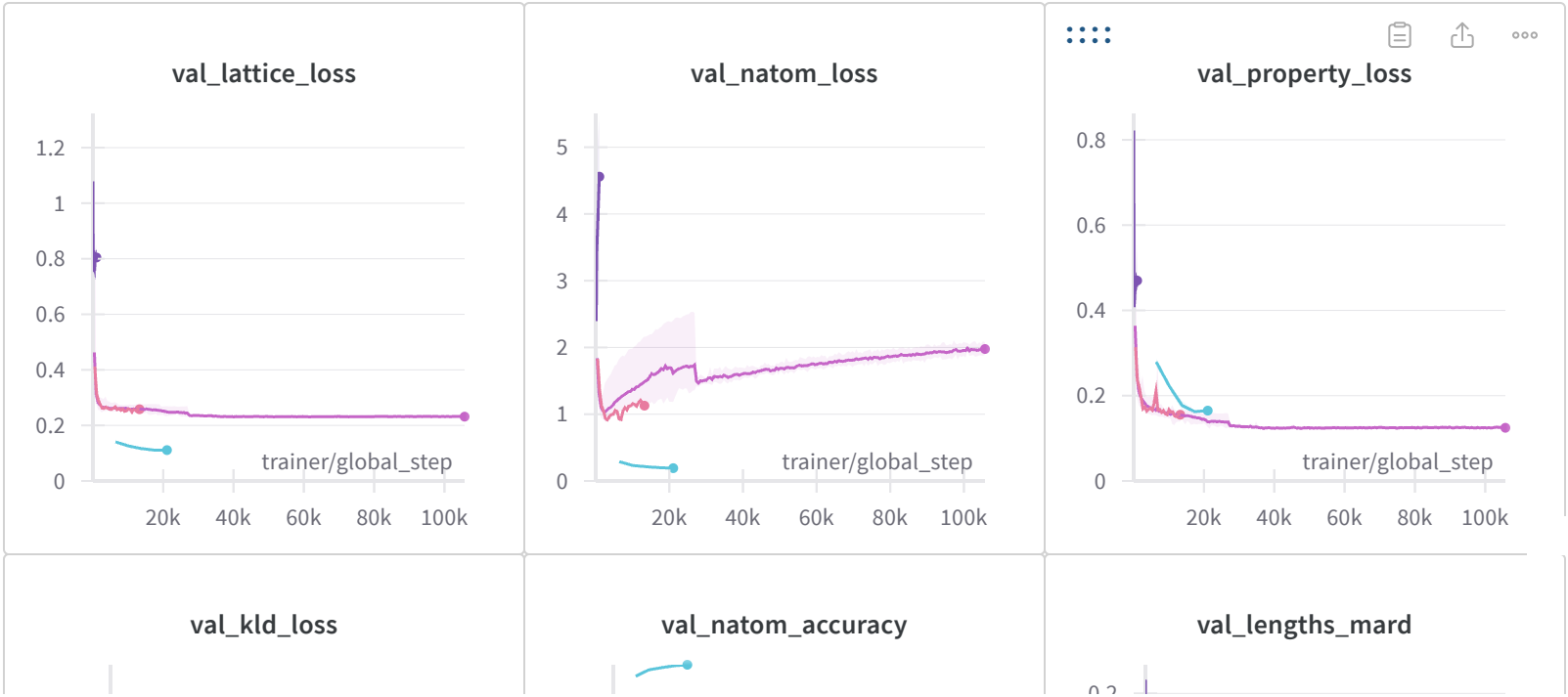
Autosaving... Edits visible only to you Publish to project

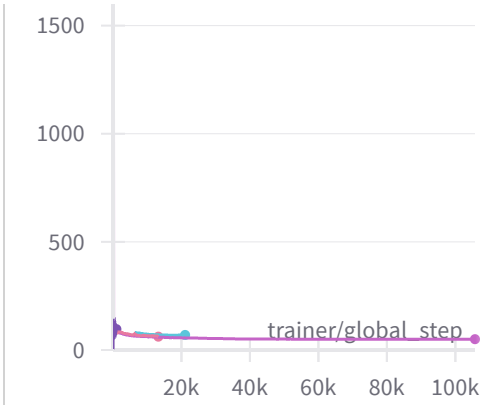
CDVAE Training Data Comparison

Comparing Training, Testing, and Validation number of atoms and types of atoms accuracy, along with measuring lattice, property, composition, and coordination Loss

