**training\_data=100, t=0->t=0.5**

A picture containing chart

Description automatically generated

Output pos: tensor([-0.2754, 1.6873, -1.7812, -0.5301, 1.9747, 0.5647, -1.8981, 1.4825,

1.1633, -1.1162], device='cuda:0')

Actual pos: tensor([-2.1900, 3.6610, -0.6610, -0.6277, 1.9556, -1.0905, -2.9526, 2.0430,

2.0230, -2.2324], device='cuda:0')

Baseline pos: tensor([-2.1965, 3.6863, -0.1967, -1.0901, 1.9350, -1.0902, -2.9674, 1.6473,

2.4179, -2.2169], device='cuda:0')

RMSE Loss after 400 simulations: 1.8935250337421894

RMSE Loss on test data: 1.8935, RMSE loss compared with baseline: 1.9018

R2\_score: 0.3998, R2\_score compared with baseline: 0.4065

**training\_data=100, t=0->t=1**

Graphical user interface

Description automatically generated with low confidence

Output pos: tensor([-0.4694, 1.8360, -1.9909, -0.8083, 2.2029, 0.7504, -2.1727, 1.7604,

1.3063, -1.4384], device='cuda:0')

Actual pos: tensor([-2.4174, 3.9788, -0.7478, -0.7317, 2.4002, -0.8706, -3.1489, 2.1728,

2.4587, -2.7947], device='cuda:0')

Baseline pos: tensor([-2.4378, 4.0912, -0.0060, -1.4693, 2.3040, -0.8683, -3.2049, 1.6674,

2.9617, -2.7387], device='cuda:0')

RMSE Loss after 400 simulations: 2.0854160392284395

RMSE Loss on test data: 2.0854, RMSE loss compared with baseline: 2.1259

R2\_score: 0.4250, R2\_score compared with baseline: 0.4340

**training\_data=100, t=0->t=1.5**

Graphical user interface, text, application

Description automatically generated

Output pos: tensor([-0.9200, 1.9571, -1.8479, -0.6275, 2.1203, 1.0415, -2.7484, 2.6129,

0.9054, -1.5100], device='cuda:0')

Actual pos: tensor([-2.6417, 4.2059, -0.6923, -0.9775, 2.9318, -0.6528, -3.3275, 2.7840,

2.4131, -3.3730], device='cuda:0')

Baseline pos: tensor([-2.6790, 4.4960, 0.1848, -1.8486, 2.6730, -0.6465, -3.4424, 1.6875,

3.5055, -3.2604], device='cuda:0')

RMSE Loss after 400 simulations: 2.363865911513567

RMSE Loss on test data: 2.3639, RMSE loss compared with baseline: 2.4515

R2\_score: 0.4093, R2\_score compared with baseline: 0.4186

**training\_data=1000, t=0->t=0.5**

A picture containing graphical user interface

Description automatically generated

Output pos: tensor([-1.9630, 2.9878, -0.5428, -0.9217, 1.8518, -1.7050, -3.3732, 1.8005,

3.0872, -2.4549], device='cuda:0')

Actual pos: tensor([-2.1900, 3.6610, -0.6610, -0.6277, 1.9556, -1.0905, -2.9526, 2.0430,

2.0230, -2.2324], device='cuda:0')

Baseline pos: tensor([-2.1965, 3.6863, -0.1967, -1.0901, 1.9350, -1.0902, -2.9674, 1.6473,

2.4179, -2.2169], device='cuda:0')

RMSE Loss after 400 simulations: 0.5682070615515112

RMSE Loss on test data: 0.5682, RMSE loss compared with baseline: 0.5560

R2\_score: 0.9386, R2\_score compared with baseline: 0.9453

**training\_data=1000, t=0->t=1**

**A picture containing text

Description automatically generated**

Output pos: tensor([-2.1047, 3.4174, -0.7876, -1.1074, 1.6961, -1.7881, -3.7871, 2.0276,

3.3256, -2.9356], device='cuda:0')

Actual pos: tensor([-2.4174, 3.9788, -0.7478, -0.7317, 2.4002, -0.8706, -3.1489, 2.1728,

