

# Sharing data from molecular simulations

Session: Standardization of file formats

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# Workshop objectives reminder

Discuss

Find best practice

Highlight issues / find new solutions

Write a whitepaper

# Evolving standard file formats

- understand user and community needs
- target extensibility and modular schemas, rather than up-front breadth of coverage
- build a community responsible for maintaining the description of any new standard
- have a reference implementation in mind
- make available sample files in the format
- assume the models and formats you're most familiar with are unsuitable to be standards ;-)

# What we're not concerned about today!

- citability of data sets
- workflows
- simulation management (simulating, visualizing, analyzing, archiving, sharing)
- actually agreeing on particular community standards (new or old)

# Do we agree on basic user needs?

## Inputs

- coordinates (low and high precision),
- descriptions of model physics,
- descriptions of chemical content (e.g. charges through to macro)
- descriptions of sampling algorithms,
- descriptions of output requirements,
- experimental data

# Do we agree on basic user needs?

## Outputs

- sets of coordinates (MD trajectories, docked ensembles, minimized states, eigensystems),
- post-processing analysis,
- log files

# Mark's take on community needs

- Container-style approach needed
- Extensibility is paramount
- Generally need both human and machine readability
- Compression
- Able to describe the input that produced it
- Able to be annotated
- Separate solutions for different needs, e.g. force field descriptions, molecular topologies, trajectory output
- Who aren't we learning from? QM, astronomy, bioinformatics, materials science, A/V

# Use cases



# Gamestorming time!

How should the molecular simulation community approach the need to store data?

- (+) What makes it possible?
- (-) What makes it complex?
- (I) What initiatives are going in useful directions?
- (A) What actions do we need to take?