Adaptive Multilevel Splitting Method: Isomerization of the alanine dipeptide

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Advisors:

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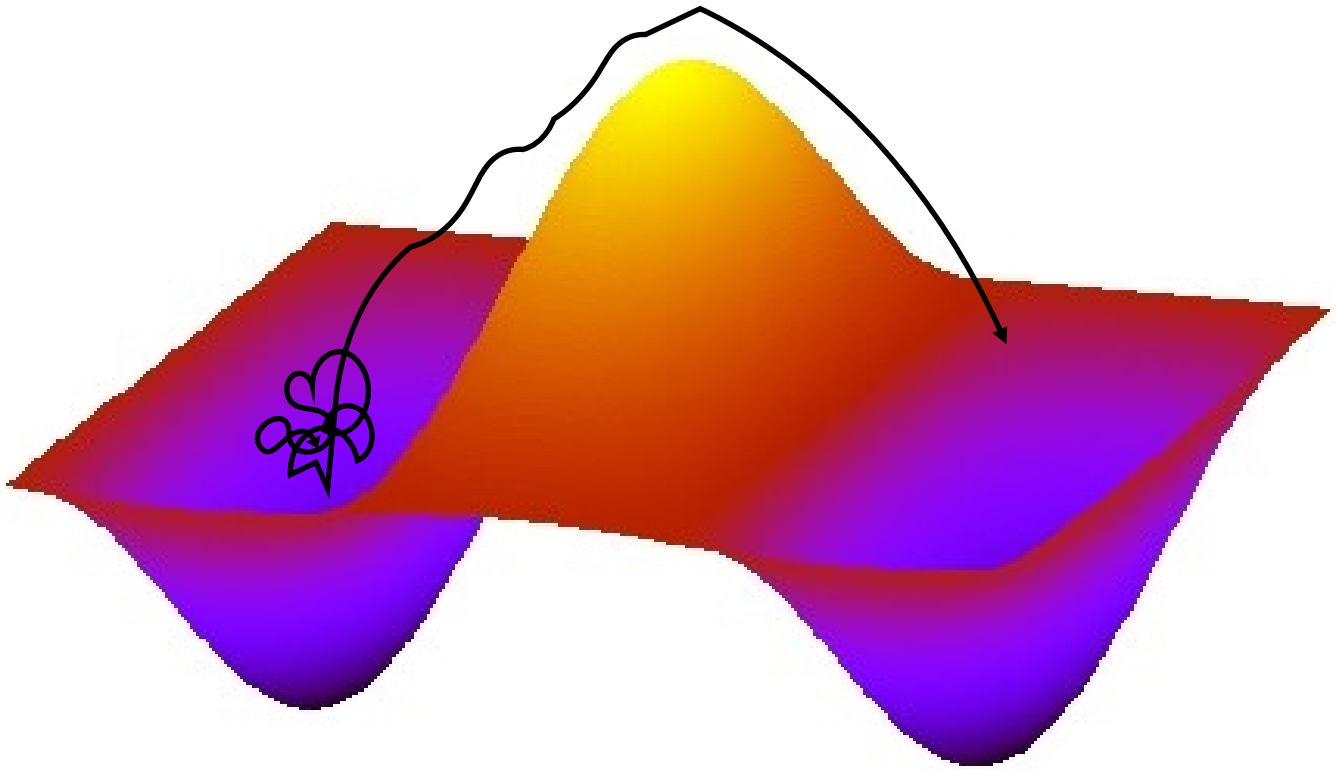
high barrier

