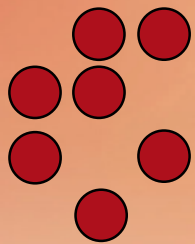
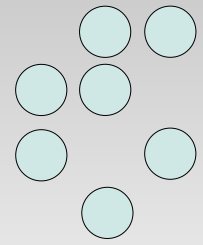

MAX School on Advanced Materials and Molecular Modelling
with QUANTUM ESPRESSO

Chasing saddle points: the NEB method

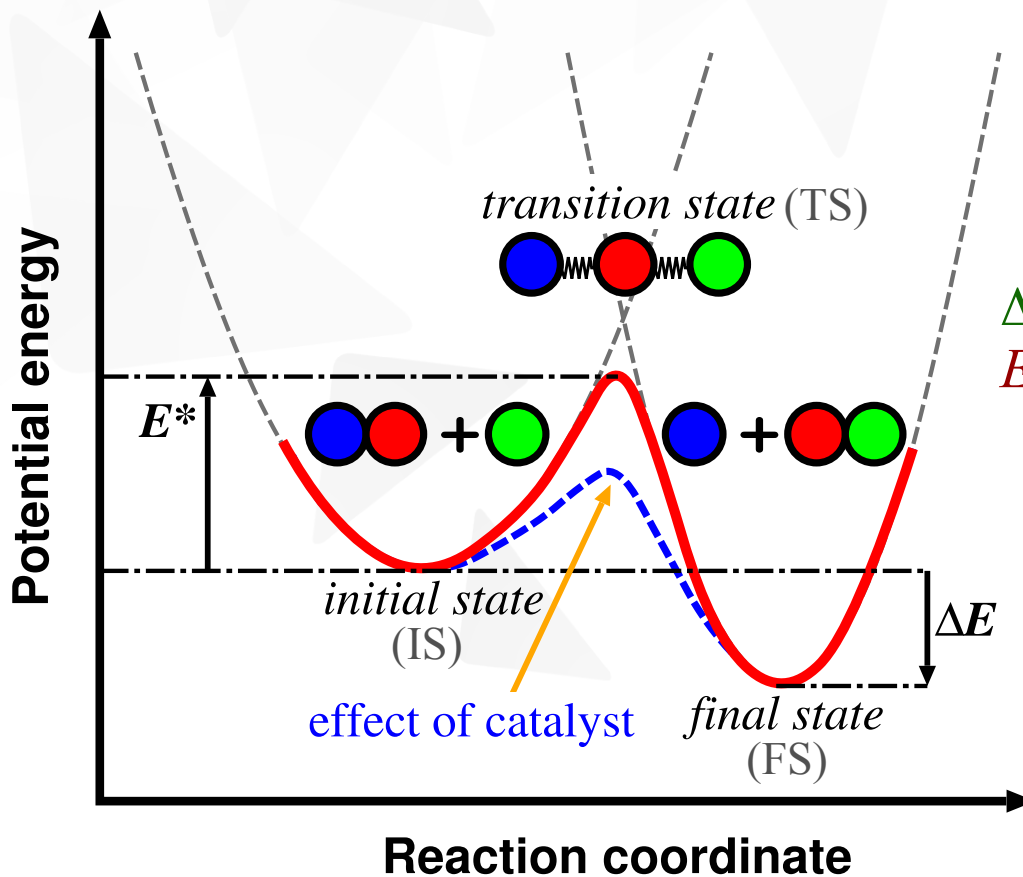


Anton Kokalj
Department of Physical and Organic Chemistry
Jožef Stefan Institute

Chemical reaction



- ▼ **bond-breaking** and **bond-making** → activated process
(there is an energy barrier)



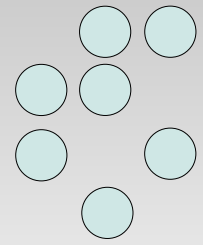
$\Delta E \equiv$ reaction energy → thermodynamics
 $E^* \equiv$ activation energy → kinetics

↓
reaction rate constant:

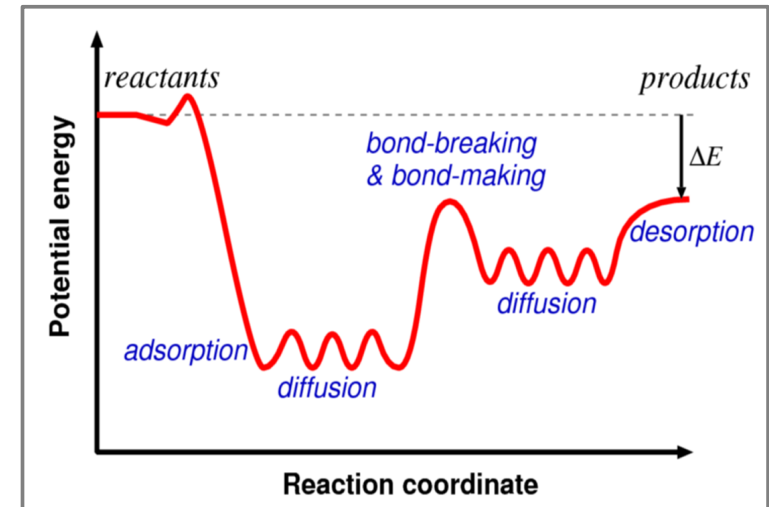
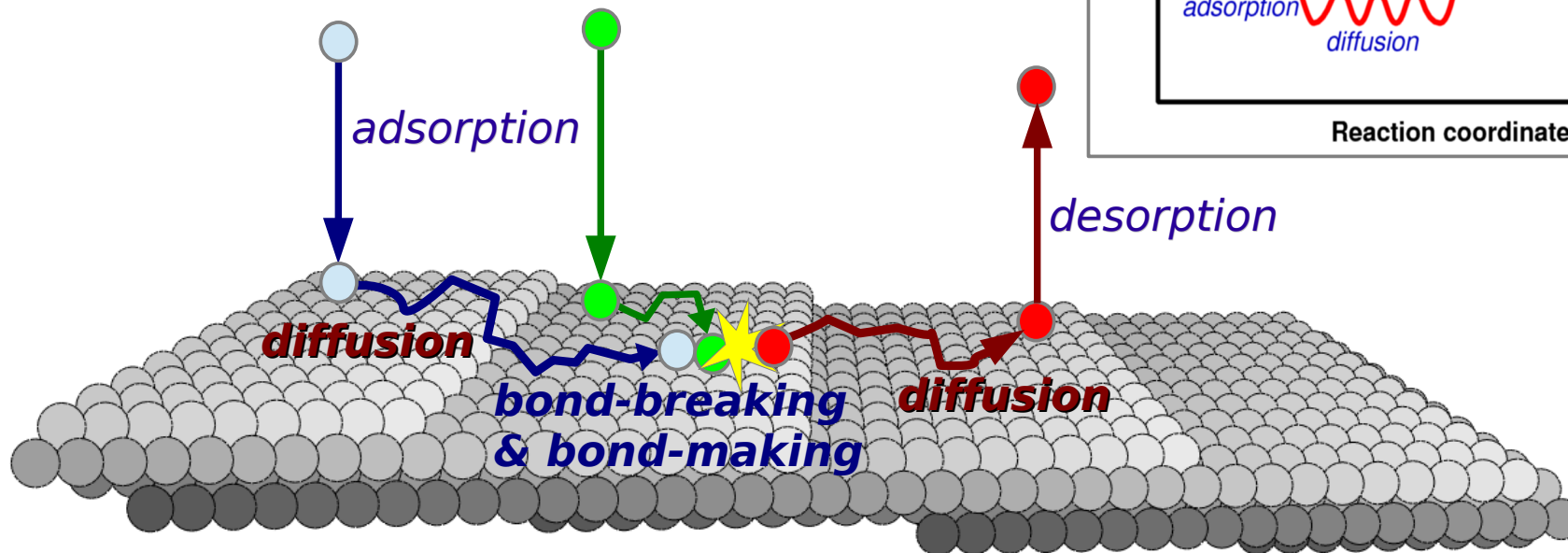
$$k = \nu \exp(-E^*/kT)$$

$$\nu = \frac{\prod_j^{3N} \nu_j^{\text{IS}}}{\prod_j^{3N-1} \nu_j^{\text{TS}}}$$

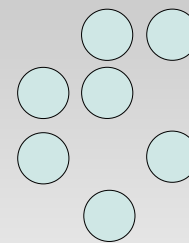
Heterogeneous catalysis



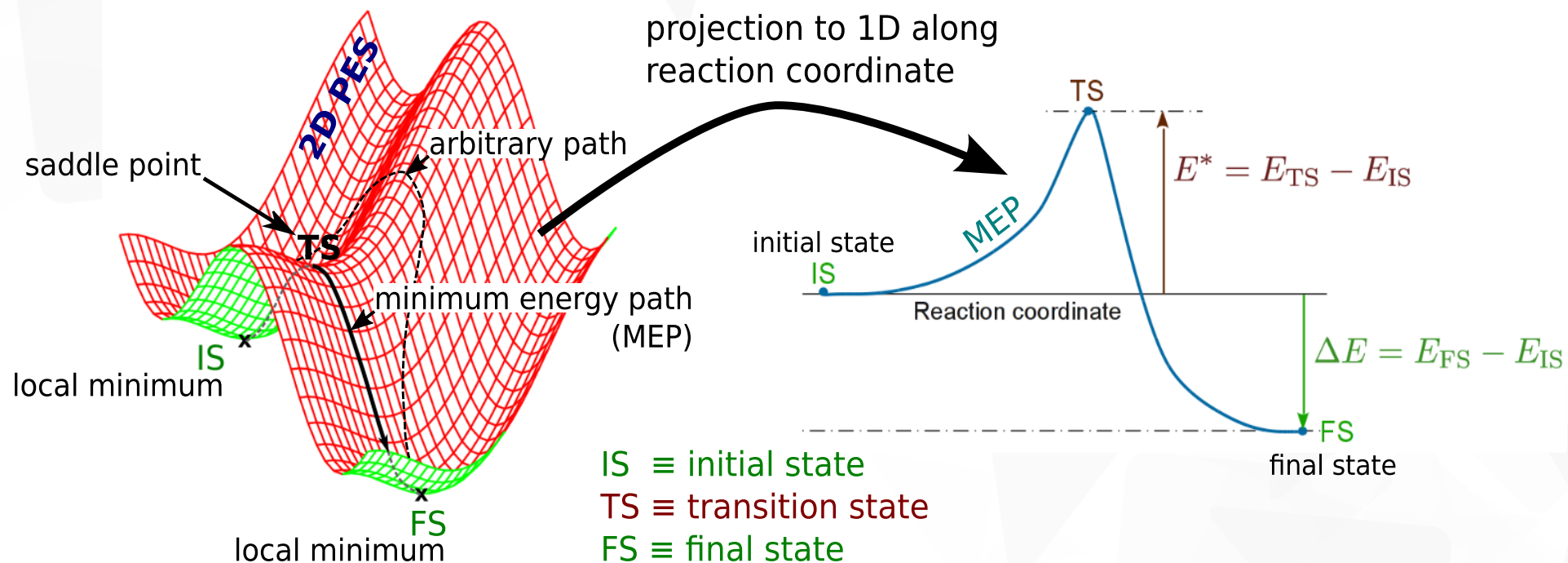
Langmuir-Hinshelwood mechanism



Elementary activated reaction step

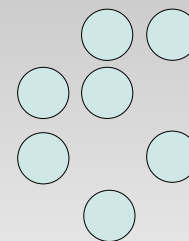


- potential energy surface (PES) is highly multidimensional (except for trivial examples)

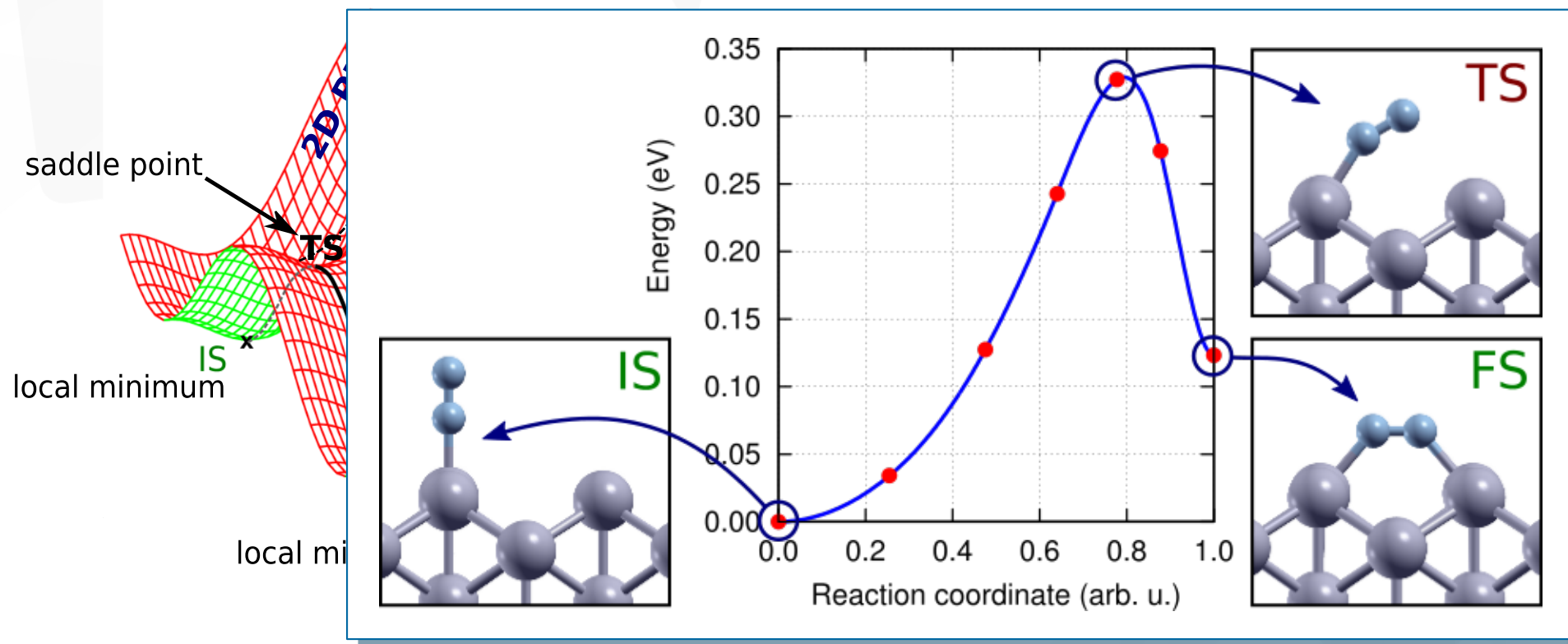


saddle points are unstable configurations and their location is a difficult task

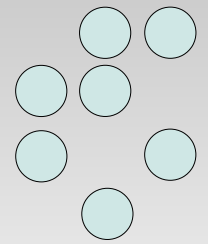
Elementary activated reaction step



- potential energy surface (PES) is highly multidimensional
(except for trivial examples)



Why is activation energy so important



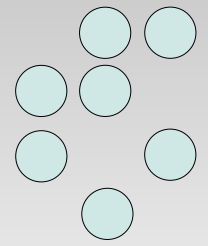
- ▶ Activation energy is a very good criterion to tell if a given activated process (or chemical reaction) is kinetically feasible at given temperature or how fast is it ...