Ayush Mahapatra

Section 1

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500
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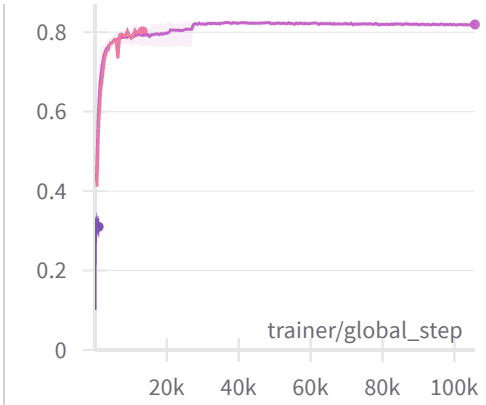
trainer/global_step
20k
40k
60k
80k
100k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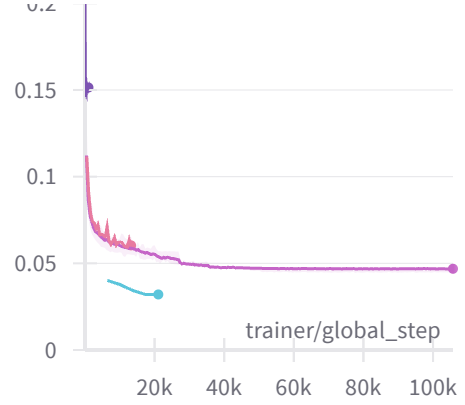
20k
40k
60k
80k
100k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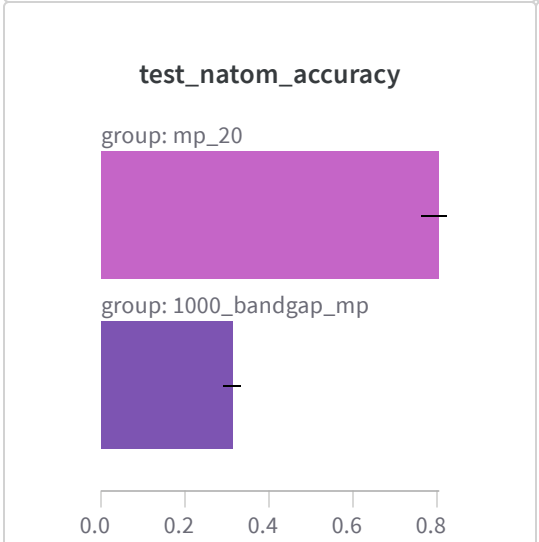
40k
60k
80k
100k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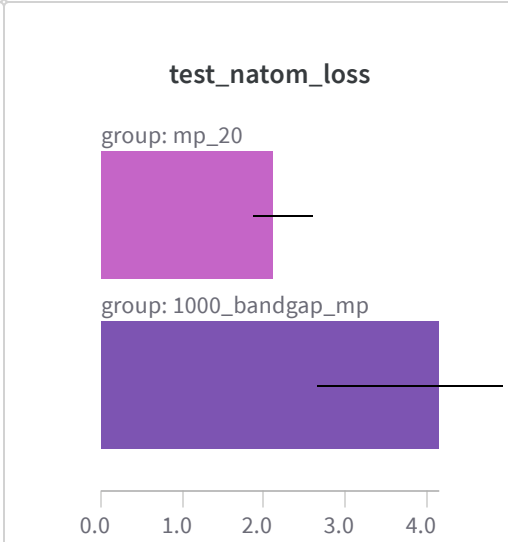
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group: 1000_bandgap_mp
0.0
1.0
2.0
3.0
4.0

test_property_loss
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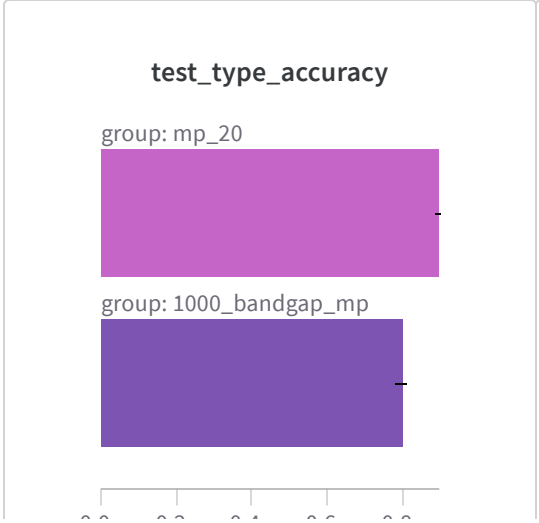
0.20
0.40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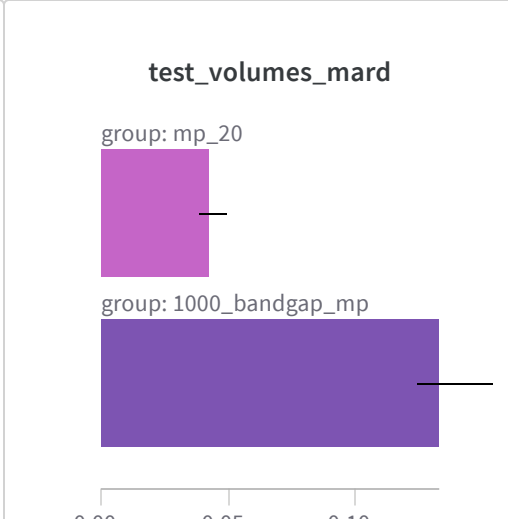
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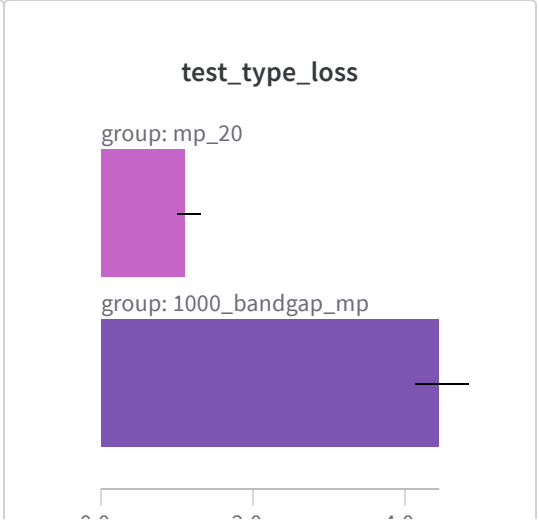
test_type_loss
group: mp_20
group: 1000_bandgap_mp