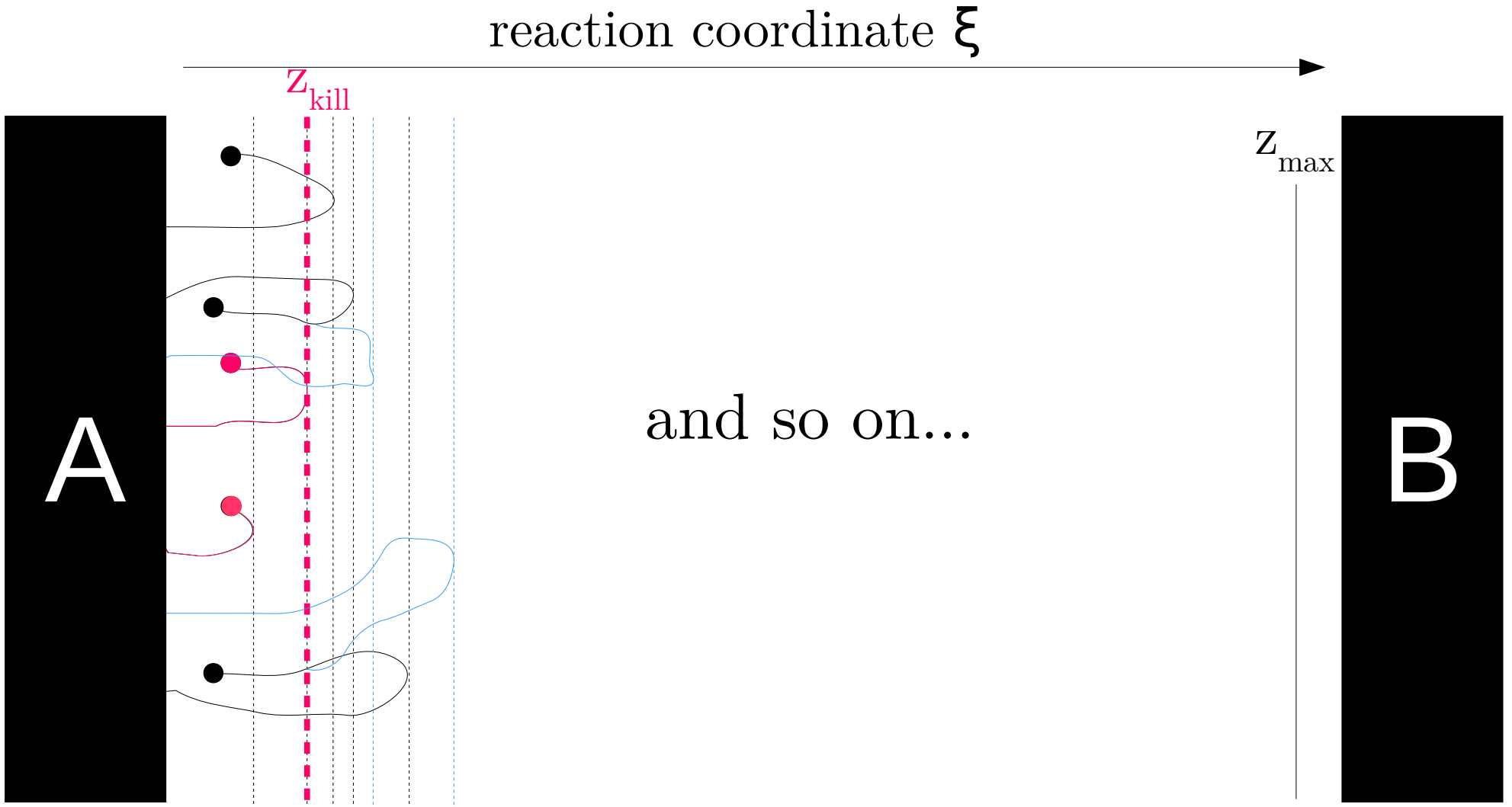


metastable states

The AMS algorithm

number of replicas N=5

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



