Adaptive Multilevel Splitting Method: Isomerization of the alanine dipeptide

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high barrier

metastable states
The AMS algorithm

number of replicas $N=5$

minimum number of replicas to kill at each iteration $k=2$

reaction coordinate $\xi$

and so on...
The AMS algorithm

number of replicas $N=5$

minimum number of replicas to kill at each iteration $k=2$

reaction coordinate $\xi$

How many replicas passed $z_{\text{kill}}$?

$$p^0 = \frac{N3k}{N}$$
The AMS algorithm

\[ p_{AMS} = \frac{r}{N} \prod_{q=1}^{Q_{iter}} p^{q-1} = \frac{r}{N} \prod_{q=1}^{Q_{iter}} \left( \frac{N - k^q}{N} \right) \]

The expected value is unbiased towards the choice of the algorithm parameter!
How to obtain the transition time?
How to obtain the transition time?

\[ T_{AB} = \sum_{k=1}^{n} T_{\text{loop}}^k + T_{\text{reac}} \]
How to obtain the transition time?

The secret lies in the initial conditions!

$$\mathbb{E}(T_{AB}) = \left(\frac{1}{p} - 1\right) \mathbb{E}(T_{\text{loop}}) + \mathbb{E}(T_{\text{react}})$$
Isomerization of the alanine dipeptide
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\[ \xi(\varphi, \psi) = \min(d_A, 6.4) - \min(d_B, 3.8) \]
Hands-on!

Tcl, bash and C programs make your life easier!
The files to provide

```plaintext
# STANDARD NAMD SETTING #

set temperature 300
set path /home/laurajoana/Desktop/cernics/dtalanine/tutoriel/common

paraTypeCharmm on parameters ${path}/par_all27_prot_lipid.inp
structure ${path}/A.psd
coordinates ${path}/A.pdb

exclude scaled1-4
1-4scaling 1.0
cutoff 12.0
switching on
switchdist 10.0
pairlistdist 14
timestep 1.0
rigidbonds all
nonbondedFreq 1
fullElectFrequency 2
stepspercycle 5 # flxed!!!

langevin on
langevinDamping 1.0
langevinTemp $temperature
langevinHydrogen on
langevinPiston off

# COLVAR SETTINGS #

# COLVARS module is used to measure the reaction coordinate
colvars on
colvarsConfig ${path}/dihedral_20.colv
```
The files to provide

\begin{verbatim}
proc ams_measure { } 
proc zone { } 
proc variables { }
\end{verbatim}

Colvars is practical!
The files to provide

```bash
# conf file to run ams in parallel
path="/home/laurajoana/Desktop/cermics/dialanine/tutoriel"
outdir="${path}="/1-point/ams2"
tokill="1"
amstype="single"
numinst="10"
numrep="100"
zmax="4.90"
timelimit="240"
icprefix="${path}="/1-point/point"
zone="${path}"/common/inzone.tcl"
measure="${path}"/common/coord.tcl"
variables="${path}"/common/variables.tcl"
inifile="${path}"/common/namd.conf"
amsteptime="20"
parallel="8"
getpaths="on"
charmrnpe="0"
removefiles="yes"
```
The tutorial

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The tutorial

Probability from one point
Transition time
Flux of reactive trajectories
Thanks to Chris Chipot, Tony Lelièvre and Jérôme Hénin!

Good luck!

I’m here to answer your questions.