- ▶ Reaction rate constant: $k = \nu \exp(-E^* / kT)$

$$\nu = \frac{\prod_{j=1}^{3N} \nu_j^{\text{IS}}}{\prod_{j=1}^{3N-1} \nu_j^{\text{TS}}} \approx 10^{13} \text{ s}^{-1}$$

- ▶ “Frequency” prefactors ν depend on reaction type (e.g. for desorption $\nu \approx 10^{16} \text{ s}^{-1}$) and were tabulated by V. P. Zhdanov (Surf. Sci. Rep. **12**, 183–242 (1991))

Why is activation energy so important

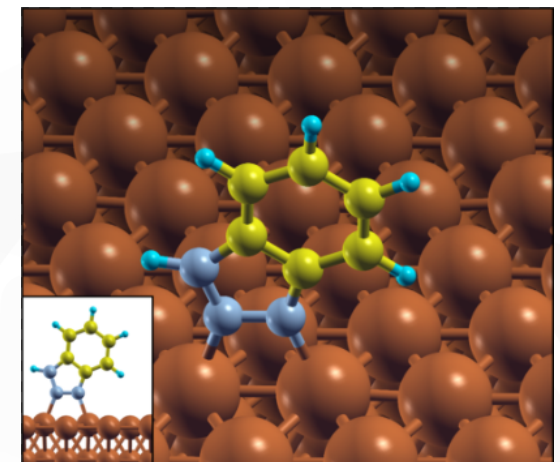


- ▶ Activation energy is a very good criterion to tell if a given activated process (or chemical reaction) is kinetically feasible at given temperature or how fast it is ...
- ▶ **Example:** typical residence time of a molecule with desorption energy (E_{des}) of 0.6 eV on the surface at $T = 300$ K

$$\tau = \nu^{-1} \exp\left(\frac{E_{\text{des}}}{kT}\right) \approx 10^{-6} \text{ s}$$

- ▶ For $E_{\text{des}} = 1$ eV: $\tau = 10$ s

molecule must adsorb stronger than 1 eV to persist on the surface at room T !



$$E_{\text{des}} = 0.60 \text{ eV}$$

Jargon terminology – “image”

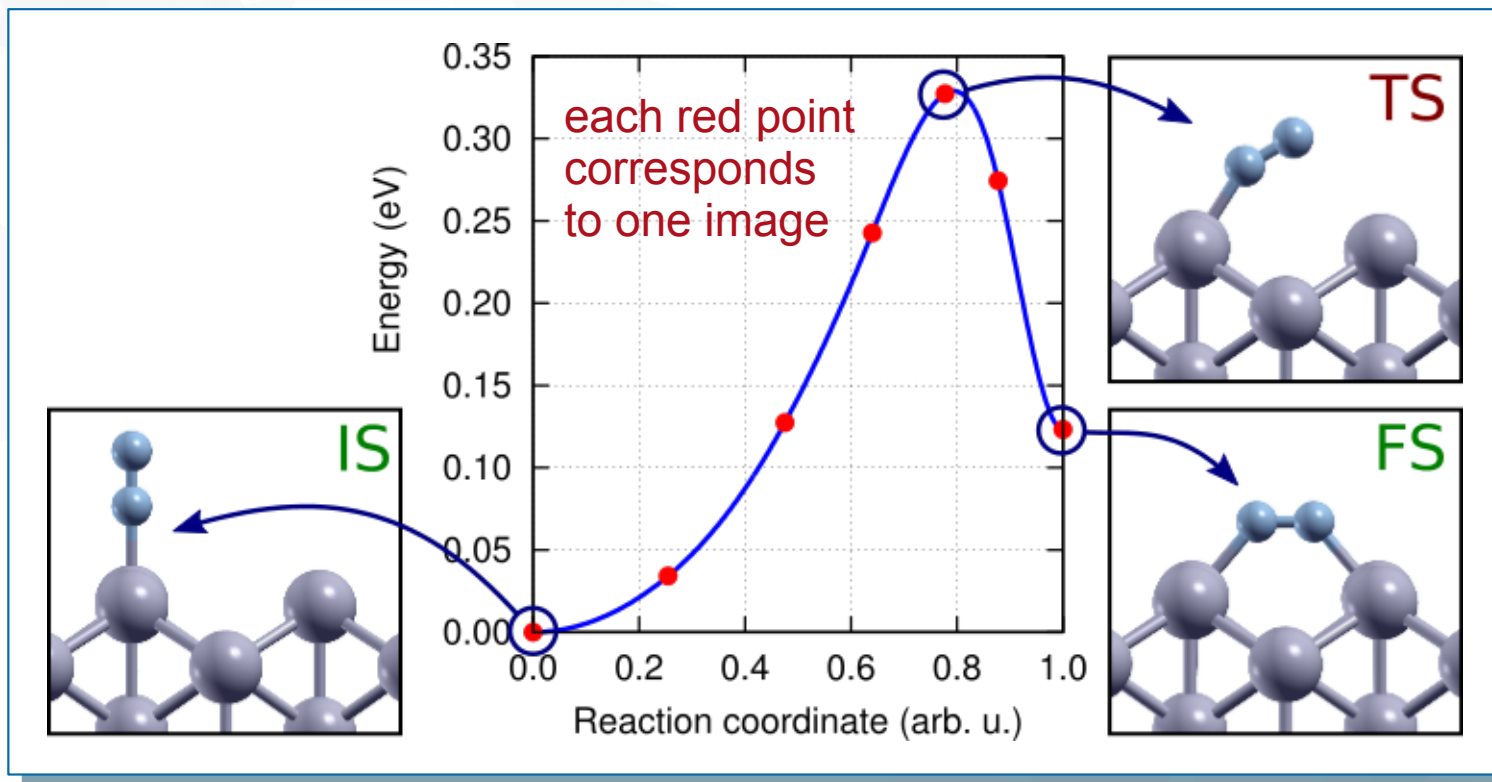
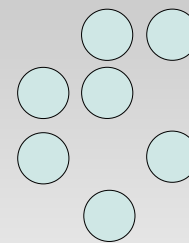
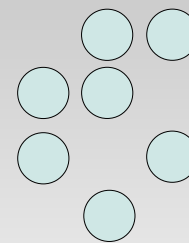


image is a given snapshot (configuration) of the whole system

Jargon terminology – “image”



images

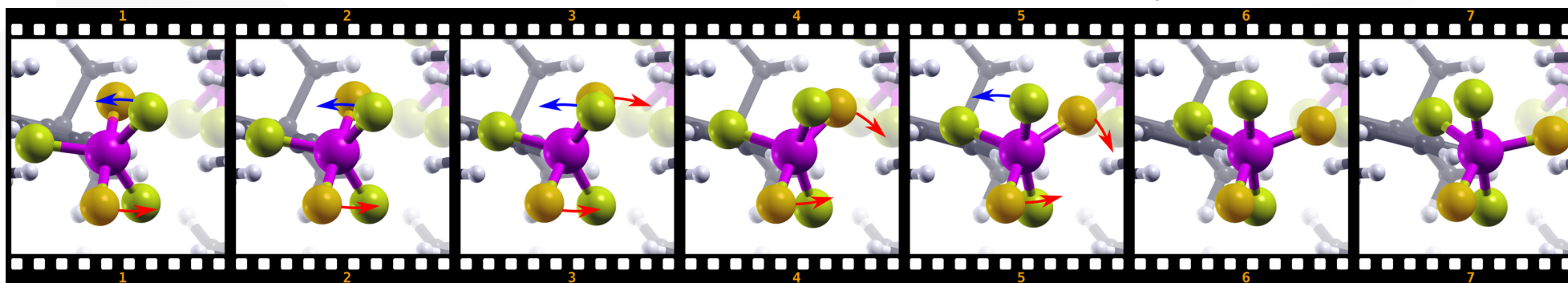
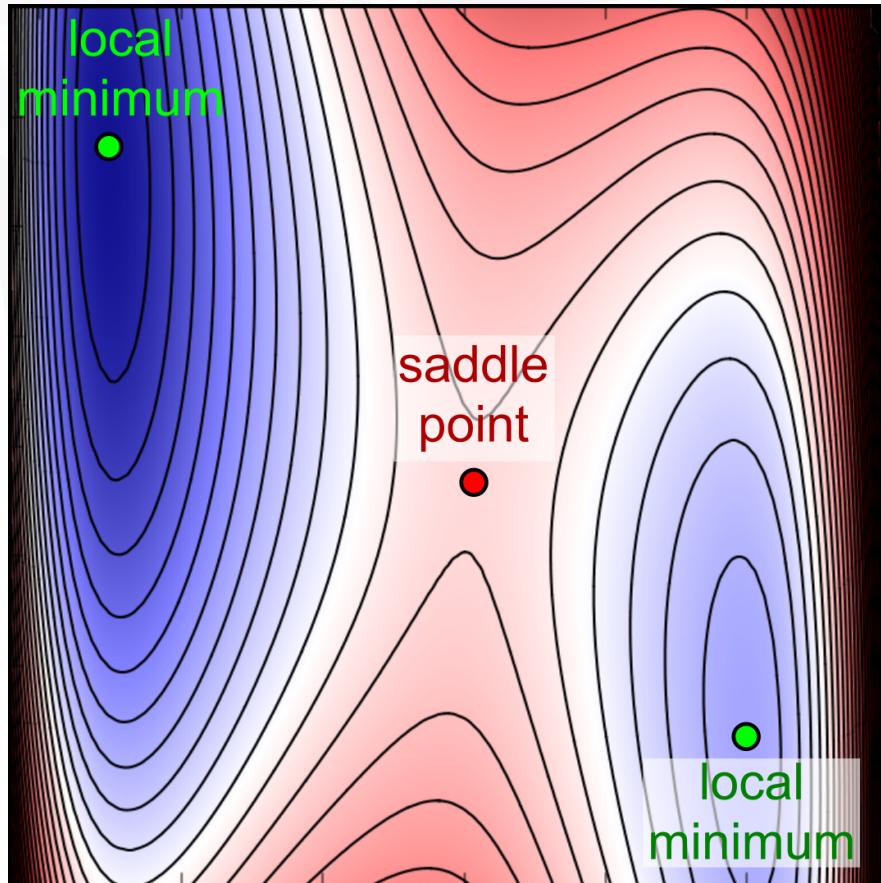
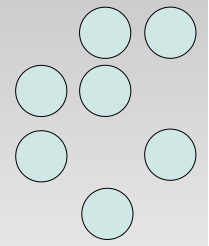


image is a given snapshot (configuration) of the whole system

PES – potential energy surface $E(\mathbf{R})$



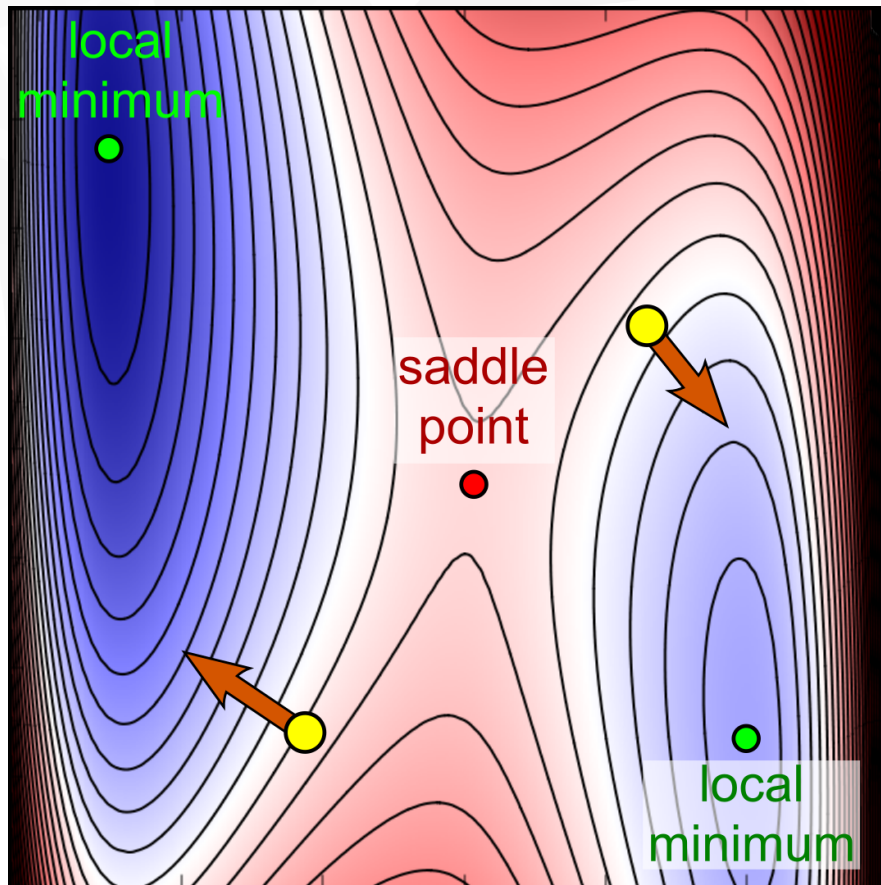
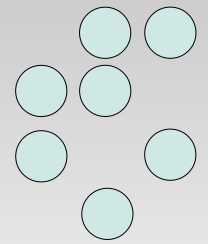
each point on this graph is an image

▼ Remarks:

- ▼ for obvious reasons, only 2D PES can be visualized
- ▼ For real examples, PES is highly multidimensional: $3N$ dimensional for N atoms

$\mathbf{R} \equiv 3N$ dimensional vector
(coordinates of all atoms)

Finding local minima



- ▼ Finding local minima is routine (provided the code can calculate first derivatives – forces)

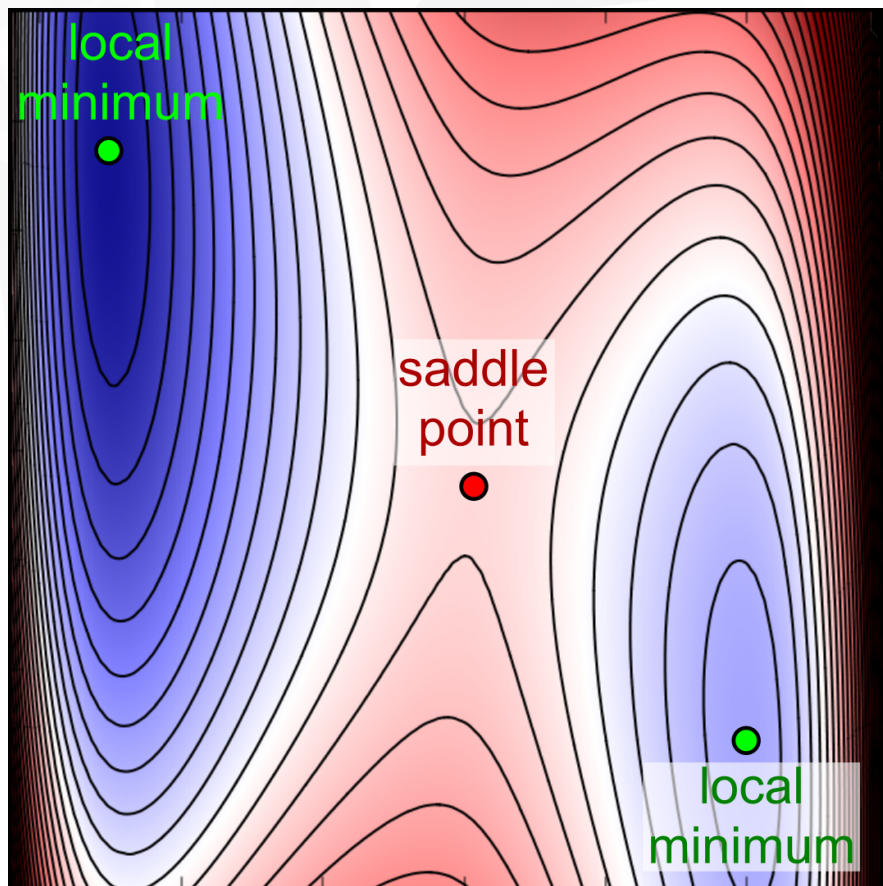
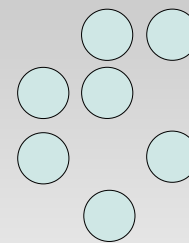
... by steepest descent

$$\mathbf{R}^{(n+1)} = \mathbf{R}^{(n)} - \lambda \nabla E(\mathbf{R}^{(n)})$$

or any other more efficient method (see the preceding talk)

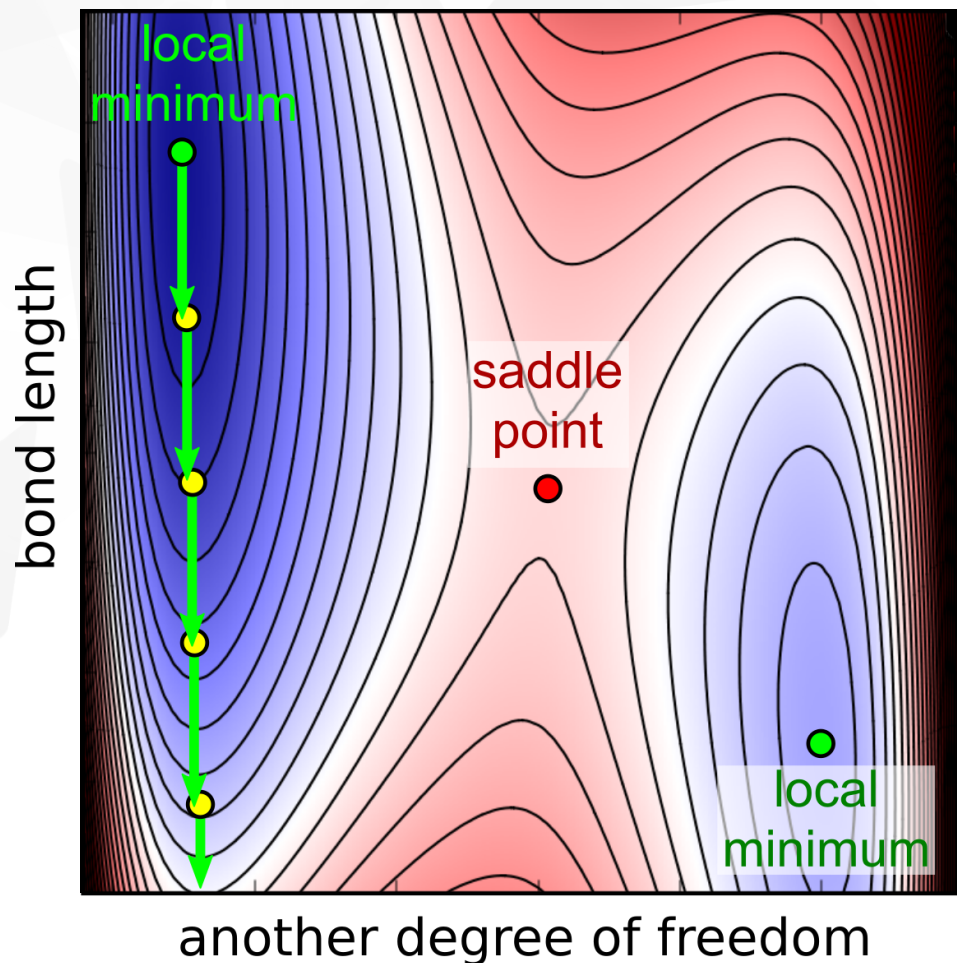
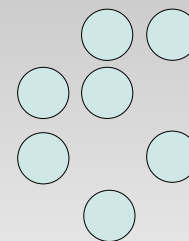
$\mathbf{R}^{(n)} \equiv$ coordinates at iteration n

How to find saddle points?