The AMS algorithm

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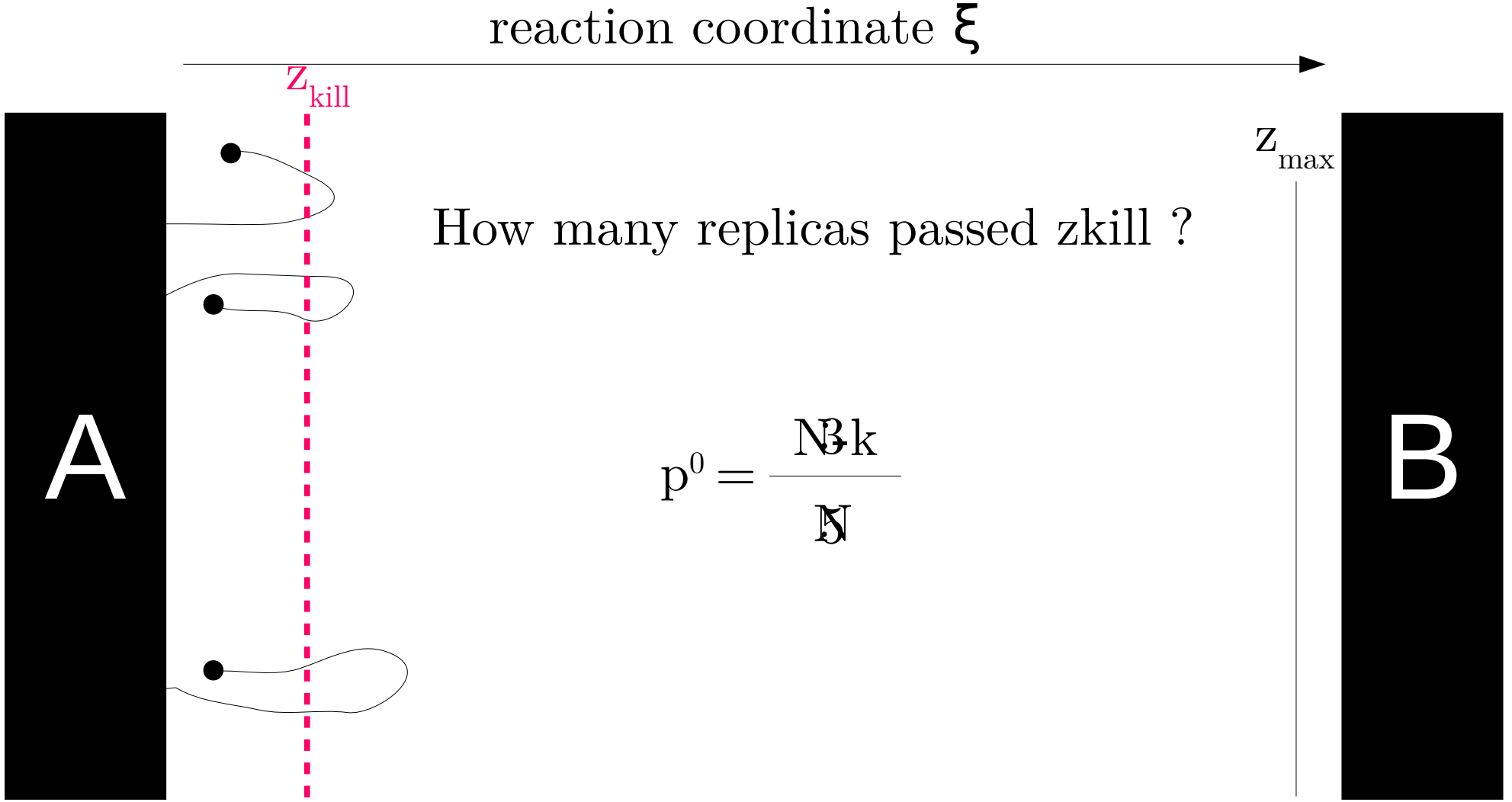
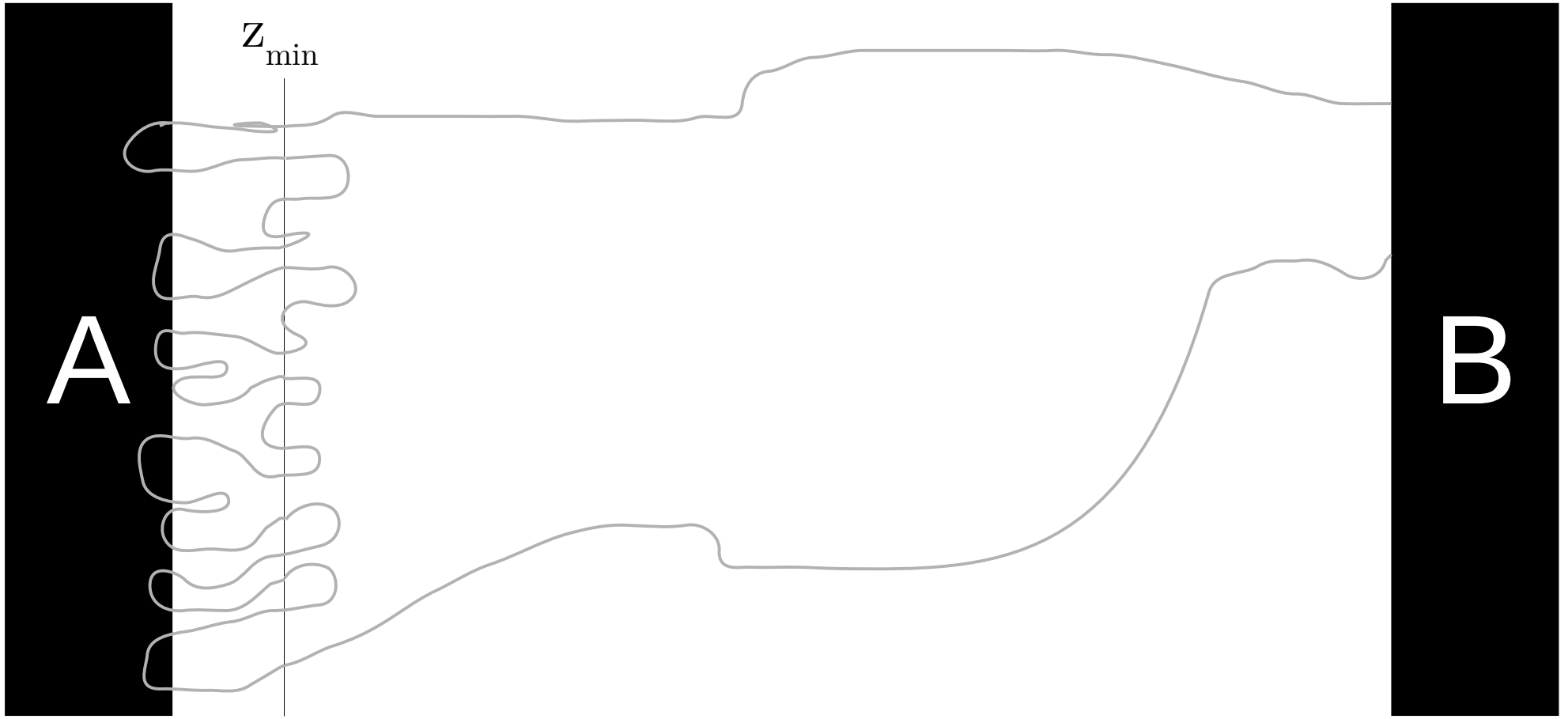