0.0
0.2
0.4
0.6
0.8
0.00
0.05
0.10
0.0
2.0
4.0
test_angles_mae
group: mp_20
group: 1000_bandgap_mp
0
5
10
test_composition_loss
group: mp_20
group: 1000_bandgap_mp
0.0
1.0
2.0
test_coord_loss
group: mp_20
group: 1000_bandgap_mp
0.0
0.5
1.0
1.5
test_kld_loss
group: mp_20
group: 1000_bandgap_mp
0
20
40
60
80
test_lattice_loss
group: mp_20
group: 1000_bandgap_mp
0.0
0.2
0.4
0.6
test_lengths_mard
group: mp_20
group: 1000_bandgap_mp
0.00
0.05
0.10
test_loss
group: mp_20
group: 1000_bandgap_mp
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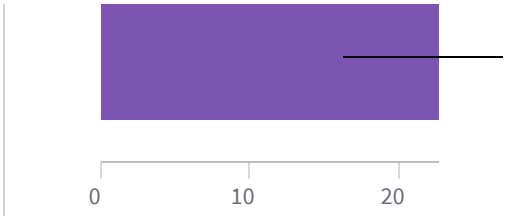
1e+11
8e+10
6e+10
train_composition_loss_step
4e+19
3e+19
2e+19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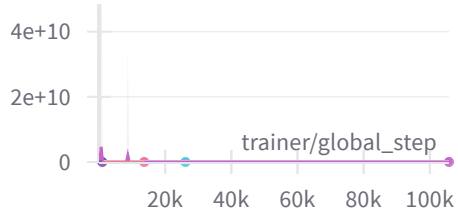
10
20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2e+10
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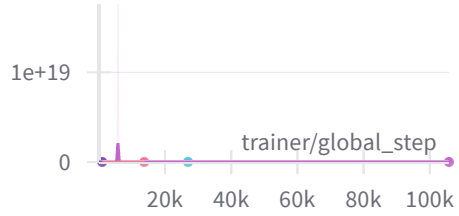
trainer/global_step
20k
40k
60k
80k
100k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40k
60k
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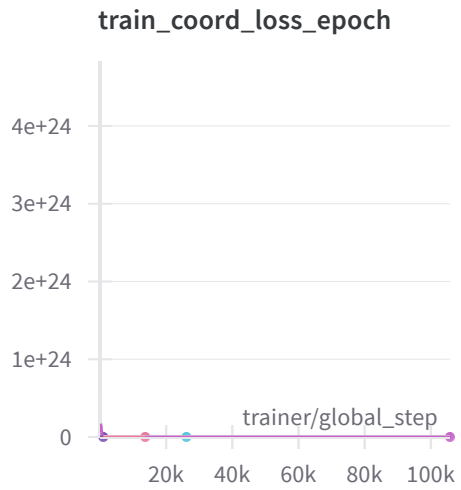
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3e+24
2e+24
1e+24
