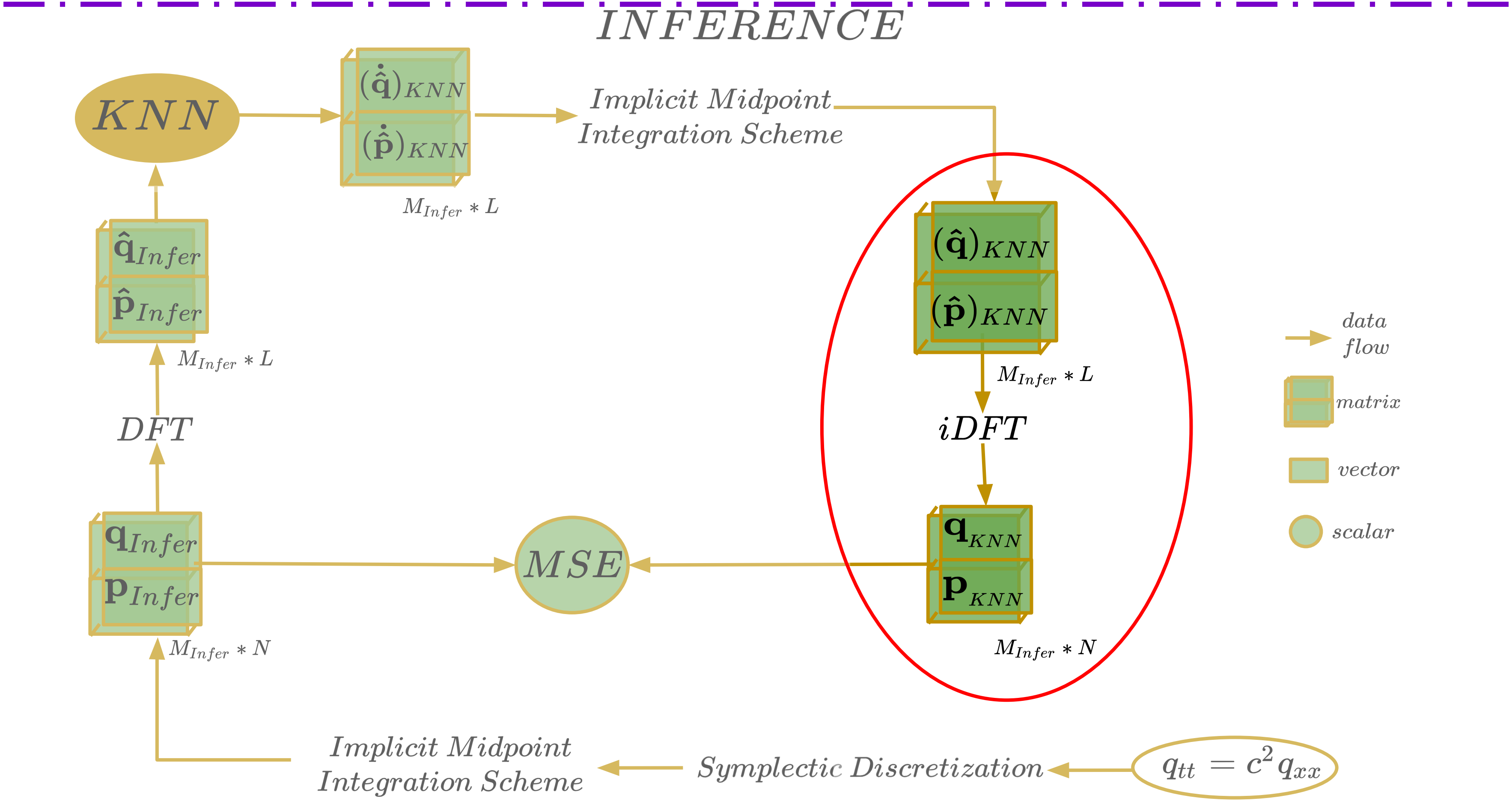
2:Kamiltonian Neural Networks



2:Kamiltonian Neural Networks



2:Kamiltonian Neural Networks



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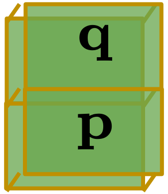
3.Results: Wave Pulse

