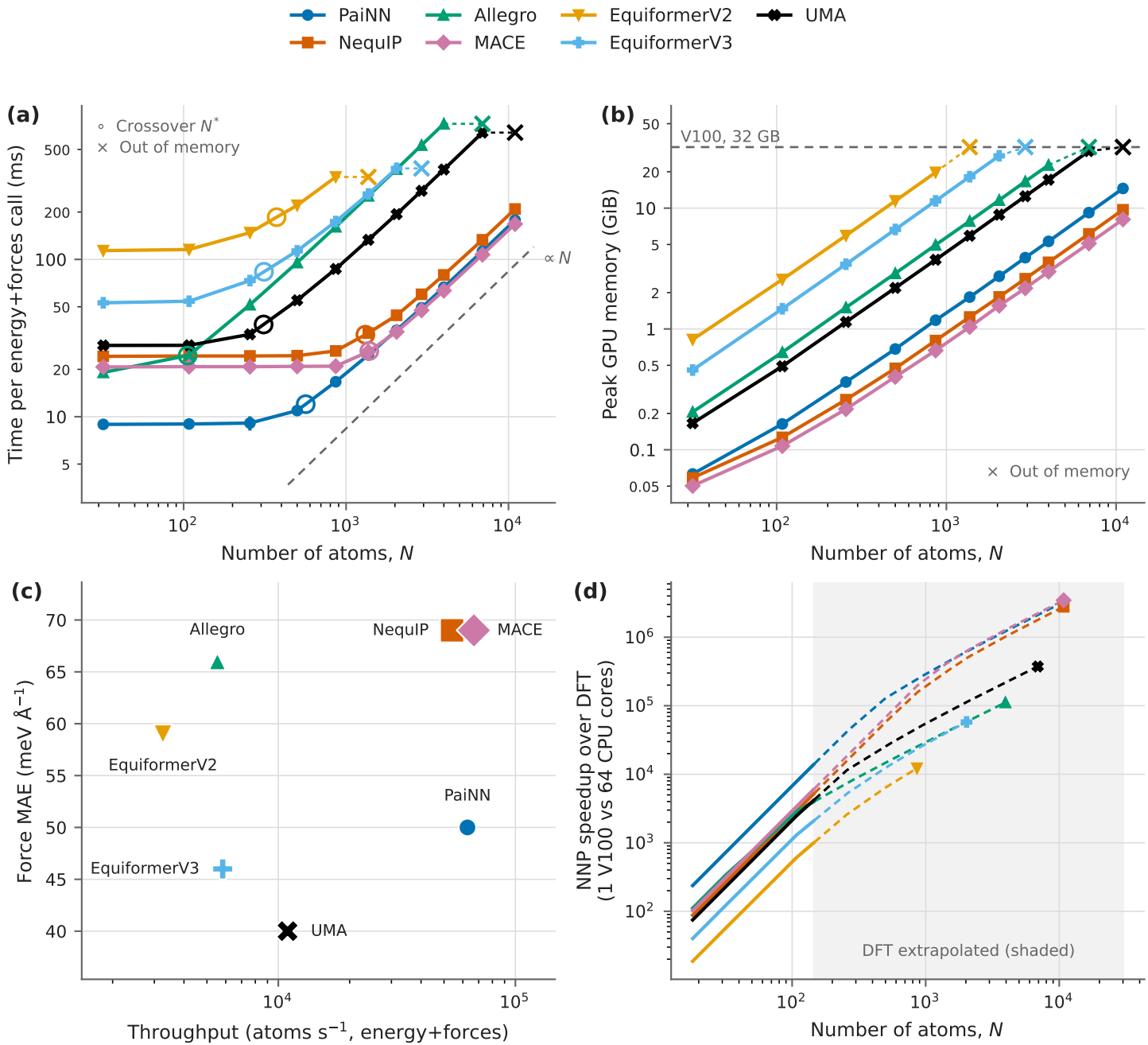

PaiNN
NequIP
Allegro
MACE
EquiformerV2
EquiformerV3
UMA
(a)
Crossover N^*
Out of memory
Time per energy+forces call (ms)
$\propto N$
Number of atoms, N
(b)
V100, 32 GB
Peak GPU memory (GiB)
Out of memory
Number of atoms, N
(c)
Allegro
NequIP
MACE
EquiformerV2
PaiNN
EquiformerV3
UMA
Force MAE (meV Å^{-1})
Throughput (atoms s^{-1}, energy+forces)
(d)
NNP speedup over DFT
(1 V100 vs 64 CPU cores)
DFT extrapolated (shaded)
Number of atoms, N