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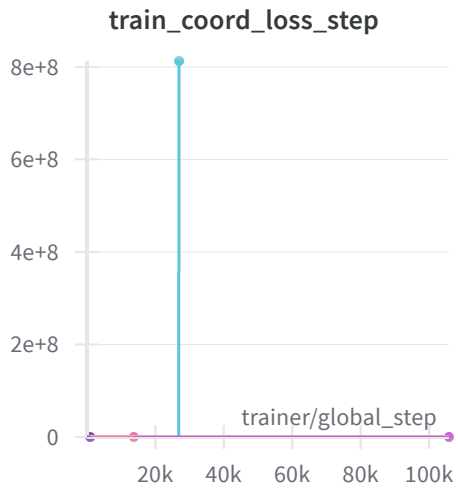
trainer/global_step
20k
40k
60k
80k
100k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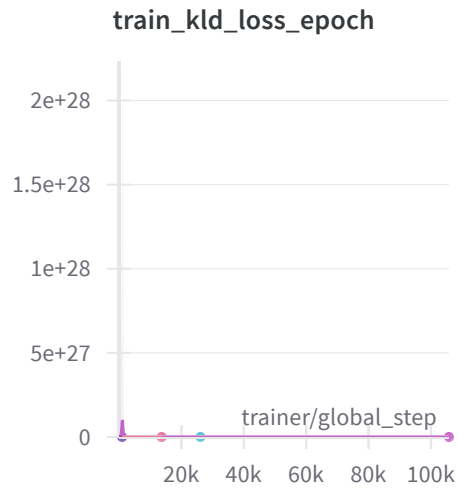
trainer/global_step
20k
40k
60k
80k
100k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1e+28
5e+27
0
trainer/global_step
20k
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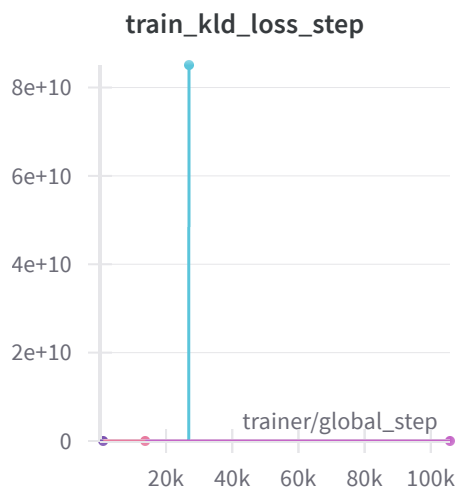
60k
80k
100k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trainer/global_step
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60k
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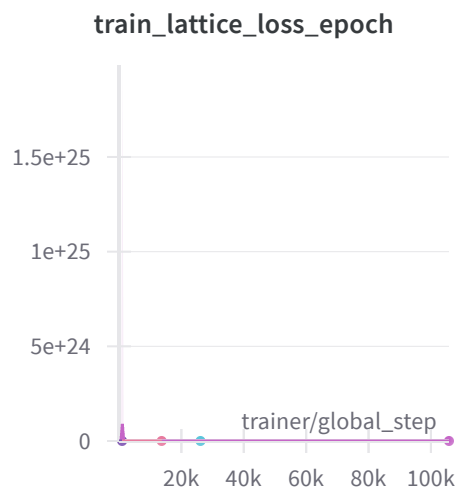
100k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5e+24
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trainer/global_step
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40k
60k
80k
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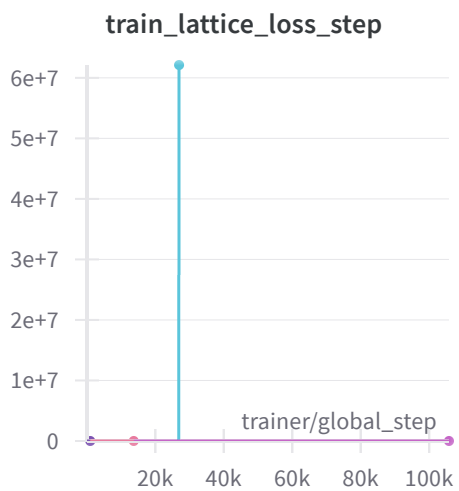
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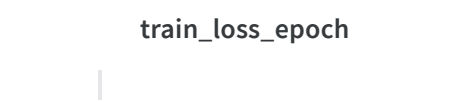
0
trainer/global_step
20k
40k
60k
80k
100k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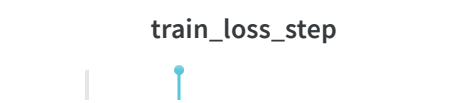
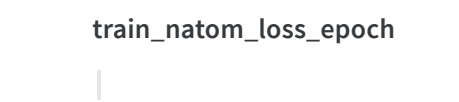

train_loss_step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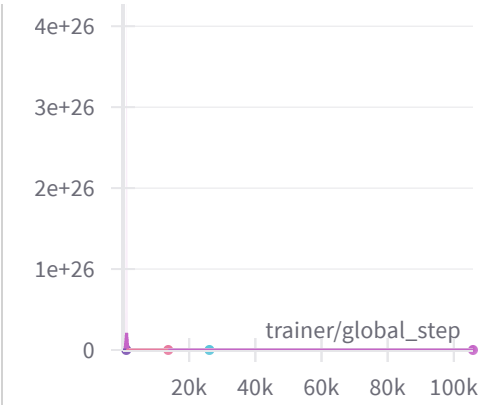

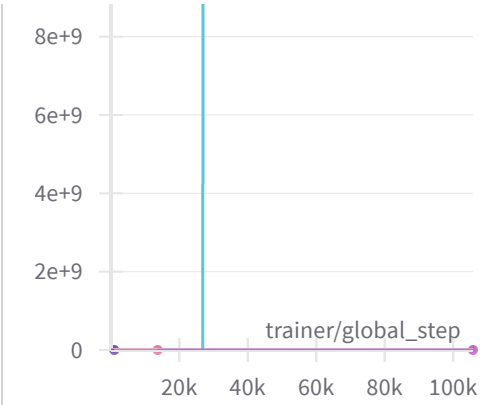

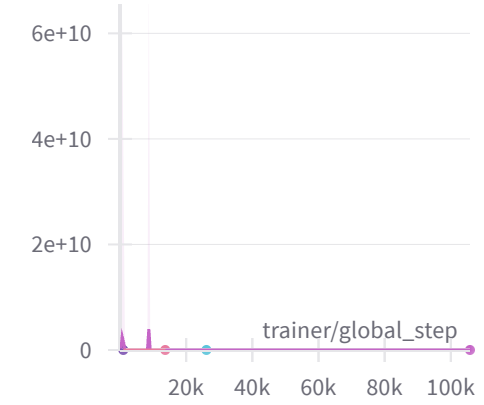

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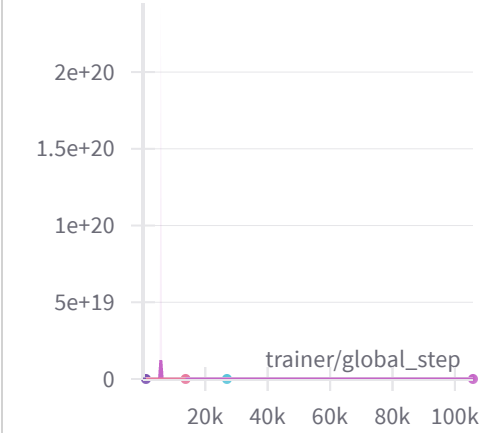

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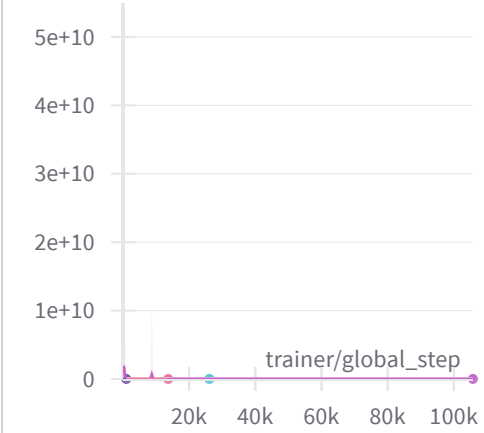

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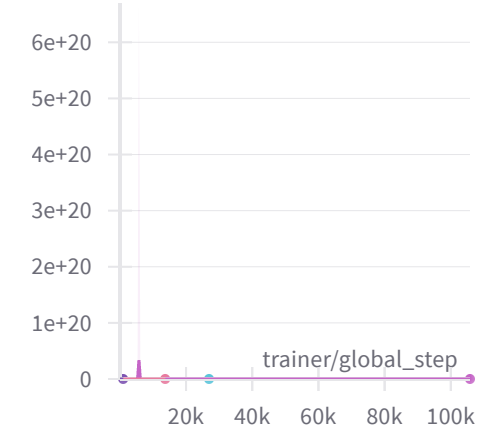

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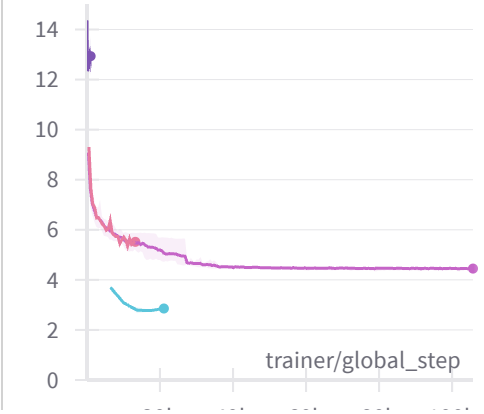

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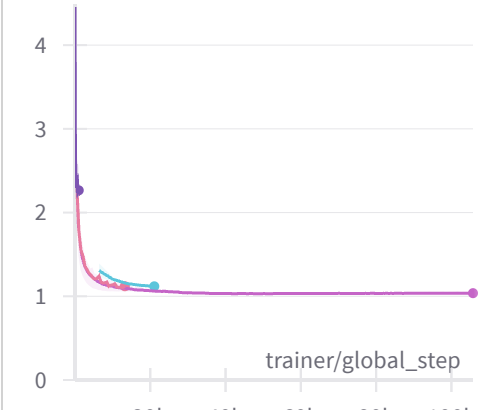

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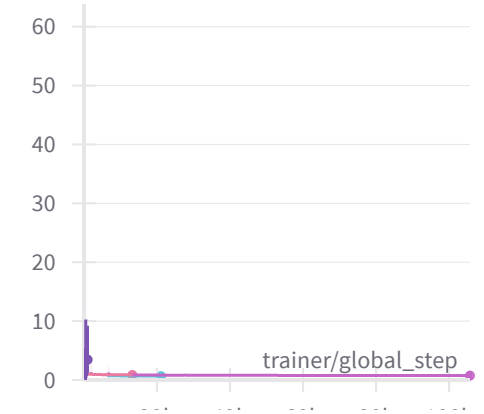

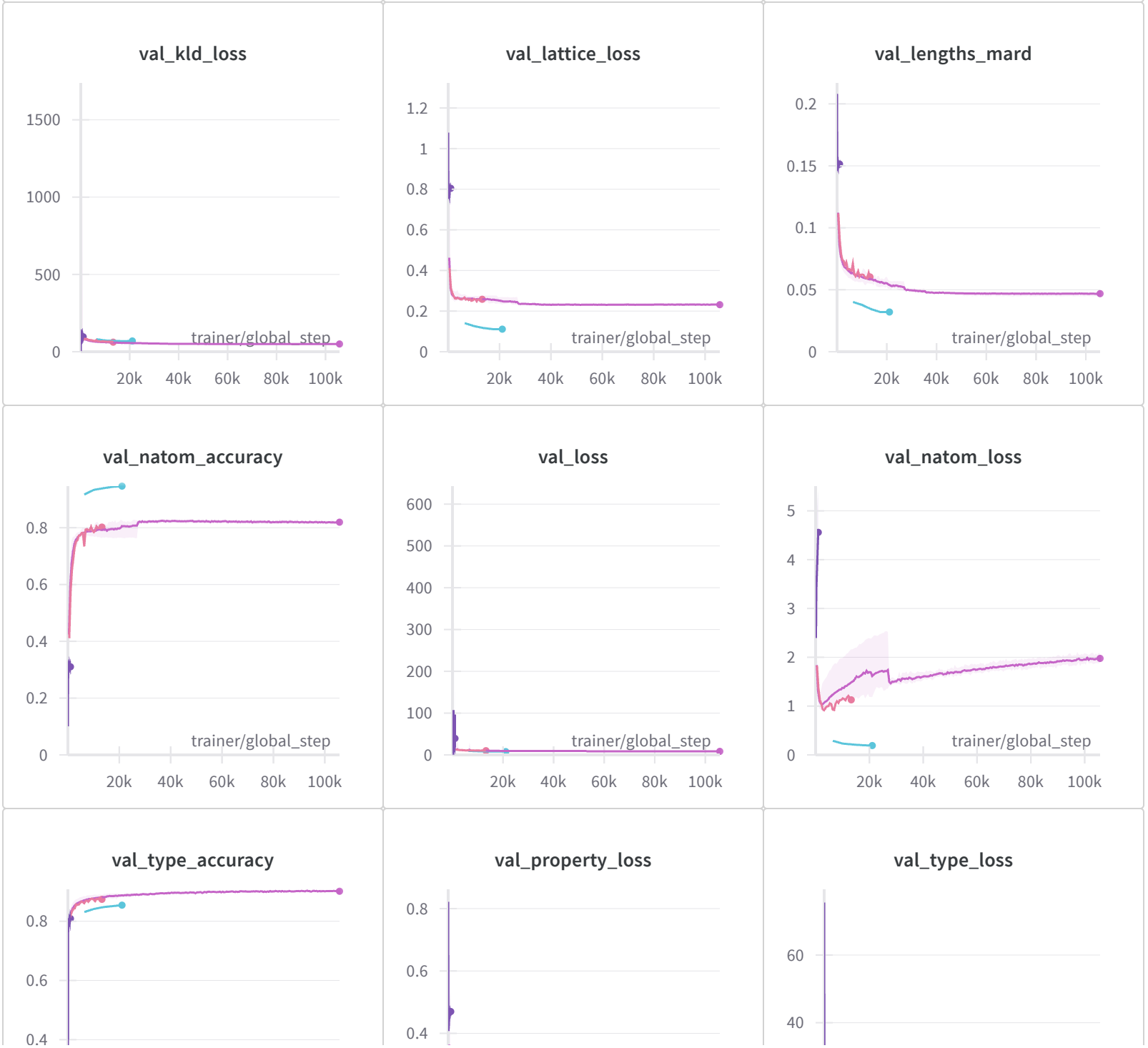
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val_kld_loss
1500
1000
500
0
trainer/global_step
20k 40k 60k 80k 100k
val_lattice_loss
1.2
1
0.8
0.6
0.4
0.2
0
trainer/global_step
20k 40k 60k 80k 100k
val_lengths_mard
0.2
0.15
0.1
0.05
0
trainer/global_step
20k 40k 60k 80k 100k
val_natom_accuracy
0.8
0.6
0.4
0.2
0
trainer/global_step
20k 40k 60k 80k 100k
val_loss
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500
400
300
200
100
0
trainer/global_step
20k 40k 60k 80k 100k
val_natom_loss
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4
3
2
1
0
trainer/global_step
20k 40k 60k 80k 100k
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0.6
0.4
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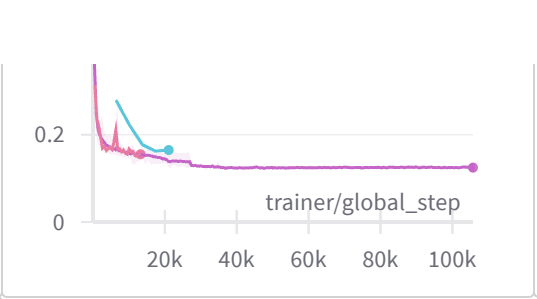

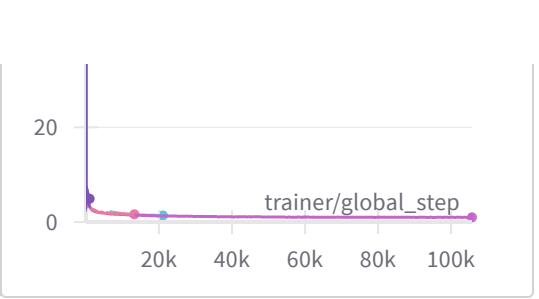

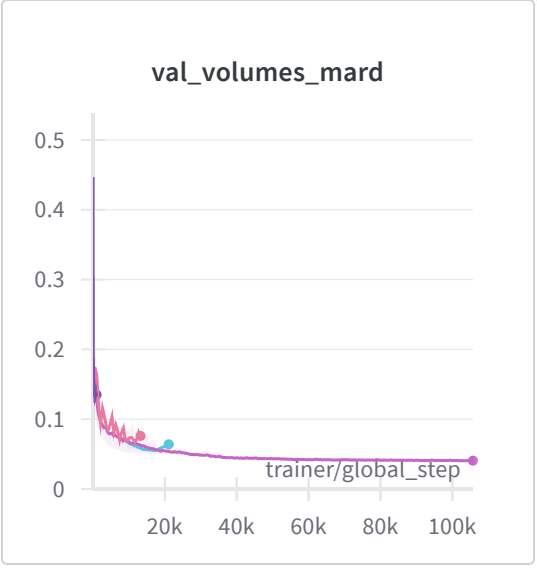

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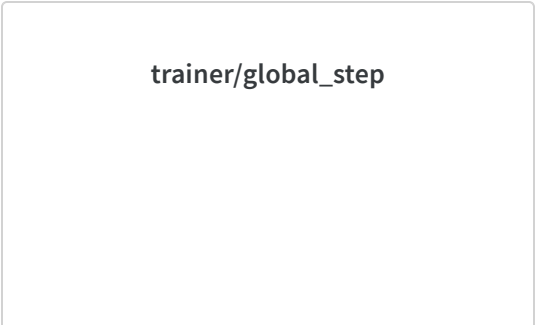
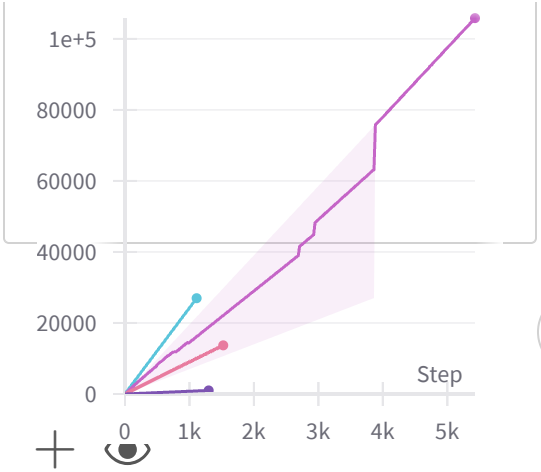
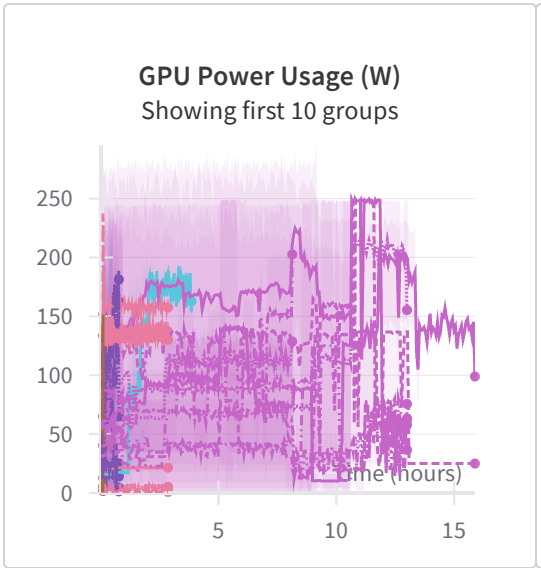
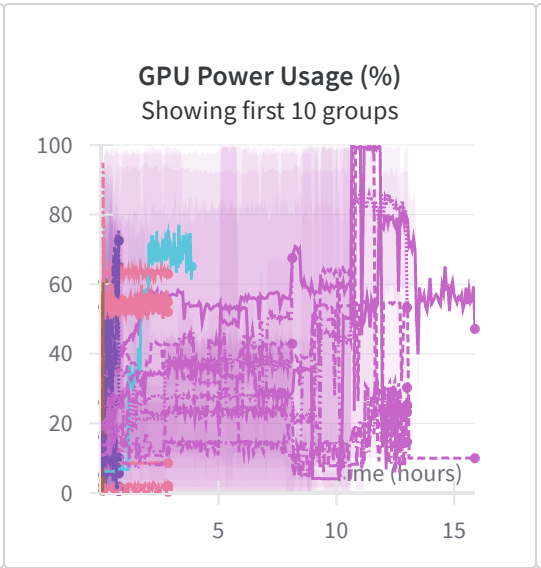


