AIM 20 entries

February 23, 2021

```
[1]: %matplotlib inline
  import laim.read_config as reader
  from laim.laim_db import *
  import laim.laim_db_solve as AIM_solver
  import laim.ml.nn as neural_net
  input = "config.ini"
  system_param, db_param, aim_param, learn_param = reader.get_config(input)
```

Starting run with 1 MPI rank(s) at : 2021-02-23 16:20:08.994372

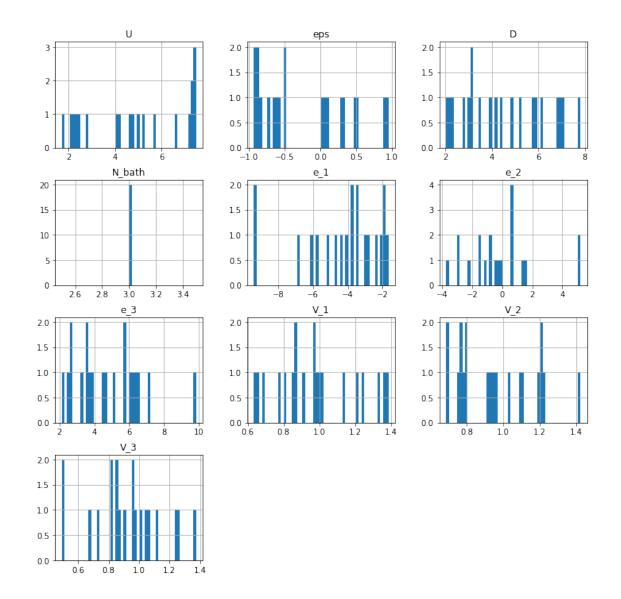
The above lines of code imports all of the necessary LAIM libraries and input files needed to create a database of 20 AIM solutions.

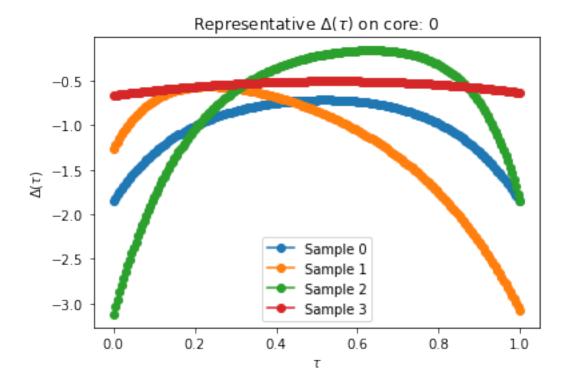
1 Generating the database

The first step is to generate the database of AIM parameters and hybridisation functions.

```
[2]: gen_db(system_param, db_param)
```

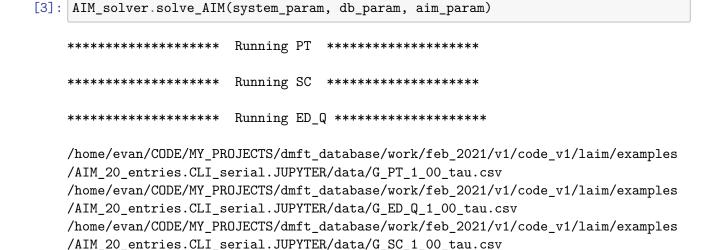
```
Checking if ./data/ exists on root node
Database already exists, we delete
Database is here: /home/evan/CODE/MY_PROJECTS/dmft_database/work/feb_2021/v1/co
de_v1/laim/examples/AIM_20_entries.CLI_serial.JUPYTER/data/
----- Database viz ------
```

