

```
2024-08-28 11:42:37.913 INFO: MACE version: 0.3.6
2024-08-28 11:42:37.913 INFO: Configuration: Namespace(config=None,
name='Mace_model', seed=123, log_dir='logs', model_dir='.',
checkpoints_dir='checkpoints', results_dir='results', downloads_dir='downloads',
device='cpu', default_dtype='float32', distributed=False, log_level='INFO',
error_table='PerAtomRMSE', model='ScaleShiftMACE', r_max=4.0, radial_type='bessel',
num_radial_basis=8, num_cutoff_basis=5, pair_repulsion=False,
distance_transform='None', interaction='RealAgnosticResidualInteractionBlock',
interaction_first='RealAgnosticResidualInteractionBlock', max_ell=3, correlation=3,
num_interactions=2, MLP_irreps='16x0e', radial_MLP='[64, 64, 64]',
hidden_irreps='32x0e', num_channels=None, max_L=None, gate='silu',
scaling='rms_forces_scaling', avg_num_neighbors=1, compute_avg_num_neighbors=True,
compute_stress=False, compute_forces=True,
train_file='C:\\botnetdata\\BOTNet-datasets\\dataset_3BPA\\train_300K.xyz',
valid_file=None, valid_fraction=0.05,
test_file='C:\\botnetdata\\BOTNet-datasets\\dataset_3BPA\\test_300K.xyz',
test_dir=None, multi_processed_test=False, num_workers=0, pin_memory=True,
atomic_numbers=None, mean=None, std=None, statistics_file=None,
E0s='{1:-13.663181292231226, 6:-1029.2809654211628, 7:-1484.1187695035828,
8:-2042.0330099956639}', keep_isolated_atoms=False, energy_key='energy',
forces_key='forces', virials_key='virials', stress_key='stress',
dipole_key='dipole', charges_key='charges', loss='weighted', forces_weight=100.0,
swa_forces_weight=100.0, energy_weight=1.0, swa_energy_weight=1000.0,
virials_weight=1.0, swa_virials_weight=10.0, stress_weight=1.0,
swa_stress_weight=10.0, dipole_weight=1.0, swa_dipole_weight=1.0,
config_type_weights='{"Default":1.0}', huber_delta=0.01, optimizer='adam',
beta=0.9, batch_size=2, valid_batch_size=10, lr=0.01, swa_lr=0.001,
weight_decay=5e-07, amsgrad=True, scheduler='ReduceLRonPlateau', lr_factor=0.8,
scheduler_patience=50, lr_scheduler_gamma=0.9993, swa=True, start_swa=None,
ema=True, ema_decay=0.99, max_num_epochs=4, patience=2048, foundation_model=None,
foundation_model_readout=True, eval_interval=2, keep_checkpoints=False,
save_all_checkpoints=False, restart_latest=False, save_cpu=False, clip_grad=10.0,
wandb=False, wandb_dir=None, wandb_project='', wandb_entity='', wandb_name='',
wandb_log_hypers=['num_channels', 'max_L', 'correlation', 'lr', 'swa_lr',
'weight_decay', 'batch_size', 'max_num_epochs', 'start_swa', 'energy_weight',
'forces_weight'])
2024-08-28 11:42:37.913 INFO: Using CPU
2024-08-28 11:42:38.226 INFO: Error accessing Git repository: C:\
2024-08-28 11:42:38.508 INFO: Since ASE version 3.23.0b1, using energy_key 'energy'
is no longer safe when communicating between MACE and ASE. We recommend using a
different key, rewriting energies to 'REF_energy'. You need to use
--energy_key='REF_energy', to tell the key name chosen.
2024-08-28 11:42:38.571 INFO: Since ASE version 3.23.0b1, using forces_key 'forces'
is no longer safe when communicating between MACE and ASE. We recommend using a
different key, rewriting energies to 'REF_forces'. You need to use
--forces_key='REF_forces', to tell the key name chosen.
2024-08-28 11:42:38.634 INFO: Since ASE version 3.23.0b1, using stress_key 'stress'
is no longer safe when communicating between MACE and ASE. We recommend using a
different key, rewriting energies to 'REF_stress'. You need to use
--stress_key='REF_stress', to tell the key name chosen.
```