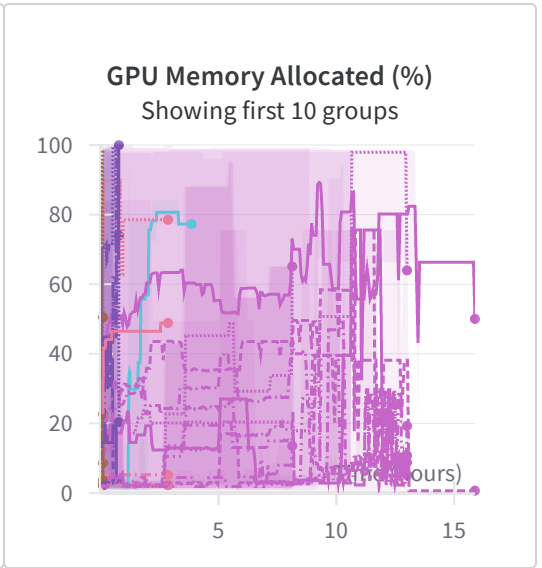


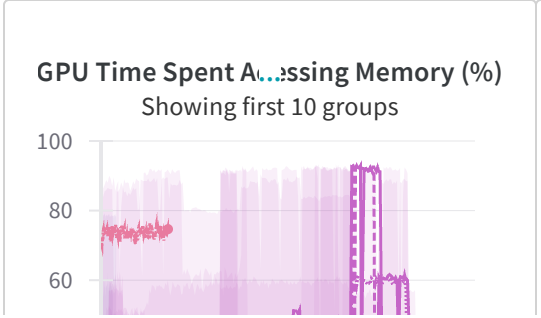
Import panel

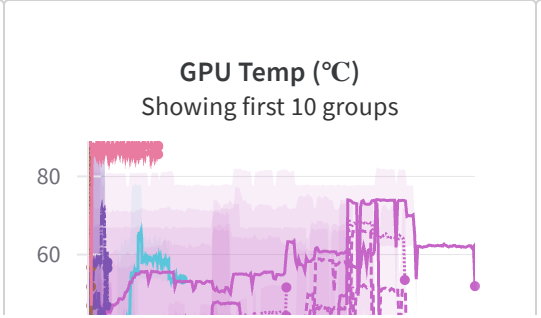
Add panel

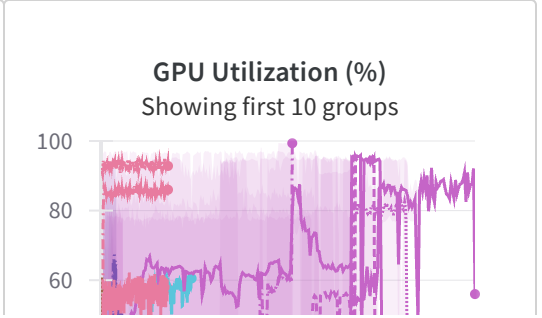


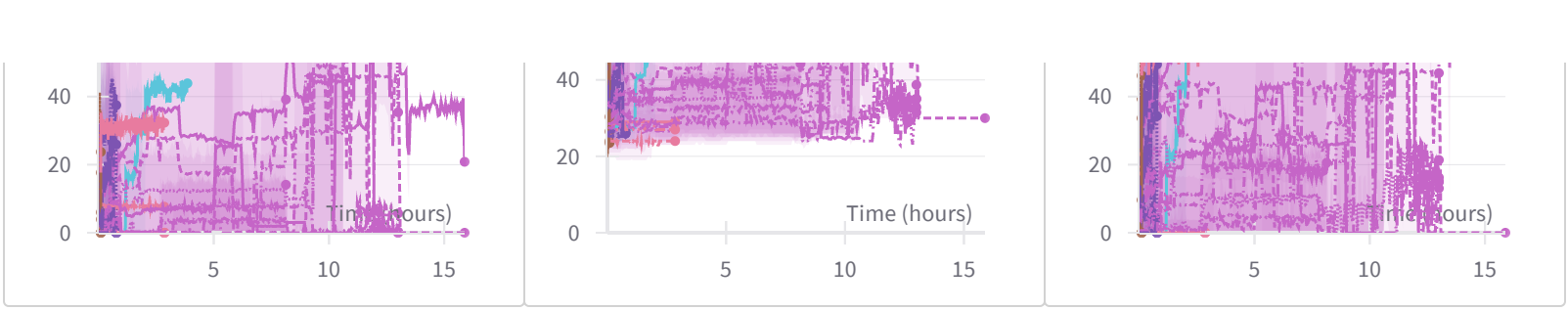












Import panel

Add panel