ReaDDy software overview

July 26, 2017

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Functionality

Particle propagation

Motion of selected particles by isotropic Brownian dynamics:

$$\frac{d\mathbf{x}(t)}{dt} = \underbrace{-D\frac{\nabla V(\mathbf{x}(t))}{k_B T}}_{\text{deterministic force}} + \underbrace{\sqrt{2D}\frac{d\eta(t)}{dt}}_{\text{stochastic force}}, \quad D = \frac{k_B T}{\gamma m}$$

Euler discretization:

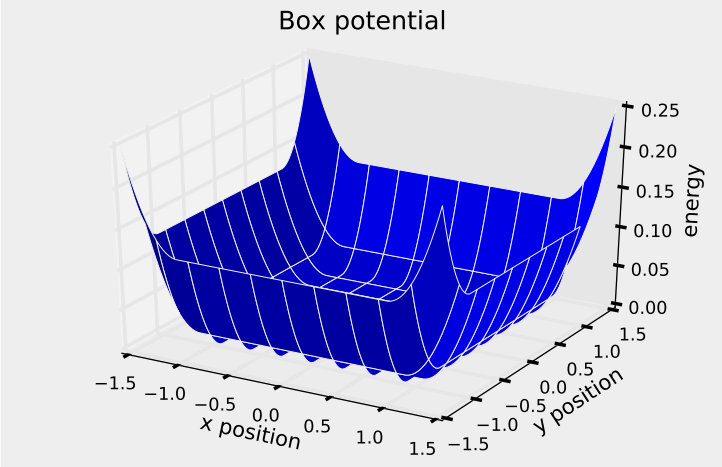
$$\mathbf{x}_{t+\tau} = \mathbf{x} - \tau D\frac{\nabla V(\mathbf{x}_t)}{k_B T} + \sqrt{2D\tau}\eta_t,$$

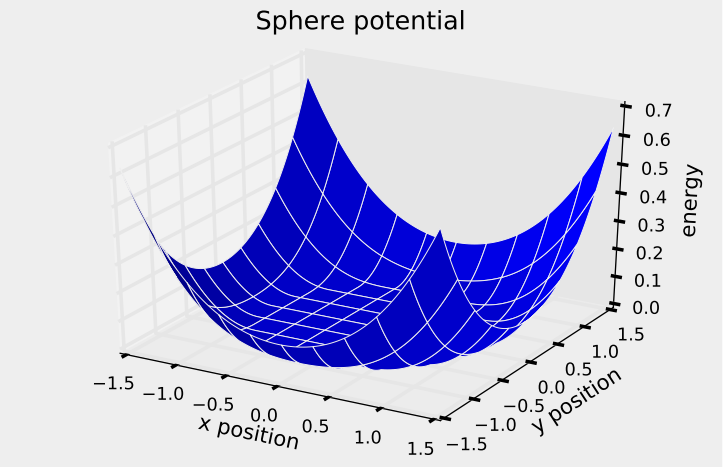
where

$$\eta_t \sim \begin{pmatrix} \mathcal{N}(0,1) & \dots & \mathcal{N}(0,1) \end{pmatrix}^T$$

