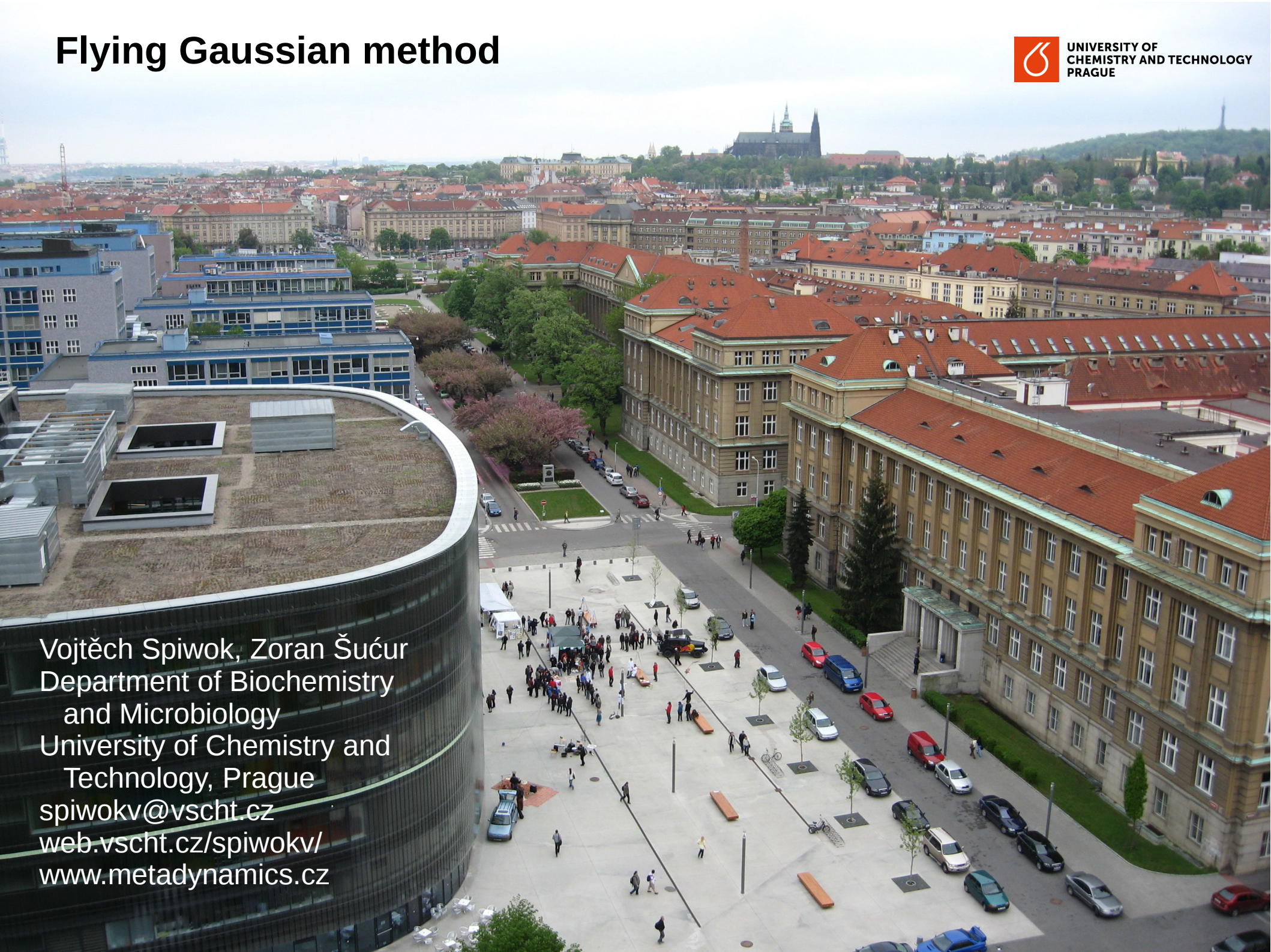
Flying Gaussian method



Vojtěch Spiwok, Zoran Šućur
Department of Biochemistry and Microbiology
University of Chemistry and Technology, Prague
spiwokv@vscht.cz
web.vscht.cz/spiwokv/
www.metadynamics.cz