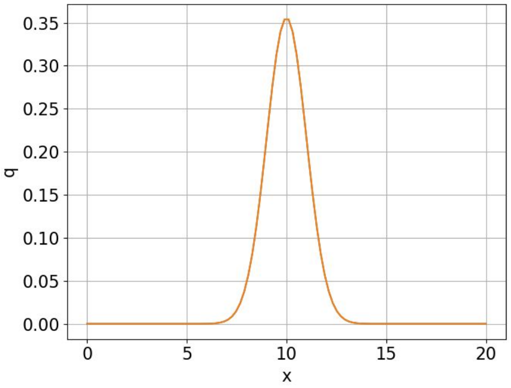


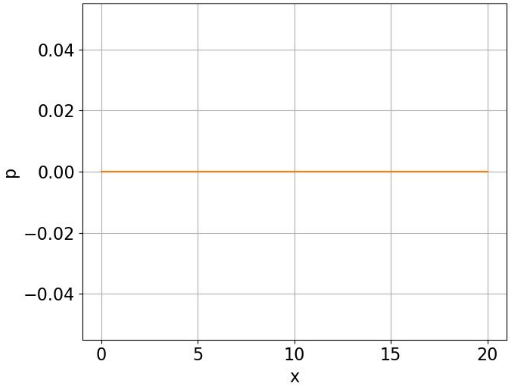
200 * 100

$x_i = i * 0.2, \quad i = 0, 1, \ldots, 100$

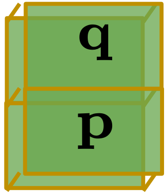
$t_j = j * 0.05, \quad j = 0, 1, \ldots, 200$