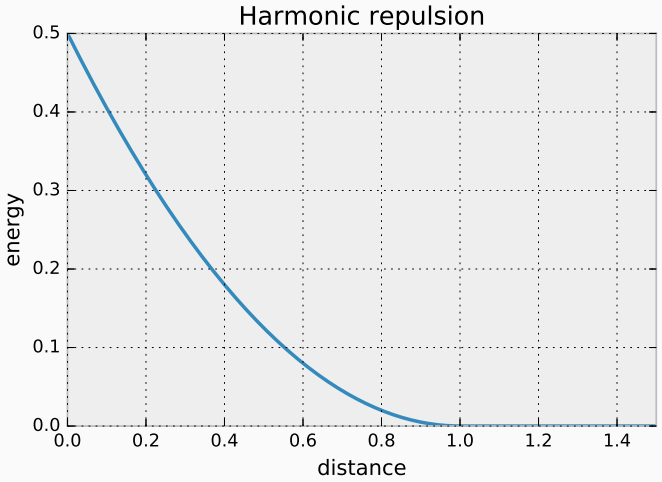
External and pair potentials

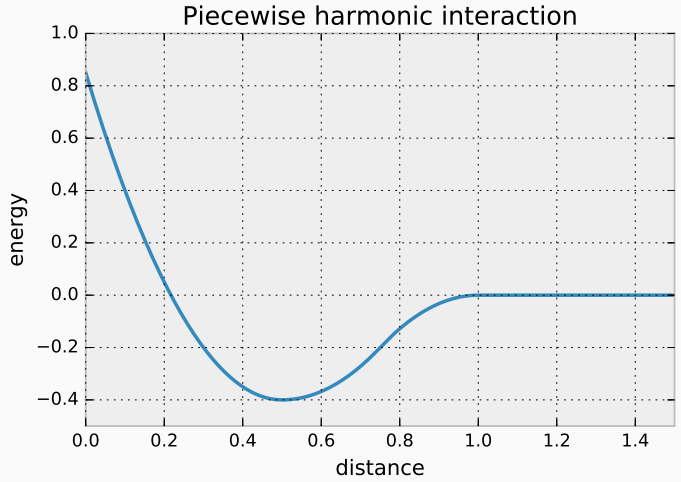
Depending only on the position of a particle:





Depending on the position of two particles relative to each other:





Reactions

Reactions are implemented unidirectionally with microscopic rates:

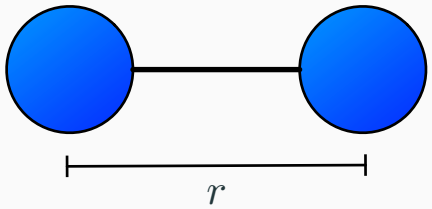
- *Fusion, Fission*: $A_1 +_d A_2 \underset{\lambda_2}{\overset{\lambda_1}{\rightleftharpoons}} B$
- *Conversion*: $A \underset{\lambda_2}{\overset{\lambda_1}{\rightleftharpoons}} B$
- *Enzymatic*: $A +_d C \underset{\lambda_2}{\overset{\lambda_1}{\rightleftharpoons}} B +_d C$
- *Decay*: $A \xrightarrow{\lambda} \emptyset$

If there is more than one educt, the particles have to be closer than d so that the reaction can occur.