- ▼ Finding a saddle point is much more difficult than finding a local minimum
- ▼ An old, easy to realize method (“slowest ascend”):
 - ▼ step-wise stretch the bond
 - ▼ at each step perform constrained optimization

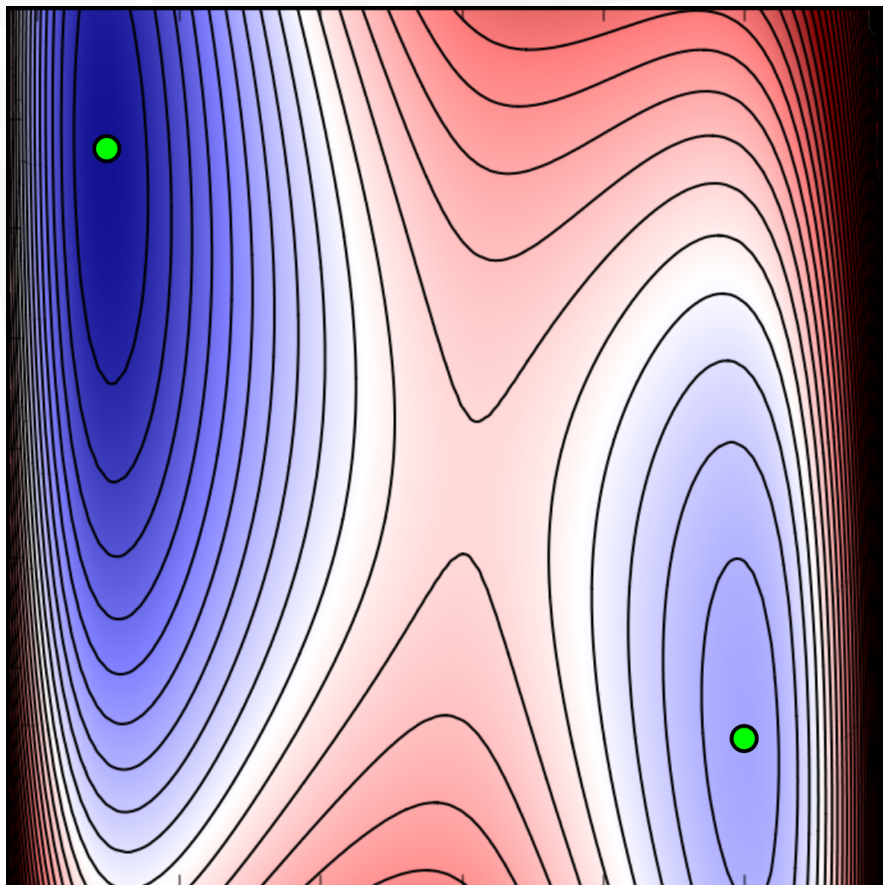
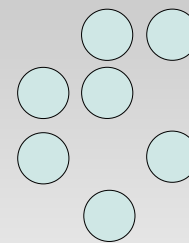
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 - ▼ step-wise stretch the bond
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May work well for dissociation reactions, but may also **fail badly**.

The NEB method – step by step explanation



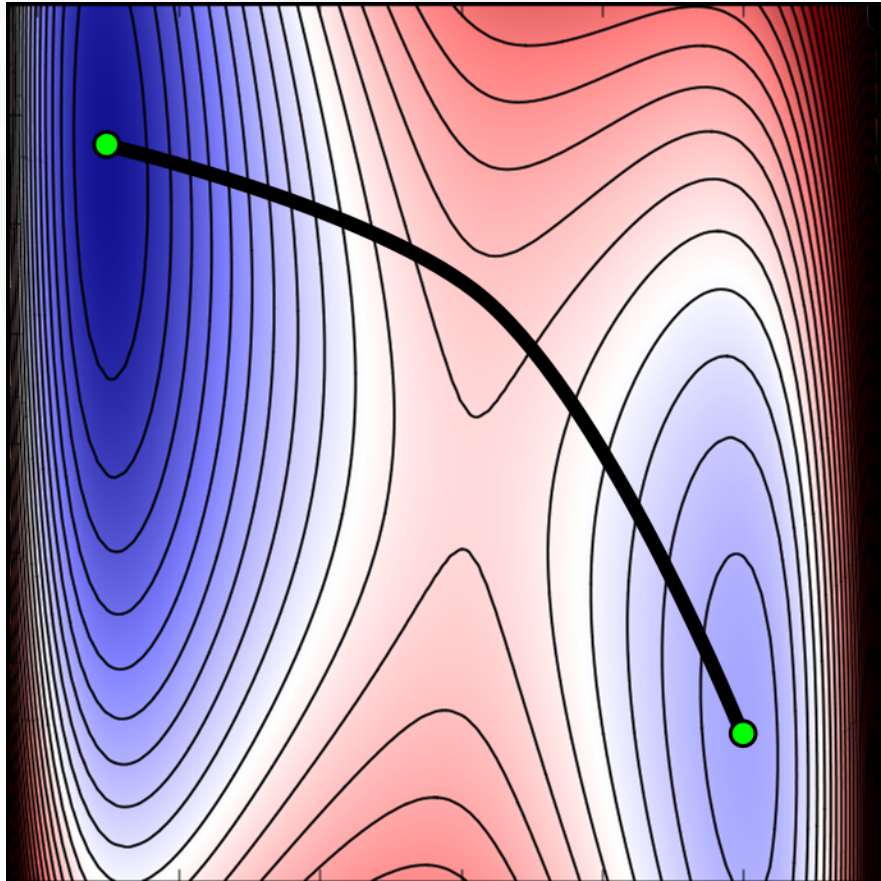
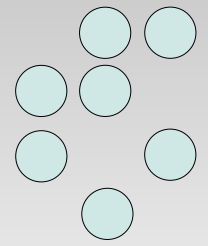
▼ **NEB** \equiv nudged elastic band

NEB references:

G. Henkelman, H. Jonsson, J. Chem Phys. **113**, 9978–9985 (2000)

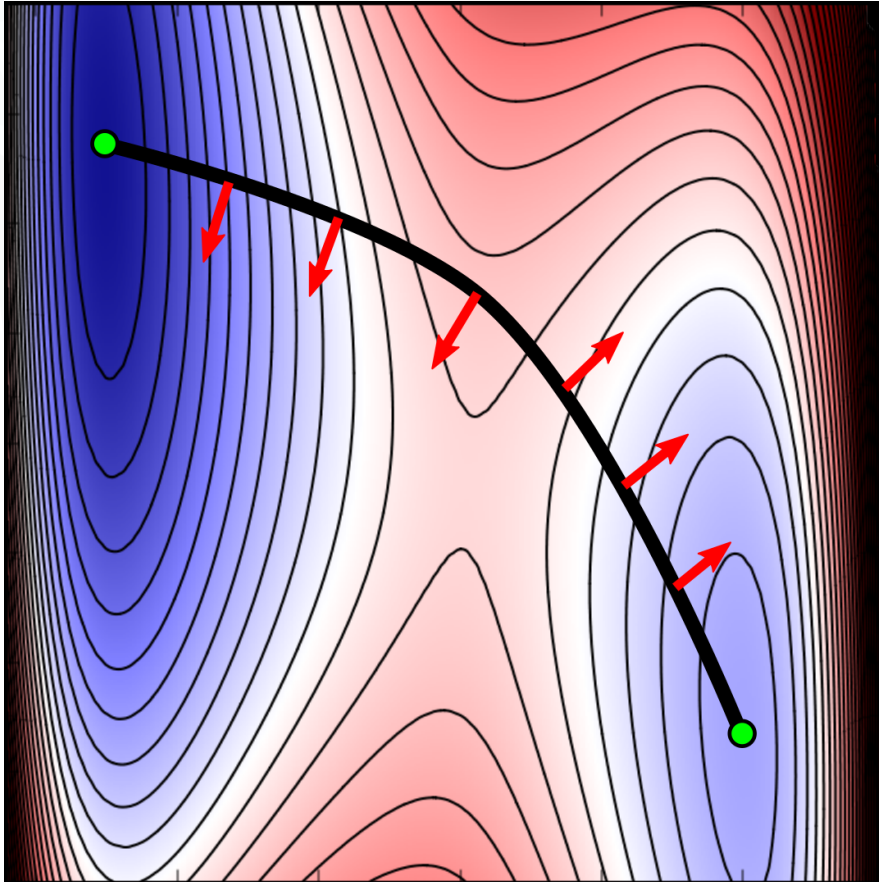
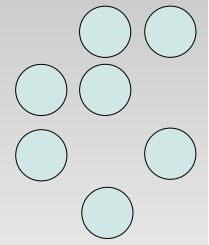
G. Henkelman, B. P. Uberuaga, H. Jonsson, J. Chem Phys. **113**, 9901–9904 (2000)

The NEB method – step by step explanation



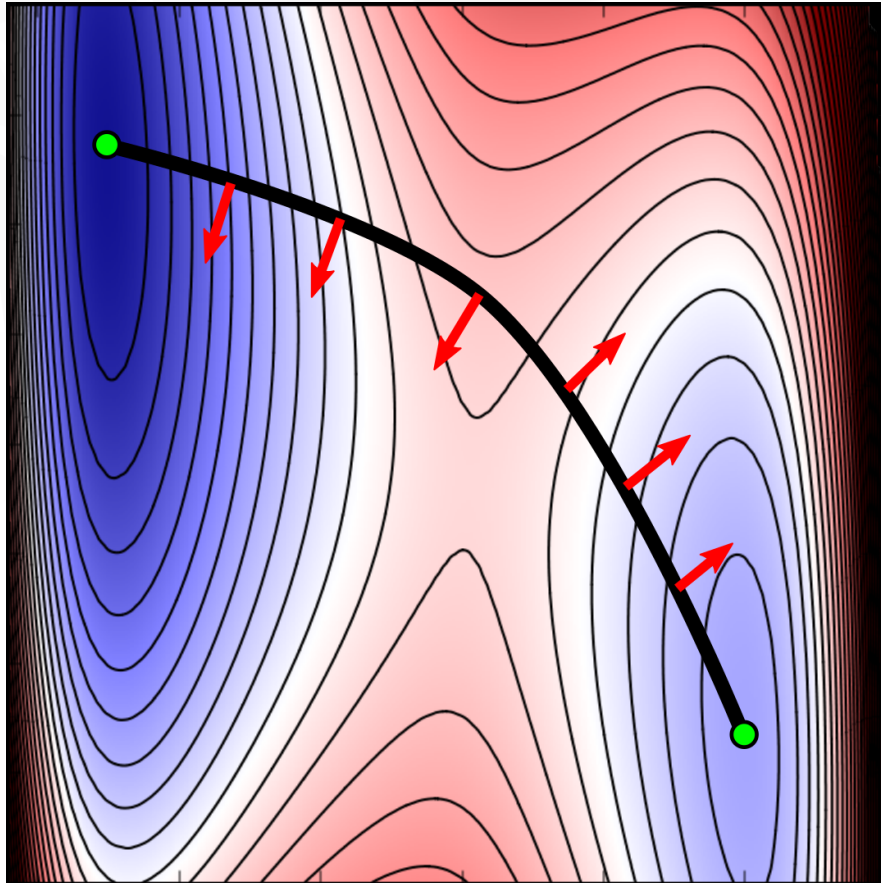
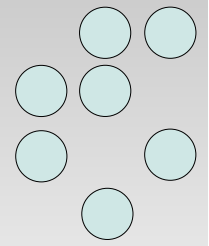
- ▼ 1. connect two minima with an elastic band

The NEB method – step by step explanation

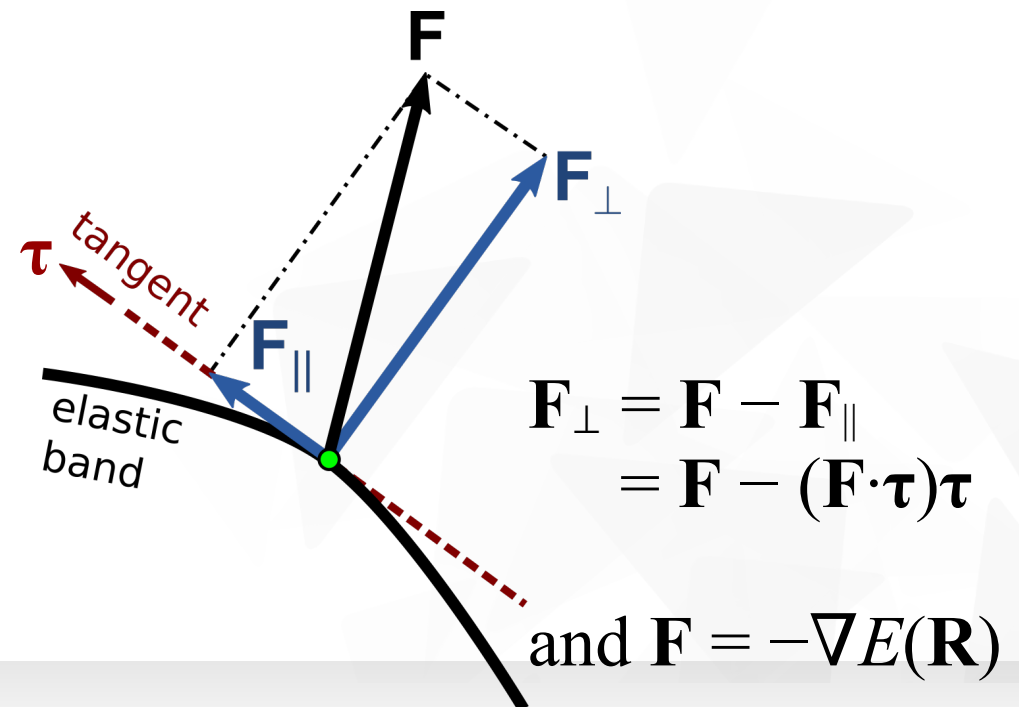


- ▼ 1. connect two minima with an elastic band
- ▼ 2. relax the band with *orthogonal* forces (\mathbf{F}_{\perp})

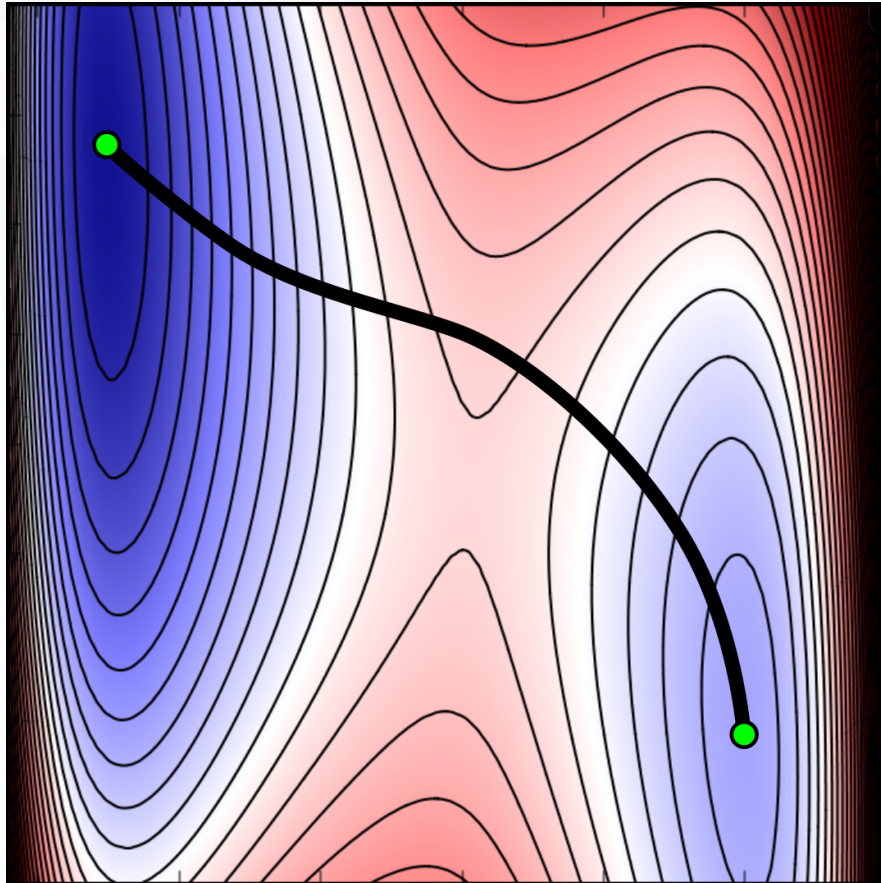
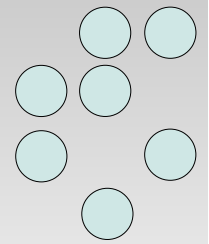
The NEB method – step by step explanation