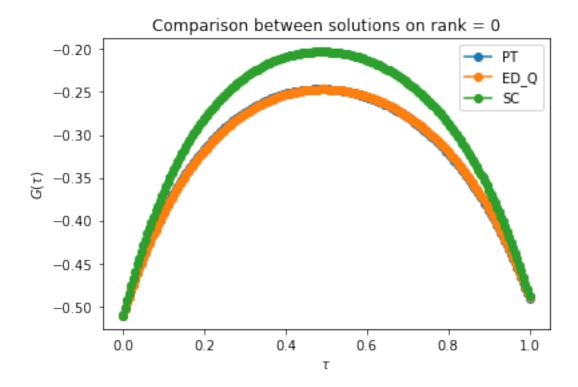




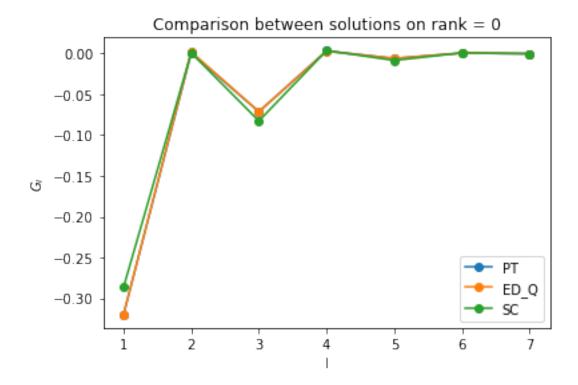
This has created a database of AIM solutions with 20 entries. The first image illustrates the distribution of selected AIM parameters. In production, 20 entries is not nearly enough to obtain meaningful statistics, but in this case I am illustrating the workflow. The second image is a representative sample of the hybridisation functions generated.

2 Populating the database with solutions





 $\label{lem:code_v1/laim/examples} $$ / \text{home/evan/CODE/MY_PROJECTS/dmft_database/work/feb_2021/v1/code_v1/laim/examples} $$ / \text{AIM_20_entries.CLI_serial.JUPYTER/data/G_PT_1_00_legendre.csv} $$ / \text{home/evan/CODE/MY_PROJECTS/dmft_database/work/feb_2021/v1/code_v1/laim/examples} $$ / \text{AIM_20_entries.CLI_serial.JUPYTER/data/G_ED_Q_1_00_legendre.csv} $$ / \text{home/evan/CODE/MY_PROJECTS/dmft_database/work/feb_2021/v1/code_v1/laim/examples} $$ / \text{AIM_20_entries.CLI_serial.JUPYTER/data/G_SC_1_00_legendre.csv} $$$



The previous action solves the AIM for each entry in the database using 3 separate solvers: (i) perturbation theory (ii) strong coupling expansion and (iii) exact diagonalisation. (iii) is the true answer and (i) and (ii) are approximations. The idea of the neural network is to learn the error between the approximations and the true answer.

I show example solutions for 1 entry in the database above in both the τ and legendre polynomial bases.

