Predicting Molecular Trajectories of a Nanomotor with Neural Networks

WHK Research Project

Ferdinand Tölkes

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Presentation outline

1. Scope of my work
2. Dataset overview
3. Training the network
4. Results
5. Possible next steps

Scope of current work

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- Work on one specific dataset: MOTOR_MD_XTB/T300_1
- Prediction of **energy** and **forces** given atomic positions
- Molecule is only examined in **ground state**

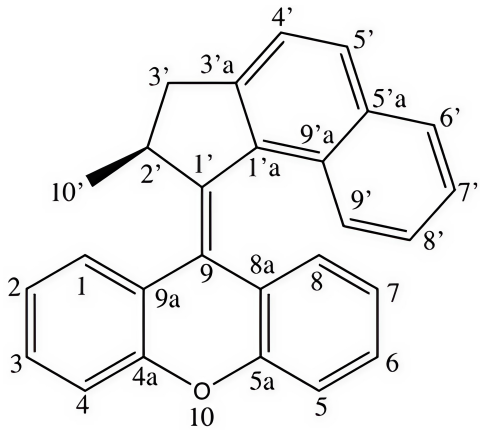

Figure: Figure adapted from [1, p.13]

Dataset overview

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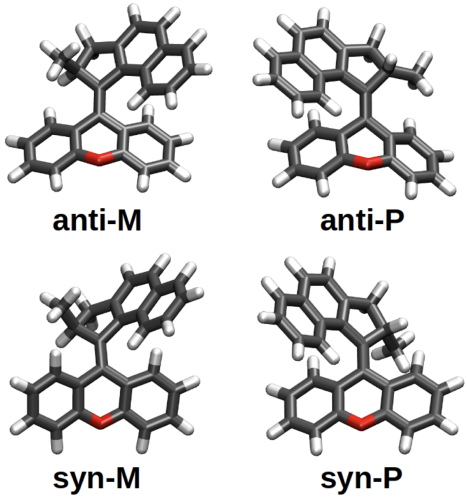

Figure: Figure adapted from [1, p.11]

- **Four** important **conformations**: anti-M, syn-M, anti-P and syn-P
- Can be roughly clustered by using **dihedral angles**, e.g.

$$\text{M: } \beta < 0, \quad \text{P: } \beta > 0$$

and furthermore

$$\text{syn-M: } \beta < 0 \quad \& \quad \delta < 0,$$
$$\textbf{anti-M: } \beta < 0 \quad \& \quad \delta > 0$$

Dataset overview

- Data sampled in **NVT ensemble**
- Split in train (12615), validation (3154) and test data (3943)
- **Center of mass** and **energy offset** substracted
- Configurations in T300_1 mostly in **anti-M**

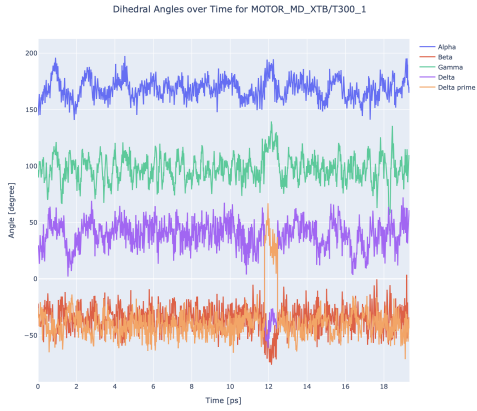

Figure: Plot of dihedral angles for T300_1 taken from [3].

Training the network

Training the network

- Training using SchNetPack (see [2] and Pragati's talk)
- Mean squared error (MSE) is underlying loss function
- Energies weighted with 0.01 and forces with 0.99
- Runs with 1000 epochs take roughly six hours and don't converge

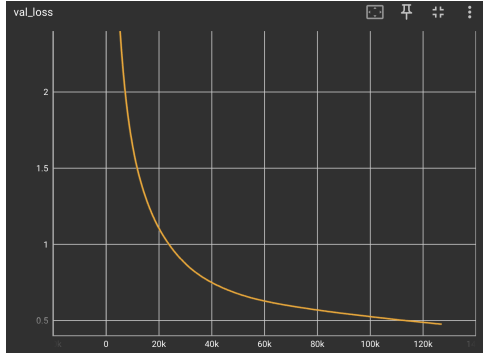

Figure: Validation loss plotted against the number of steps when training a model on Angstrom and kcal/mol for 1000 epochs.