2024-08-28 11:42:38.649 INFO: Loaded 500 training configurations from
'C:\botnetdata\BOTNet-datasets\dataset_3BPA\train_300K.xyz'
2024-08-28 11:42:38.649 INFO: Using random 5.0% of training set for validation
2024-08-28 11:42:39.322 INFO: Since ASE version 3.23.0b1, using energy_key 'energy'
is no longer safe when communicating between MACE and ASE. We recommend using a
different key, rewriting energies to 'REF_energy'. You need to use
--energy_key='REF_energy', to tell the key name chosen.
2024-08-28 11:42:39.541 INFO: Since ASE version 3.23.0b1, using forces_key 'forces'
is no longer safe when communicating between MACE and ASE. We recommend using a
different key, rewriting energies to 'REF_forces'. You need to use
--forces_key='REF_forces', to tell the key name chosen.
2024-08-28 11:42:39.745 INFO: Since ASE version 3.23.0b1, using stress_key 'stress'
is no longer safe when communicating between MACE and ASE. We recommend using a
different key, rewriting energies to 'REF_stress'. You need to use
--stress_key='REF_stress', to tell the key name chosen.
2024-08-28 11:42:39.791 INFO: Loaded 1669 test configurations from
'C:\botnetdata\BOTNet-datasets\dataset_3BPA\test_300K.xyz'
2024-08-28 11:42:39.791 INFO: Total number of configurations: train=475, valid=25,
tests=[Default: 1669]
2024-08-28 11:42:39.791 INFO: AtomicNumberTable: (1, 6, 7, 8)
2024-08-28 11:42:39.791 INFO: Atomic Energies not in training file, using command
line argument E0s
2024-08-28 11:42:39.791 INFO: Atomic energies: [-13.663181292231226,
-1029.2809654211628, -1484.1187695035828, -2042.0330099956639]
2024-08-28 11:42:40.153 INFO: WeightedEnergyForcesLoss(energy_weight=1.000,
forces_weight=100.000)
2024-08-28 11:42:40.341 INFO: Average number of neighbors: 11.989529609680176
2024-08-28 11:42:40.341 INFO: Selected the following outputs: {'energy': True,
'forces': True, 'virials': False, 'stress': False, 'dipoles': False}
2024-08-28 11:42:40.559 INFO: Building model
2024-08-28 11:42:40.559 INFO: Hidden irreps: 32x0e
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.

```
warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
  warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
  warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
  warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
  warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
  warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
  warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
  warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
  warnings.warn(
C:\Users\2mris\AppData\Roaming\Python\Python311\site-packages\torch\jit\_check.py:1
77: UserWarning: The TorchScript type system doesn't support instance-level
annotations on empty non-base types in `__init__`. Instead, either 1) use a type
annotation in the class body, or 2) wrap the type in `torch.jit.Attribute`.
```

```

warnings.warn(
2024-08-28 11:42:42.546 INFO: Using stochastic weight averaging (after 3 epochs)
with energy weight : 1000.0, forces weight : 100.0 and learning rate : 0.001
2024-08-28 11:42:42.842 INFO: ScaleShiftMACE(
  (node_embedding): LinearNodeEmbeddingBlock(
    (linear): Linear(4x0e -> 32x0e | 128 weights)
  )
  (radial_embedding): RadialEmbeddingBlock(
    (bessel_fn): BesselBasis(r_max=4.0, num_basis=8, trainable=False)
    (cutoff_fn): PolynomialCutoff(p=5.0, r_max=4.0)
  )
  (spherical_harmonics): SphericalHarmonics()
  (atomic_energies_fn): AtomicEnergiesBlock(energies=[-13.6632, -1029.2810,
-1484.1188, -2042.0330])
  (interactions): ModuleList(
    (0-1): 2 x RealAgnosticResidualInteractionBlock(
      (linear_up): Linear(32x0e -> 32x0e | 1024 weights)
      (conv_tp): TensorProduct(32x0e x 1x0e+1x1o+1x2e+1x3o ->
32x0e+32x1o+32x2e+32x3o | 128 paths | 128 weights)
      (conv_tp_weights): FullyConnectedNet[8, 64, 64, 128]
      (linear): Linear(32x0e+32x1o+32x2e+32x3o -> 32x0e+32x1o+32x2e+32x3o | 4096
weights)
      (skip_tp): FullyConnectedTensorProduct(32x0e x 4x0e -> 32x0e | 4096 paths |
4096 weights)
      (reshape): reshape_irreps()
    )
  )
  (products): ModuleList(
    (0-1): 2 x EquivariantProductBasisBlock(
      (symmetric_contractions): SymmetricContraction(
        (contractions): ModuleList(
          (0): Contraction(
            (contractions_weighting): ModuleList(
              (0-1): 2 x GraphModule()
            )
            (contractions_features): ModuleList(
              (0-1): 2 x GraphModule()
            )
            (weights): ParameterList(
              (0): Parameter containing: [torch.float32 of size 4x4x32]
              (1): Parameter containing: [torch.float32 of size 4x1x32]
            )
            (graph_opt_main): GraphModule()
          )
        )
      )
    )
  )
  (linear): Linear(32x0e -> 32x0e | 1024 weights)
)
(readouts): ModuleList(