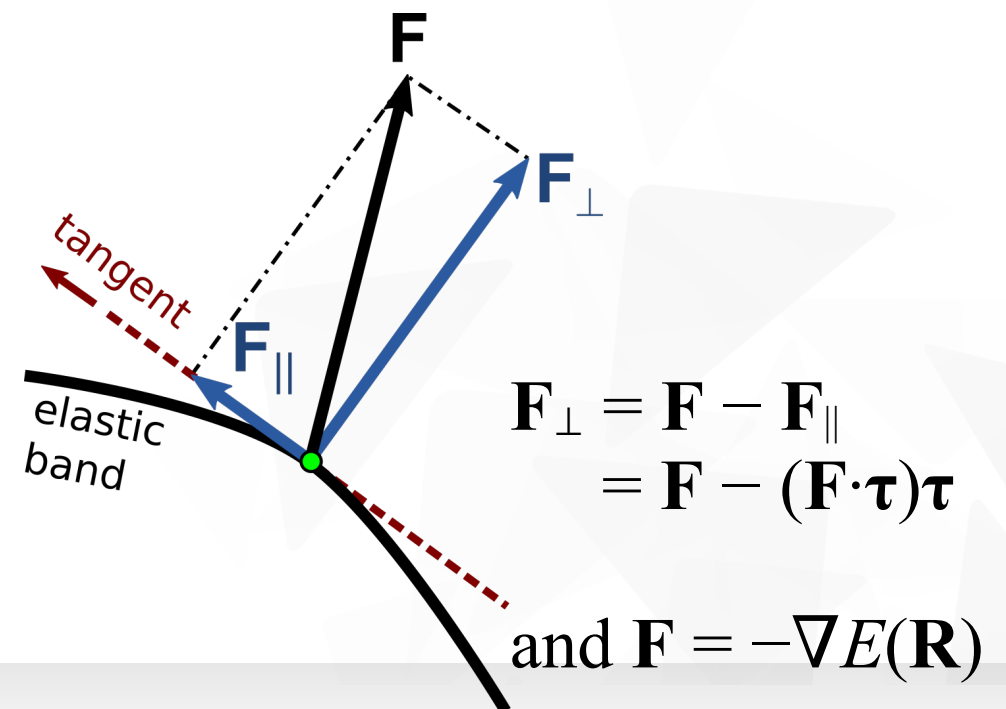
- 1. connect two minima with an elastic band
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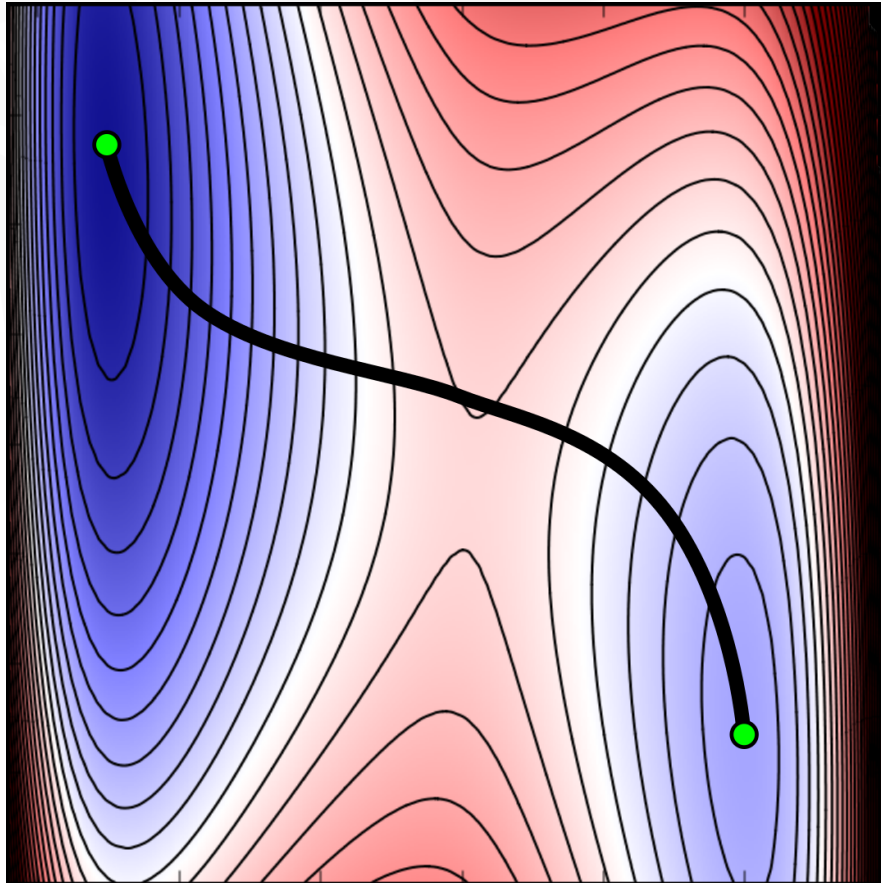
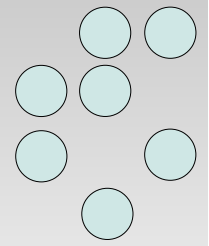
The NEB method – step by step explanation



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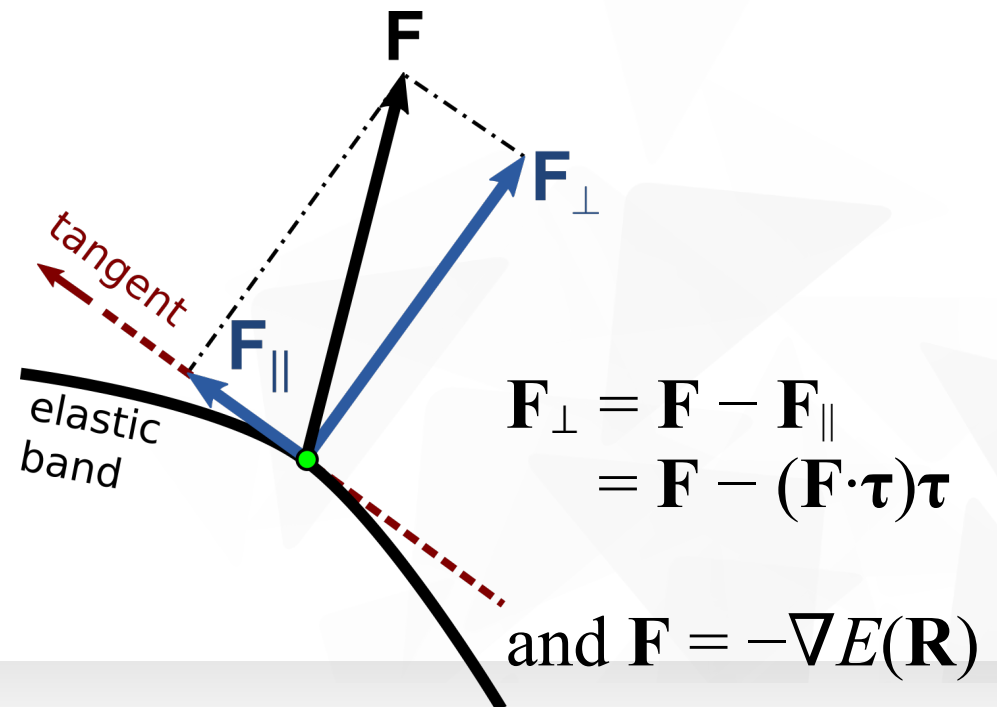


The NEB method – step by step explanation

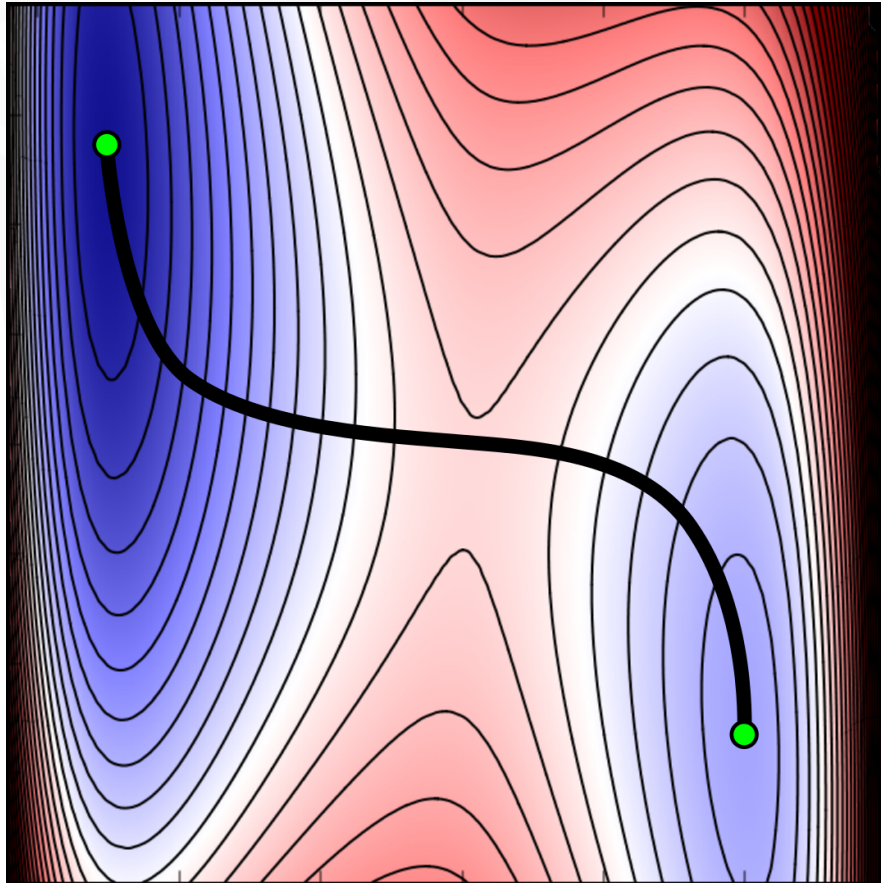
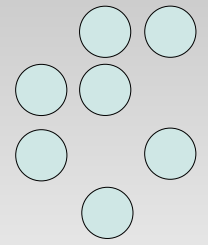


we assume elastic band is super stretchable
(no „corner cutting“)

- 1. connect two minima with an elastic band
- 2. relax the band with *orthogonal* forces (\mathbf{F}_\perp)

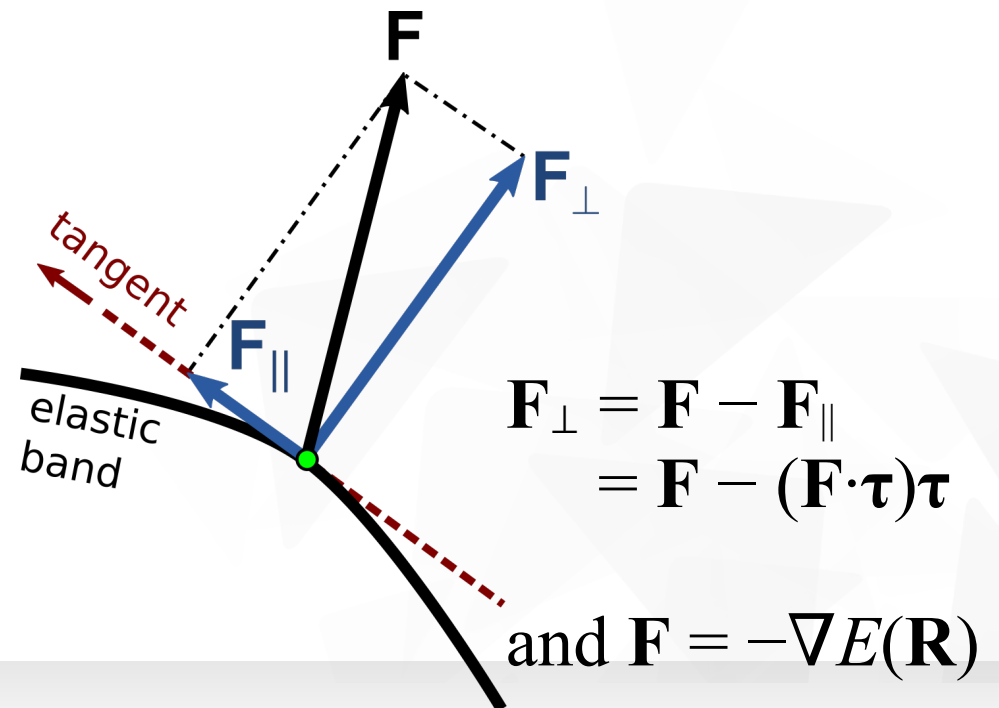


The NEB method – step by step explanation

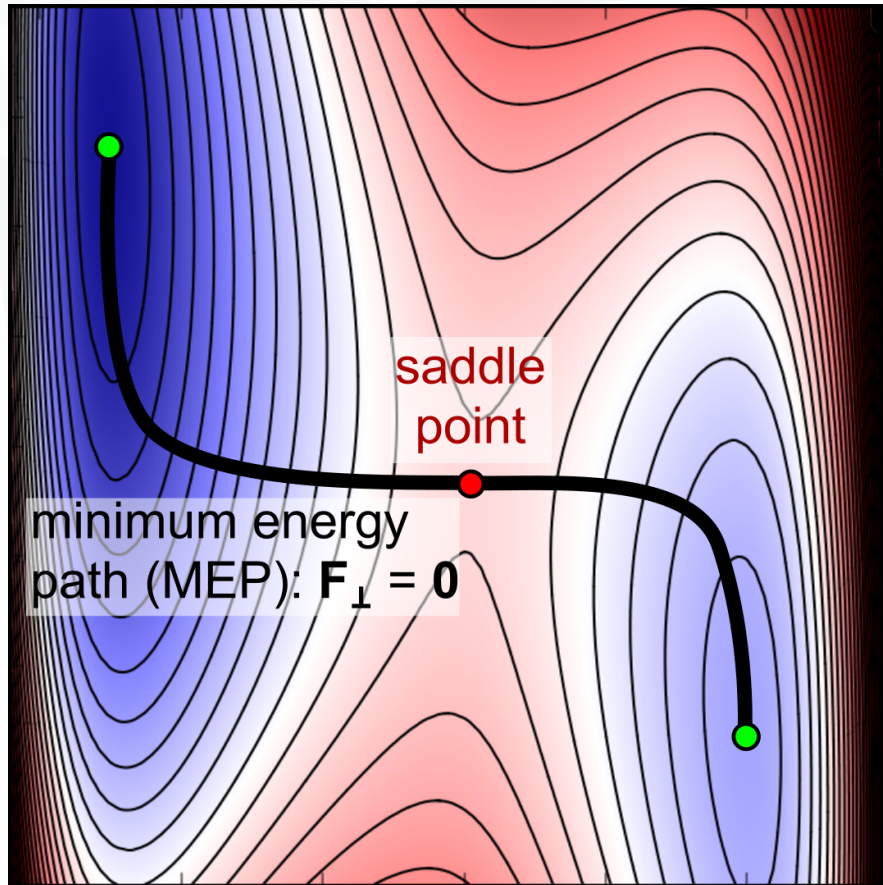
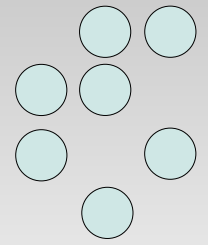


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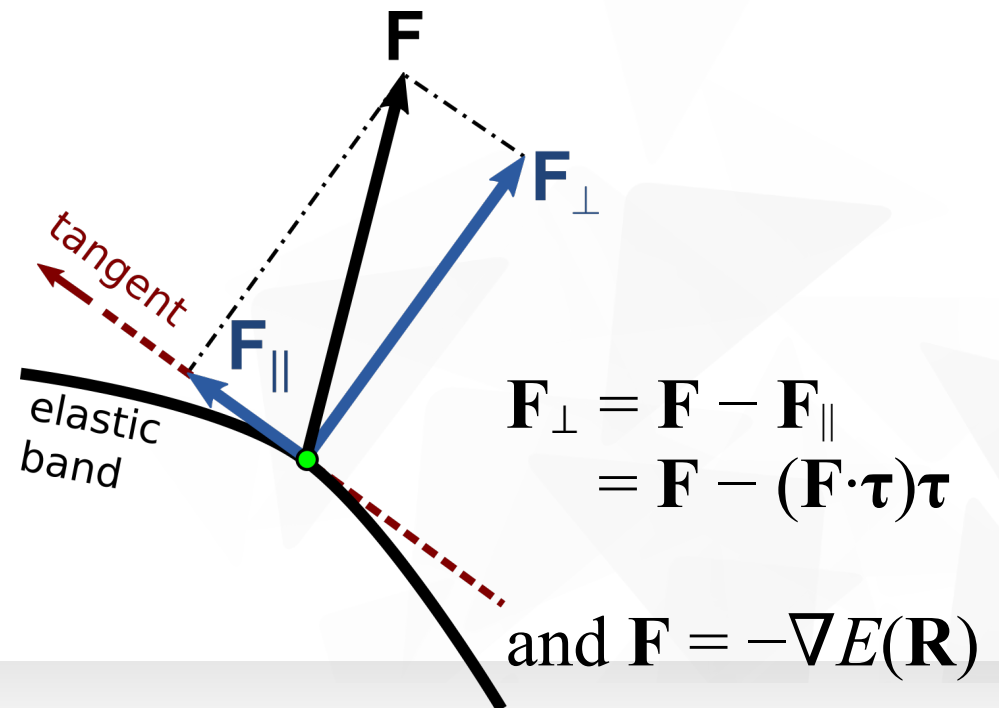