Impact of units

- Change of units (COU) **affects model performance** (see results section)
- Possible explanation: COU **affects weights** of energies and forces within the MSE
- Trying to counteract this effect, is not yet fruitful (see starred entry in results section)
- More on this later, if you are interested!

Results

Performance on Validation Data

Molecule	Training Units	Energy MAE [kcal/mol]	Forces MAE [kcal/mol/Å]
CPNX	Å, kcal/mol	0.1896 ± 0.0134	0.2999 ± 0.0110
CPNX	Å, eV	0.1581 ± 0.0027	0.3174 ± 0.0067
CPNX	Å, Hartree	0.2960 ± 0.0050	0.5154 ± 0.0100
CPNX	Å, Hartree*	0.3053 ± 0.0085	0.4993 ± 0.0119
$C_9O_8H_4$	Å, kcal/mol	$0.11 - 0.38$	$0.14 - 1.17$

Table: Mean absolute errors (MAEs) with corresponding standard errors on the validation data, for models trained in three different unit systems. The reference values for Acetylsalicylic ($C_9O_8H_4$) are taken from [2, p.453]. Note that the chemical accuracy is more or less defined as 1 kcal/mol

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XTB vs. NN Trajectory

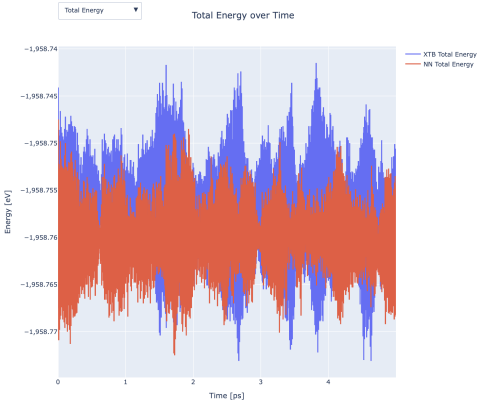


Figure: Plot of predicted energies from XTB and the neural network taken from [3].

- Take last sample of test data as starting configuration
- Using its velocities should ensure that **trajectory is equilibrated**
- Predict trajectory with XTB and neural network for 5000 steps à one femtosecond
- Simulating this with NN takes around five minutes

Correlation

- How similar are the trajectories around a certain point?
- Correlation as **measure of similarity**
- At step s take the next n steps to compute the **Pearson correlation**
- Repeat for each time step

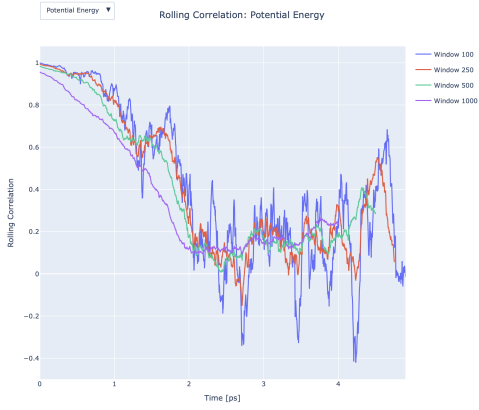


Figure: Plot of correlations between predicted energies from XTB and the neural network taken from [3].

