GROMACS 2023-2024: New features and improvements

Magnus Lundborg

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About GROMACS

- Molecular dynamics simulation package
- User-driven development
- High performance
  - Good scalability
  - GPU acceleration
  - Runs on most platforms and hardware
- Suite of analysis tools
- Tutorials
- Interfaces to other software
- Free Software

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- General information: https://www.gromacs.org
- Documentation: https://manual.gromacs.org
- Tutorials: https://tutorials.gromacs.org
- Forums: https://gromacs.bioexcel.eu
- Development: https://gitlab.com/gromacs/gromacs

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2024 release

- 2024.0 was released January 30th
- 2024.1 was released February 28th

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News in 2024

- Colvars integration
- AWH improvements
  - Automatic scaling of the target distribution
  - Improved control of the exponential growth of histograms
- Improved deform option, now suitable for calculating viscosities
- Reduced artifacts, on pressure, from Lennard-Jones pair interactions
- Performance improvements
  - Hydrogen mass repartitioning in `gmx grompp`
  - Configurable multi-GPU FFT options

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Native Colvars integration

- Use collective variables
  - Apply restraint or bias
  - Enhanced sampling

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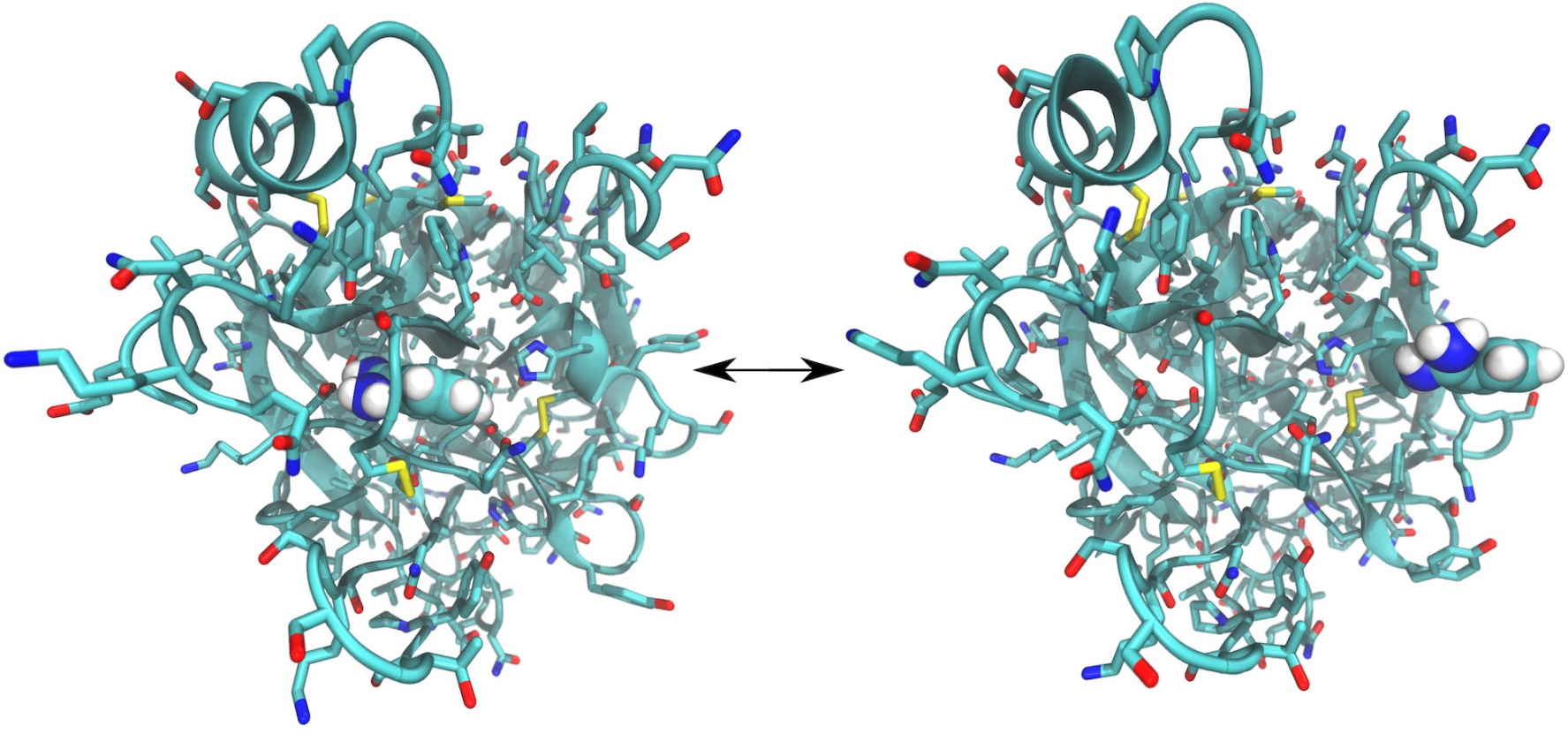

Input data from Aho N, Groenhof G, Buslaev P. ChemRxiv. 2023; doi:10.26434/chemrxiv-2023-2pqls.