Bonds, Angles, Dihedrals

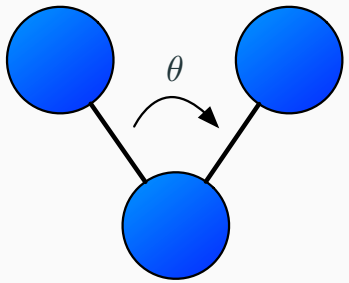
Harmonic bonds

$$V_{\text{bond}} = k(r - r_0)^2$$



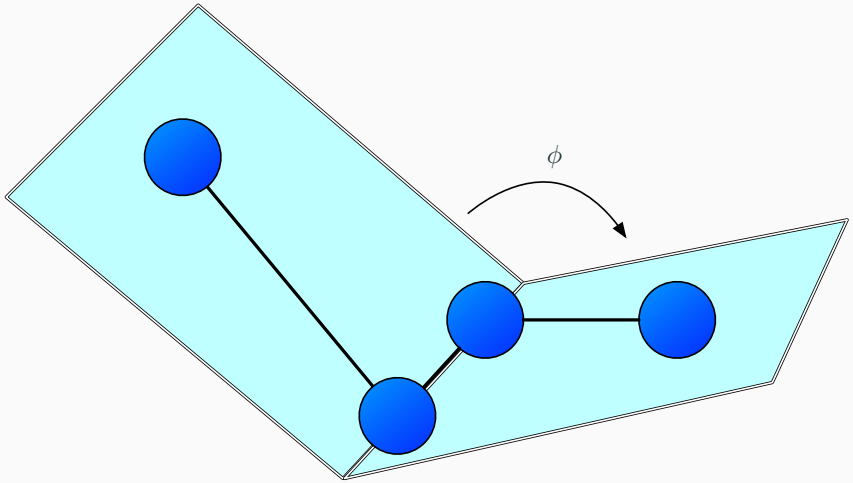
Harmonic angles

$$V_{\text{angle}} = k(\theta - \theta_0)^2$$



Proper dihedrals

$$V_{\text{dihedral}} = k(\phi - \phi_0)^2$$

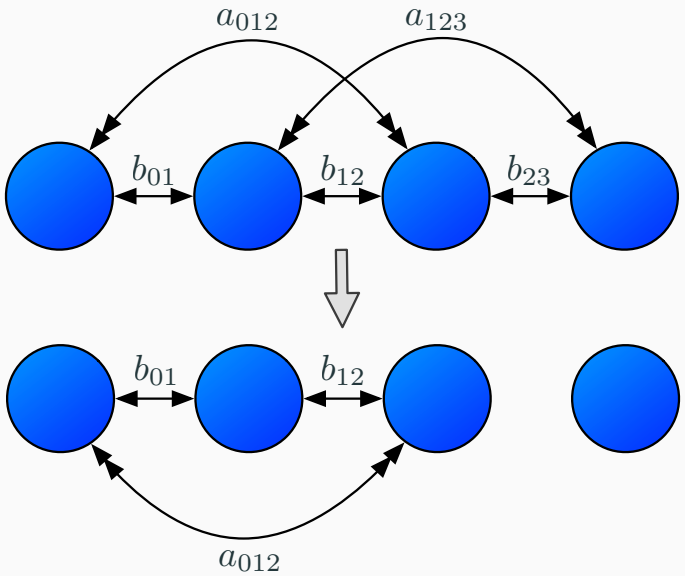


Topology reactions

There are two types of possible topology reactions:

- “Fission-type” reactions, in which the inner structure of the topology can change.
- “Fusion-type” reactions, i.e., attaching of particles or merging of two topologies. (not yet implemented)

The structural changes are applied via the topology’s connectivity graph, e.g.,



Handling reactions

Uncontrolled Approximation

1. Gather a list of possible reactions
2. Shuffle the list
3. For each reaction: If the educts are still present, execute it and proceed