The AMS algorithm

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

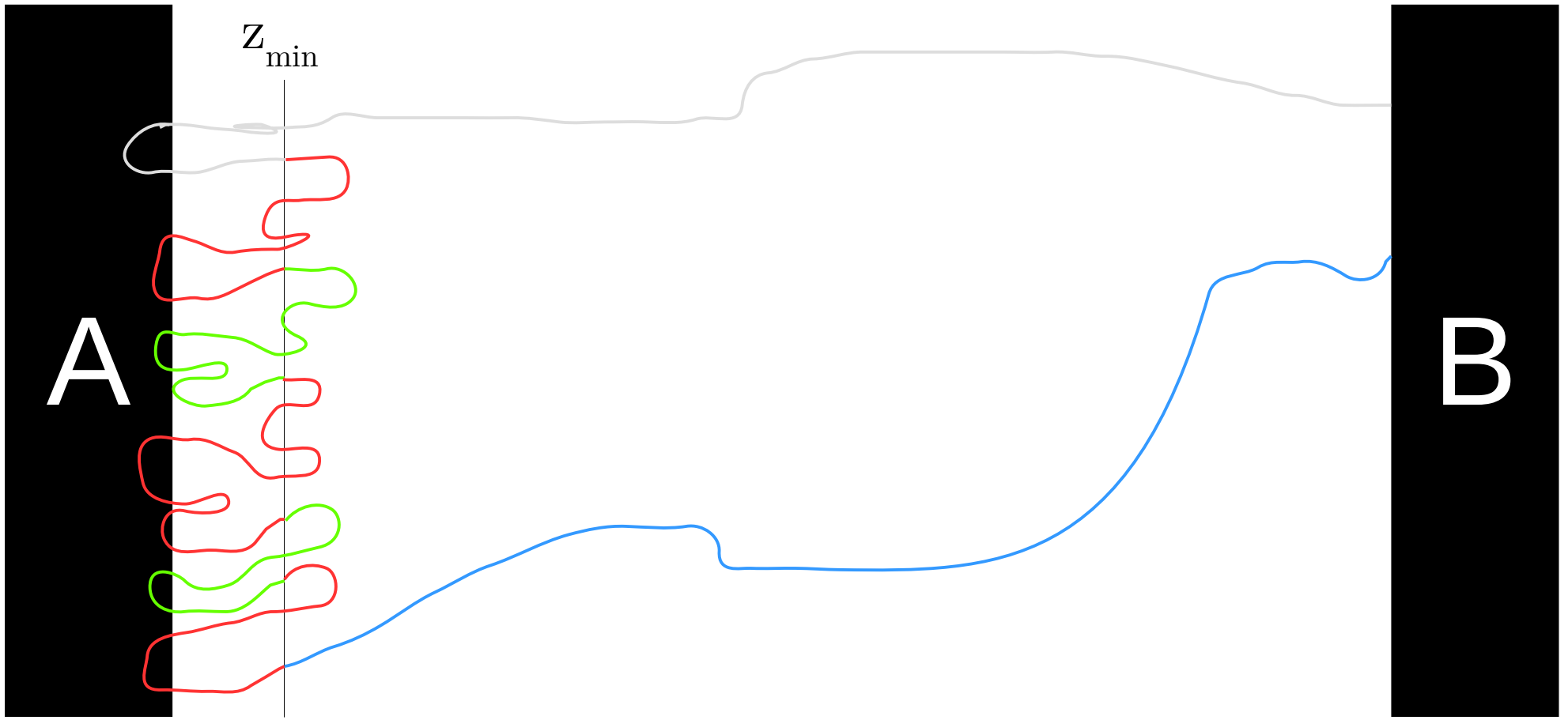
The expected value is unbiased towards the choice of the algorithm parameter !

How to obtain the transition time?



How to obtain the transition time?