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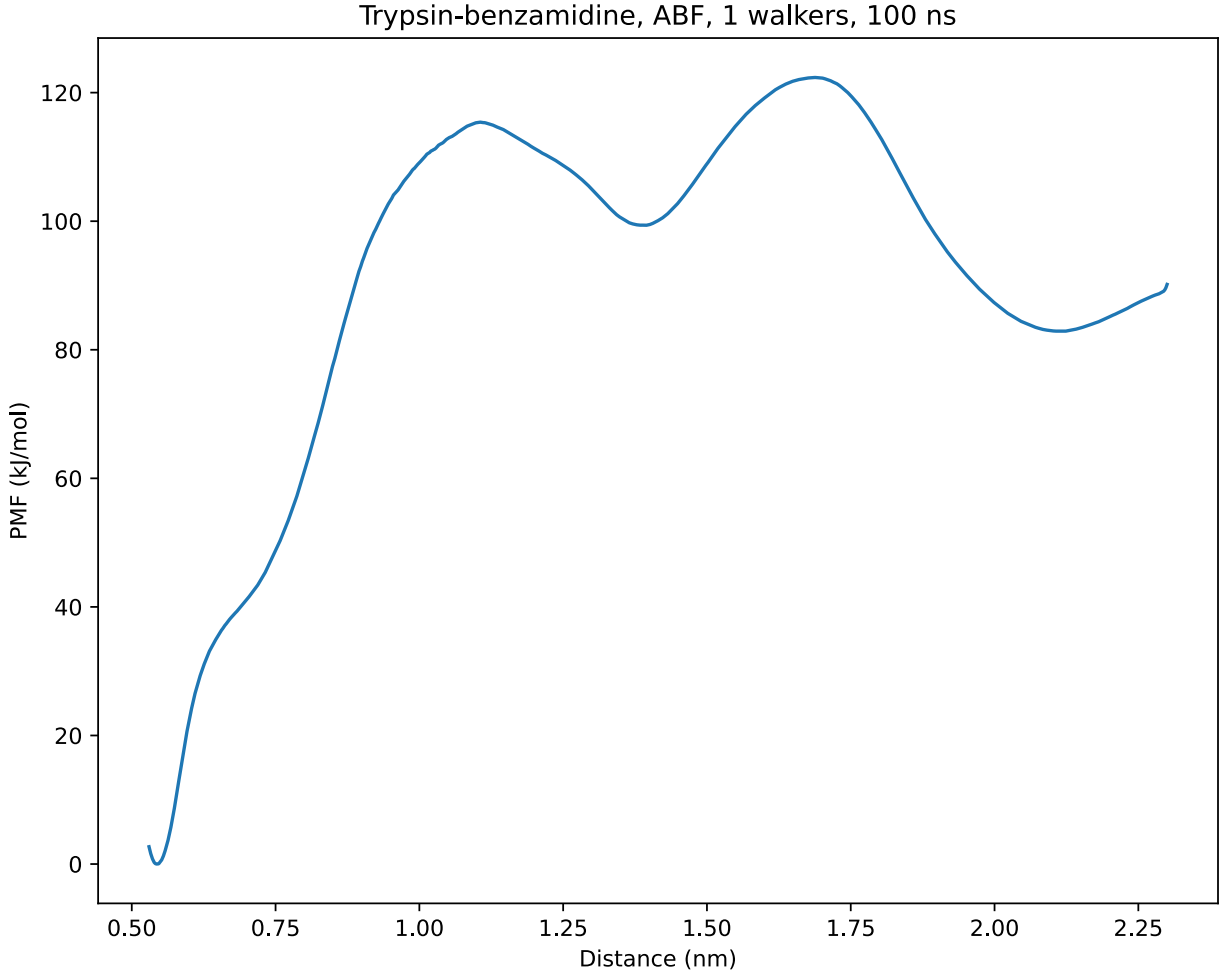
Using Colvars from GROMACS

```
colvars-active        = true
colvars-configfile    = colvars.cfg
```

```
colvarsTrajFrequency 1000
indexFile ../../awh/awh_sw/index.ndx

colvar {
  name binding
  width 0.001

  lowerBoundary 0.53
  upperBoundary 2.3

  distanceZ {
    ref { indexGroup chainB }
    main { indexGroup chainA }
    axis (0.0, 0.0, 1.0)
  }
  extendedLagrangian on
  extendedFluctuation 0.005
}

abf {
  colvars binding
  fullSamples 200
}

harmonicWalls {
  name wall_binding
  colvars binding
  lowerWalls 0.53
  upperWalls 2.3
  forceConstant 1
}
```



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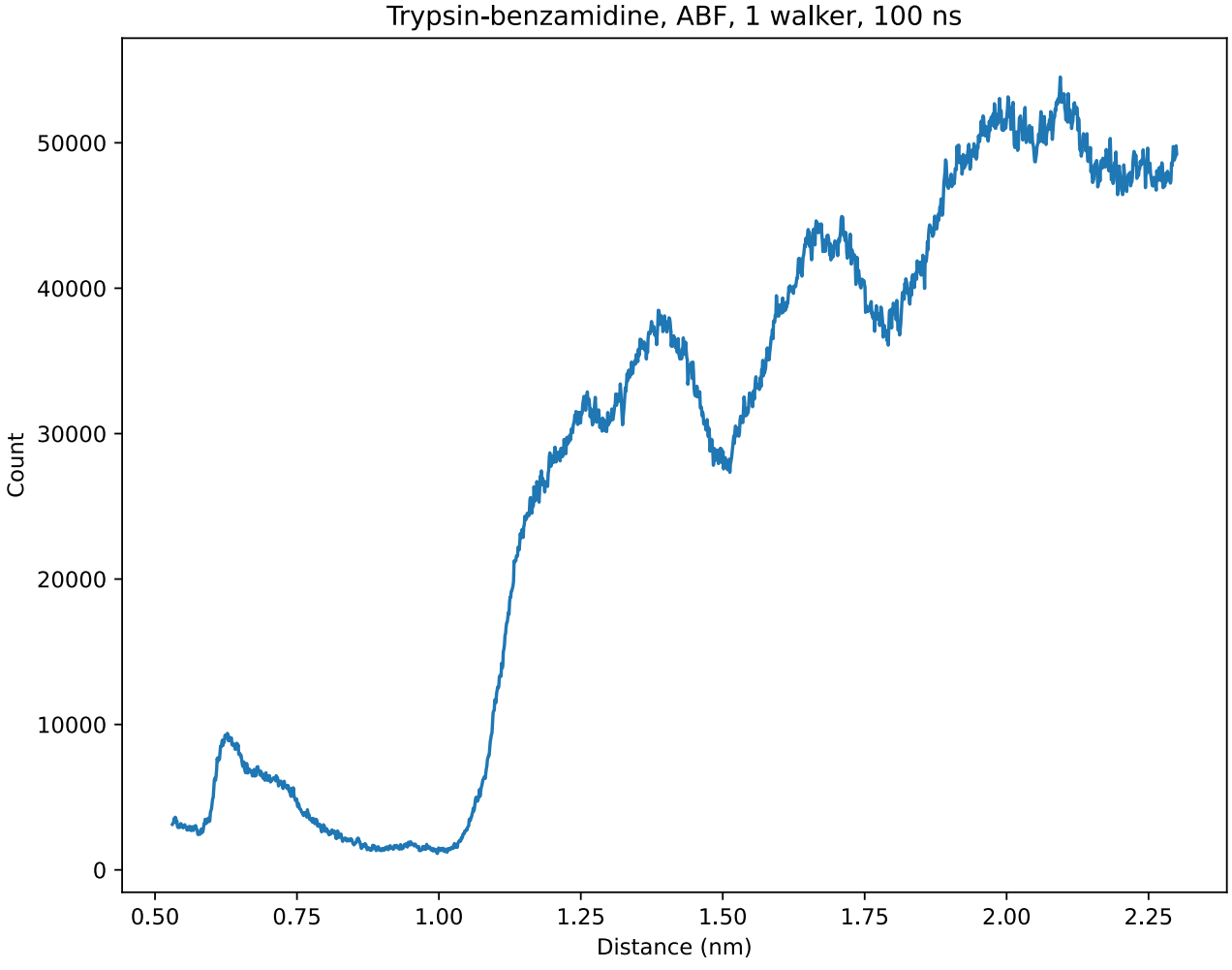