t = t0





3.Results: Wave Pulse



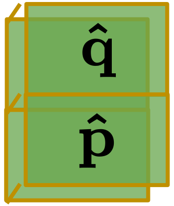
200 * 100

$$(q_i, p_i), \quad i = 0, 1, \ldots, 100$$

Discrete Fourier Transform

$$(\hat{q}_i, \hat{p}_i), \quad i = 0, 1, \ldots, 51$$

$$(\hat{q}_i, \hat{p}_i), \quad i = 0, 1, \ldots, 15$$



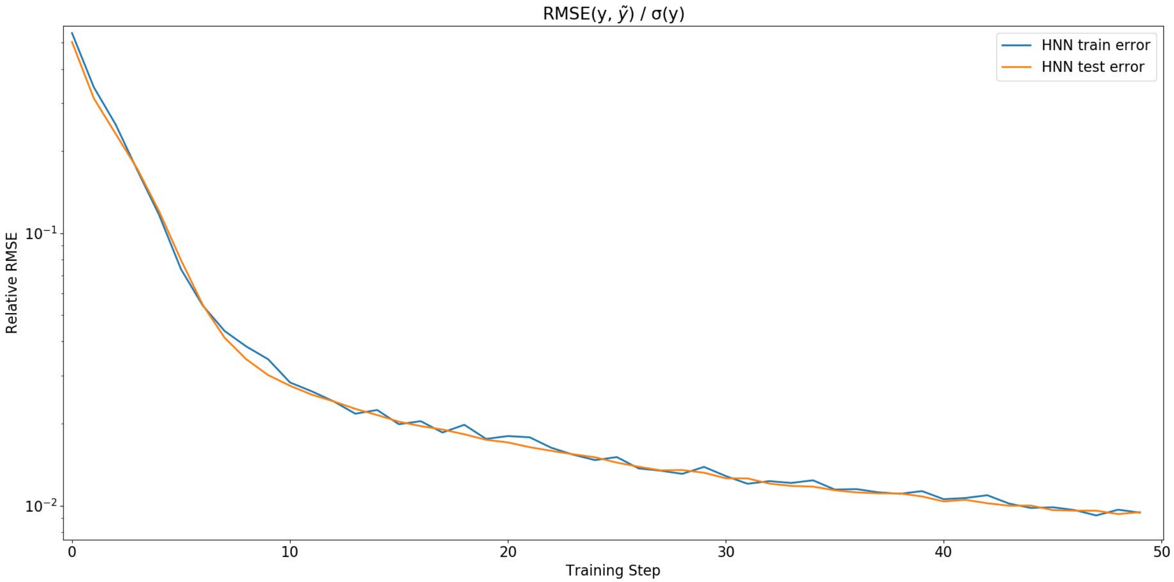
200 * 15

3.Results: Fourier Space

$$KNN\ OUTPUT$$

$$\tilde{y} = [\dot{\hat{q}}, \dot{\hat{p}}]$$

$$Relative\ RMSE = \frac{RMSE[y,\tilde{y}]}{\sigma(y)}$$



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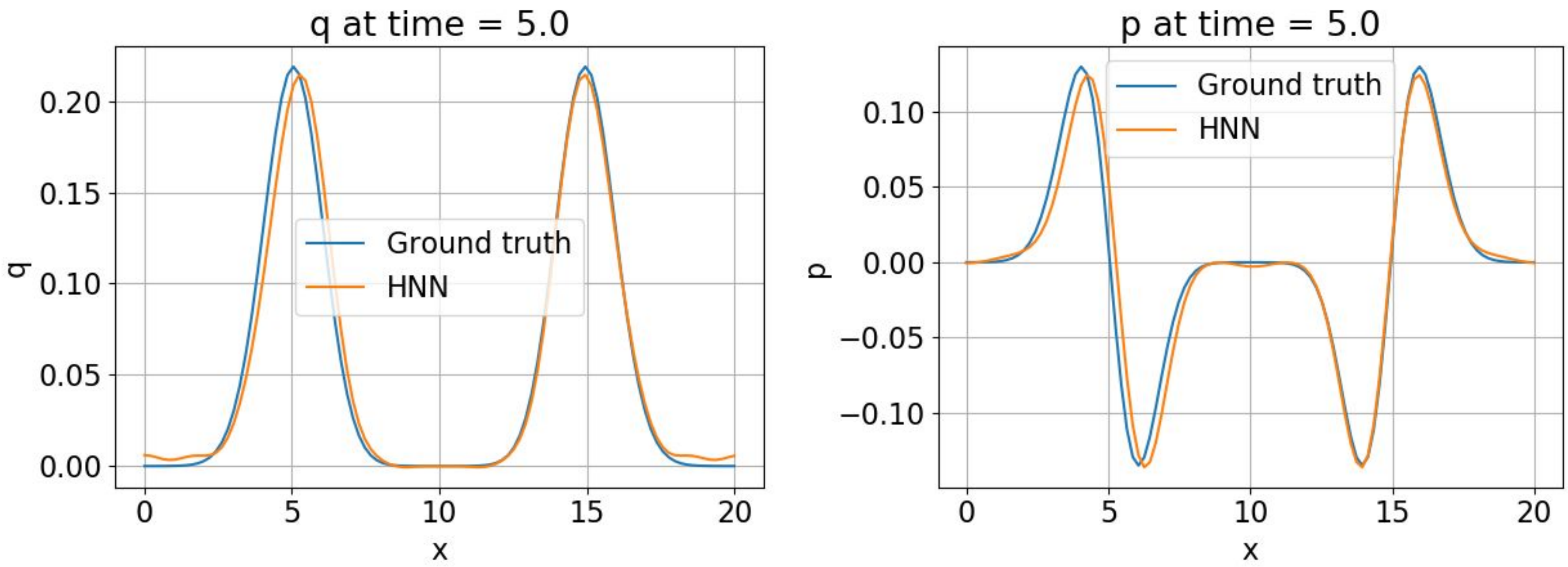
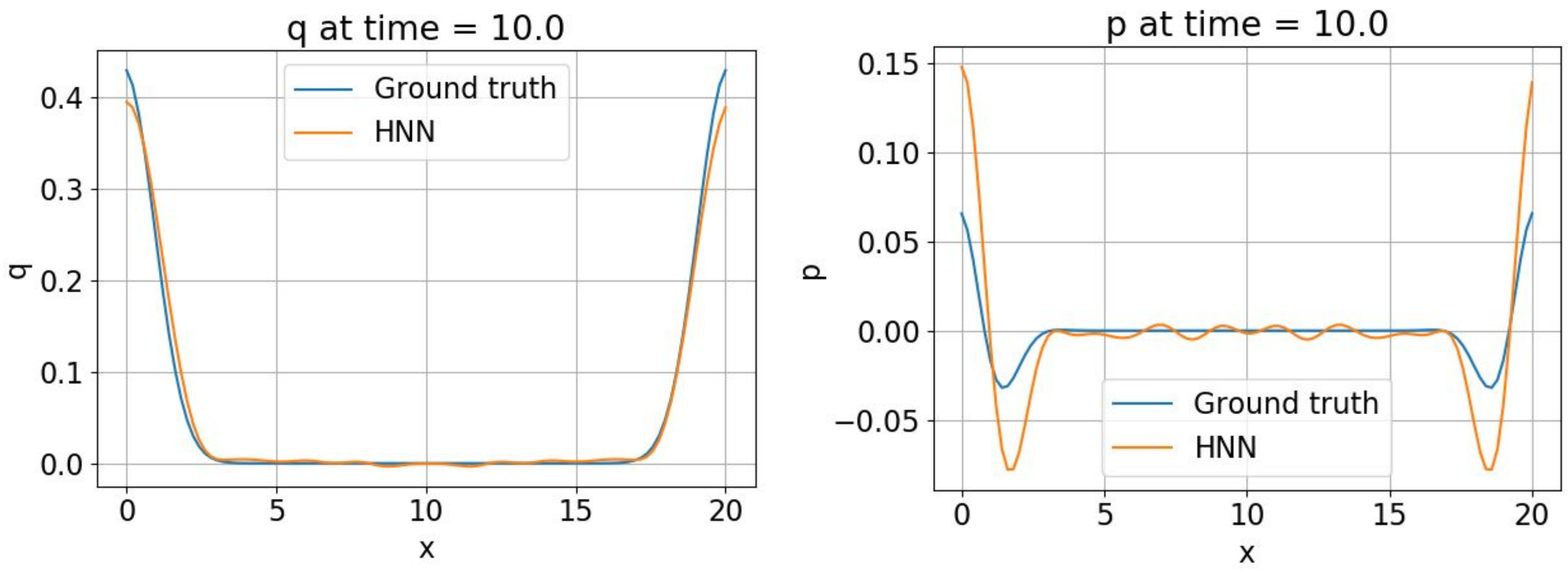
3.Results: Physical Space