$$T_{AB} = \sum_{k=1}^{\overset{?}{n}} T_{\text{loop}}^{k} + T_{\text{reac}}$$

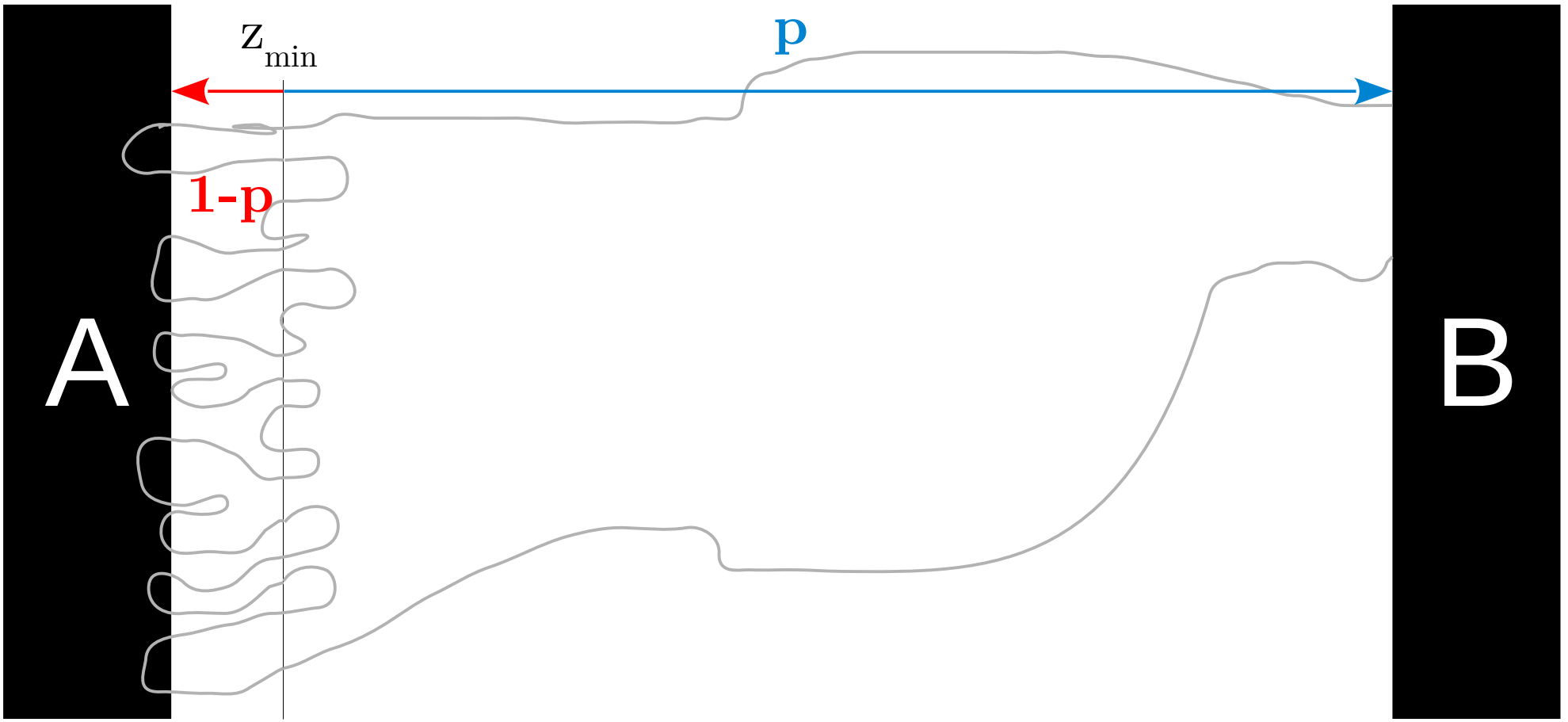


How to obtain the transition time?

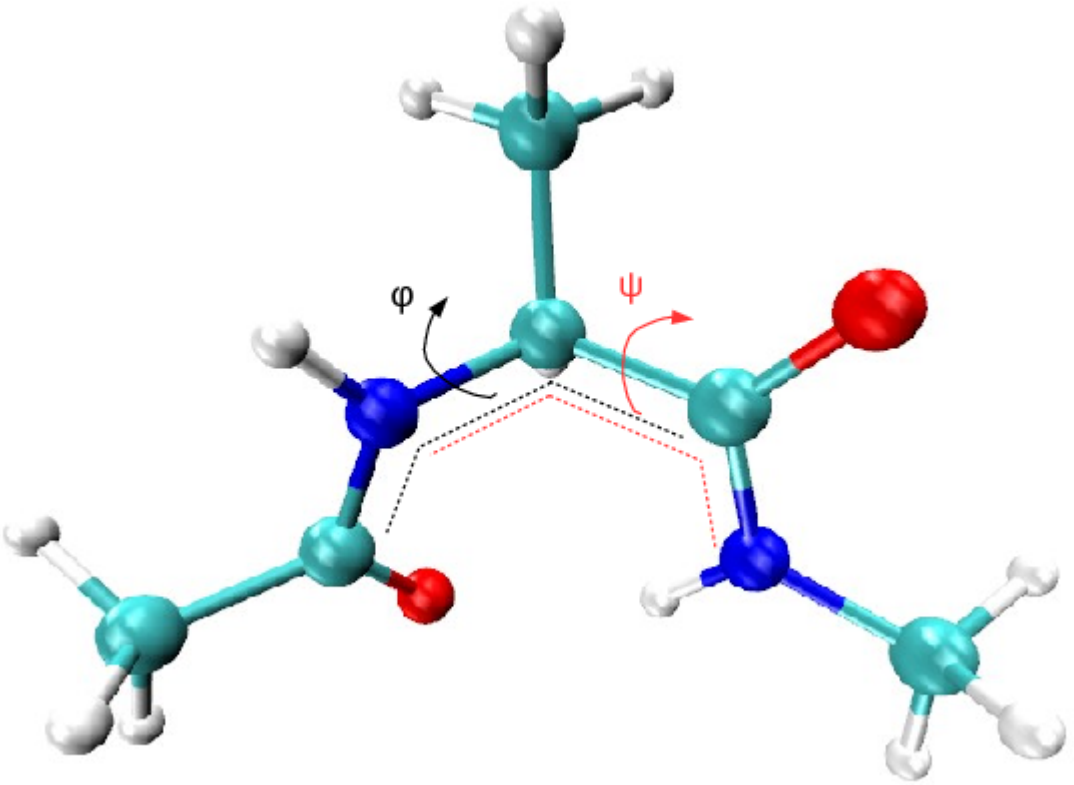
The secret lies in the initial conditions !

$$\mathbb{E}(T_{AB}) = \left(\frac{1}{p} - 1\right) \mathbb{E}(T_{\text{loop}}) + \mathbb{E}(T_{\text{reac}})$$