https://commons.wikimedia.org/wiki/File:ASDA_in_Keighley.jpg

https://commons.wikimedia.org/wiki/File:ASDA_in_Keighley.jpg

“Molecular” dynamics simulation

https://commons.wikimedia.org/wiki/File:ASDA_in_Keighley.jpg

“Molecular” dynamics simulation

$$F(s) = -kT \log(P(s))$$

https://commons.wikimedia.org/wiki/File:ASDA_in_Keighley.jpg

Metadynamics

$$F(s) = -V_{bias}(s)$$

https://commons.wikimedia.org/wiki/File:ASDA_in_Keighley.jpg

Multiple walker metadynamics

$$F(s) = -V_{bias}(s) = -\sum_i V_{bias,i}(s)$$

https://commons.wikimedia.org/wiki/File:ASDA_in_Keighley.jpg

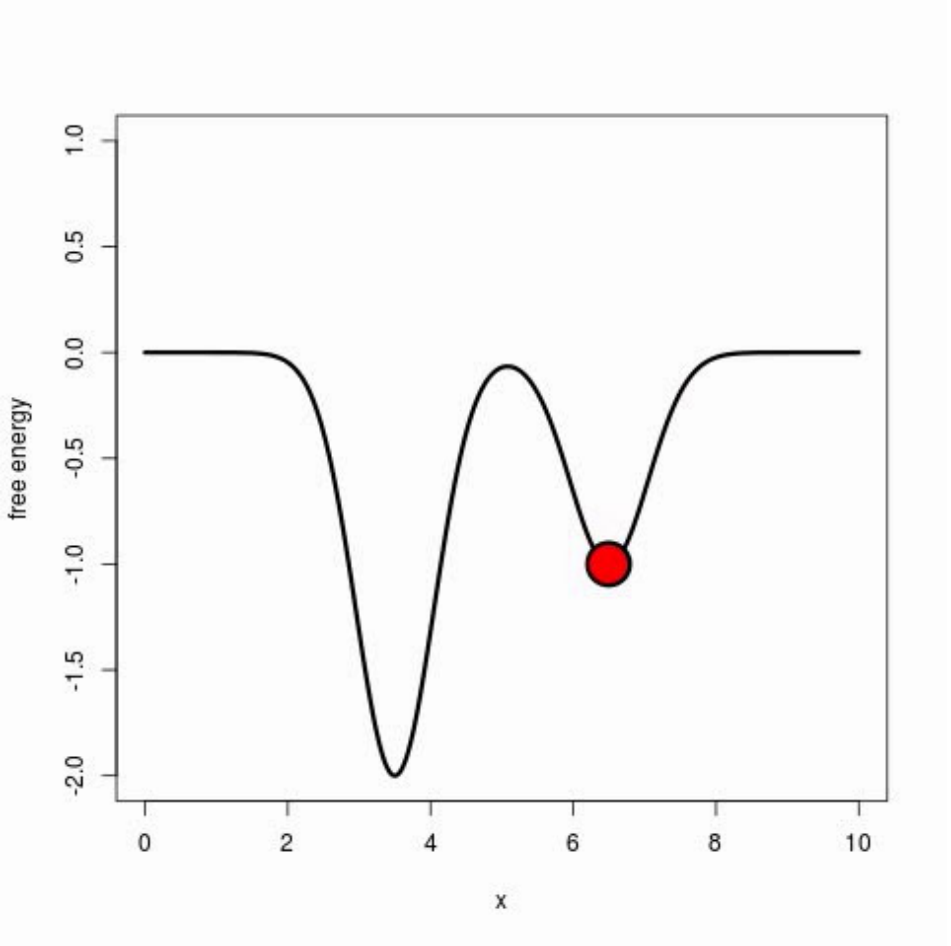
Flying Gaussian method

$$V_{bias,j}(s) = \sum_{i=1}^{N} w \exp\left(-\frac{(s_i - s_j)^2}{2\delta s^2}\right)$$