3 Training a neural network

```
[4]: net = neural_net.NN(system_param, learn_param)
net.train()
```

Training the neural network

```
- val_max_error: 0.5757 - val_boundary_cond: 6.9934e-04
Epoch 3/100
- max_error: 0.6211 - boundary_cond: 4.8204e-04 - val_loss: 0.0961 - val_mae:
0.2751 - val_max_error: 0.5741 - val_boundary_cond: 4.0531e-04
Epoch 4/100
- max_error: 0.6192 - boundary_cond: 7.5555e-04 - val_loss: 0.0933 - val_mae:
0.2707 - val_max_error: 0.5717 - val_boundary_cond: 0.0012
Epoch 5/100
- max_error: 0.6019 - boundary_cond: 0.0015 - val_loss: 0.0894 - val_mae: 0.2646
- val_max_error: 0.5675 - val_boundary_cond: 0.0017
Epoch 6/100
- max_error: 0.5910 - boundary_cond: 0.0019 - val_loss: 0.0840 - val_mae: 0.2557
- val_max_error: 0.5606 - val_boundary_cond: 0.0021
Epoch 7/100
- max_error: 0.5946 - boundary_cond: 0.0024 - val_loss: 0.0770 - val_mae: 0.2438
- val_max_error: 0.5503 - val_boundary_cond: 0.0024
Epoch 8/100
- max_error: 0.5714 - boundary_cond: 0.0026 - val_loss: 0.0682 - val_mae: 0.2282
- val_max_error: 0.5352 - val_boundary_cond: 0.0025
Epoch 9/100
- max_error: 0.5811 - boundary_cond: 0.0027 - val_loss: 0.0580 - val_mae: 0.2092
- val_max_error: 0.5143 - val_boundary_cond: 0.0024
Epoch 10/100
- max_error: 0.5453 - boundary_cond: 0.0025 - val_loss: 0.0471 - val_mae: 0.1870
- val_max_error: 0.4874 - val_boundary_cond: 0.0019
Epoch 11/100
- max_error: 0.4484 - boundary_cond: 0.0015 - val_loss: 0.0366 - val_mae: 0.1631
- val_max_error: 0.4554 - val_boundary_cond: 0.0013
Epoch 12/100
- max_error: 0.4278 - boundary_cond: 0.0010 - val_loss: 0.0274 - val_mae: 0.1385
- val_max_error: 0.4195 - val_boundary_cond: 8.8441e-04
Epoch 13/100
- max_error: 0.4391 - boundary_cond: 8.3917e-04 - val_loss: 0.0199 - val_mae:
0.1160 - val_max_error: 0.3806 - val_boundary_cond: 5.8568e-04
Epoch 14/100
- max_error: 0.3809 - boundary_cond: 5.6517e-04 - val_loss: 0.0146 - val_mae:
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0.0977 - val_max_error: 0.3404 - val_boundary_cond: 5.1761e-04
Epoch 15/100
- max_error: 0.3537 - boundary_cond: 6.2019e-04 - val_loss: 0.0109 - val_mae:
0.0832 - val max error: 0.3009 - val boundary cond: 6.6161e-04
Epoch 16/100
- max_error: 0.3048 - boundary_cond: 7.5287e-04 - val_loss: 0.0087 - val_mae:
0.0726 - val_max_error: 0.2638 - val_boundary_cond: 8.6808e-04
Epoch 17/100
- max_error: 0.2868 - boundary_cond: 9.6273e-04 - val_loss: 0.0073 - val_mae:
0.0654 - val_max_error: 0.2305 - val_boundary_cond: 0.0010
Epoch 18/100
- max_error: 0.2476 - boundary_cond: 0.0011 - val_loss: 0.0064 - val_mae: 0.0605
- val_max_error: 0.2240 - val_boundary_cond: 0.0011
Epoch 19/100
- max_error: 0.2422 - boundary_cond: 0.0012 - val_loss: 0.0059 - val_mae: 0.0570
- val_max_error: 0.2234 - val_boundary_cond: 0.0012
Epoch 20/100
- max_error: 0.2401 - boundary_cond: 0.0012 - val_loss: 0.0056 - val_mae: 0.0547