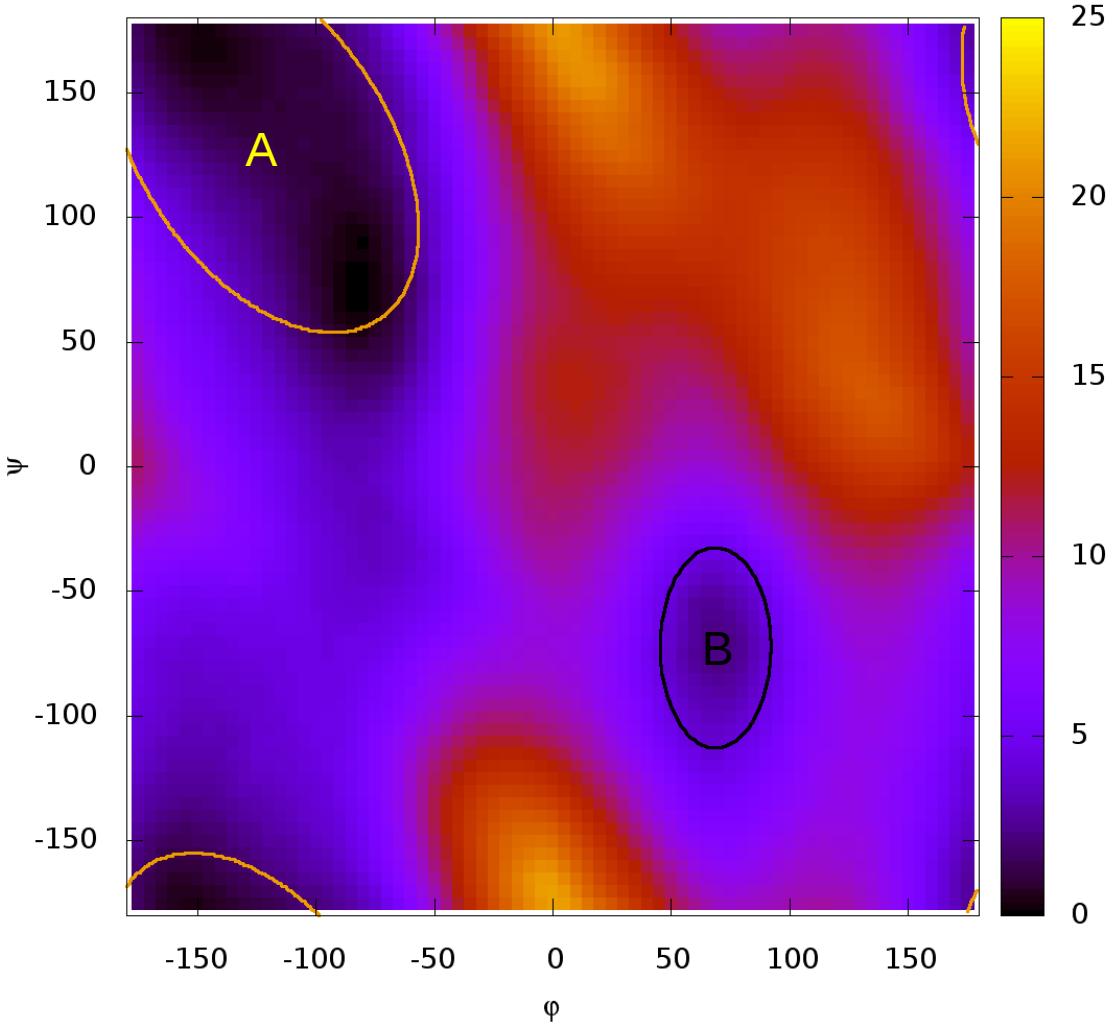
AMS

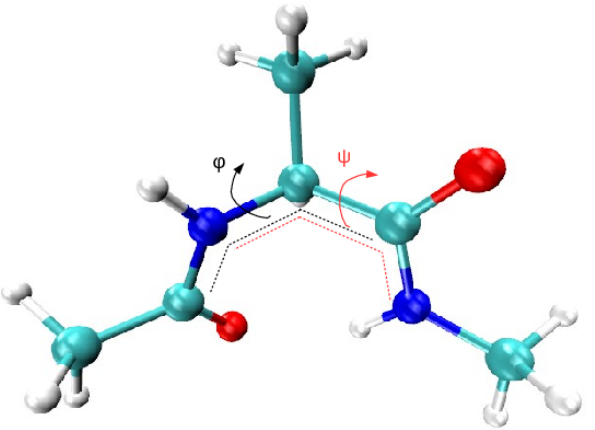


Isomerization of the alanine dipeptide

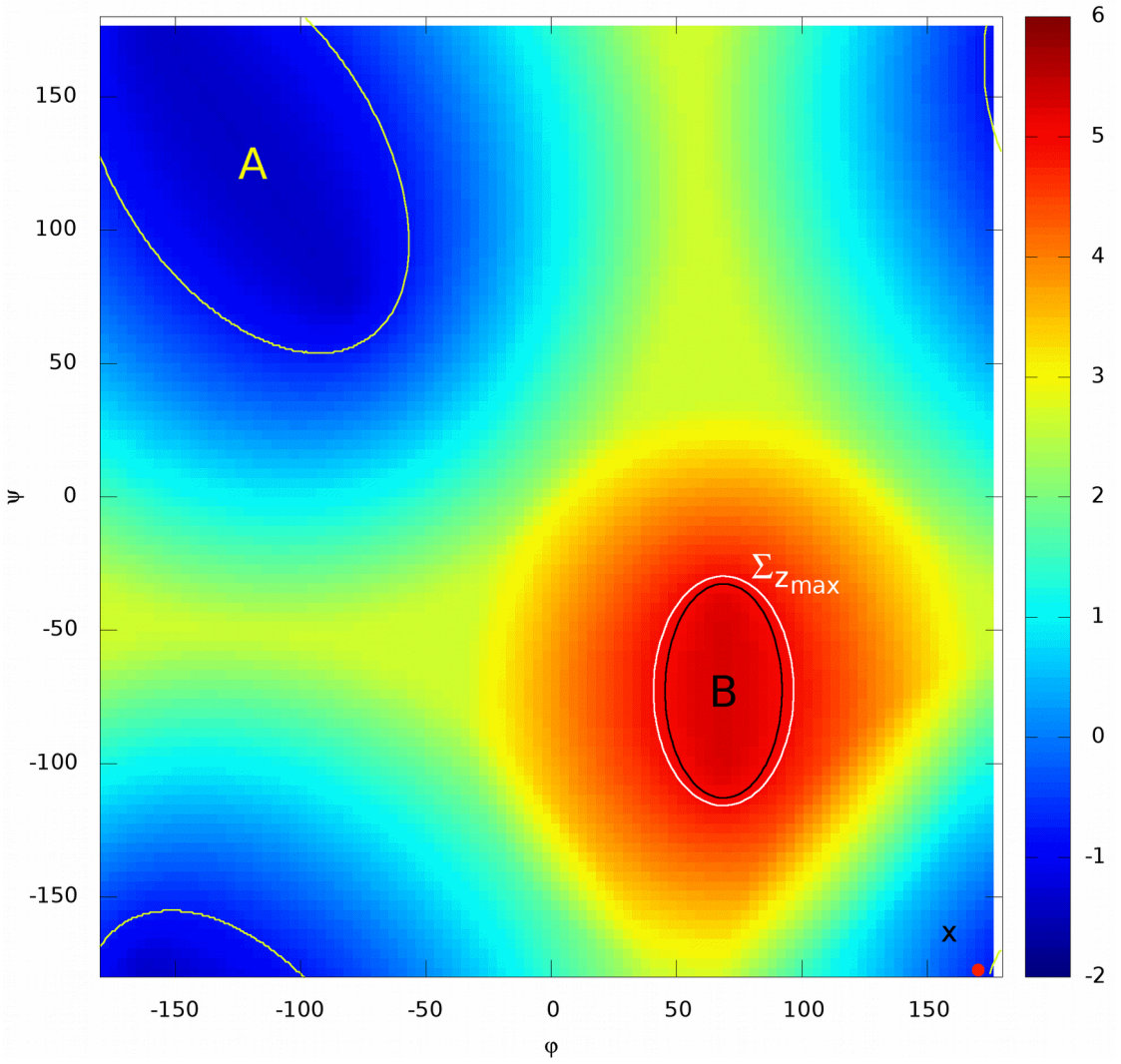


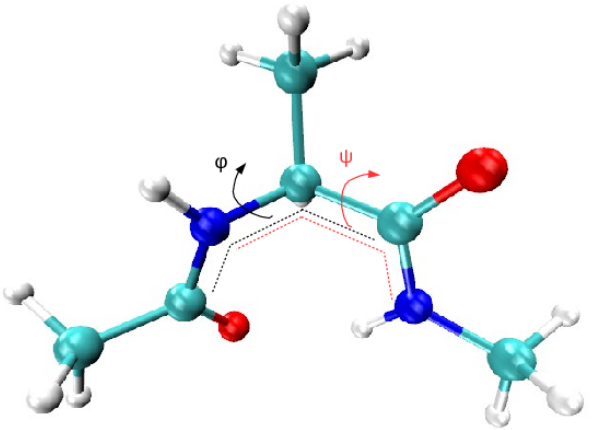
Isomerization of the alanine dipeptide





Isomerization of the alanine dipeptide





$$\xi(\varphi, \psi) = \min(d_A, 6.4) - \min(d_B, 3.8)$$

Hands-on !

Tcl, bash and C programs make your life easier !

The files to provide

```
##############################################################################
#                          STANDARD NAMD SETTINGS                            #
##############################################################################

set temperature 300
set path        /home/laurajoana/Desktop/cermics/dialanine/tutoriel/common

paraTypeCharmm          on
parameters              ${path}/par_all27_prot_lipid.inp
structure                           ${path}/A.psf
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 # fixed!!!

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

```
proc ams_measure { }
proc zone { }
proc variables { }
```

Colvars is practical !

The files to provide

