



MDX

Version 1.0.0

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Overview

MDX is collection of C libraries for MD

- object-based, "clean C"
- simple, flexible design
- easy to understand and modify

Focus on developing new methods



New Methods

MSM (multilevel summation method)

- fast method for electrostatics

MDAPI

- interfaces front end with MD engine



Libraries

force: Evaluate force field

mgrid: MSM implementation

step: Time integration

mdio: MD file I/O

random: Random number generator

adt: Container classes

HTML documentation via *doxygen*



MDSim Application

Config file driven MD program, “NAMD-lite”

mdsim: Front end (uses *mdio*, *adt*)

mdapi: Interface layer (uses *adt*)

deven: MD engine (uses *step*, *force*, *mgrid*)



Your Projects

MDAPI is well-documented, but difficult to use

Recommendation for scientists:

- start with *step*, *force*, *mgrid*, *mdio*
- later extend *mdsim* and/or *deven*



Limitations

step: constant energy, leapfrog (velocity Verlet)

force: cutoff nonbonded, orthogonal domains

mgrid: cubic domains, fully nonperiodic or
periodic



Future Work

- MSM: orthogonal and orthorhombic cells
- polarizable force fields
- multiple time stepping
- modified Hamiltonian approximation