- val_max_error: 0.2233 - val_boundary_cond: 0.0011
Epoch 21/100
- max_error: 0.2041 - boundary_cond: 0.0011 - val_loss: 0.0053 - val_mae: 0.0532
- val_max_error: 0.2236 - val_boundary_cond: 8.7118e-04
Epoch 22/100
- max_error: 0.2207 - boundary_cond: 8.1447e-04 - val_loss: 0.0052 - val_mae:
0.0526 - val max_error: 0.2243 - val_boundary_cond: 7.5746e-04
Epoch 23/100
- max_error: 0.2220 - boundary_cond: 7.3251e-04 - val_loss: 0.0051 - val_mae:
0.0523 - val_max_error: 0.2247 - val_boundary_cond: 6.3646e-04
Epoch 24/100
- max_error: 0.2220 - boundary_cond: 5.7831e-04 - val_loss: 0.0050 - val_mae:
0.0522 - val_max_error: 0.2247 - val_boundary_cond: 5.4264e-04
Epoch 25/100
- max_error: 0.2156 - boundary_cond: 5.2762e-04 - val_loss: 0.0050 - val_mae:
0.0521 - val_max_error: 0.2244 - val_boundary_cond: 4.5073e-04
Epoch 26/100
- max_error: 0.1855 - boundary_cond: 5.5104e-04 - val_loss: 0.0050 - val_mae:
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0.0519 - val_max_error: 0.2240 - val_boundary_cond: 3.7646e-04
Epoch 27/100
- max_error: 0.1929 - boundary_cond: 5.6696e-04 - val_loss: 0.0049 - val_mae:
0.0517 - val max error: 0.2236 - val boundary cond: 4.0126e-04
Epoch 28/100
- max_error: 0.2146 - boundary_cond: 5.0531e-04 - val_loss: 0.0049 - val_mae:
0.0515 - val_max_error: 0.2234 - val_boundary_cond: 4.1461e-04
Epoch 29/100
- max_error: 0.1830 - boundary_cond: 5.5005e-04 - val_loss: 0.0049 - val_mae:
0.0512 - val_max_error: 0.2232 - val_boundary_cond: 4.4775e-04
Epoch 30/100
- max_error: 0.2215 - boundary_cond: 5.9430e-04 - val_loss: 0.0049 - val_mae:
0.0509 - val_max_error: 0.2230 - val_boundary_cond: 4.5991e-04
Epoch 31/100
- max_error: 0.2198 - boundary_cond: 5.8734e-04 - val_loss: 0.0049 - val_mae:
0.0506 - val_max_error: 0.2227 - val_boundary_cond: 4.7851e-04
Epoch 32/100
- max_error: 0.1882 - boundary_cond: 5.7639e-04 - val_loss: 0.0048 - val_mae:
0.0504 - val_max_error: 0.2224 - val_boundary_cond: 4.8500e-04
Epoch 33/100
- max_error: 0.2226 - boundary_cond: 5.8517e-04 - val_loss: 0.0048 - val_mae:
0.0502 - val_max_error: 0.2222 - val_boundary_cond: 4.6140e-04
Epoch 34/100
- max_error: 0.2224 - boundary_cond: 5.6221e-04 - val_loss: 0.0048 - val_mae:
0.0500 - val_max_error: 0.2222 - val_boundary_cond: 4.7058e-04
Epoch 35/100
- max_error: 0.1967 - boundary_cond: 5.9678e-04 - val_loss: 0.0048 - val_mae:
0.0500 - val max error: 0.2226 - val boundary cond: 4.5216e-04
Epoch 36/100
- max_error: 0.1948 - boundary_cond: 5.6674e-04 - val_loss: 0.0048 - val_mae:
0.0499 - val_max_error: 0.2226 - val_boundary_cond: 4.3297e-04
Epoch 37/100
- max_error: 0.2243 - boundary_cond: 5.5194e-04 - val_loss: 0.0048 - val_mae:
0.0500 - val_max_error: 0.2229 - val_boundary_cond: 4.0501e-04
Epoch 38/100
- max_error: 0.1851 - boundary_cond: 4.9593e-04 - val_loss: 0.0048 - val_mae:
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0.0499 - val_max_error: 0.2229 - val_boundary_cond: 4.0281e-04
Epoch 39/100
- max_error: 0.1735 - boundary_cond: 5.5172e-04 - val_loss: 0.0048 - val_mae:
0.0500 - val_max_error: 0.2228 - val_boundary_cond: 3.9184e-04
Epoch 40/100
- max_error: 0.2211 - boundary_cond: 5.1965e-04 - val_loss: 0.0047 - val_mae:
0.0498 - val_max_error: 0.2226 - val_boundary_cond: 4.3344e-04
Epoch 41/100
- max_error: 0.1946 - boundary_cond: 5.9077e-04 - val_loss: 0.0047 - val_mae:
0.0497 - val_max_error: 0.2226 - val_boundary_cond: 4.2808e-04
Epoch 42/100
- max_error: 0.2056 - boundary_cond: 5.3567e-04 - val_loss: 0.0047 - val_mae:
0.0497 - val_max_error: 0.2226 - val_boundary_cond: 4.0561e-04
Epoch 43/100
- max_error: 0.1879 - boundary_cond: 4.8485e-04 - val_loss: 0.0047 - val_mae:
0.0495 - val_max_error: 0.2225 - val_boundary_cond: 4.3237e-04
Epoch 44/100
- max_error: 0.2206 - boundary_cond: 5.2603e-04 - val_loss: 0.0047 - val_mae:
0.0493 - val_max_error: 0.2224 - val_boundary_cond: 4.5413e-04
Epoch 45/100
- max_error: 0.2117 - boundary_cond: 5.3236e-04 - val_loss: 0.0047 - val_mae:
0.0493 - val_max_error: 0.2226 - val_boundary_cond: 4.3184e-04
Epoch 46/100
- max_error: 0.2141 - boundary_cond: 5.5918e-04 - val_loss: 0.0047 - val_mae:
0.0492 - val_max_error: 0.2229 - val_boundary_cond: 4.5276e-04
Epoch 47/100
- max_error: 0.2198 - boundary_cond: 5.7018e-04 - val_loss: 0.0047 - val_mae:
0.0491 - val max error: 0.2232 - val boundary cond: 4.6790e-04
Epoch 48/100
- max_error: 0.2045 - boundary_cond: 4.9274e-04 - val_loss: 0.0046 - val_mae:
0.0490 - val_max_error: 0.2232 - val_boundary_cond: 4.6676e-04
Epoch 49/100
- max_error: 0.2206 - boundary_cond: 6.2439e-04 - val_loss: 0.0046 - val_mae:
0.0488 - val_max_error: 0.2231 - val_boundary_cond: 4.8244e-04
Epoch 50/100
- max_error: 0.2010 - boundary_cond: 6.1649e-04 - val_loss: 0.0046 - val_mae:
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0.0487 - val_max_error: 0.2228 - val_boundary_cond: 4.8006e-04
Epoch 51/100
- max_error: 0.2139 - boundary_cond: 5.9623e-04 - val_loss: 0.0046 - val_mae:
0.0485 - val max error: 0.2224 - val boundary cond: 4.8697e-04
Epoch 52/100
- max_error: 0.1783 - boundary_cond: 5.8244e-04 - val_loss: 0.0046 - val_mae:
0.0482 - val_max_error: 0.2220 - val_boundary_cond: 5.2595e-04
Epoch 53/100
- max_error: 0.1864 - boundary_cond: 5.6078e-04 - val_loss: 0.0046 - val_mae:
0.0480 - val_max_error: 0.2218 - val_boundary_cond: 5.5540e-04
Epoch 54/100
- max_error: 0.2187 - boundary_cond: 6.3872e-04 - val_loss: 0.0045 - val_mae:
0.0479 - val_max_error: 0.2218 - val_boundary_cond: 5.4979e-04
Epoch 55/100
- max_error: 0.2095 - boundary_cond: 7.0056e-04 - val_loss: 0.0045 - val_mae:
0.0480 - val_max_error: 0.2219 - val_boundary_cond: 6.1154e-04
Epoch 56/100