The NEB method – step by step explanation

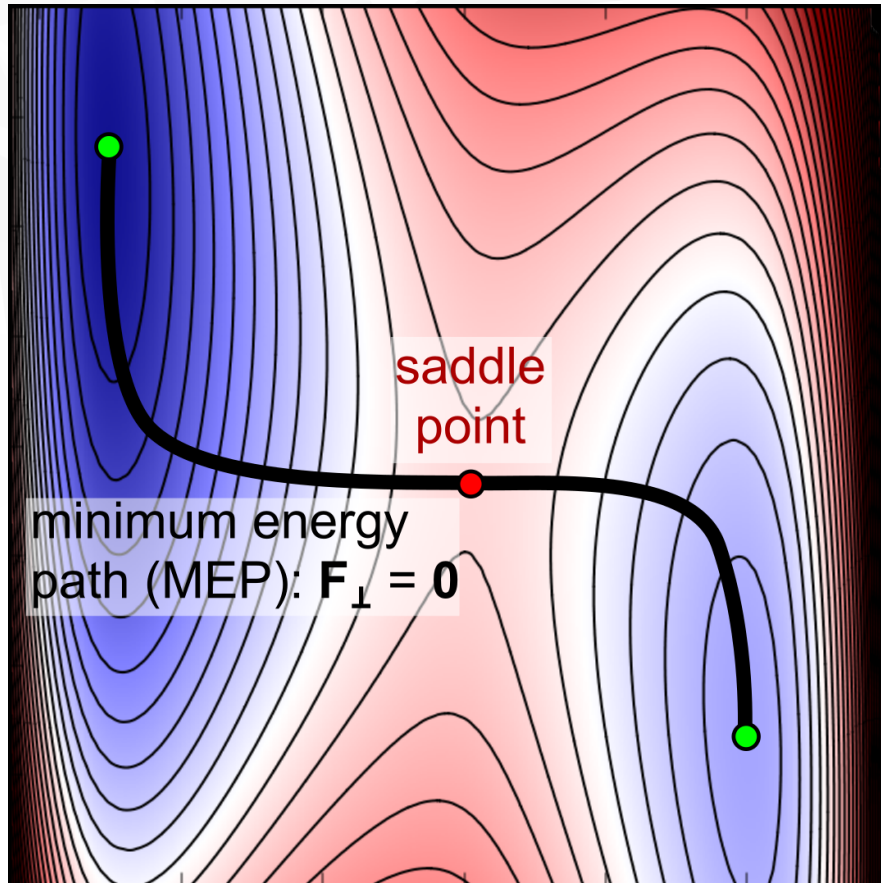
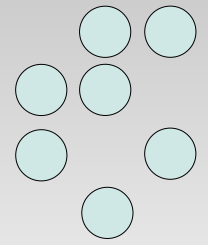


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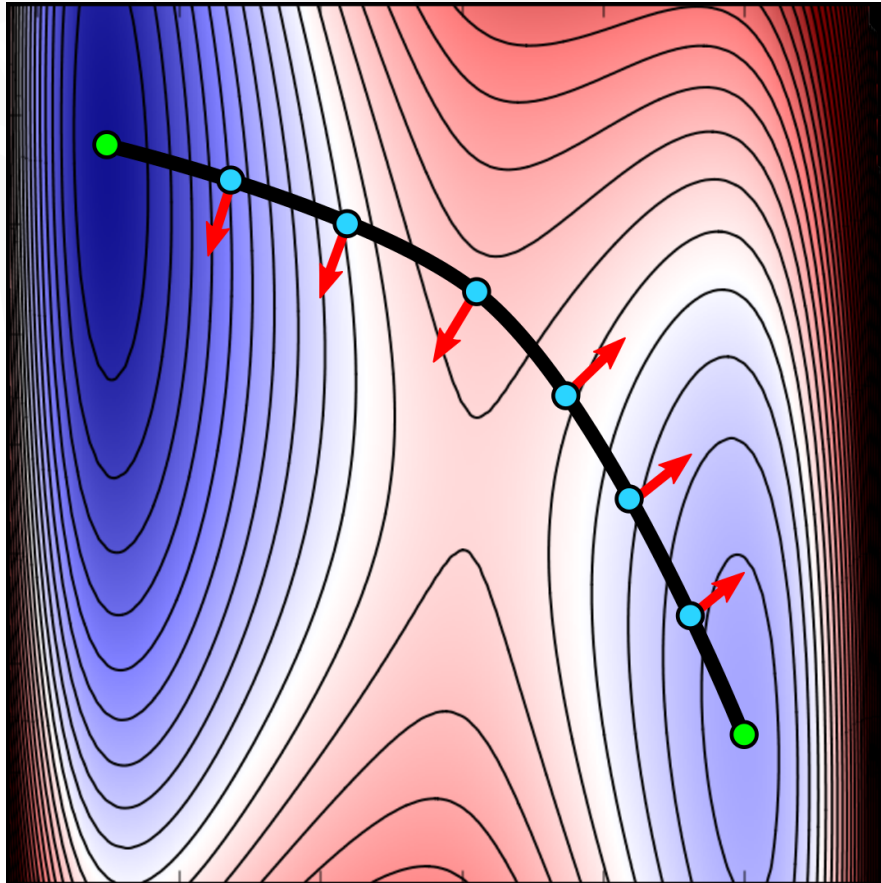
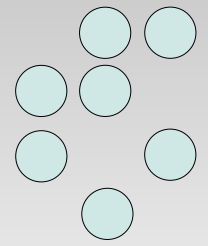
The NEB method – step by step explanation



we assume elastic band is super stretchable
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- 1. connect two minima with an elastic band
- 2. relax the band with *orthogonal* forces (F_{\perp})
- 3. but this was only thought experiment!

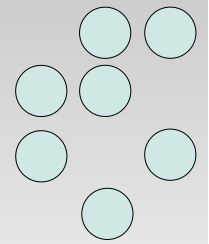
The NEB method – step by step explanation



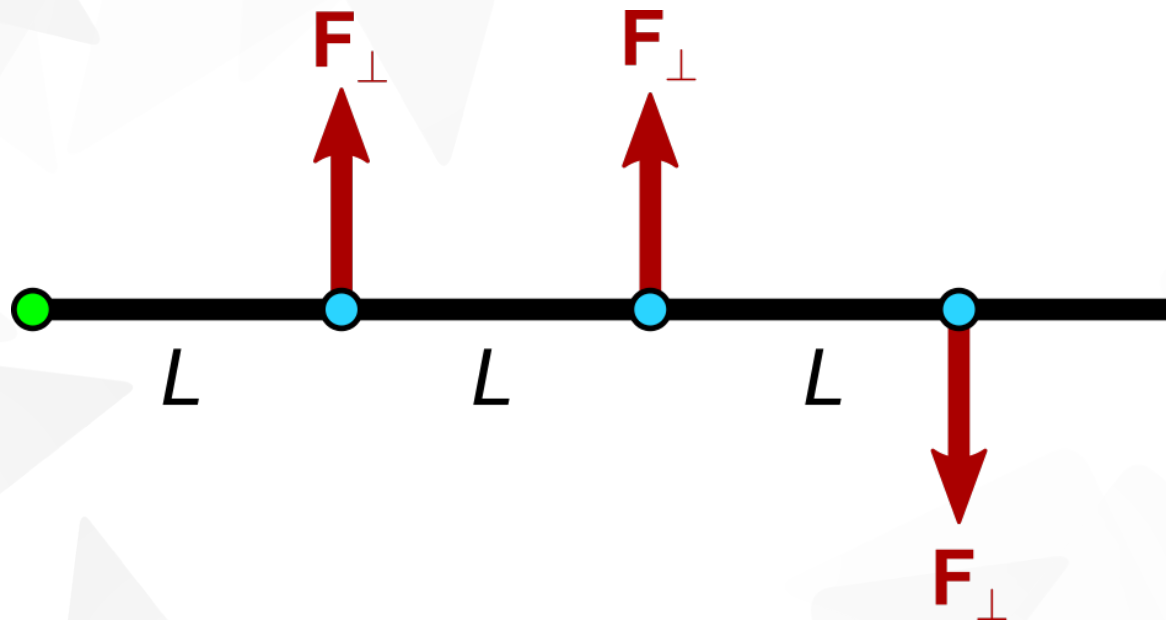
- 1. connect two minima with an elastic band
- 2. relax the band with *orthogonal* forces (F_{\perp})
- 3. but this was only thought experiment!

In computer, for obvious reasons, the elastic band is discretized into several “images”!

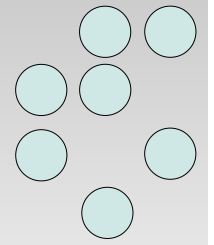
The NEB method – step by step explanation



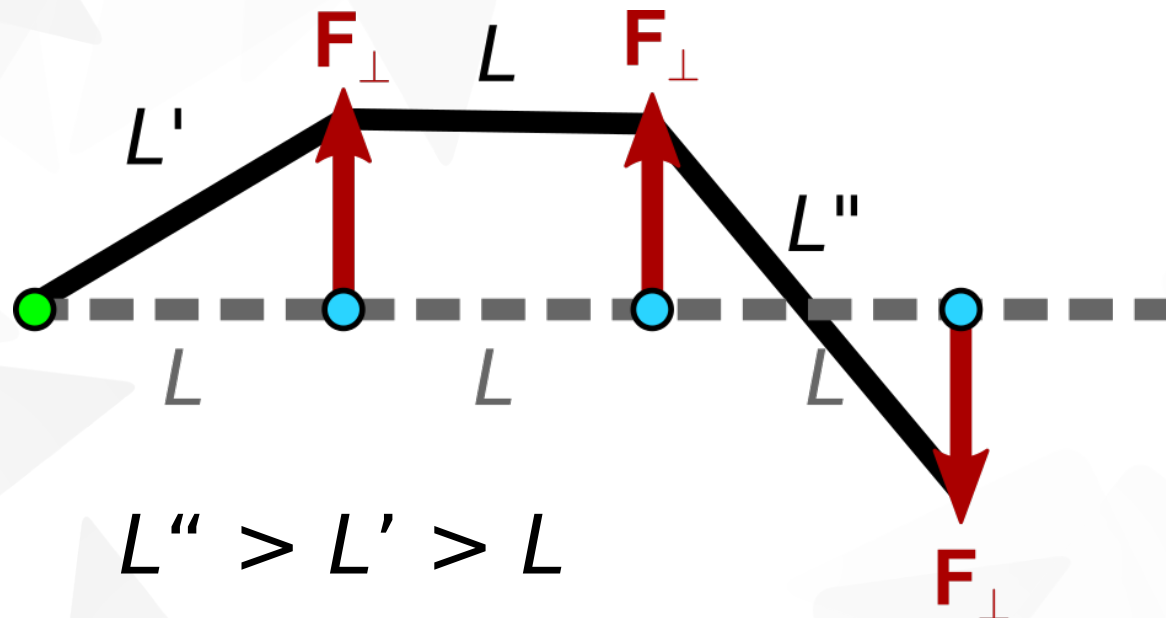
- ▼ A problem with path discretization ...



The NEB method – step by step explanation

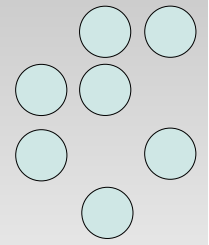


- ▶ A problem with path discretization ...

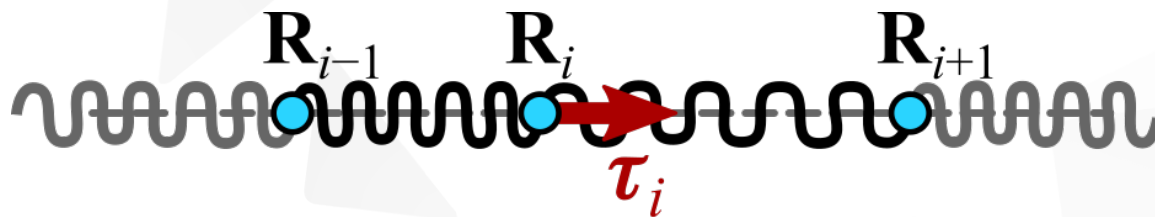


- ▶ Path dynamics does not preserve inter-image distances (after many iterations severe problems can emerge)
- ▶ **Solution:** connect images by springs

The NEB method – step by step explanation



- ▼ A problem with path discretization ...
- ▼ Path dynamics does not preserve inter-image distance (after many iterations severe problems can emerge)
- ▼ **Solution:** connect images by springs that act only along reaction path

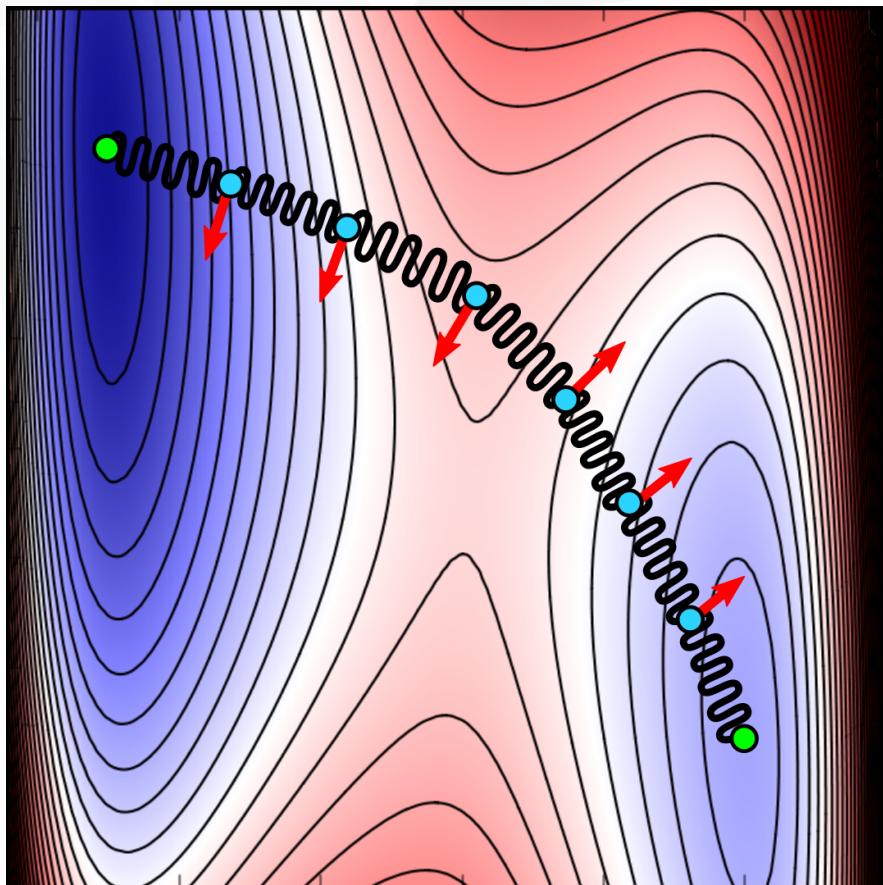
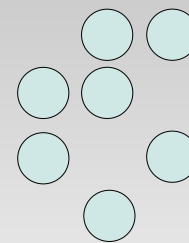


$$F_i^{\text{spring}}|_{\parallel} = k(|\mathbf{R}_{i+1} - \mathbf{R}_i| - |\mathbf{R}_i - \mathbf{R}_{i-1}|)\boldsymbol{\tau}_i$$