```
# 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=${path}"/common/variables.tcl"
initfile=${path}"/common/namd.conf"
amssteptime="20"
parallel="8"
getpaths="on"
charmrunp="0"
removefiles="yes"
```

`smart_parallel.sh`

The tutorial

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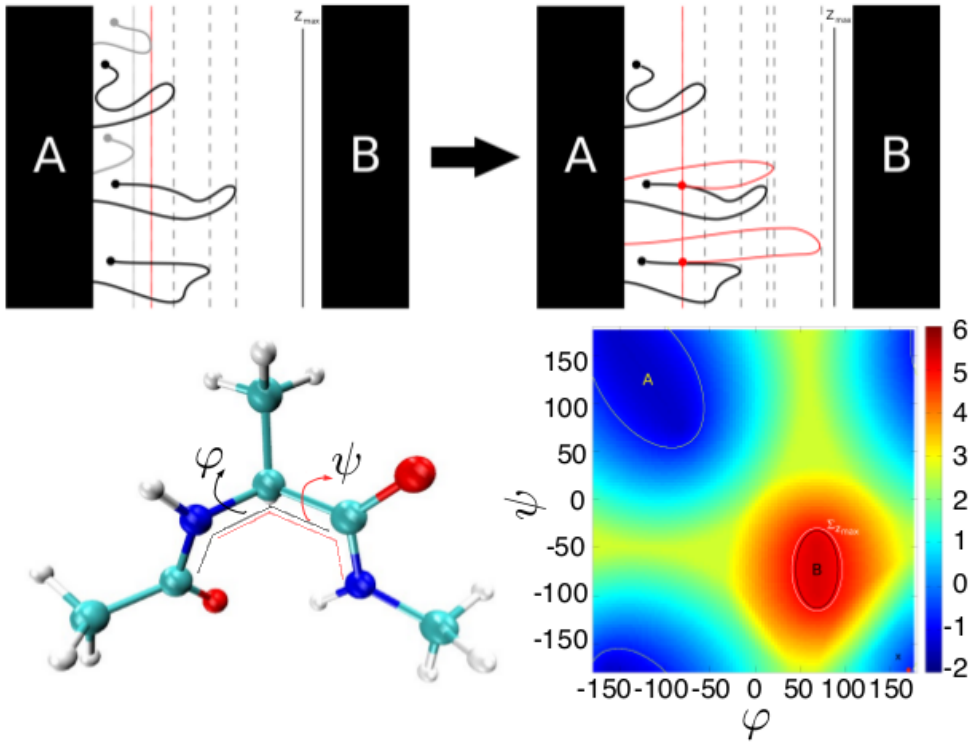

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Christophe Chipot
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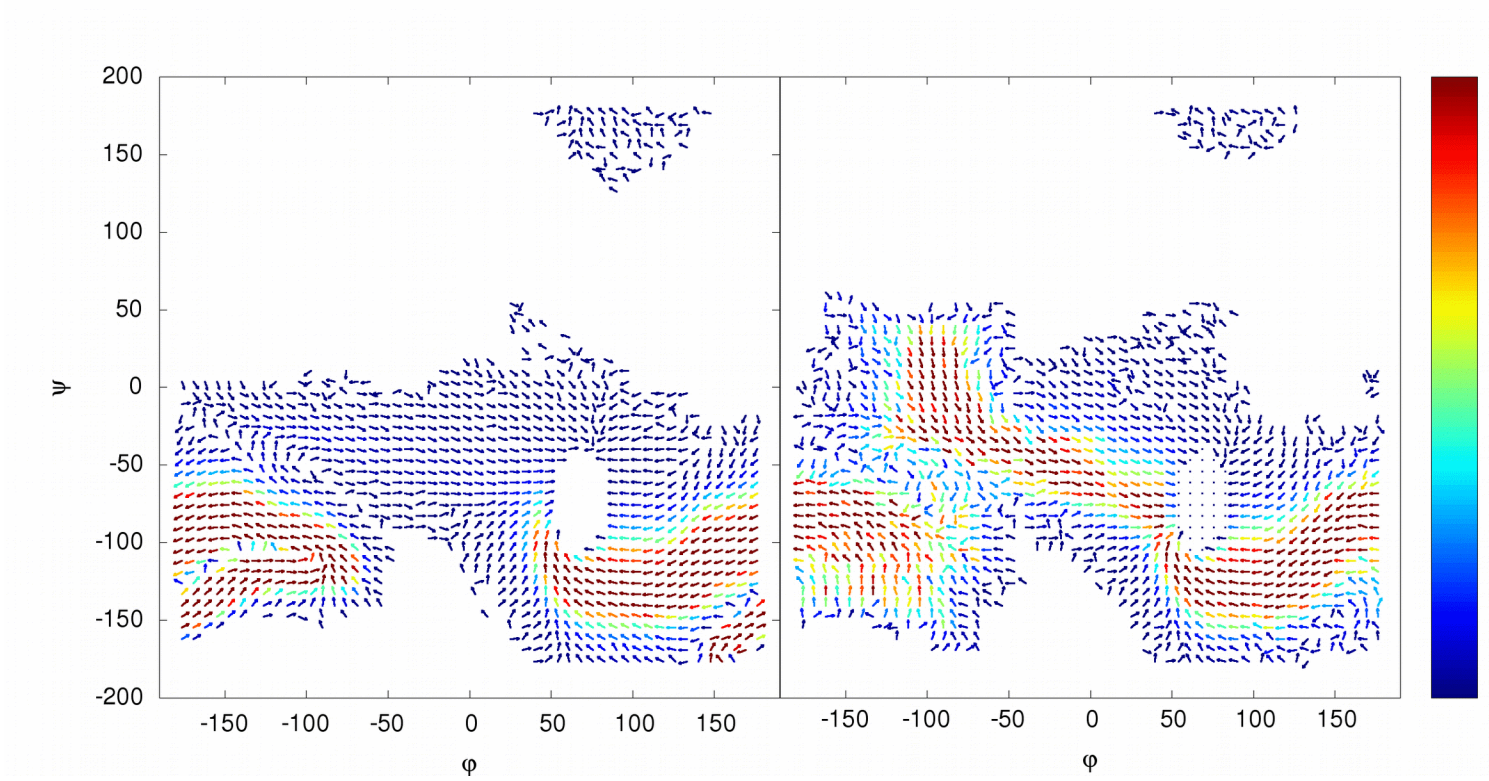
September 25, 2017

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