- max_error: 0.1926 - boundary_cond: 6.9265e-04 - val_loss: 0.0045 - val_mae:
0.0480 - val_max_error: 0.2217 - val_boundary_cond: 6.6793e-04
Epoch 57/100
- max_error: 0.2004 - boundary_cond: 7.6336e-04 - val_loss: 0.0045 - val_mae:
0.0478 - val_max_error: 0.2214 - val_boundary_cond: 6.9618e-04
Epoch 58/100
- max_error: 0.1713 - boundary_cond: 6.4431e-04 - val_loss: 0.0045 - val_mae:
0.0474 - val_max_error: 0.2212 - val_boundary_cond: 7.0477e-04
Epoch 59/100
- max_error: 0.2212 - boundary_cond: 8.4153e-04 - val_loss: 0.0045 - val_mae:
0.0472 - val max error: 0.2213 - val boundary cond: 7.2885e-04
Epoch 60/100
- max_error: 0.1920 - boundary_cond: 8.0612e-04 - val_loss: 0.0045 - val_mae:
0.0471 - val_max_error: 0.2214 - val_boundary_cond: 7.9095e-04
Epoch 61/100
- max_error: 0.2025 - boundary_cond: 8.0426e-04 - val_loss: 0.0044 - val_mae:
0.0470 - val_max_error: 0.2213 - val_boundary_cond: 8.3423e-04
Epoch 62/100
- max_error: 0.2037 - boundary_cond: 8.8239e-04 - val_loss: 0.0044 - val_mae:
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0.0470 - val_max_error: 0.2214 - val_boundary_cond: 9.0778e-04
Epoch 63/100
- max_error: 0.2180 - boundary_cond: 9.6473e-04 - val_loss: 0.0044 - val_mae:
0.0470 - val max error: 0.2211 - val boundary cond: 9.8979e-04
Epoch 64/100
- max_error: 0.1990 - boundary_cond: 8.8330e-04 - val_loss: 0.0044 - val_mae:
0.0469 - val_max_error: 0.2208 - val_boundary_cond: 0.0010
Epoch 65/100
- max_error: 0.2168 - boundary_cond: 0.0010 - val_loss: 0.0044 - val_mae: 0.0467
- val_max_error: 0.2206 - val_boundary_cond: 0.0011
Epoch 66/100
- max_error: 0.2174 - boundary_cond: 0.0011 - val_loss: 0.0044 - val_mae: 0.0465
- val_max_error: 0.2203 - val_boundary_cond: 0.0011
Epoch 67/100
- max_error: 0.2049 - boundary_cond: 0.0010 - val_loss: 0.0043 - val_mae: 0.0463
- val_max_error: 0.2201 - val_boundary_cond: 0.0012
Epoch 68/100
- max_error: 0.1984 - boundary_cond: 0.0010 - val_loss: 0.0043 - val_mae: 0.0461
- val_max_error: 0.2199 - val_boundary_cond: 0.0012
Epoch 69/100
- max_error: 0.2013 - boundary_cond: 0.0010 - val_loss: 0.0043 - val_mae: 0.0461
- val_max_error: 0.2200 - val_boundary_cond: 0.0013
Epoch 70/100
- max_error: 0.2205 - boundary_cond: 0.0012 - val_loss: 0.0043 - val_mae: 0.0460
- val_max_error: 0.2200 - val_boundary_cond: 0.0014
Epoch 71/100
- max_error: 0.2164 - boundary_cond: 0.0013 - val_loss: 0.0043 - val_mae: 0.0458
- val_max_error: 0.2197 - val_boundary_cond: 0.0014
Epoch 72/100
- max_error: 0.2167 - boundary_cond: 0.0013 - val_loss: 0.0043 - val_mae: 0.0456
- val_max_error: 0.2192 - val_boundary_cond: 0.0015
Epoch 73/100
- max_error: 0.2101 - boundary_cond: 0.0014 - val_loss: 0.0042 - val_mae: 0.0452
- val_max_error: 0.2188 - val_boundary_cond: 0.0015
Epoch 74/100
- max_error: 0.2070 - boundary_cond: 0.0014 - val_loss: 0.0042 - val_mae: 0.0451
```