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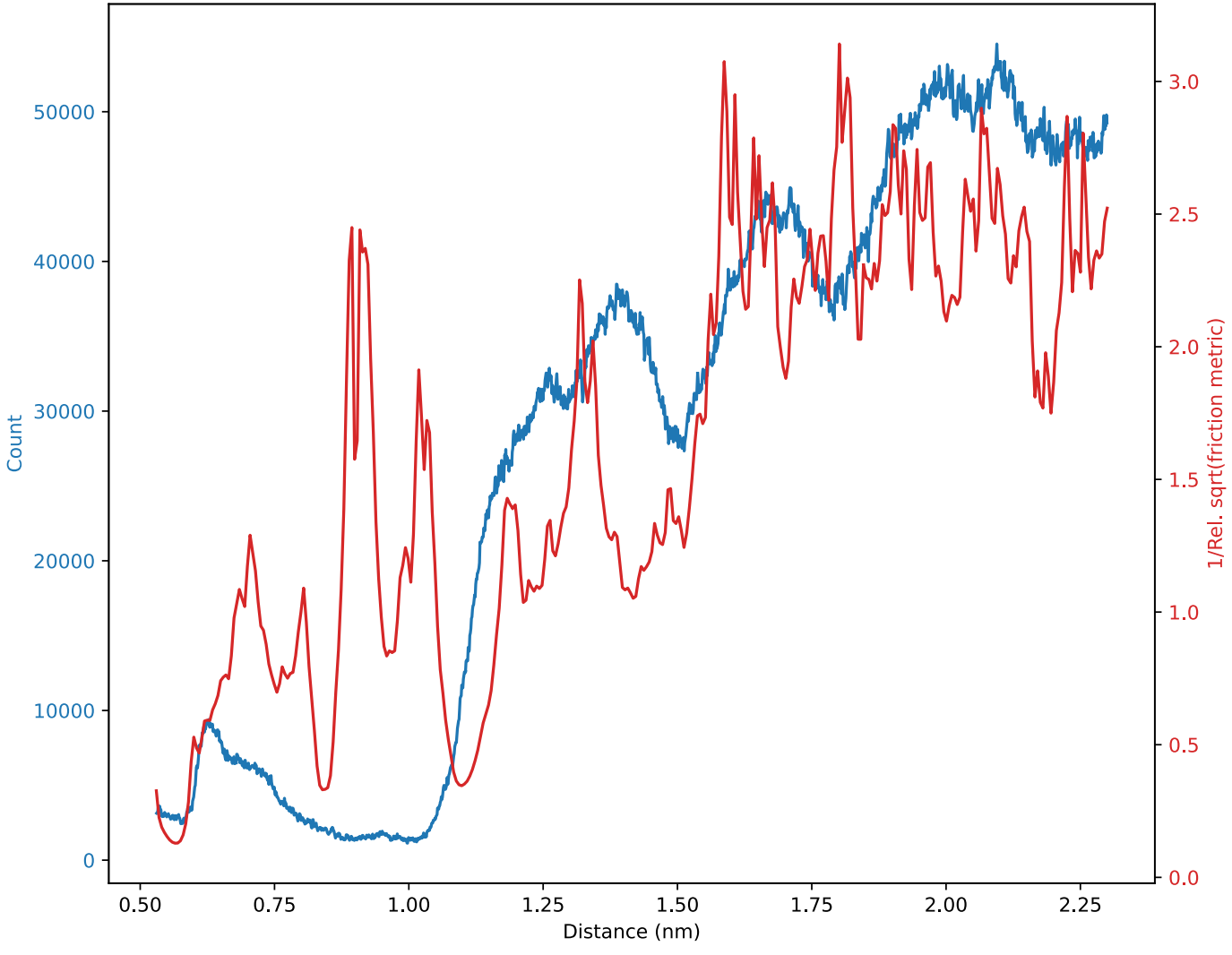