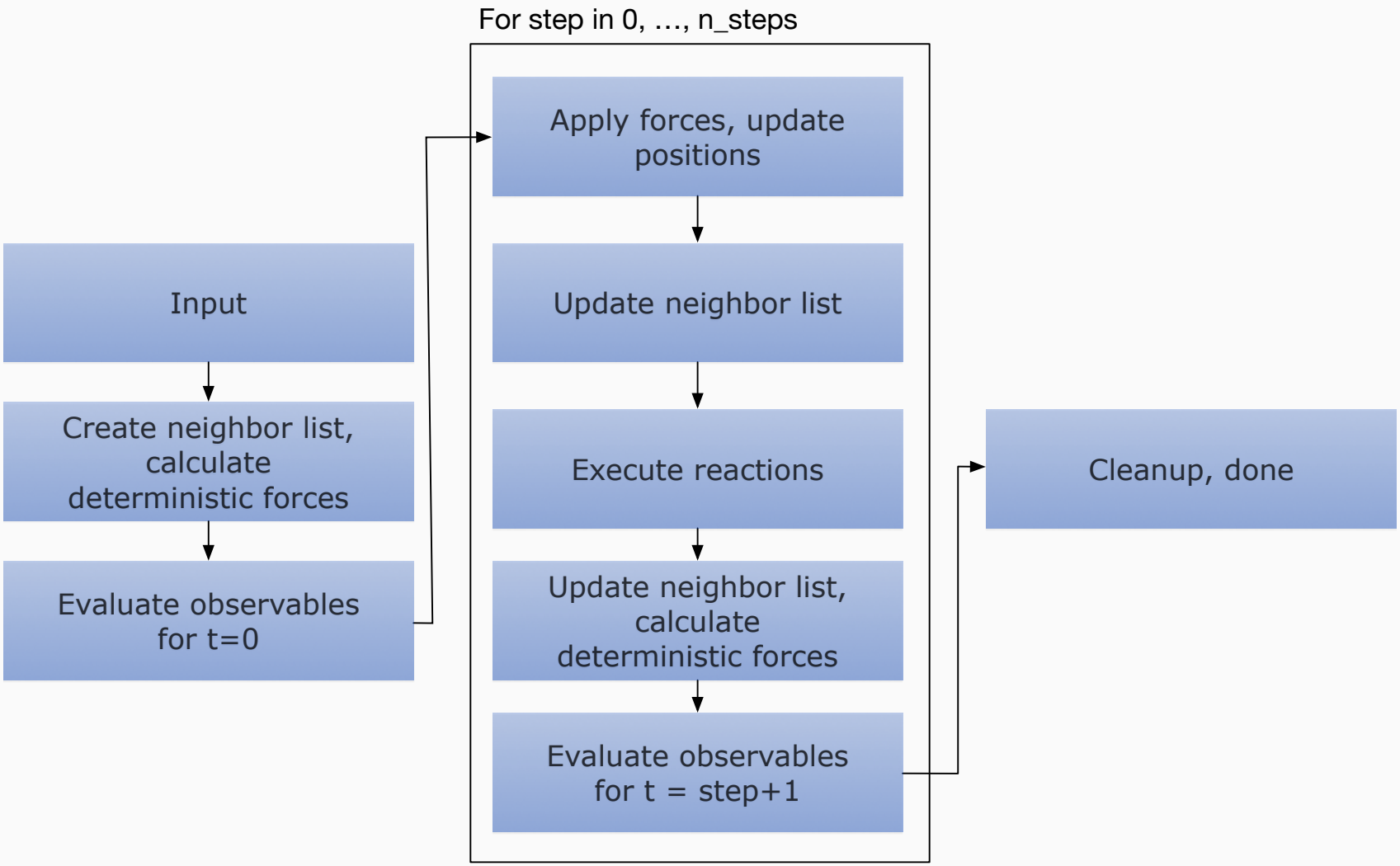
Gillespie reaction order

1. Gather a list of possible reactions events
2. Weight each event by its rate
3. Select and execute an event based on the weighted list
4. Remove the event (and all conflicting ones), repeat.

Example conflict:

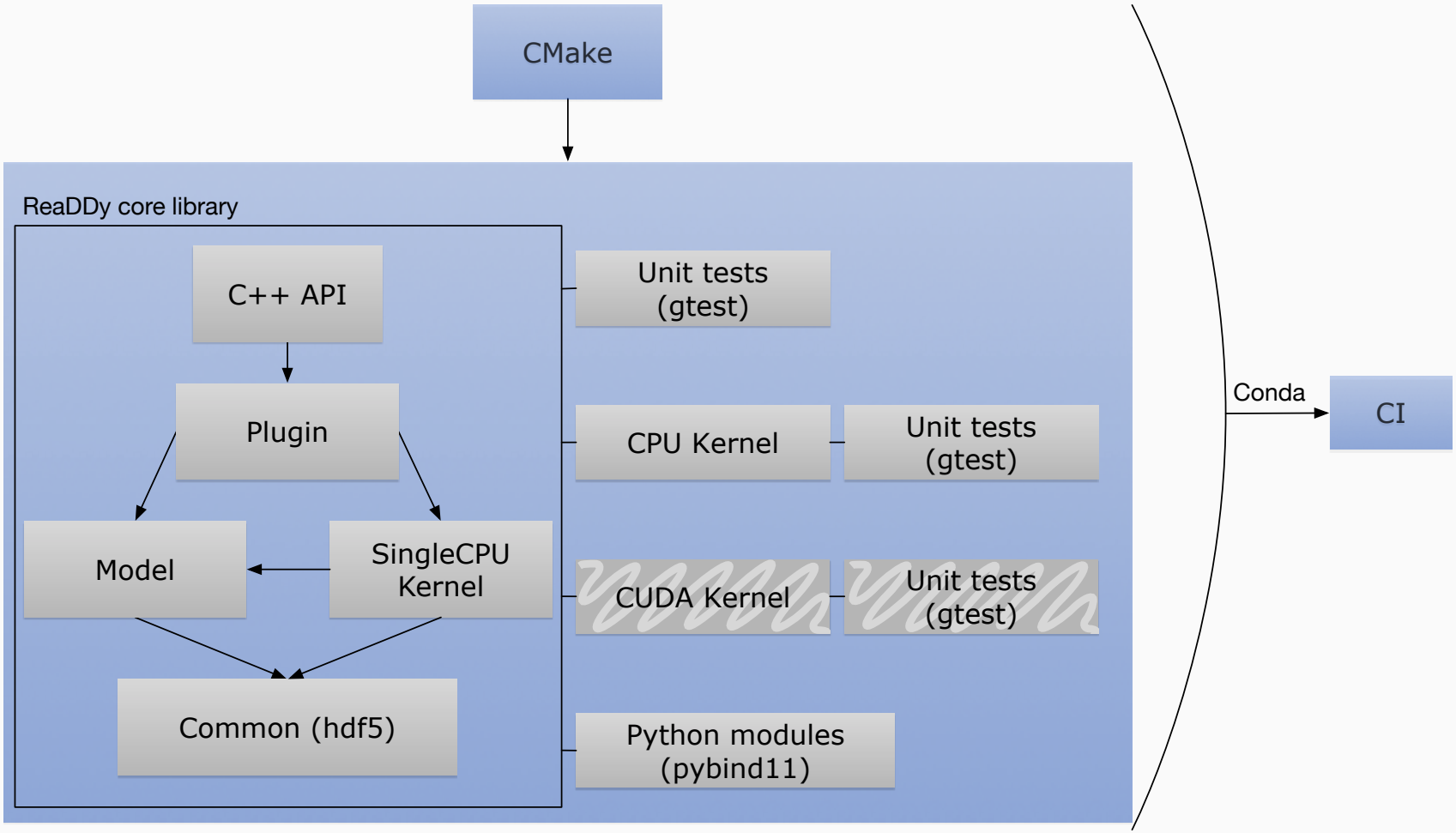
$$\left\{\begin{array}{rcl} A+B & \rightharpoonup & C \\ A & \rightharpoonup & D \end{array}\right. \rightarrow \left\{\begin{array}{rcl} A+B & \rightharpoonup & C \\ \cancel{A} & \cancel{\rightharpoonup} & \cancel{D} \end{array}\right.$$

The default simulation loop

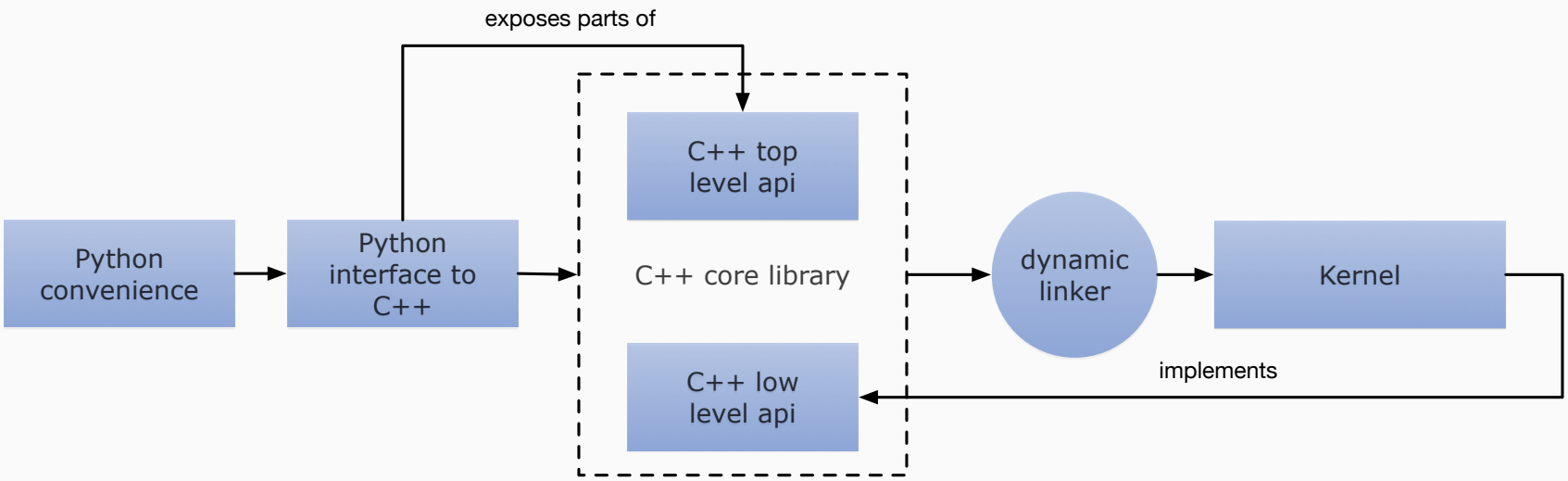


Architecture

Build and execution

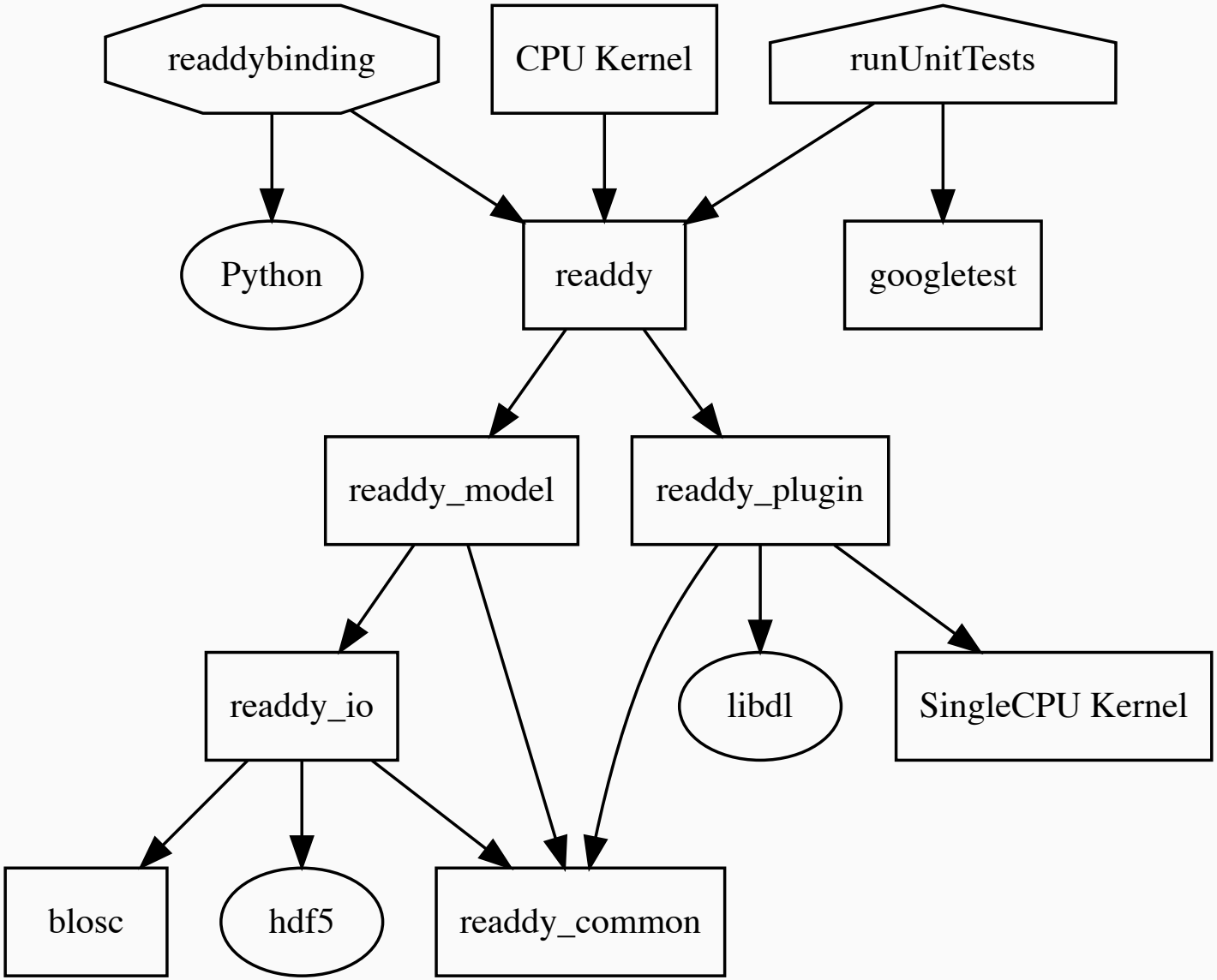


Software structure



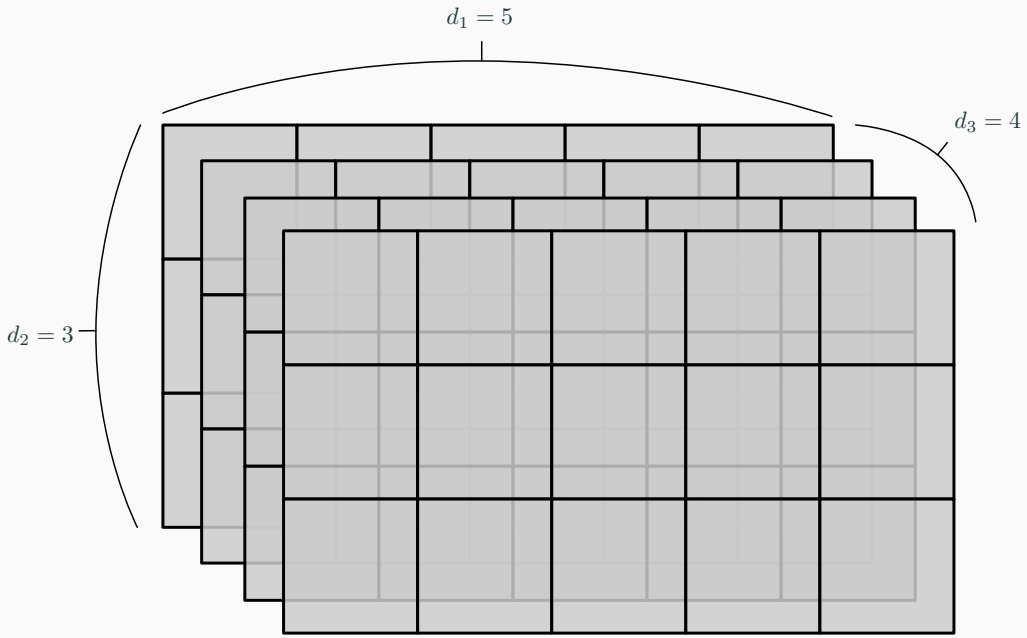
- Python interface as well as Kernels (with the exception of SingleCPU) are optional
- Kernels (with the exception of SingleCPU) can be loaded at runtime

CMake dependency graph



HDF5? Blosc?

- HDF5:
  - File format that offers a file tree like structure, data is stored binary in extensible tensors.
  - Data sets can be compressed, allows for variable length dimensions



- Blosc metacompressor: Perform compression on chunks that fit into the CPU L1 cache.

The kernels

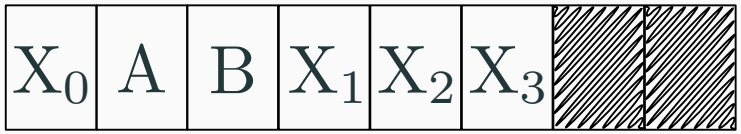
SingleCPU Kernel

- always included in the software package
- always runs with exactly one thread
- internal data structures are exposed to python
- can be used for prototyping

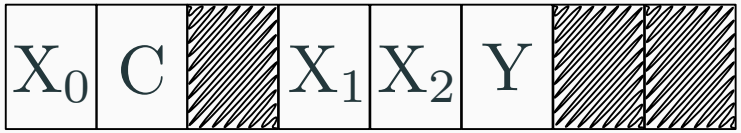
```
# extends the c++ abstract class PotentialOrder2
class MyPot2(pr.PotentialOrder2):
    def __init__(self):
        super(MyPot2, self).__init__("my pot 2")
    def calculate_energy(self, x_ij):
        return np.sqrt(x_ij * x_ij)
    def calculate_force(self, x_ij):
        return .5 * x_ij
# register the python defined potential in the c++ library
context.register_potential_order_2(MyPot2(), "A", "B")
```

CPU Kernel

- employs shared-memory thread-pool based parallelization for neighbor list, integrator, and (sort of) reaction handler
- persisting indices make the construction of Verlet lists easier
- particle indices persist between time steps when particle number changes due to “ghost” particles
  1. Initial situation:



  2. Reactions $A + B \rightharpoonup C$ and $X_3 \rightharpoonup Y$ occur:



ReaDDy outlook / todos

Outlook / todos

- Topology fusion reactions
- Descriptor language for reactions like

myReaction:A+(r)B ->(k) C

- Mohsen's membrane model (more about that tomorrow)
- Snapshotting
- GPU and MPI kernel
- high-level python API