\mathbf{R}_i = atomic coordinates of image i

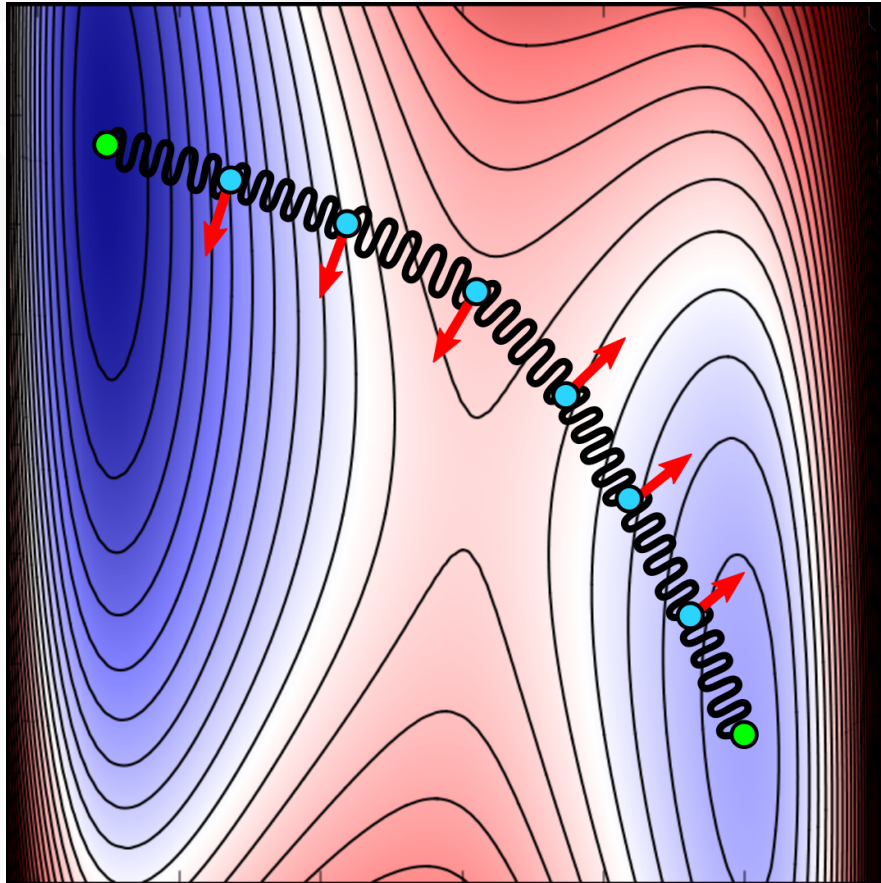
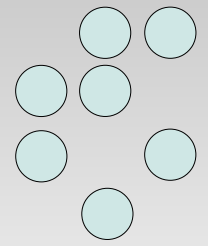
$\boldsymbol{\tau}_i$ = normalized tangent to reaction path for image i

The NEB method – step by step explanation



- ▼ 1. connect two minima with a “guessed” reaction path (can be linear)
- ▼ 2. discretize reaction path into several images: \mathbf{R}_1 , \mathbf{R}_2 , \mathbf{R}_3 ...
- ▼ 3. connect images by springs
- ▼ 4. minimize reaction path using the NEB recipe

The NEB method – step by step explanation



- 4. minimize reaction path using the NEB recipe:
 - true forces, $-\nabla E(\mathbf{R}_i)$, act only perpendicular to the reaction path
 - spring forces act only along the reaction path

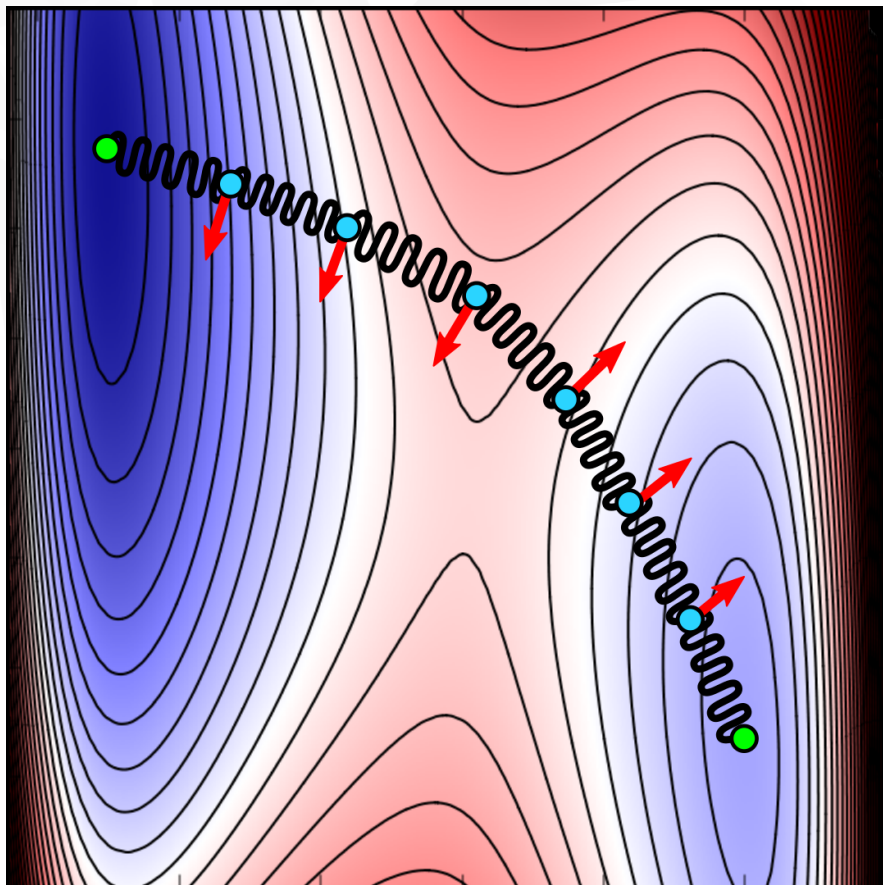
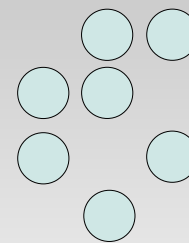
$$\mathbf{F}_i = -\nabla E(\mathbf{R}_i)|_{\perp} + \mathbf{F}_i^{\text{spring}}|_{\parallel}$$

where

$$\nabla E(\mathbf{R}_i)|_{\perp} = \nabla E(\mathbf{R}_i) - (\nabla E(\mathbf{R}_i) \cdot \boldsymbol{\tau}_i) \boldsymbol{\tau}_i$$

$$\mathbf{F}_i^{\text{spring}}|_{\parallel} = k(|\mathbf{R}_{i+1} - \mathbf{R}_i| - |\mathbf{R}_i - \mathbf{R}_{i-1}|) \boldsymbol{\tau}_i$$

The NEB method – step by step explanation



- 4. minimize reaction path using the NEB recipe:

- true forces, $-\nabla E(\mathbf{R}_i)$, act only perpendicular to the reaction path
- spring forces act only along the reaction path

»nudging«

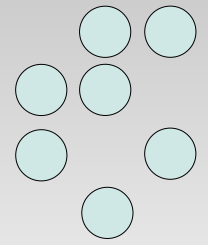
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$$\mathbf{F}_i^{\text{spring}}|_{\parallel} = k(|\mathbf{R}_{i+1} - \mathbf{R}_i| - |\mathbf{R}_i - \mathbf{R}_{i-1}|) \boldsymbol{\tau}_i$$

The NEB method – step by step explanation



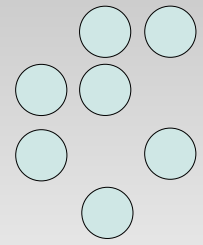
- Choice of the tangent $\boldsymbol{\tau}_i$ is crucial for convergence!


A good choice is a *local* tangent taken only with respect to the adjacent image with the higher energy:

$$\mathbf{T}_i = \begin{cases} \mathbf{T}_i^+ = \mathbf{R}_{i+1} - \mathbf{R}_i & \text{if } E_{i+1} > E_i > E_{i-1} \\ \mathbf{T}_i^- = \mathbf{R}_i - \mathbf{R}_{i-1} & \text{if } E_{i+1} < E_i < E_{i-1} \end{cases} \quad \text{and} \quad \boldsymbol{\tau}_i = \frac{\mathbf{T}_i}{|\mathbf{T}_i|}$$

(if $E_{i+1} > E_i < E_{i-1}$ or $E_{i+1} < E_i > E_{i-1}$ then \mathbf{T}_i is an energy-weighted sum of \mathbf{T}_i^+ and \mathbf{T}_i^-)

The NEB method – step by step explanation



- Transition state (TS) – the saddle point on the MEP – is the most *interesting* point
 - Hence:** higher resolution of points around TS is preferable
- 
- Variable spring constants** (between k_{\min} & k_{\max})

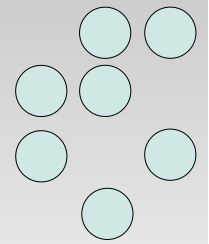
$$k_i = \begin{cases} k_{\max} - \Delta k \frac{E_{\max} - \tilde{E}_i}{E_{\max} - E_{\text{ref}}} & \text{if } \tilde{E}_i > E_{\text{ref}} \\ k_{\min} & \text{if } \tilde{E}_i < E_{\text{ref}} \end{cases}$$

where $E_{\text{ref}} = \max(E_{\text{IS}}, E_{\text{FS}})$ ← IS = initial state
FS = final state

$k_i \equiv$ spring constant between images $i - 1$ and i

$$\tilde{E}_i \equiv \max(E_{i-1}, E_i) \quad \Delta k = k_{\max} - k_{\min}$$

Climbing image NEB (CI NEB)



- Even with many images and variable spring constants no image may lie sufficiently close to the saddle point
- Hence:** let the image with the highest energy **climb up** (this image is decoupled from the springs)
- Climbing-up means that F_{\parallel} is reverted

force on the climbing image

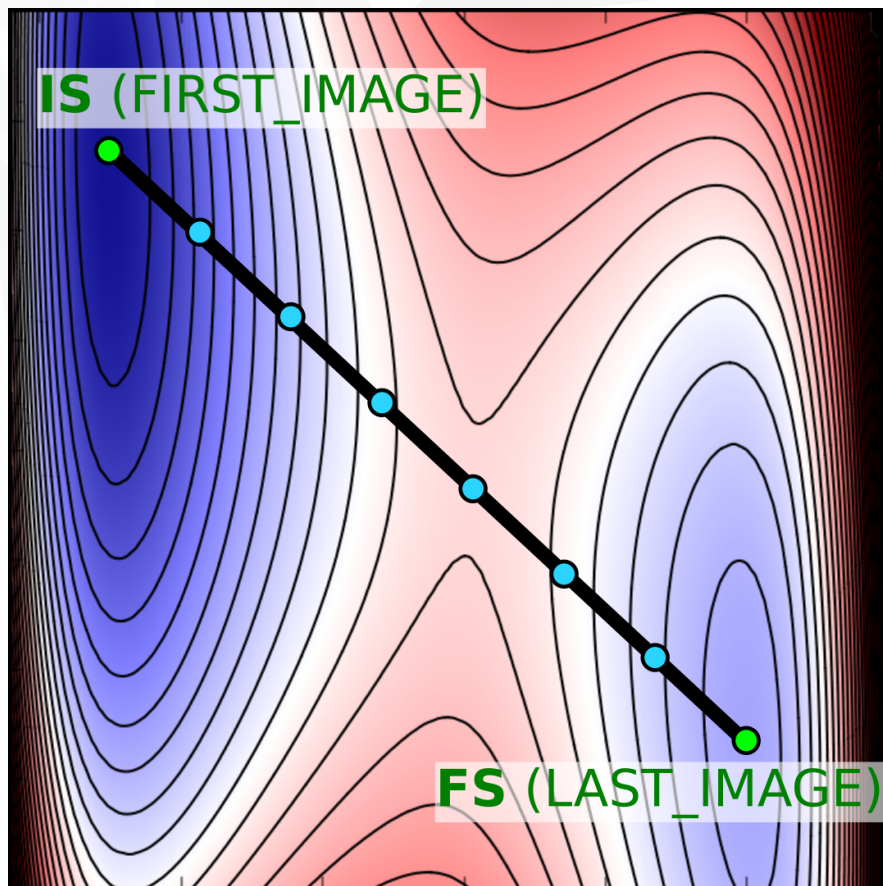
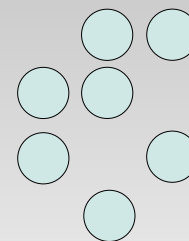
$$F_{i_{\max}} = F_{\perp} - F_{\parallel}$$

$$= F - 2F_{\parallel}$$

$$= -\nabla E(\mathbf{R}_{i_{\max}}) + 2(\nabla E(\mathbf{R}_{i_{\max}}) \cdot \boldsymbol{\tau}_{i_{\max}}) \boldsymbol{\tau}_{i_{\max}}$$

$$F = F_{\perp} + F_{\parallel}$$

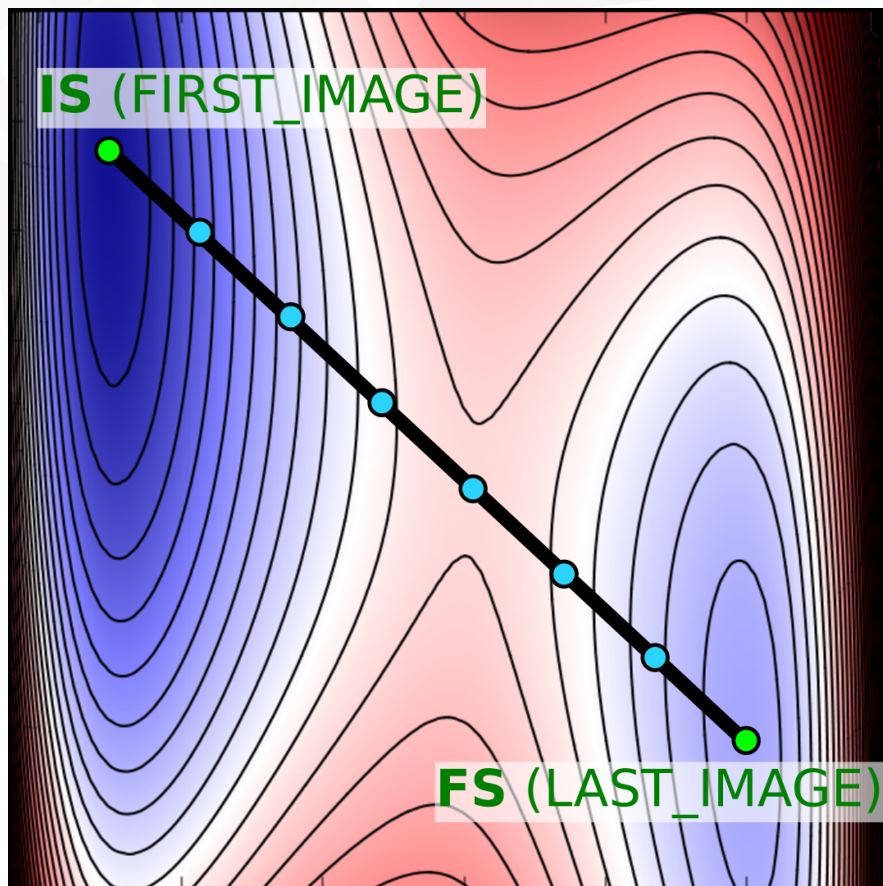
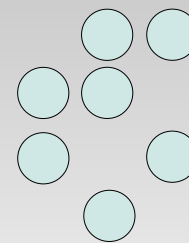
NEB calculations – practical aspects



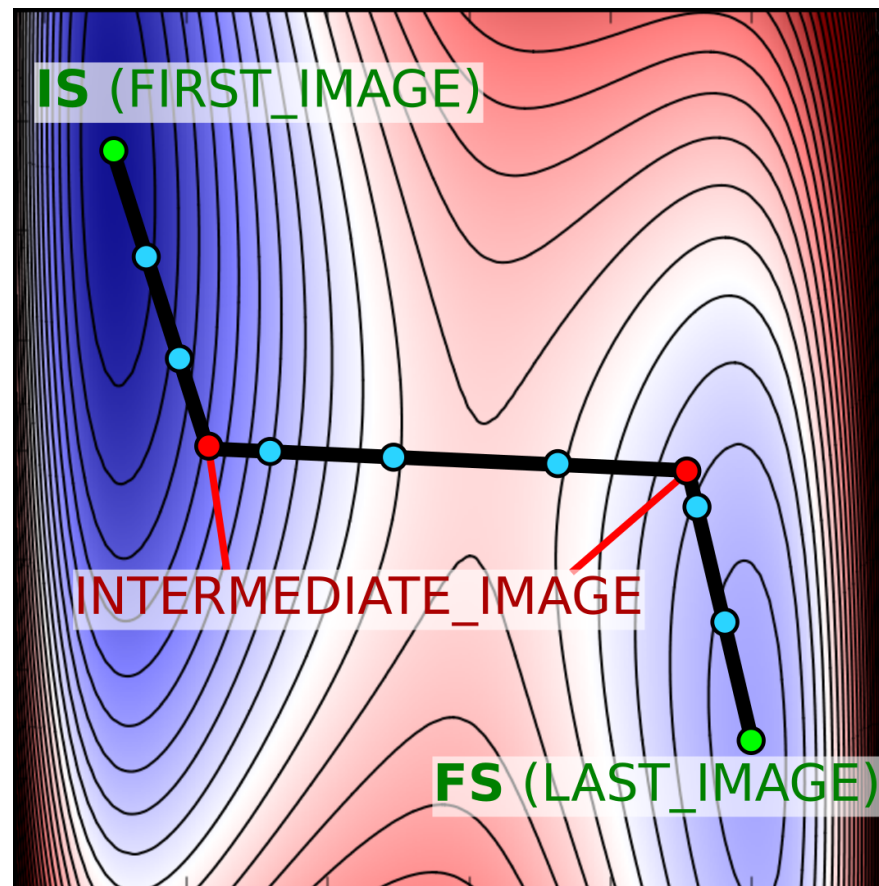
- ▼ **IS** \equiv initial state
FS \equiv final state
- ▼ default initial guess for the reaction path:
linear interpolation

here linearly interpolated reaction path passes very close to the saddle point, but in real cases this is seldom the case