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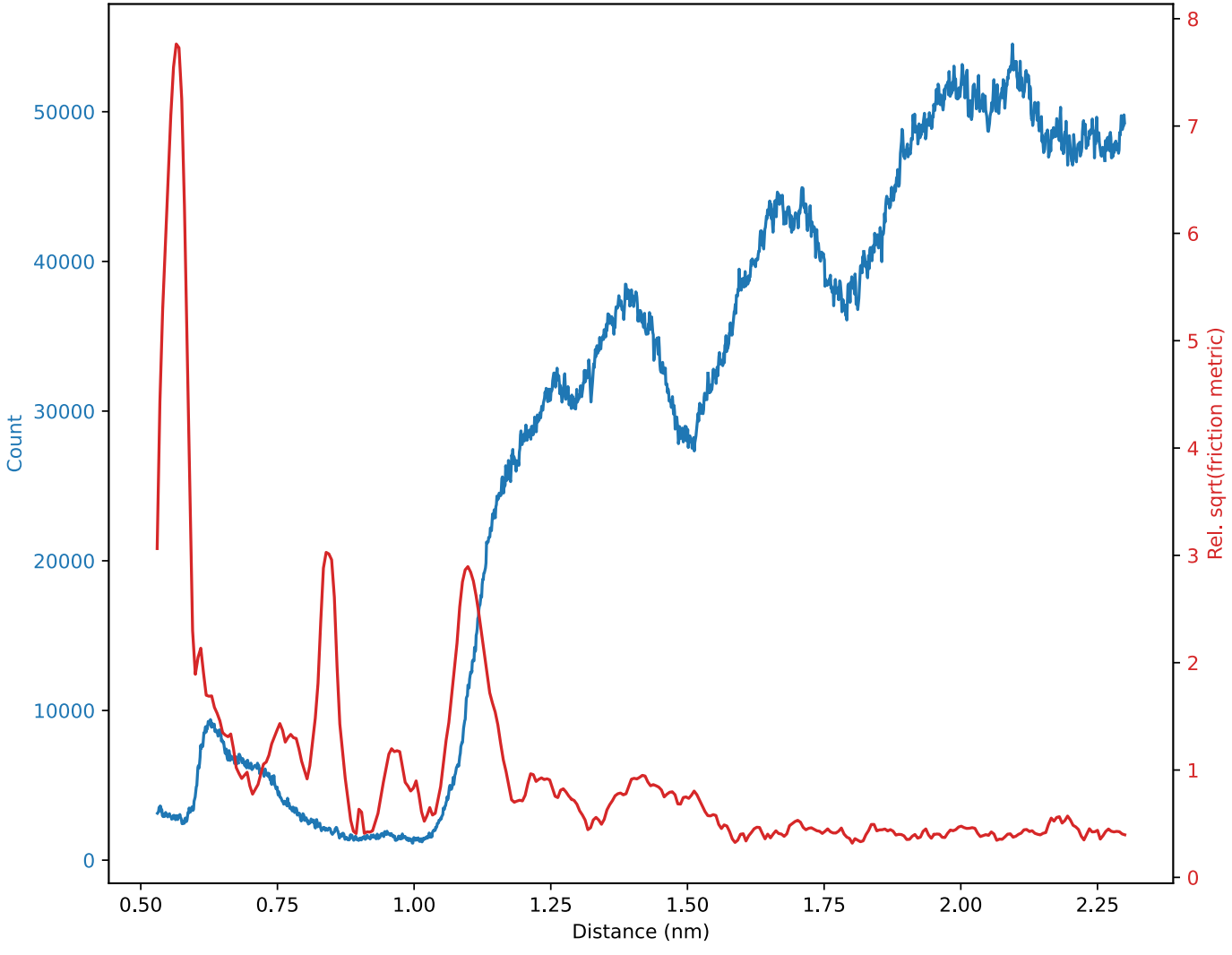

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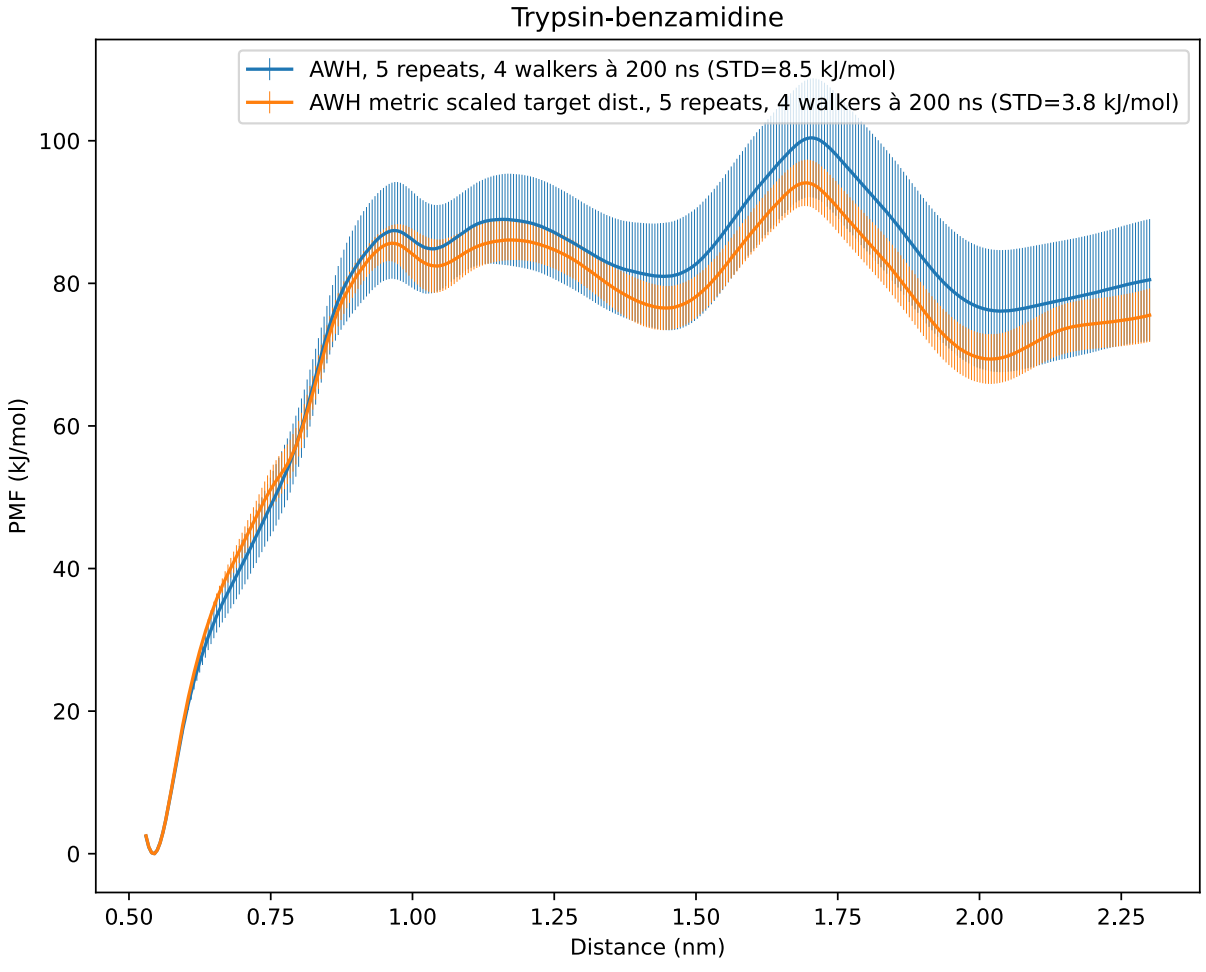
Accelerated Weight Histogram (AWH) method

- Automatic scaling of the target distribution based on the AWH friction metric

```
awh1-target-metric-scaling = yes
```



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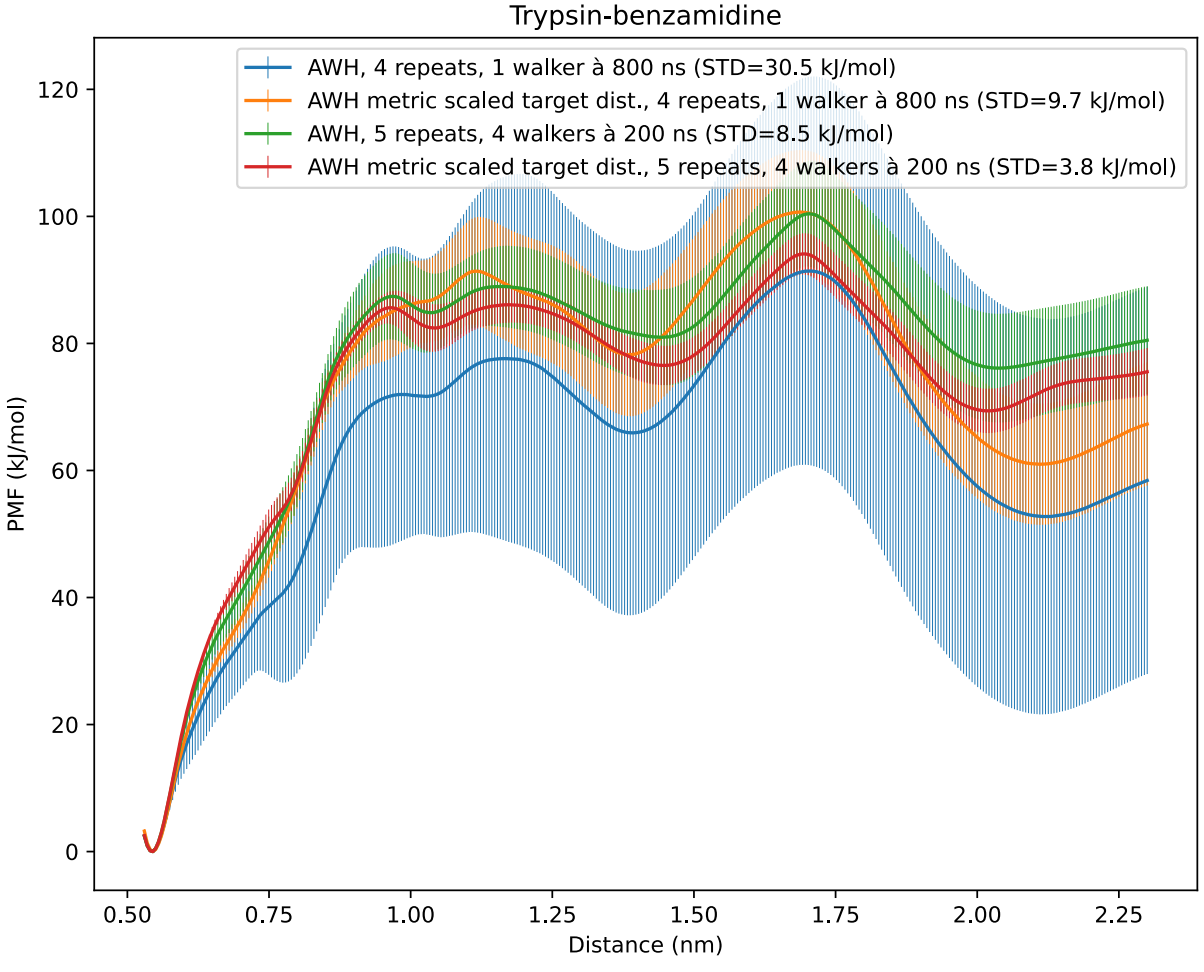

Accelerated Weight Histogram (AWH) method

- Set the exponential growth factor during the initial stage

```
awh1-growth-factor              = 2
```

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Box deformation and viscosity calculations

- The deform option now only deforms the box without modifying particle positions.
- Uses a velocity profile (flow field), that can be automatically generated at the beginning of the simulation.

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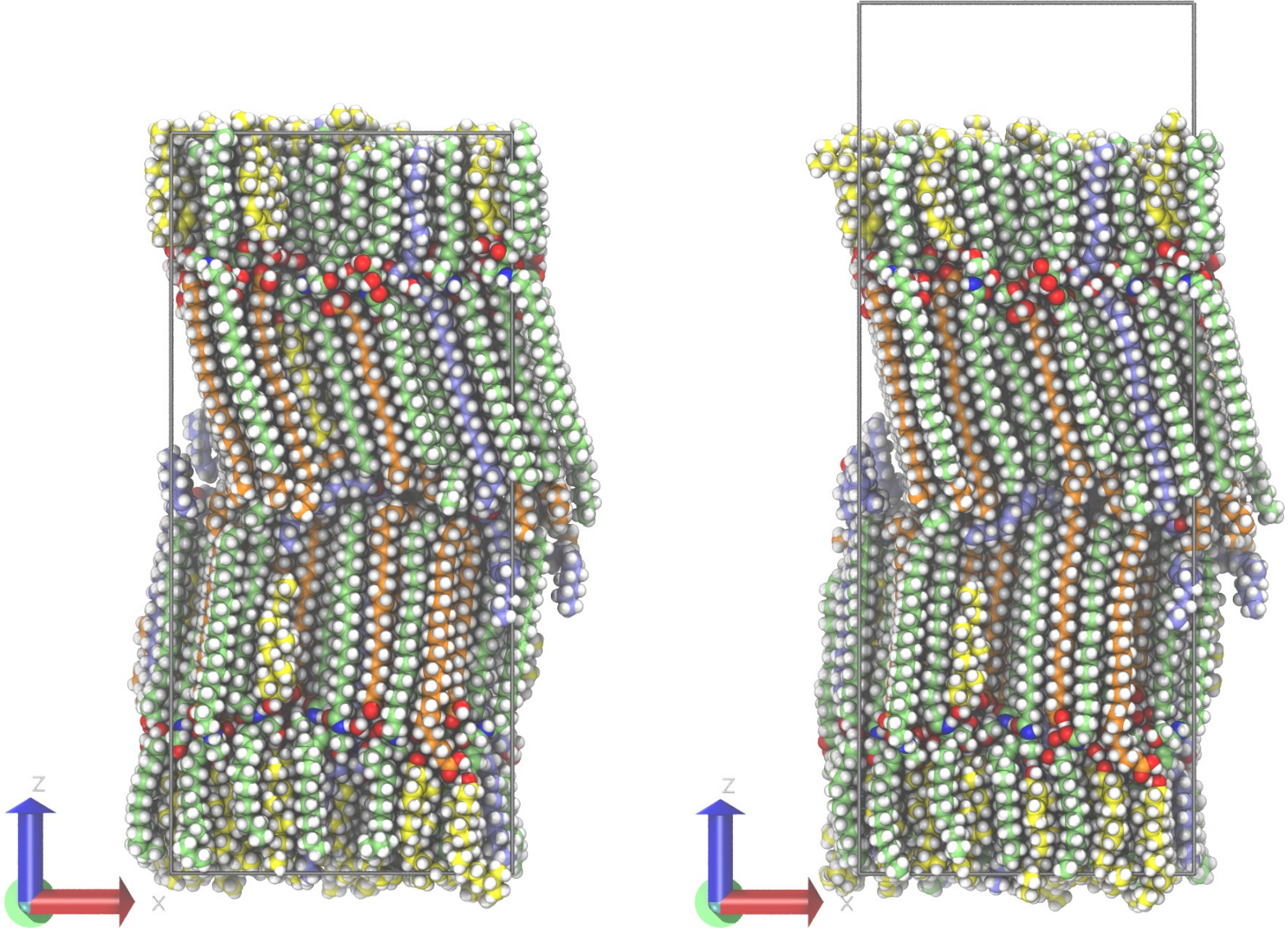
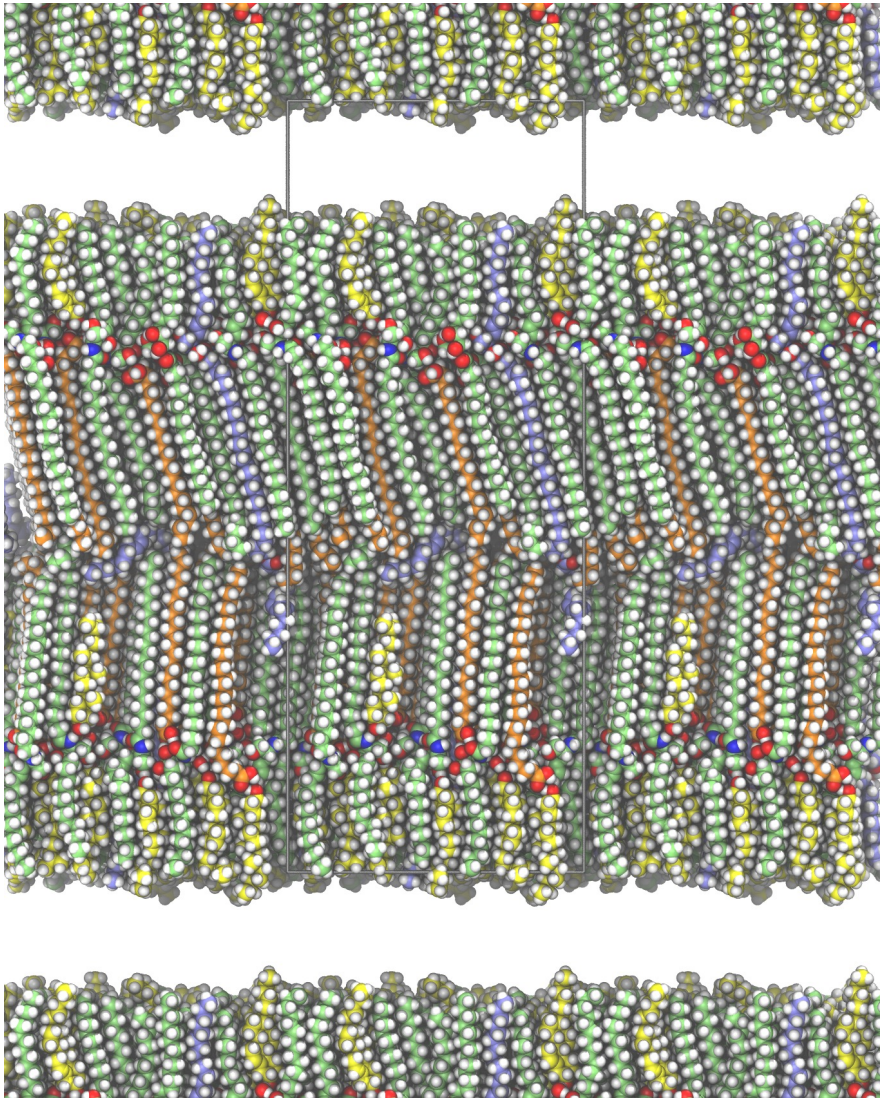
- MDP example

```
deform              = 0 0 0.001 0 0 0
deform-init-flow    = yes
```





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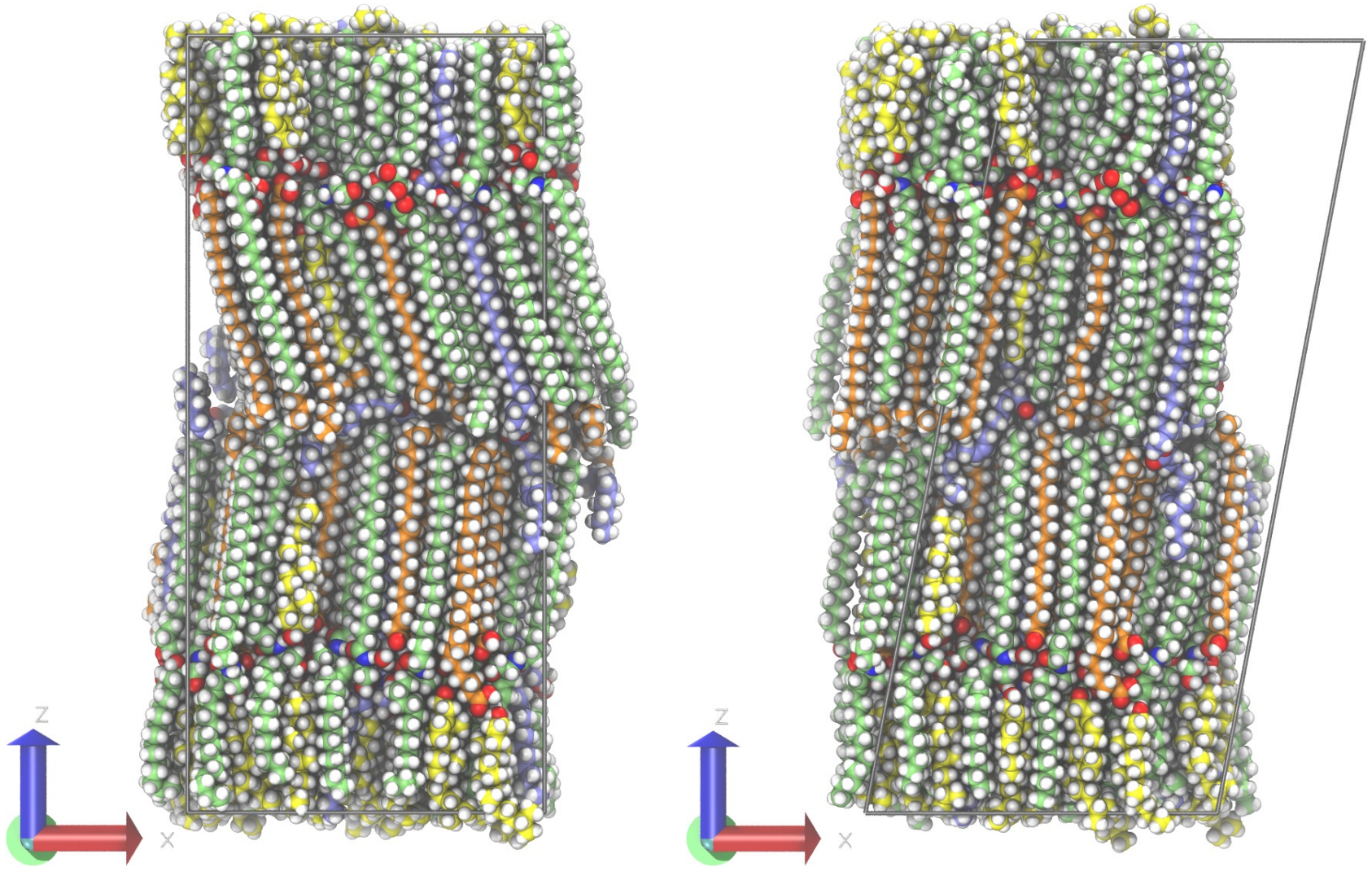
- MDP example

```
deform              = 0 0 0 0 0.001 0
deform-init-flow = yes
```



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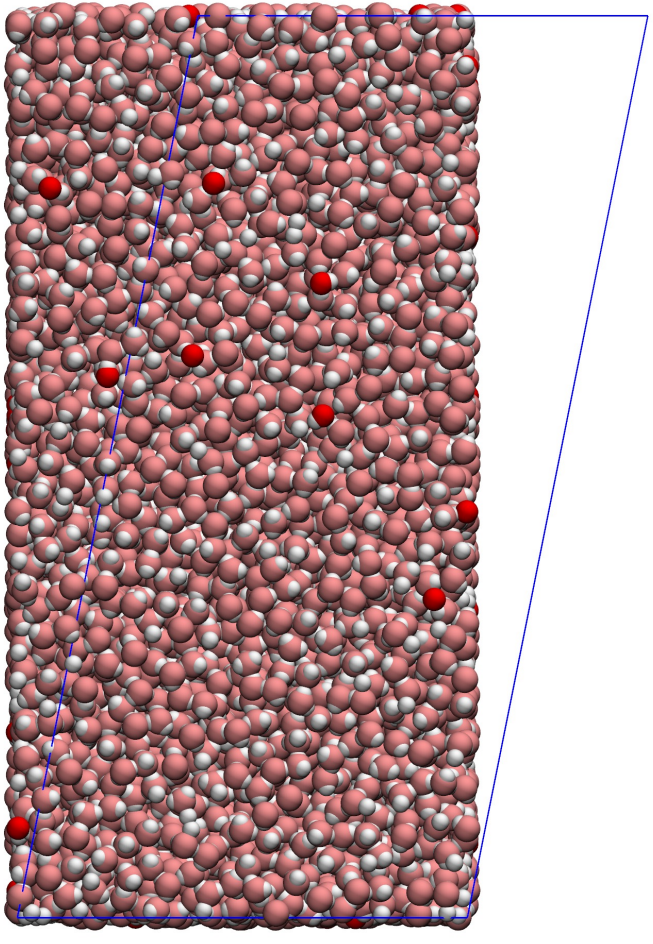

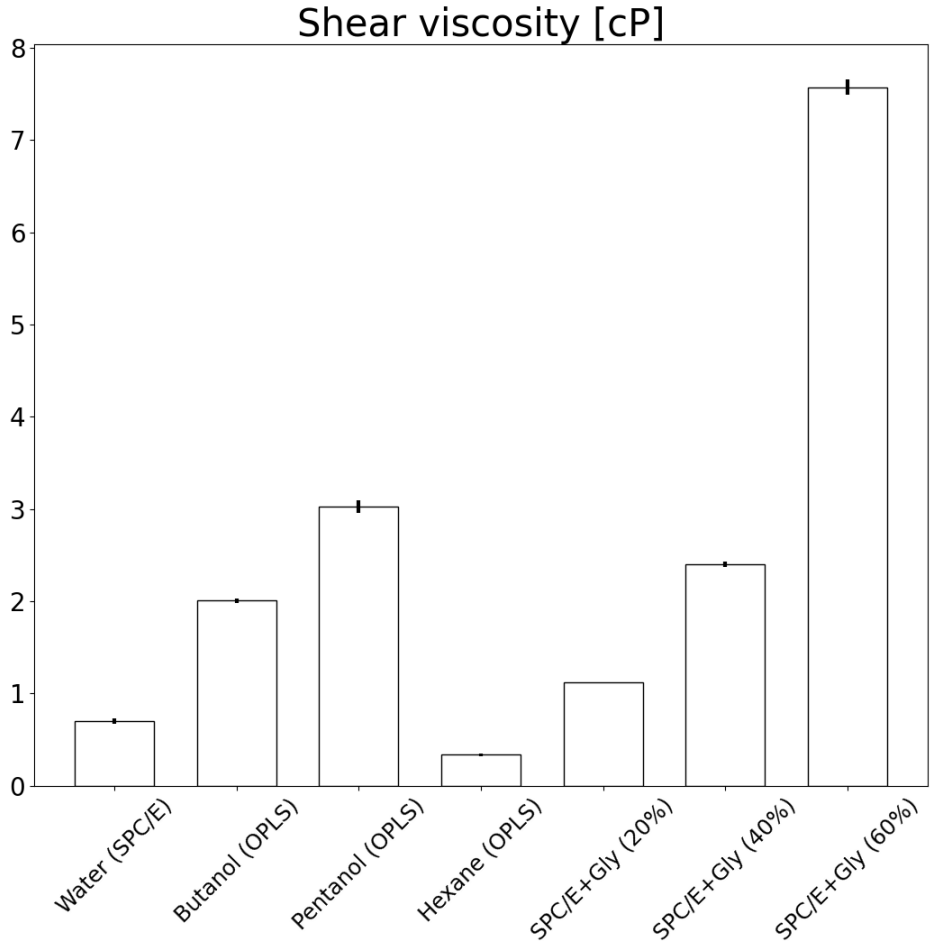

- Reduced artifacts from LJ interactions on the pressure
  - The Verlet pair list buffer was based only on energy drift.
  - Missing Lennard-Jones interactions could lead to incorrectly increasing pressure over the life time of the pairlist.
  - Affected systems without charge.

  - Can lead to a slight performance loss, especially for coarse-grained systems.
  - The tolerance to pressure deviation over the lifetime of the pair list can be set by an mdp parameter:

```
verlet-buffer-pressure-tolerance (0.5) [bar]
```

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Performance improvements 2023

- Major SYCL GPU extensions
  - Working on important HPC platforms
- CUDA Graphs
  - When all force and updates are run on GPU
  - Record activities to a graph
  - Reduced overhead when launching a graph instead of each activity
  - Enabled using `GMX_CUDA_GRAPH` environment variable
- PME decomposition support with CUDA and SYCL
- Updates run on GPU by default
- Higher default coupling intervals for thermostats and barostats

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Performance improvements 2024

- Hydrogen mass repartitioning in `gmx grompp`
  - New mdp option

    `mass-repartitioning-factor = 1`
- HeFFTe multi-GPU FFT plan options are configurable
  - Using environment variables
  - Users can find and use suitable settings for their setup.

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Contributors to the 2024 release

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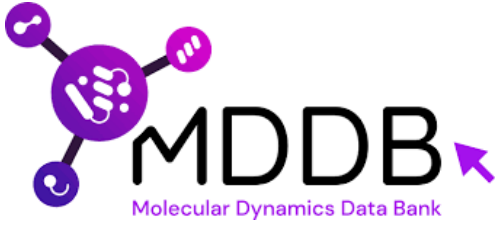

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