2.4587, -2.7947], device='cuda:0')

Baseline pos: tensor([-2.4378, 4.0912, -0.0060, -1.4693, 2.3040, -0.8683, -3.2049, 1.6674,

2.9617, -2.7387], device='cuda:0')

RMSE Loss after 400 simulations: 0.7096436027437448

RMSE Loss on test data: 0.7096, RMSE loss compared with baseline: 0.7397

R2\_score: 0.9193, R2\_score compared with baseline: 0.9215

**training\_data=1000, t=0->t=1.5**

**Text

Description automatically generated**

Output pos: tensor([-2.6136, 4.4888, -0.7220, -1.3487, 1.7043, -2.2001, -4.3560, 1.8925,

3.6118, -2.4009], device='cuda:0')

Actual pos: tensor([-2.6417, 4.2059, -0.6923, -0.9775, 2.9318, -0.6528, -3.3275, 2.7840,

2.4131, -3.3730], device='cuda:0')

Baseline pos: tensor([-2.6790, 4.4960, 0.1848, -1.8486, 2.6730, -0.6465, -3.4424, 1.6875,

3.5055, -3.2604], device='cuda:0')

RMSE Loss after 400 simulations: 1.0620239997655154

RMSE Loss on test data: 1.0620, RMSE loss compared with baseline: 1.1304

R2\_score: 0.8566, R2\_score compared with baseline: 0.8603

**training\_data=10000, t=0->t=0.5**

**Graphical user interface

Description automatically generated**

Output pos: tensor([-2.3039, 3.6434, -0.4173, -0.8486, 2.0014, -1.2690, -3.0198, 1.9088,

2.4184, -2.0874], device='cuda:0')

Actual pos: tensor([-2.1900, 3.6610, -0.6610, -0.6277, 1.9556, -1.0905, -2.9526, 2.0430,

2.0230, -2.2324], device='cuda:0')

Baseline pos: tensor([-2.1965, 3.6863, -0.1967, -1.0901, 1.9350, -1.0902, -2.9674, 1.6473,

2.4179, -2.2169], device='cuda:0')

RMSE Loss after 400 simulations: 0.2797224322706461

RMSE Loss on test data: 0.2797, RMSE loss compared with baseline: 0.2713

R2\_score: 0.9821, R2\_score compared with baseline: 0.9842

**training\_data=10000, t=0->t=1**

**Chart, line chart

Description automatically generated**

Output pos: tensor([-2.5458, 4.1285, -0.3633, -1.0946, 2.3120, -1.4278, -3.5177, 2.0790,

2.7789, -2.2373], device='cuda:0')

Actual pos: tensor([-2.4174, 3.9788, -0.7478, -0.7317, 2.4002, -0.8706, -3.1489, 2.1728,

2.4587, -2.7947], device='cuda:0')

Baseline pos: tensor([-2.4378, 4.0912, -0.0060, -1.4693, 2.3040, -0.8683, -3.2049, 1.6674,

2.9617, -2.7387], device='cuda:0')

RMSE Loss after 400 simulations: 0.4309442748501897

RMSE Loss on test data: 0.4309, RMSE loss compared with baseline: 0.4769

R2\_score: 0.9640, R2\_score compared with baseline: 0.9574

**training\_data=10000, t=0->t=1.5**

**A picture containing shape

Description automatically generated**

Output pos: tensor([-2.7650, 4.2510, -0.2271, -1.7640, 3.3430, -1.8915, -3.7781, 2.7376,

2.8176, -2.8697], device='cuda:0')

Actual pos: tensor([-2.6417, 4.2059, -0.6923, -0.9775, 2.9318, -0.6528, -3.3275, 2.7840,

2.4131, -3.3730], device='cuda:0')

Baseline pos: tensor([-2.6790, 4.4960, 0.1848, -1.8486, 2.6730, -0.6465, -3.4424, 1.6875,

3.5055, -3.2604], device='cuda:0')

RMSE Loss after 400 simulations: 0.8198399741947651

RMSE Loss on test data: 0.8198, RMSE loss compared with baseline: 0.8909

R2\_score: 0.9085, R2\_score compared with baseline: 0.9040