

Engine

Context

Param

DataSet

Write

Input

Handler

1st Solver

Kernel

Kernel

Kernel

Kernel

Kernel

Kernel

.....

.....

2nd Solver

Execute

.....

Mth Solver

Dynamics & Application

Platform/Env/Device

(Parallel Optimized, MPI etc)

Various Kernels

Sampling

Integrator

Model/Force

Ab Initio Interface

Recorder & RuleSet

Load/Dump

Analyzer

.....

Send

Recieve

Output

Results & Dumpfiles

Scripts

Utils

- Normal Mode Analysis
- Select/Filter Initial Condition
- Convert Data Format
- ...

QM Interface

- MNDO, BAGEL, Gaussian, OpenMolcas
- ...

QMMM Interface

- Cobramm Interface
- External Forcefield: Amber / OpenMM etc.
- External Ab Initio: MNDO, BAGEL, Gaussian, OpenMolcas
- ...

Python

- Smooth Integration of C++/Cython/Python
- Effortless Modular Building & Controlling
- Versatile Dynamics Algorithms Support
- Parallel High-Performance Computing
- Customizable Functionality through APIs
- Machine Learning Embedding Toolkits