$t = t_{1/2} = 5$



3.Results: Physical Space

$t = t_f = 10$



3.Results: Physical Space

$$MSE = \frac{1}{M_{Infer}} \frac{1}{N} \sum_{j=0}^{M_{Infer}} \sum_{i=0}^{N} \left[[q_i^j, p_i^j]_{Infer} - [q_i^j, p_i^j]_{KNN} \right]^2$$

$$\boxed{MSE \sim 10^{-4}}$$

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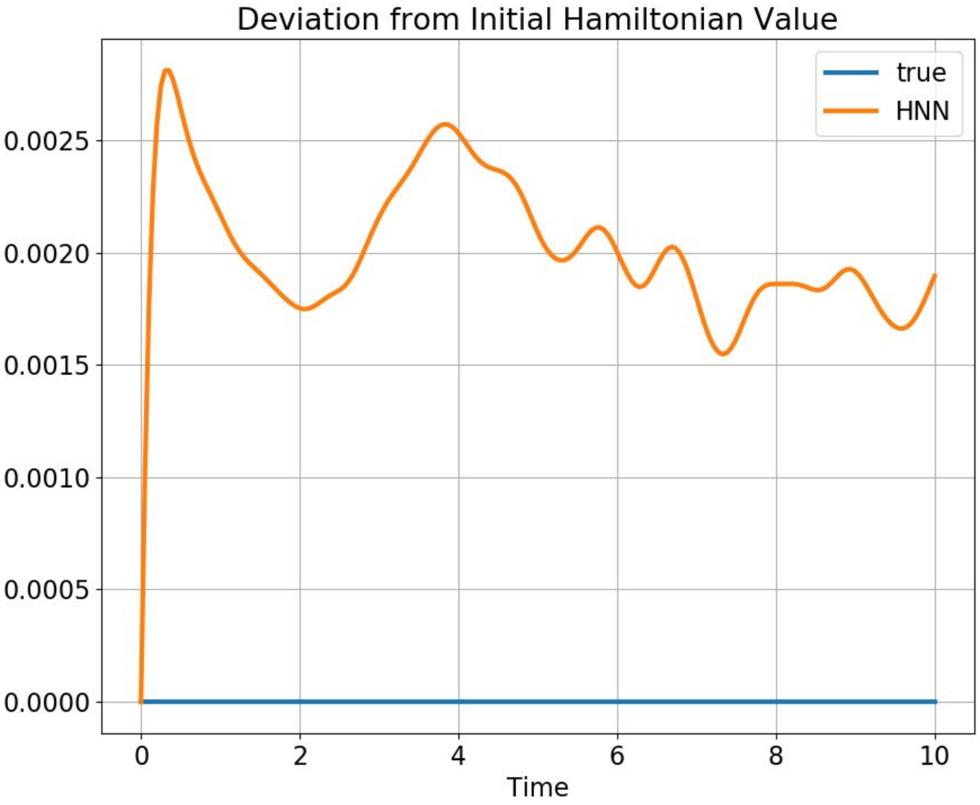
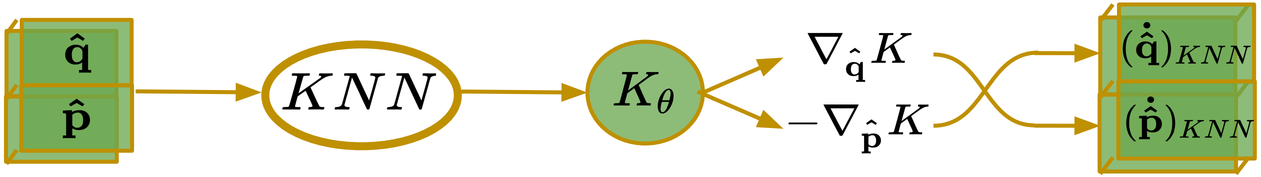
3.Results: Energy Conservation



4.Summary & Future Steps

- Hamiltonian Fluid Dynamics -> Hamilton's Equations applicable to Fluid Dynamics problems, too
- HNN variant for multidimensional problems -> KNN
- KNN -> Fourier Space -> Independent of Discretization



Thank you for your attention!