NEB calculations – intermediate images

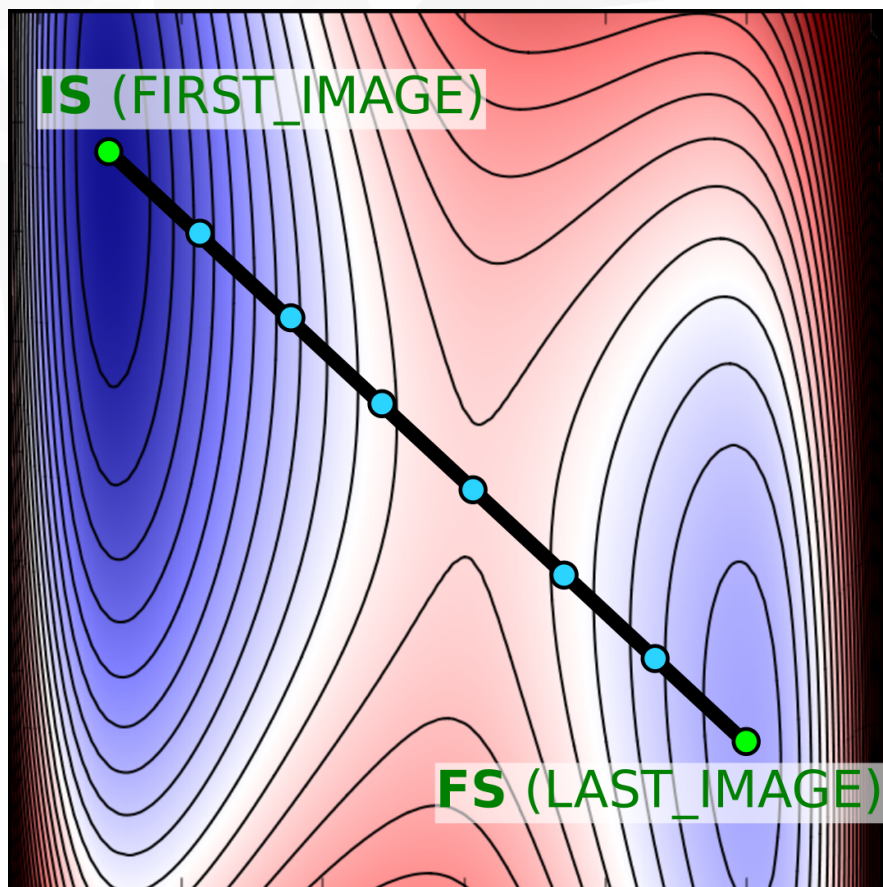
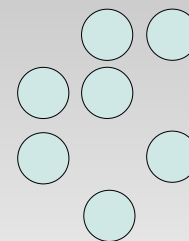


here linearly interpolated reaction path passes very close to the saddle point, but in real cases this is seldom the case

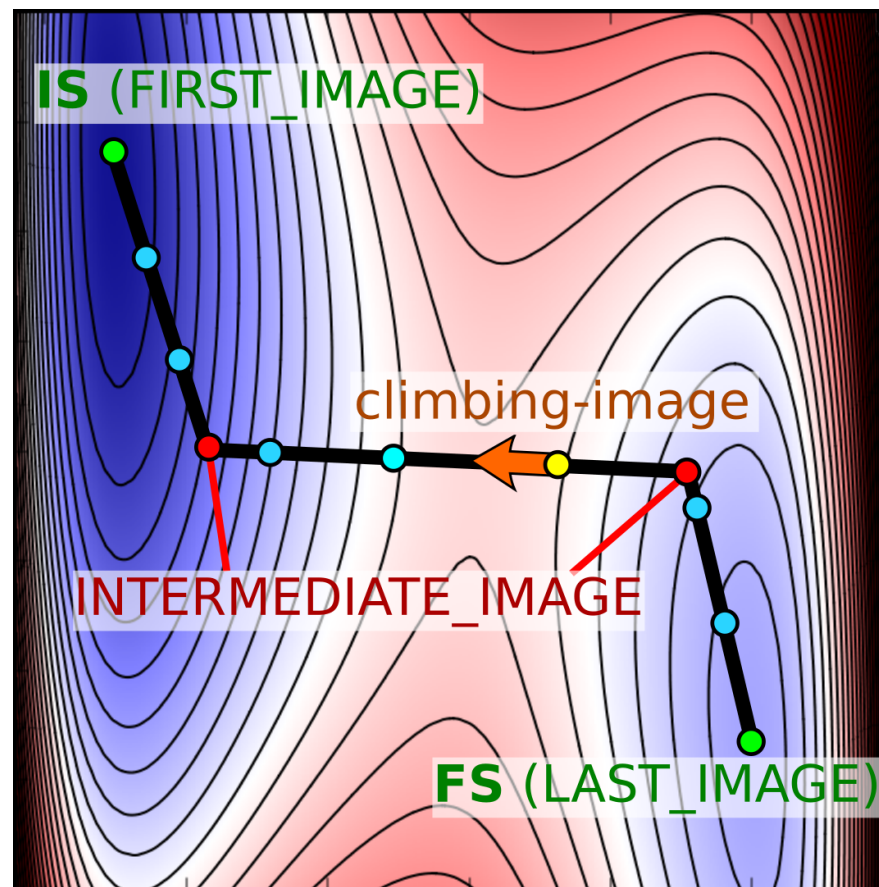


intermediate images are used to steer initial reaction path (they are not actually used); exploiting chemical intuition is a plus

NEB calculations – climbing image

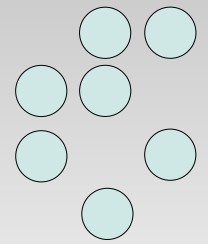


here linearly interpolated reaction path passes very close to the saddle point, but in real cases this is seldom the case



intermediate images are used to steer initial reaction path (they are not actually used); exploiting chemical intuition is a plus

Structure of the neb.x input file



BEGIN

```
BEGIN_PATH_INPUT
...
END_PATH_INPUT
```

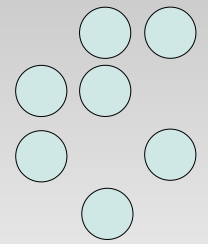
NEB specification

```
BEGIN_ENGINE_INPUT
...
END_ENGINE_INPUT
```

pw.x specification

END

Structure of the neb.x input file



BEGIN

```
BEGIN_PATH_INPUT  
...  
END_PATH_INPUT
```

```
BEGIN_ENGINE_INPUT  
...  
END_ENGINE_INPUT
```

END

```
BEGIN_PATH_INPUT
```

```
&PATH
```

```
...
```

```
/
```

```
CLIMBING_IMAGES
```

```
...
```

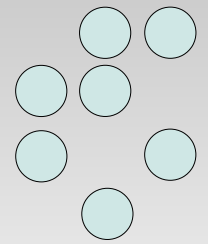
```
END_PATH_INPUT
```

mandatory

only when

CI_scheme = 'manual'

Structure of the neb.x input file



```
BEGIN
```

```
BEGIN_PATH_INPUT  
...  
END_PATH_INPUT
```

```
BEGIN_ENGINE_INPUT  
...  
END_ENGINE_INPUT
```

```
END
```

```
BEGIN_PATH_INPUT  
&PATH  
  string_method = 'neb'  
  num_of_images = 9  
  CI_scheme     = "manual"  
  path_thr      = 0.05  
  nstep_path    = 100  
/  
CLIMBING_IMAGES  
  6  
END_PATH_INPUT
```

what do these variables mean



Input File Description

Program: neb.x / NEB / Quantum Espresso

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[BEGIN_ENGINE_INPUT](#)

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BEGIN

```
BEGIN_PATH_INPUT  
...  
END_PATH_INPUT
```

```
BEGIN_ENGINE_INPUT  
...  
END_ENGINE_INPUT
```

END

```
BEGIN_ENGINE_INPUT
```

```
&CONTROL
```

```
/
```

```
&SYSTEM
```

```
/
```

```
&ELECTRONS
```

```
/
```

```
ATOMIC_SPECIES
```

```
...
```

```
K_POINTS
```

```
...
```

```
BEGIN_POSITIONS
```

```
FIRST_IMAGE
```

```
ATOMIC_POSITIONS
```

```
...
```

```
INTERMEDIATE_IMAGE
```

```
ATOMIC_POSITIONS
```

```
...
```

```
LAST_IMAGE
```

```
ATOMIC_POSITIONS
```

```
...
```

```
END_POSITIONS
```

```
END_ENGINE_INPUT
```

} pw.x specs
(mandatory)

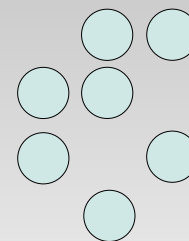
} mandatory

} optional

} mandatory

*there can be many
INTERMEDIATE_IMAGES*

Structure of the neb.x input file: PATH input



```
BEGIN_PATH_INPUT
&PATH
  string_method = 'neb' | 'smd'
  num_of_images = 9
  path_thr      = 0.05
  nstep_path   = 100
  opt_scheme    = 'broyden' | 'quick-min' | 'sd'
  ds           = 1.0
  CI_scheme    = 'no-CI' | 'auto' | 'manual'
  k_max        = 0.3
  k_min        = 0.15
  use_freezing = .true. | .false.
/
CLIMBING_IMAGES
6
END_PATH_INPUT
```

default

conv. threshold on forces

time step (for velocity Verlet opt. scheme)

climbing-image scheme

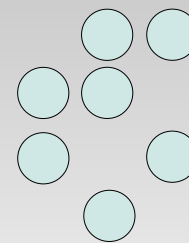
variable spring constants

in eV/Å

maximum number of optimization steps

in a given iteration move only images that have "large" error

Structure of the neb.x output file



Input variables:

```
num_of_images = 8
CI_scheme     = 'auto'
use_freezing  = .true.
```

```
----- iteration 10 -----
tcpu =    33.3    self-consistency for image  2
tcpu =    35.1    self-consistency for image  3
tcpu =    37.6    self-consistency for image  4
tcpu =    39.8    self-consistency for image  5
tcpu =    41.8    self-consistency for image  6
tcpu =    44.2    self-consistency for image  7

activation energy (->) =  1.173353 eV
activation energy (<-) =  1.426101 eV

image      energy (eV)      error (eV/A)      frozen
-----
  1      -2178.8704395      0.022370         T
  2      -2178.7915492      0.815753         F
  3      -2178.4744222      0.653550         F
  4      -2177.6970863      0.271615         T
  5      -2177.8369509      0.391123         T
  6      -2178.3473551      0.315382         T
  7      -2178.8816419      0.509630         F
  8      -2179.1231876      0.000469         T

climbing image =  4

path length      =  5.328 bohr
inter-image distance =  0.761 bohr
```

```
----- iteration 11 -----
tcpu =    46.7    self-consistency for image  2
tcpu =    48.6    self-consistency for image  3
tcpu =    50.9    self-consistency for image  7

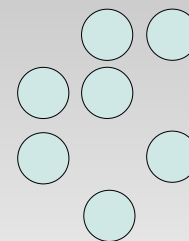
activation energy (->) =  1.173353 eV
activation energy (<-) =  1.426101 eV

image      energy (eV)      error (eV/A)      frozen
-----
  1      -2178.8704395      0.022370         T
  2      -2178.7844525      0.925352         F
  3      -2178.4348079      0.345968         T
  4      -2177.6970863      0.265414         T
  5      -2177.8369509      0.391123         T
  6      -2178.3473551      0.313012         T
  7      -2178.8978837      0.339249         T
  8      -2179.1231876      0.000469         T

climbing image =  4

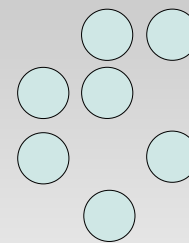
path length      =  5.369 bohr
inter-image distance =  0.767 bohr
```

NEB calculations: practical aspects



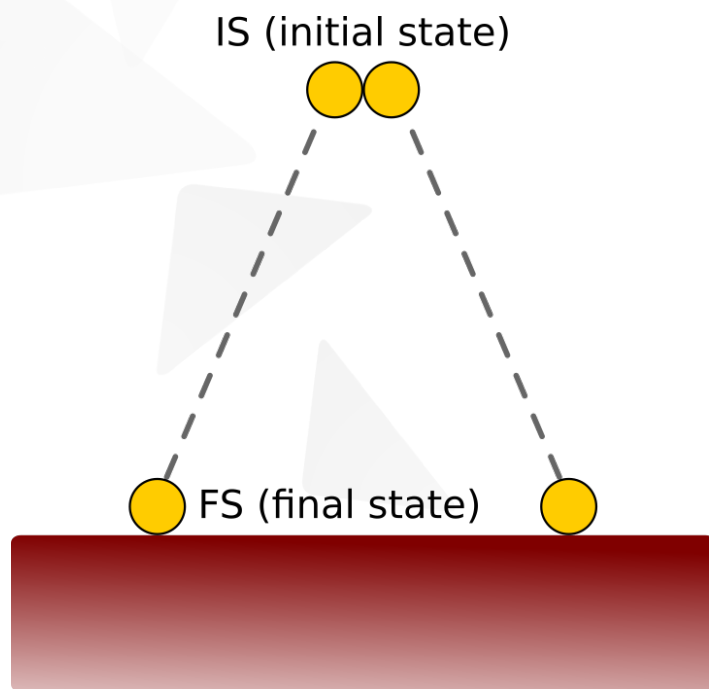
- ▼ NEB calculation may be relatively difficult to converge
(experience is a plus !)
 - ▼ **Some practical guidelines** (based on experience):
 - ▼ use **chemical intuition** to guess a “reasonable” initial reaction path:
 - ▼ start from **relaxed initial** and **final states**
(FIRST_IMAGE & LAST_IMAGE)
 - ▼ use **INTERMEDIATE_IMAGES**
- (use of `first_last_opt = .true.` is discouraged, i.e., optimization of FIRST_IMAGE and LAST_IMAGE during NEB run itself)