Per-atom fluctuations

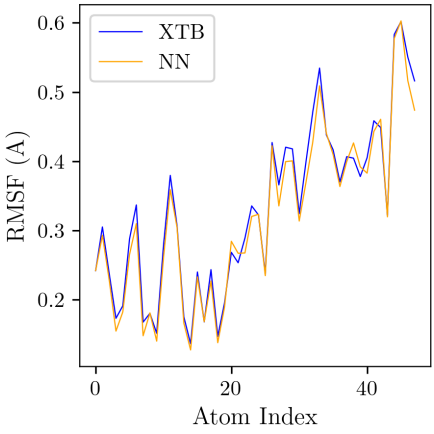
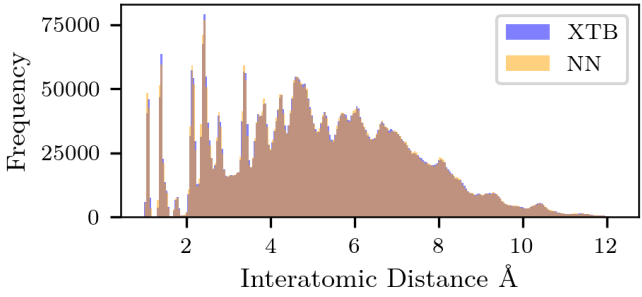


Figure: Average RMSF per atom.

- Take average over positions to compute reference structure
- Compute root mean squared fluctuations (RMSF) from reference structure per atom over time
- Indices $[0, \ldots, 47] \mathrel{\widehat{=}}$ atoms $[O, C, \ldots H, \ldots]$
- Pearson correlation of 0.9934

Interatomic distances



- Plot of distribution of interatomic distances
- $48 \cdot 47/2 = 1128$ distances per step
- Flattened into array of length $1128 \cdot \#\text{steps}$

Radius of gyration

- Radius of gyration is the distance from a systems **rotational axis** to its **center of mass**
- Describes **how masses** of system are **distributed**

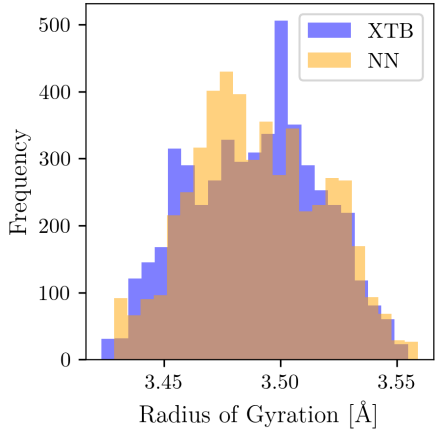
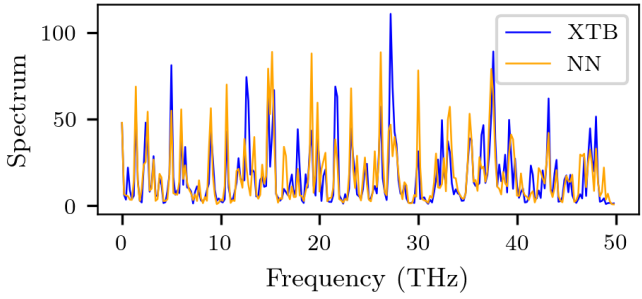


Figure: Distributions of the radius of gyration.

Power spectrum



- Excerpt of power spectra from XTB and NN trajectories, $r_{\text{Pearson}} = 0.7125$
- Calculated as Fourier transform of the velocity autocorrelation function
- Gives insights into active vibrational modes

Possible next steps

Possible next steps

- Include also the other T300 datasets in training and inference
- Train models until they converge
- Move on to exited states
- Try to use trained model as foundational model:
  - Finetune it for specific needs
  - Perform MD on the fly

Sources

[1] Jesús Lucia-Tamudo, Michelle Menkel-Lantz, and Enrico Tapavicza. "First principles prediction of wavelength-dependent isomerization quantum yields of a second-generation molecular nanomotor". In: *Physical Chemistry Chemical Physics* 27.23 (2025), pp. 12519–12531.

[2] KT Schütt et al. "SchNetPack: A deep learning toolbox for atomistic systems". In: *Journal of chemical theory and computation* 15.1 (2018), pp. 448–455.

[3] Ferdinand Tölkes. *Molecular Dynamics of a nanomotor using SchNetPack*. `https://github.com/FerdinandToelkes/whk`. GitHub repository. 2025.