Flying Gaussian method

Model profile

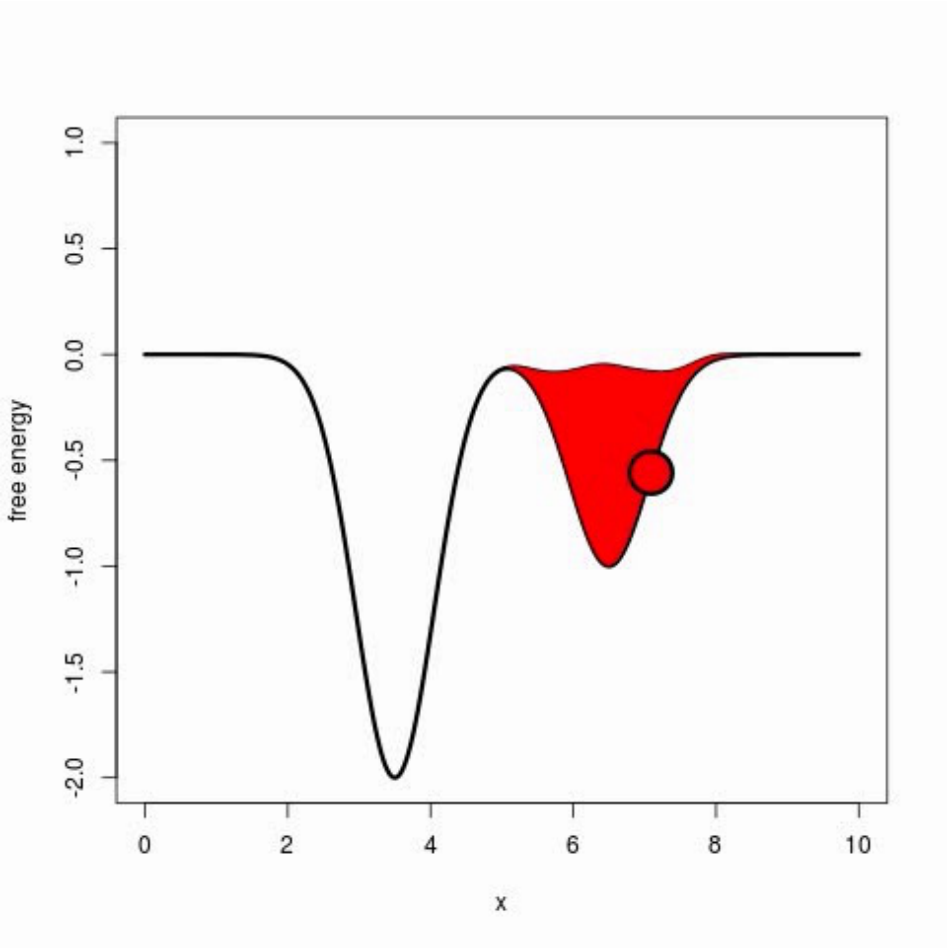
Unbiased MD



Flying Gaussian method

Model profile

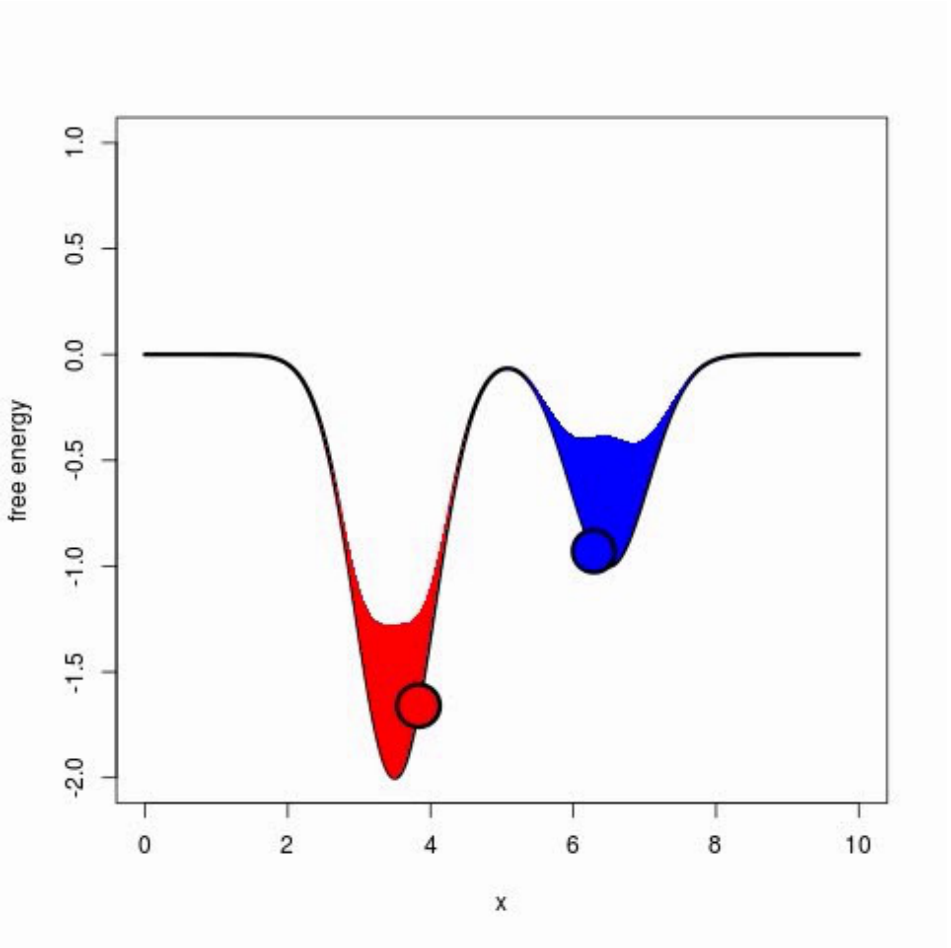
Metadynamics



Flying Gaussian method

Model profile

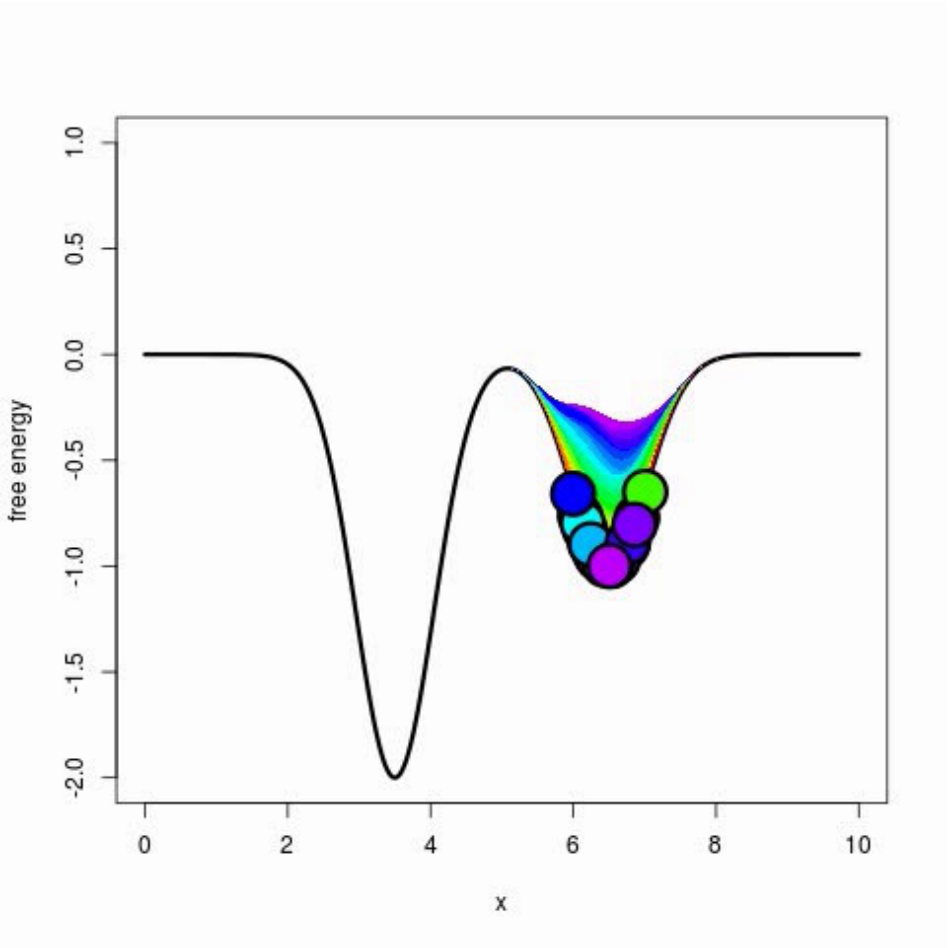
Multiple-walker metadynamics



Flying Gaussian method

Model profile

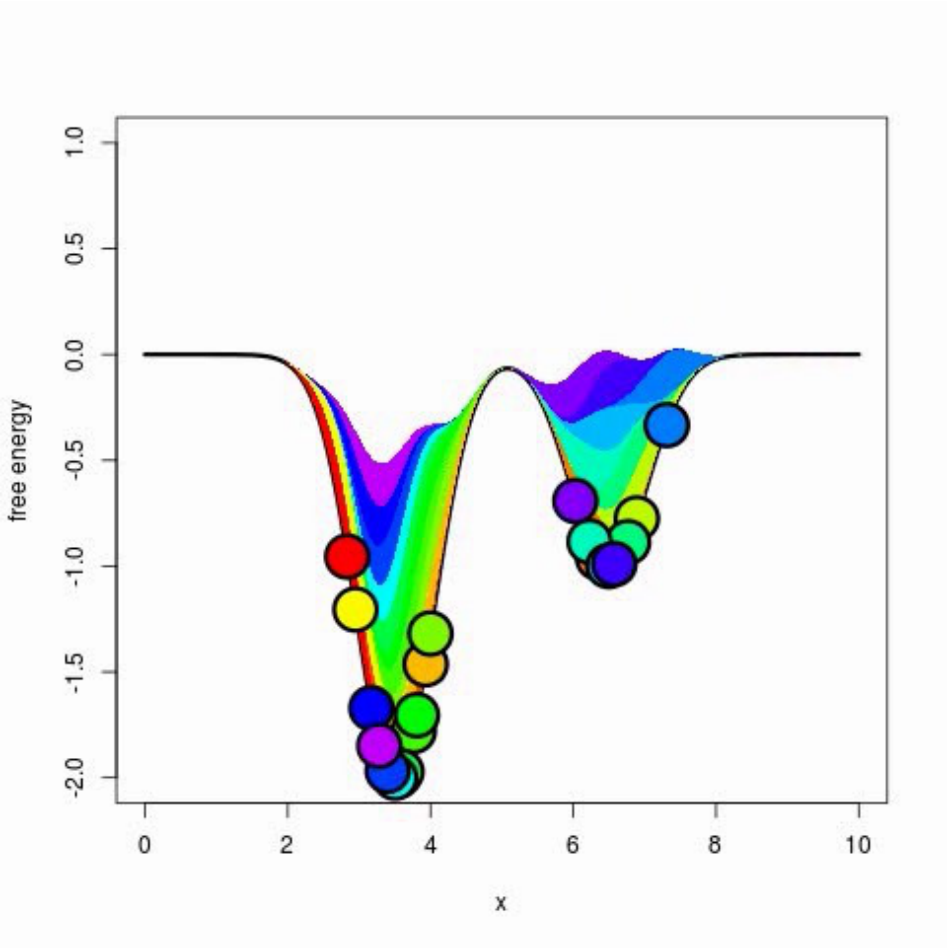
Flying Gaussian



Flying Gaussian method

Model profile

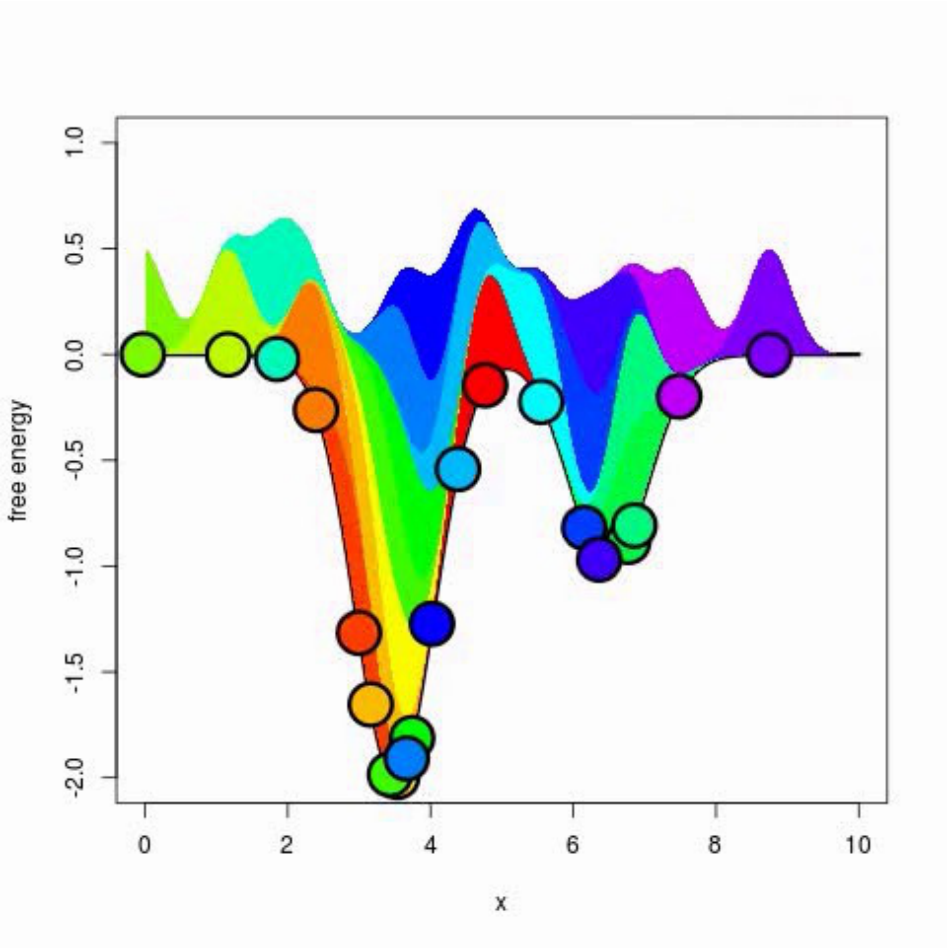
Flying Gaussian



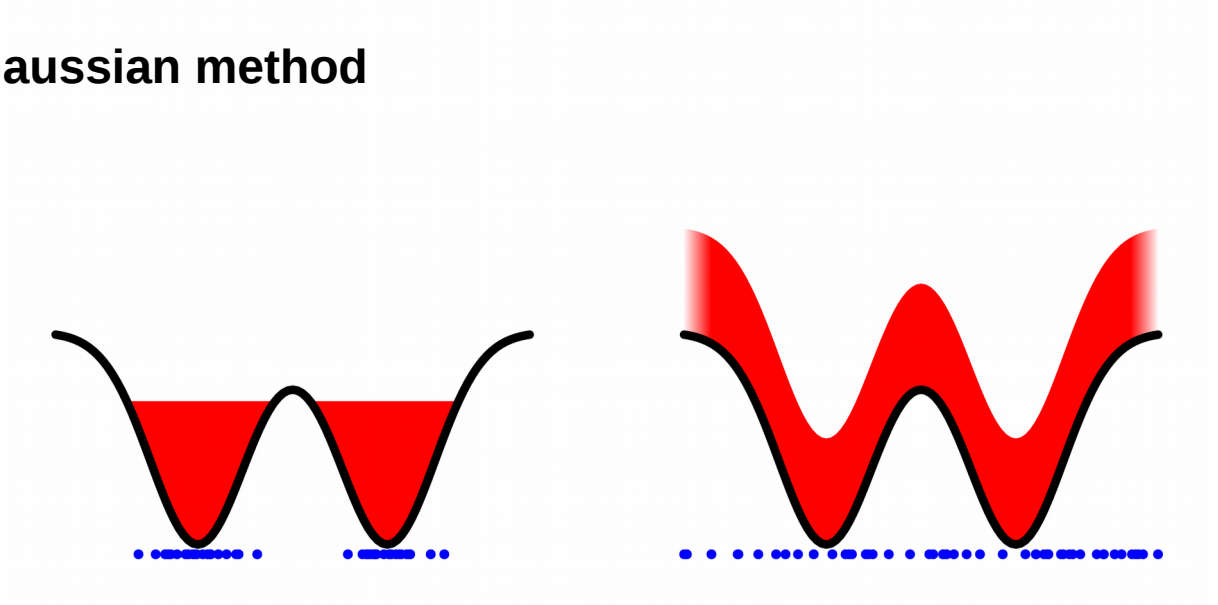