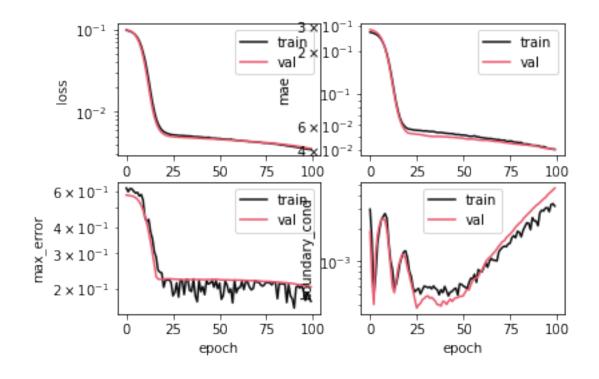
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- val_max_error: 0.2184 - val_boundary_cond: 0.0016
Epoch 75/100
- max_error: 0.2099 - boundary_cond: 0.0014 - val_loss: 0.0042 - val_mae: 0.0449
- val_max_error: 0.2182 - val_boundary_cond: 0.0017
Epoch 76/100
- max_error: 0.2168 - boundary_cond: 0.0015 - val_loss: 0.0042 - val_mae: 0.0447
- val_max_error: 0.2182 - val_boundary_cond: 0.0018
Epoch 77/100
- max_error: 0.2148 - boundary_cond: 0.0016 - val_loss: 0.0042 - val_mae: 0.0445
- val_max_error: 0.2180 - val_boundary_cond: 0.0018
Epoch 78/100
- max_error: 0.2147 - boundary_cond: 0.0017 - val_loss: 0.0042 - val_mae: 0.0444
- val_max_error: 0.2178 - val_boundary_cond: 0.0019
Epoch 79/100
- max_error: 0.2098 - boundary_cond: 0.0016 - val_loss: 0.0041 - val_mae: 0.0443
- val_max_error: 0.2174 - val_boundary_cond: 0.0020
Epoch 80/100
- max_error: 0.2169 - boundary_cond: 0.0019 - val_loss: 0.0041 - val_mae: 0.0441
- val_max_error: 0.2169 - val_boundary_cond: 0.0021
Epoch 81/100
- max_error: 0.2147 - boundary_cond: 0.0018 - val_loss: 0.0041 - val_mae: 0.0440
- val_max_error: 0.2167 - val_boundary_cond: 0.0022
Epoch 82/100
- max_error: 0.1795 - boundary_cond: 0.0017 - val_loss: 0.0041 - val_mae: 0.0437
- val_max_error: 0.2164 - val_boundary_cond: 0.0023
Epoch 83/100
- max_error: 0.2136 - boundary_cond: 0.0019 - val_loss: 0.0040 - val_mae: 0.0438
- val_max_error: 0.2162 - val_boundary_cond: 0.0024
Epoch 84/100
- max_error: 0.2125 - boundary_cond: 0.0021 - val_loss: 0.0040 - val_mae: 0.0437
- val_max_error: 0.2159 - val_boundary_cond: 0.0025
Epoch 85/100
- max_error: 0.2123 - boundary_cond: 0.0022 - val_loss: 0.0040 - val_mae: 0.0435
- val_max_error: 0.2154 - val_boundary_cond: 0.0026
- max_error: 0.2126 - boundary_cond: 0.0022 - val_loss: 0.0040 - val_mae: 0.0433
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- val_max_error: 0.2150 - val_boundary_cond: 0.0027
Epoch 87/100
- max_error: 0.1721 - boundary_cond: 0.0019 - val_loss: 0.0040 - val_mae: 0.0431
- val_max_error: 0.2145 - val_boundary_cond: 0.0028
Epoch 88/100
- max_error: 0.2108 - boundary_cond: 0.0025 - val_loss: 0.0039 - val_mae: 0.0431
