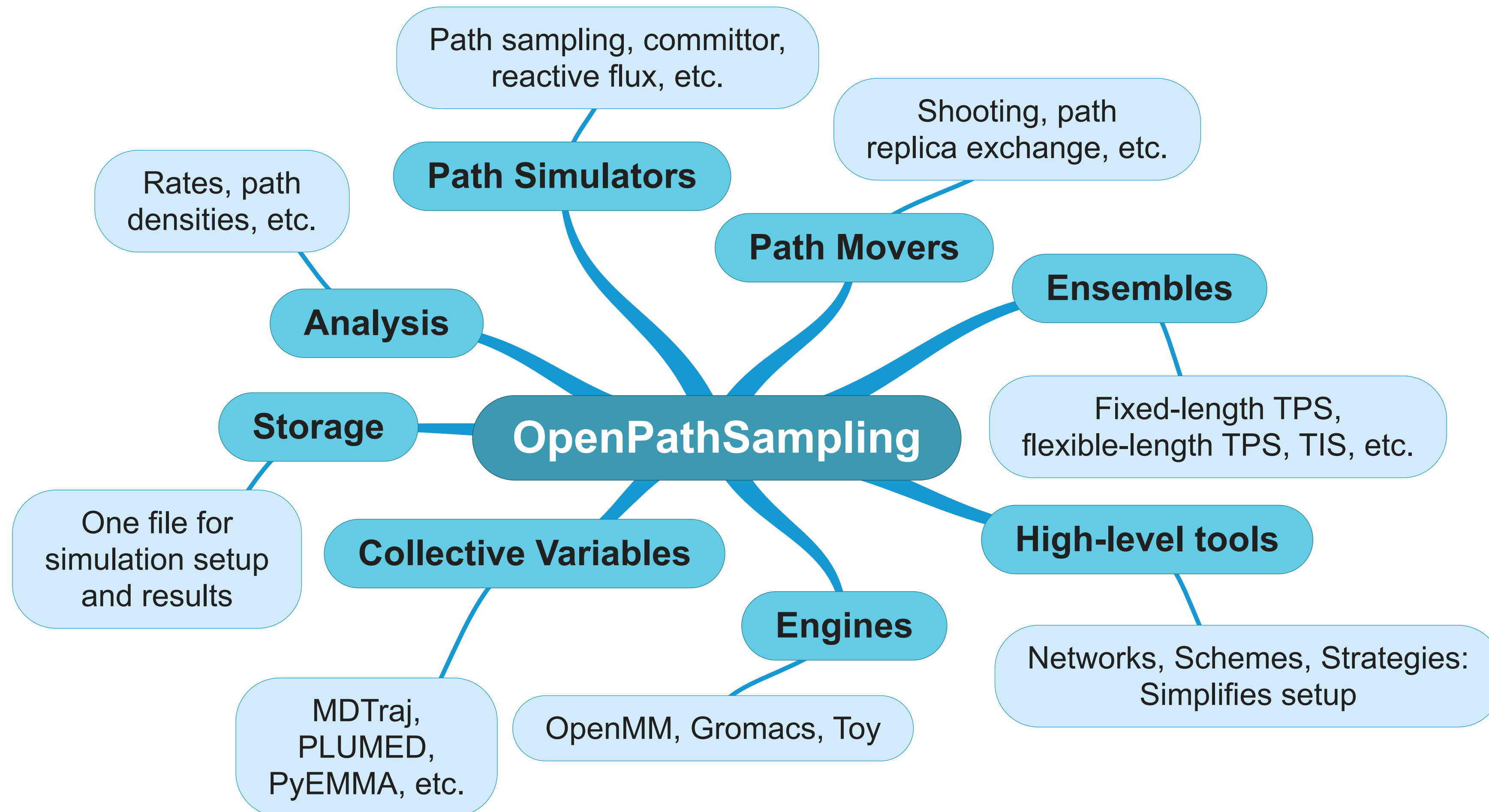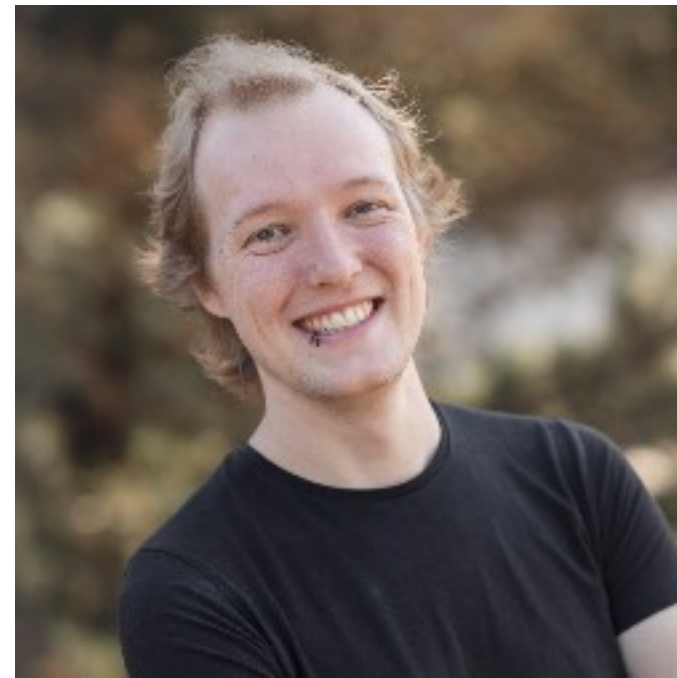# OpenPathSampling is modular

250+ Python files with 43000+ lines of code; 400+ classes; 1200+ tests.
But you can make a contribution in one part without needing to understand others.

Path sampling, committor, reactive flux, etc.

Shooting, path replica exchange, etc.

Rates, path densities, etc.

Path Simulators

Path Movers

Ensembles

Analysis

OpenPathSampling

Storage

Fixed-length TPS, flexible-length TPS, TIS, etc.

One file for simulation setup and results

Collective Variables

High-level tools

Engines

MDTraj, PLUMED, PyEMMA, etc.

OpenMM, Gromacs, Toy

Networks, Schemes, Strategies: Simplifies setup

OPS Acknowledgments

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