Practical aspects: use chemical intuition

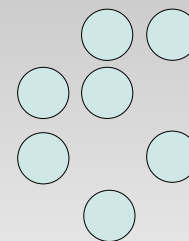


▼ Use INTERMEDIATE_IMAGES

dissociation of a molecule at a surface

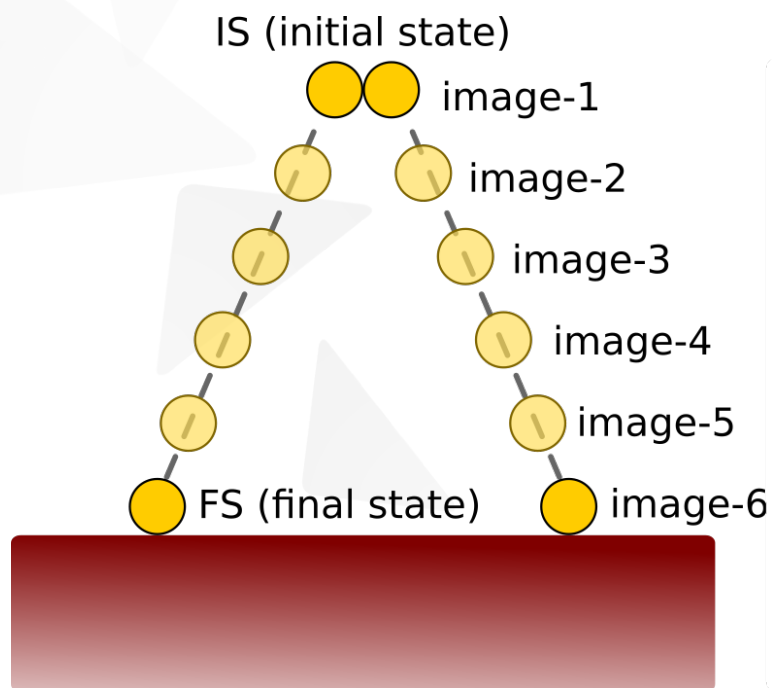


Practical aspects: use chemical intuition

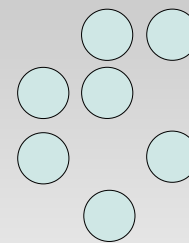


▼ Use INTERMEDIATE_IMAGES

dissociation of a molecule at a surface

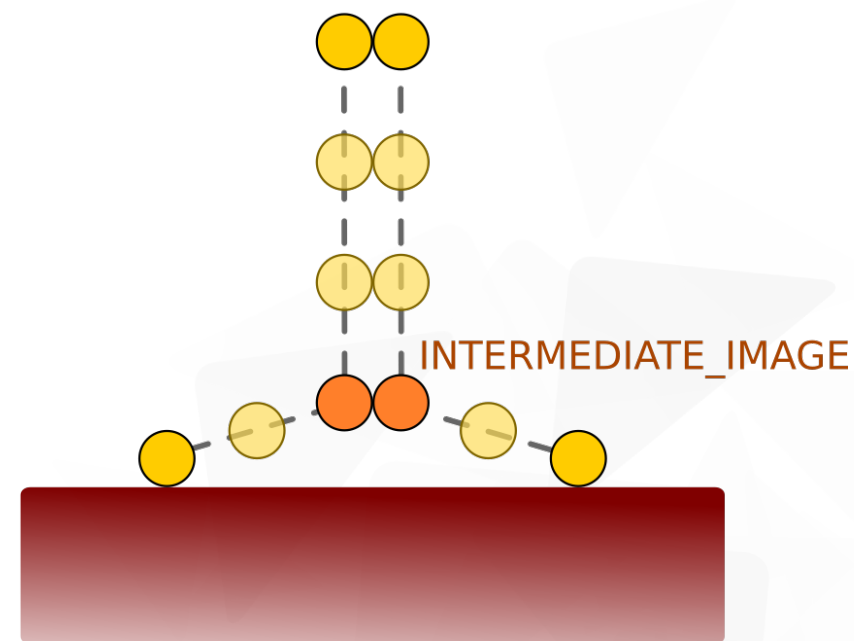
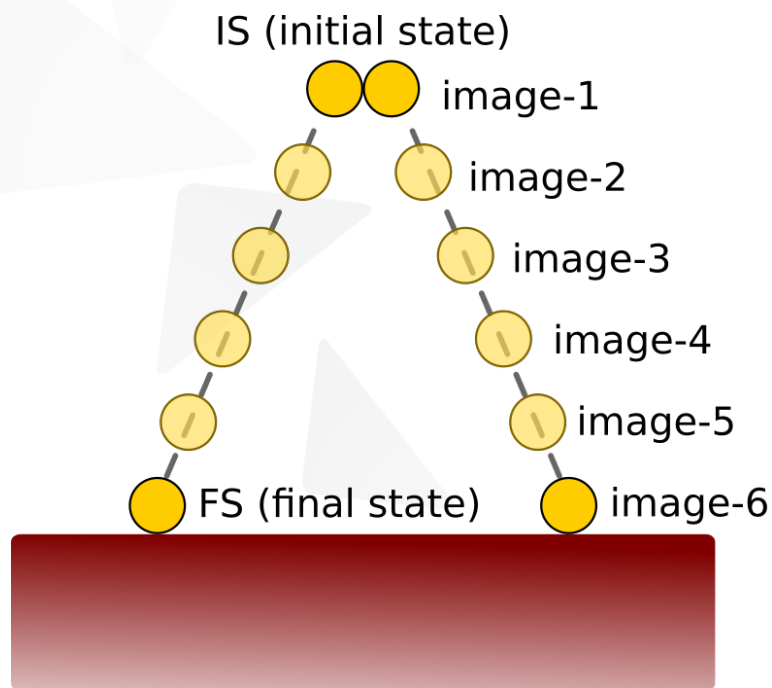


Practical aspects: use chemical intuition



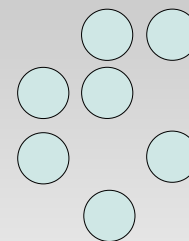
▼ Use INTERMEDIATE_IMAGES

dissociation of a molecule at a surface



much better initial guess !

NEB calculations: number of images



▼ **Question:** How many images should I use?

Answer: It depends, but usually inter-image distance in range of 1 to 2 Bohr should be OK (inter-image distance is printed in the output; make a neb.x dryrun by setting `nstep_path = 0`)

```
activation energy (->) = 0.000000 eV
activation energy (<-) = 0.000000 eV

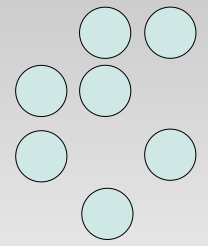
image      energy (eV)      error (eV/A)      frozen
  1         0.0000000      0.0000000         F
  2         0.0000000      0.0000000         F
  3         0.0000000      0.0000000         F
  4         0.0000000      0.0000000         F
  5         0.0000000      0.0000000         F
  6         0.0000000      0.0000000         F
  7         0.0000000      0.0000000         F
  8         0.0000000      0.0000000         F

climbing image = 0

path length      = 5.247 bohr
inter-image distance = 0.750 bohr

NEB              : 0.39s CPU 0.41s WALL
```

NEB calculations: number of images



- ▼ **Question:** How many images should I use?

Answer: It depends, but usually inter-image distance in range of 1 to 2 Bohr should be OK (inter-image distance is printed in the output; make a neb.x dryrun by setting `nstep_path = 0`)

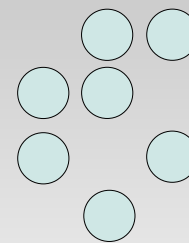
- ▼ What is the inter-image distance & how is it measured?

It is a distance in a $3N$ dimensional space, i.e.:

$$d_{i,i+1} = |\mathbf{R}_i - \mathbf{R}_{i+1}| = \sqrt{\sum_{j=1}^{3N} (x_{i,j} - x_{i+1,j})^2}$$

coordinates of all atoms of the image i

NEB calculations: number of images



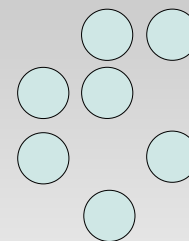
- ▼ **Question:** How many images should I use?

Answer: It depends, but usually inter-image distance in range of 1 to 2 Bohr should be OK (inter-image distance is printed in the output; make a neb.x dryrun by setting `nstep_path = 0`)

- ▼ Visualize the initial reaction path before doing a calculation, e.g.:

```
xcrysden --pwi neb.in
```

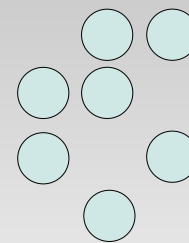
Various hints ...



- ▼ Calculate one elementary reaction step (one saddle point) at a time (note that `CI_scheme = 'manual'` allows for more saddle points simultaneously)
- ▼ `use_freezing = .true.` is usually beneficial
- ▼ **Question:** Which value of spring constants (`k_min`, `k_max`) should I use?

Answer: spring constant values are not that important, default works just fine. Otherwise, suggested values are printed in the `neb.x` output.

A problem with a climbing-image (CI)



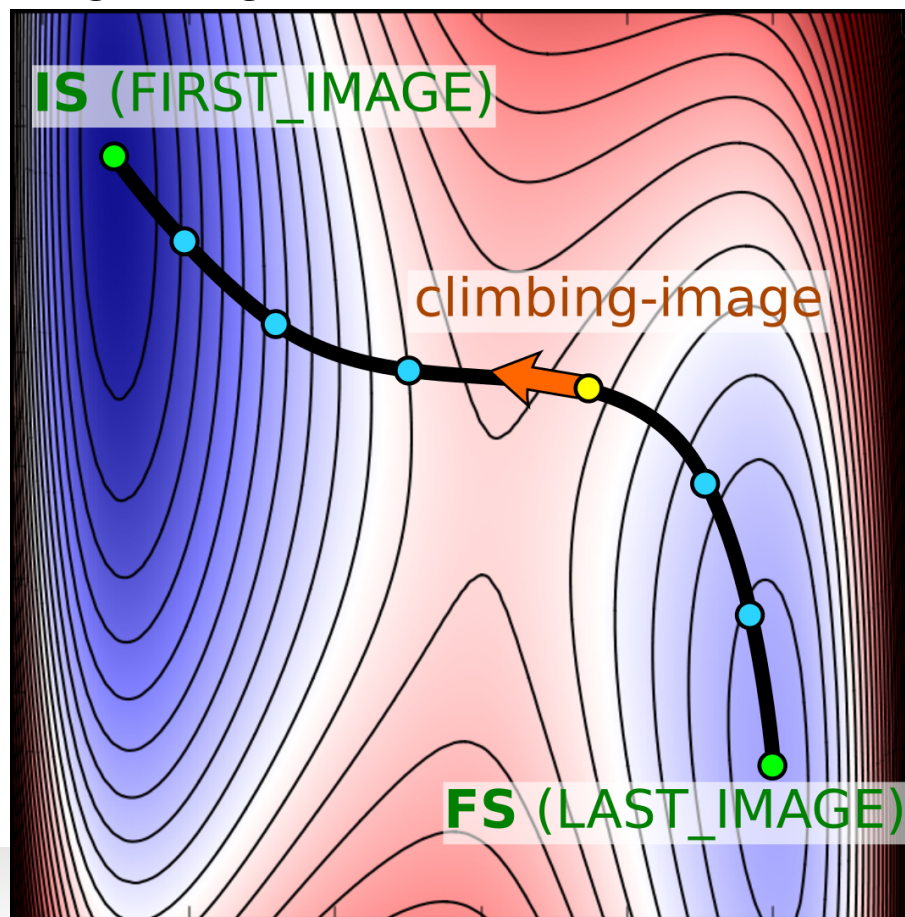
- Do not activate climbing-image NEB from the start !

The reaction path should be first relaxed to some extent as to stabilize it and only then the climbing-image should be activated (`CI_scheme = 'auto'`)

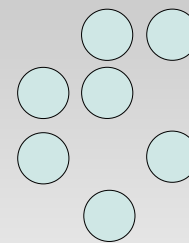
The problem:

CI-image # can oscillate from iteration to iteration

iteration *#n*:
image-5 is climbing



A problem with a climbing-image (CI)



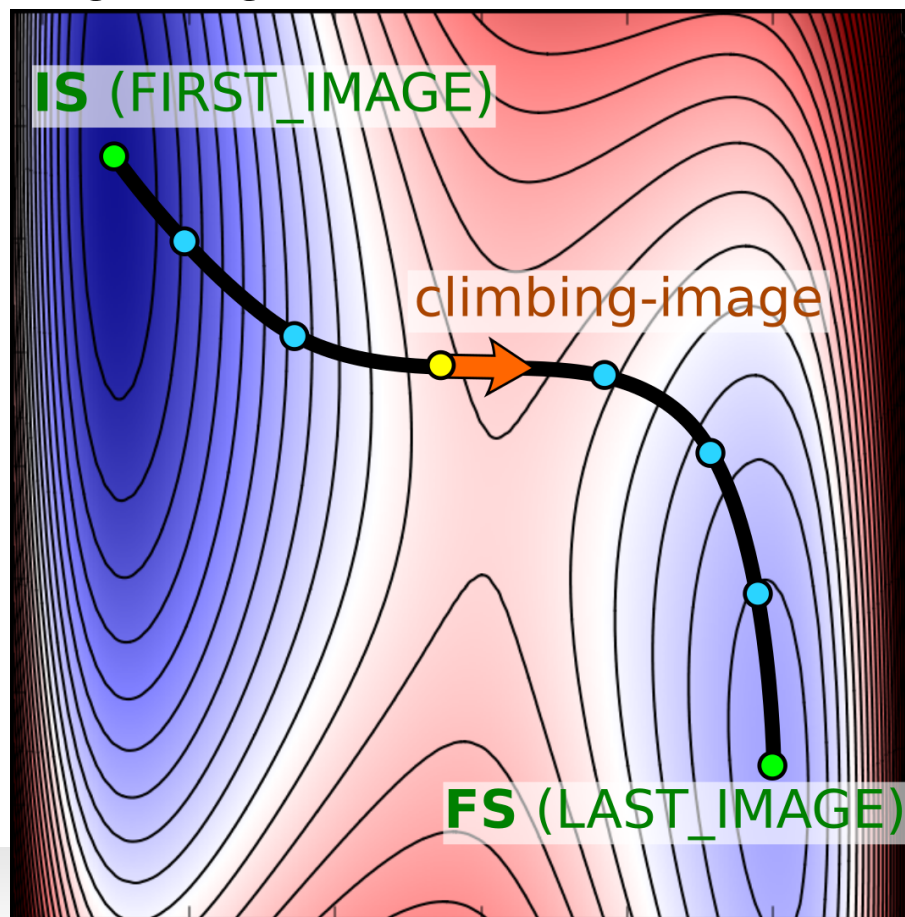
- Do not activate climbing-image NEB from the start !

The reaction path should be first relaxed to some extent as to stabilize it and only then the climbing-image should be activated (`CI_scheme = 'auto'`)

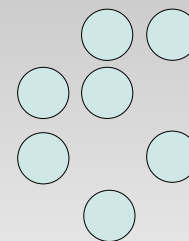
The problem:

CI-image # can oscillate from iteration to iteration

iteration $\#n+1$:
image-4 is climbing



A problem with a climbing-image (CI)



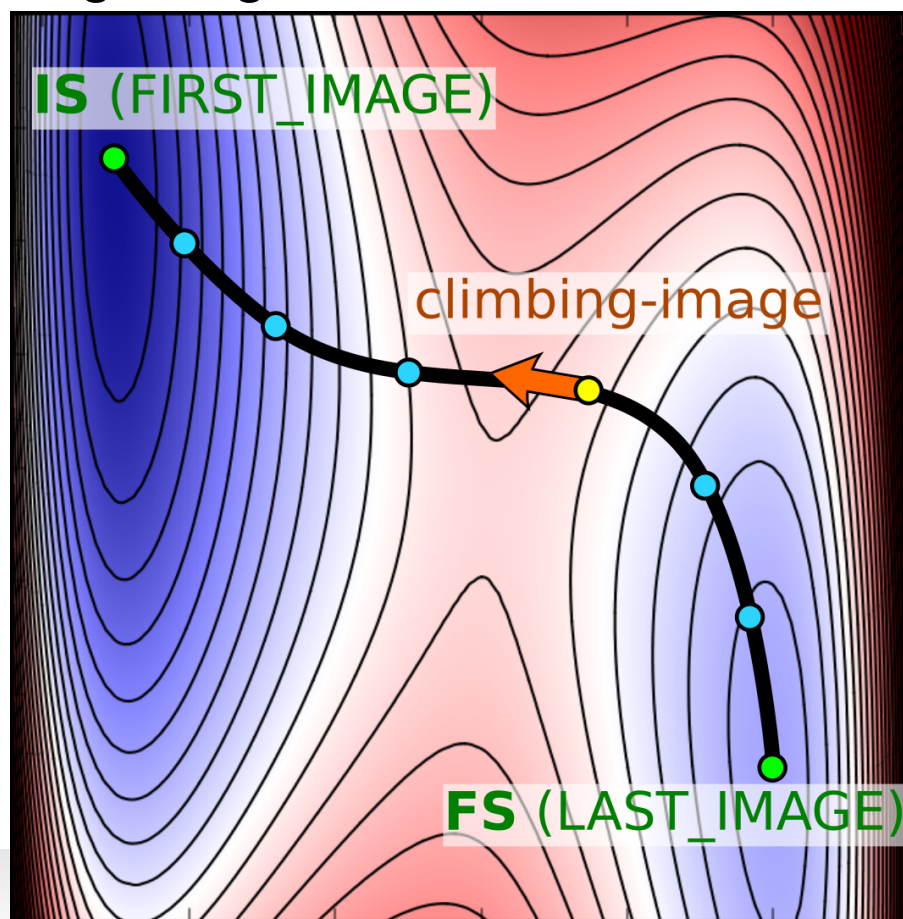
- Do not activate climbing-image NEB from the start !

The reaction path should be first relaxed to some extent as to stabilize it and only then the climbing-image should be activated (`CI_scheme = 'auto'`)

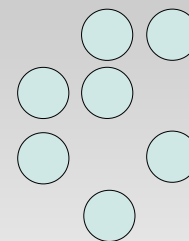
The problem:

CI-image # can oscillate from iteration to iteration

iteration $\#n+2$:
image-5 is climbing



A problem with a climbing-image (CI)



- Do not activate climbing-image NEB from the start !

The reaction path should be first relaxed to some extent as to stabilize it and only then the climbing-image should be activated (`CI_scheme = 'auto'`)

- PWTK snippet for `'no-CI' + 'auto'` NEB workflow:

```
load_fromNEBI neb.in
```

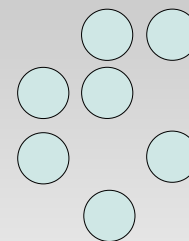
```
PATH {  
    CI_scheme = 'no-CI'  
    path_thr  = 0.8  
}
```

```
runNEB neb.noCI.in
```

```
PATH {  
    restart_mode = 'restart'  
    CI_scheme = 'auto'  
    path_thr  = 0.05  
}
```

```
runNEB neb.auto.in
```

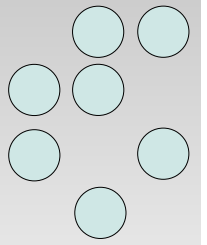
Specification of IMAGES



▼ **BEWARE:** do not swap atoms !

(keep atom indices the same for all specified images)

That's all – practice follows ...



It is time to try neb.x calculations
during hands-on !