- val_max_error: 0.2142 - val_boundary_cond: 0.0030
Epoch 89/100
- max_error: 0.1851 - boundary_cond: 0.0023 - val_loss: 0.0039 - val_mae: 0.0430
- val_max_error: 0.2136 - val_boundary_cond: 0.0031
Epoch 90/100
- max_error: 0.1793 - boundary_cond: 0.0023 - val_loss: 0.0039 - val_mae: 0.0429
- val_max_error: 0.2131 - val_boundary_cond: 0.0032
Epoch 91/100
- max_error: 0.1616 - boundary_cond: 0.0021 - val_loss: 0.0038 - val_mae: 0.0425
- val_max_error: 0.2124 - val_boundary_cond: 0.0033
Epoch 92/100
- max_error: 0.2042 - boundary_cond: 0.0028 - val_loss: 0.0038 - val_mae: 0.0421
- val_max_error: 0.2115 - val_boundary_cond: 0.0034
Epoch 93/100
- max_error: 0.2075 - boundary_cond: 0.0029 - val_loss: 0.0038 - val_mae: 0.0419
- val_max_error: 0.2107 - val_boundary_cond: 0.0036
Epoch 94/100
- max_error: 0.2024 - boundary_cond: 0.0029 - val_loss: 0.0038 - val_mae: 0.0416
- val_max_error: 0.2099 - val_boundary_cond: 0.0037
Epoch 95/100
- max_error: 0.2104 - boundary_cond: 0.0030 - val_loss: 0.0037 - val_mae: 0.0413
- val_max_error: 0.2093 - val_boundary_cond: 0.0038
Epoch 96/100
- max_error: 0.1952 - boundary_cond: 0.0031 - val_loss: 0.0037 - val_mae: 0.0413
- val_max_error: 0.2088 - val_boundary_cond: 0.0040
Epoch 97/100
- max_error: 0.1760 - boundary_cond: 0.0028 - val_loss: 0.0037 - val_mae: 0.0412
- val_max_error: 0.2081 - val_boundary_cond: 0.0041
Epoch 98/100
- max_error: 0.1930 - boundary_cond: 0.0033 - val_loss: 0.0036 - val_mae: 0.0409
```

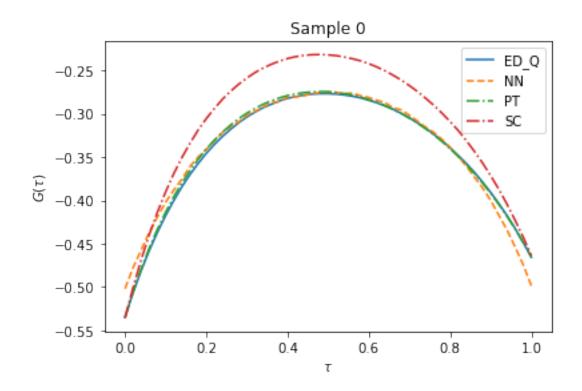
******** Performance of Neural Network

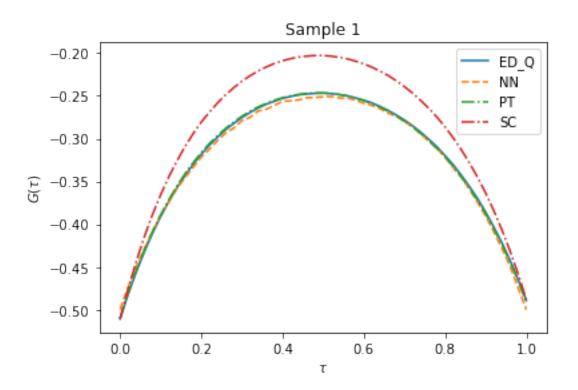
Test MSE: 0.0035388690885156393 Test MAE: 0.040402017533779144 Test max error: 0.20513738691806793

Test boundary condition 0.004629611968994141



----- > Saving image: NN-details.png <





A neural network has been trained for 100 epochs. The first plot illustrates the performance of the network and the value of the minimized metric, which in this case is the MSDE. The final two plots are samples of the neural network solving the AIM for the validation set. Clearly the NN is better than the strong coupling expansion, but for such a small database this solver will not be better than the perturbation theory result.

[]: