

A serialization solution

- There is a `to_dict` / `from_dict` method for each class that creates a shallow mapping of attributes.
- All classes that can be serialized this way inherit from a base class and carry a mechanism for creating their unique identifier.
 - OPS: UUID; OpenFE: gufe key
 - Do you want equivalent objects created at different times to have the same identifier, or different ones?
- There is a function that consumes such objects and converts them to bytes/string.

Conclusions

- Path sampling methods are a powerful tool for sampling rare events, and interfacing with OpenPathSampling might be of interest to MD engine developers.
- Alchemical free energy methods provide vital tools for the drug discovery pipeline, and Open Free Energy is a new toolkit facilitating these simulations.
- Both of these methods are “campaign-scale,” and clear APIs and good serialization mechanisms in underlying tools make our lives easier.

<http://openpathsampling.org>

<https://openfree.energy>