```

```
(0): LinearReadoutBlock(
  (linear): Linear(32x0e -> 1x0e | 32 weights)
)
(1): NonLinearReadoutBlock(
  (linear_1): Linear(32x0e -> 16x0e | 512 weights)
  (non_linearity): Activation [x] (16x0e -> 16x0e)
  (linear_2): Linear(16x0e -> 1x0e | 16 weights)
)
)
(scale_shift): ScaleShiftBlock(scale=0.946295, shift=-4.993633)
)
```

2024-08-28 11:42:42.858 INFO: Number of parameters: 62128

2024-08-28 11:42:42.858 INFO: Optimizer: Adam (

Parameter Group 0

```
amsgrad: True
betas: (0.9, 0.999)
capturable: False
differentiable: False
eps: 1e-08
foreach: None
fused: None
initial_lr: 0.01
lr: 0.01
maximize: False
name: embedding
swa_lr: 0.001
weight_decay: 0.0
```

Parameter Group 1

```
amsgrad: True
betas: (0.9, 0.999)
capturable: False
differentiable: False
eps: 1e-08
foreach: None
fused: None
initial_lr: 0.01
lr: 0.01
maximize: False
name: interactions_decay
swa_lr: 0.001
weight_decay: 5e-07
```

Parameter Group 2

```
amsgrad: True
betas: (0.9, 0.999)
capturable: False
differentiable: False
eps: 1e-08
foreach: None
```

fused: None
initial_lr: 0.01
lr: 0.01
maximize: False
name: interactions_no_decay
swa_lr: 0.001
weight_decay: 0.0

Parameter Group 3

amsgrad: True
betas: (0.9, 0.999)
capturable: False
differentiable: False
eps: 1e-08
foreach: None
fused: None
initial_lr: 0.01
lr: 0.01
maximize: False
name: products
swa_lr: 0.001
weight_decay: 5e-07

Parameter Group 4

amsgrad: True
betas: (0.9, 0.999)
capturable: False
differentiable: False
eps: 1e-08
foreach: None
fused: None
initial_lr: 0.01
lr: 0.01
maximize: False
name: readouts
swa_lr: 0.001
weight_decay: 0.0

)

2024-08-28 11:42:42.858 INFO: Using gradient clipping with tolerance=10.000
2024-08-28 11:42:42.858 INFO: Started training
2024-08-28 11:42:46.268 INFO: Epoch None: loss=11.1146, RMSE_E_per_atom=10.5 meV,
RMSE_F=976.0 meV / A
2024-08-28 11:43:57.397 INFO: Epoch 0: loss=0.4052, RMSE_E_per_atom=26.4 meV,
RMSE_F=185.1 meV / A
2024-08-28 11:46:15.184 INFO: Epoch 2: loss=0.1088, RMSE_E_per_atom=3.8 meV,
RMSE_F=94.4 meV / A
2024-08-28 11:46:15.215 INFO: Changing loss based on SWA
2024-08-28 11:47:23.745 INFO: Training complete
2024-08-28 11:47:23.745 INFO: Computing metrics for training, validation, and test
sets