Flying Gaussian method

Model profile

Flying Gaussian



Flying Gaussian method



Free energy estimate:

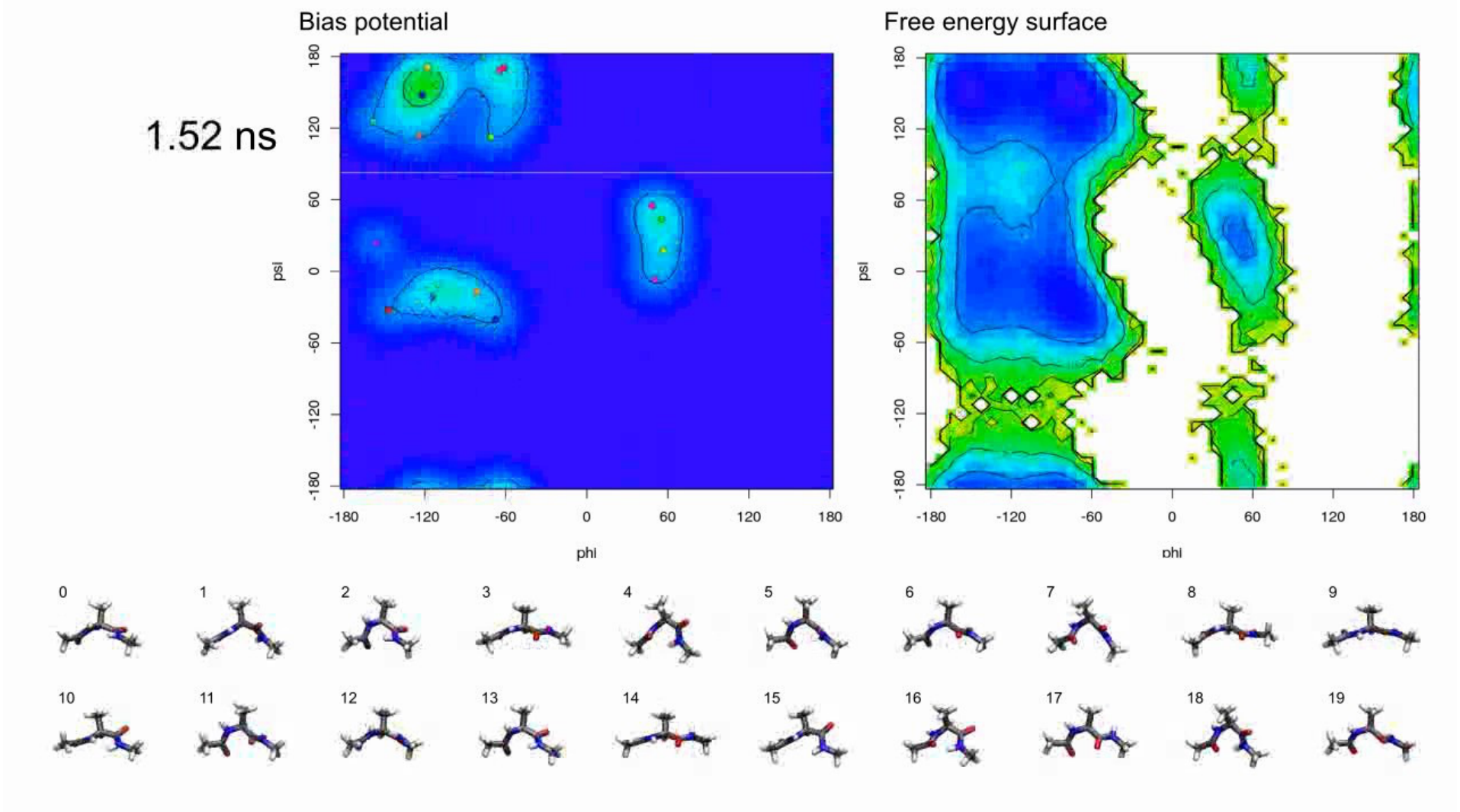
On-the-fly reweighing:

