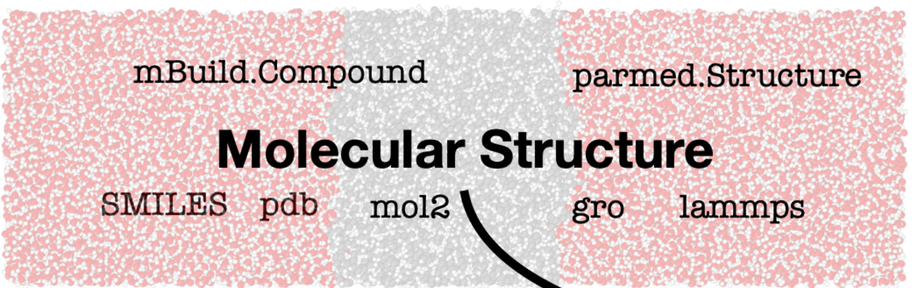
GMSO

the General Molecular
Simulation Object

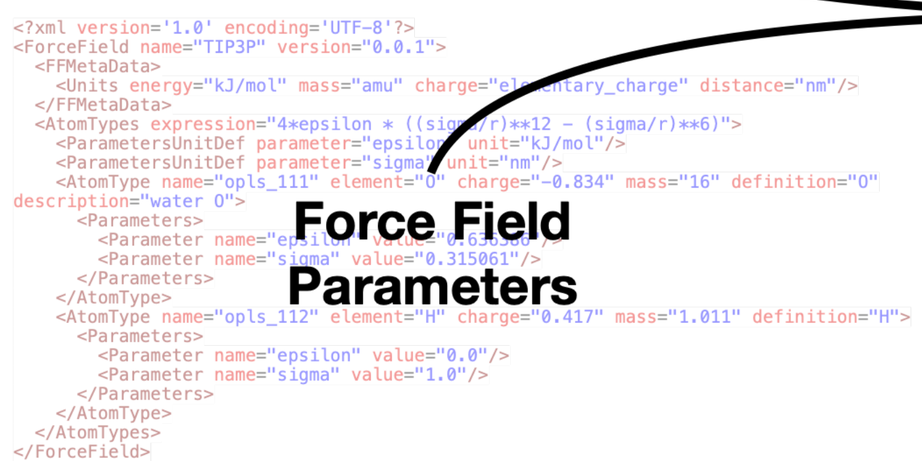


Systematic and
Flexible Unit

Extensible
Workflow

Topology

Symbolic Potential
Expression



Molecular Topology File

hoomdblue

NAMD
Scalable Molecular Dynamics

LAMMPS

Cassandra
Monte Carlo
SOFTWARE

cp2k

GOMC

GROMACS FAST. FLEXIBLE. FREE.

MoSDeF

Molecular Simulation Design Framework