$$F(s) = -kT \log \left(\frac{\sum_{i=1}^{N} \sum_{t} \delta(s_i(t) - s) \exp(+V_{bias,i}(t)/kT)}{\sum_{i=1}^{N} \sum_{t} \exp(+V_{bias,i}(t)/kT)} \right)$$

Weighted histogram analysis method

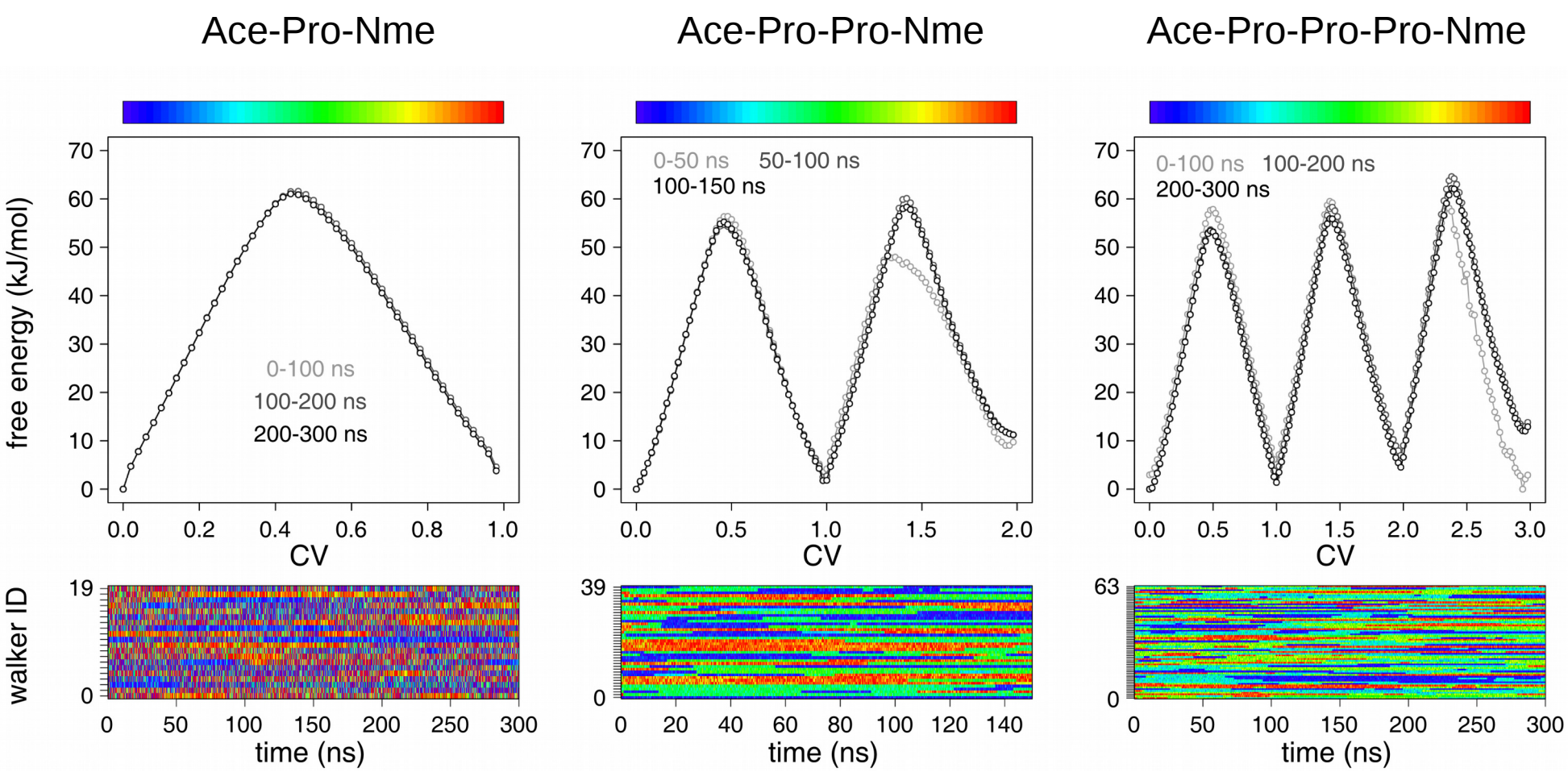
Flying Gaussian method

Ace-Ala-Nme in water, 20 walkers



Flying Gaussian method

Ace-(Pro)n-Nme in vacuum

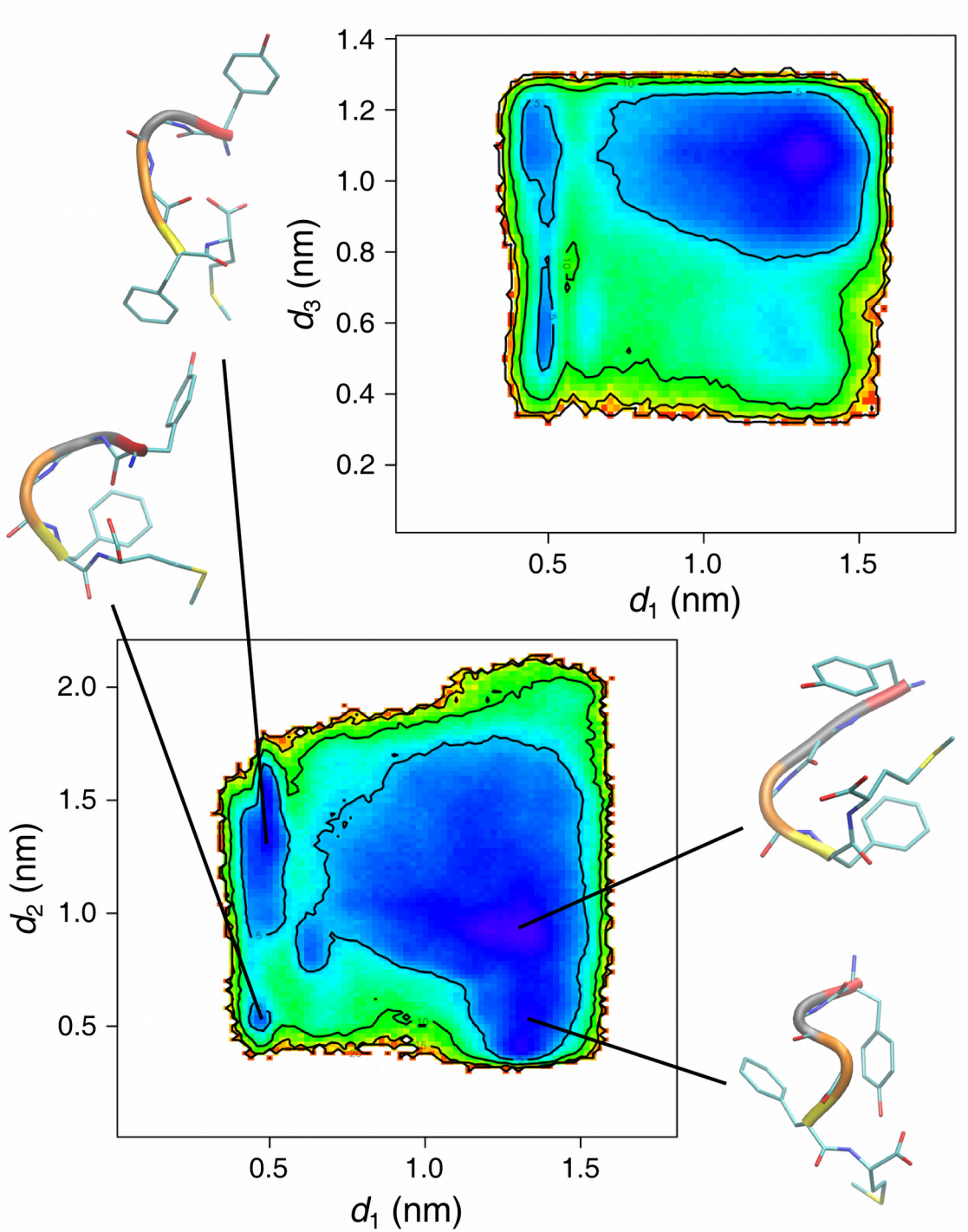


$$CV = \sum_{i=1}^{n} \cos^2\left(\omega_i / 2\right)$$

Flying Gaussian method

Met-enkephalin (YGGFM) in water

CVs:
d1: N[Tyr1]-Cα[Met5]
d2: Cζ[Tyr1]-Cζ[Phe4]
d3: Cζ[Phe4]-Sδ[Met5]



UNIVERSITY OF CHEMISTRY AND TECHNOLOGY PRAGUE

Flying Gaussian method

Advantages:

- easy to parallelize
- tunable biasing
- autonomous bias potential (CVs can be adaptive)

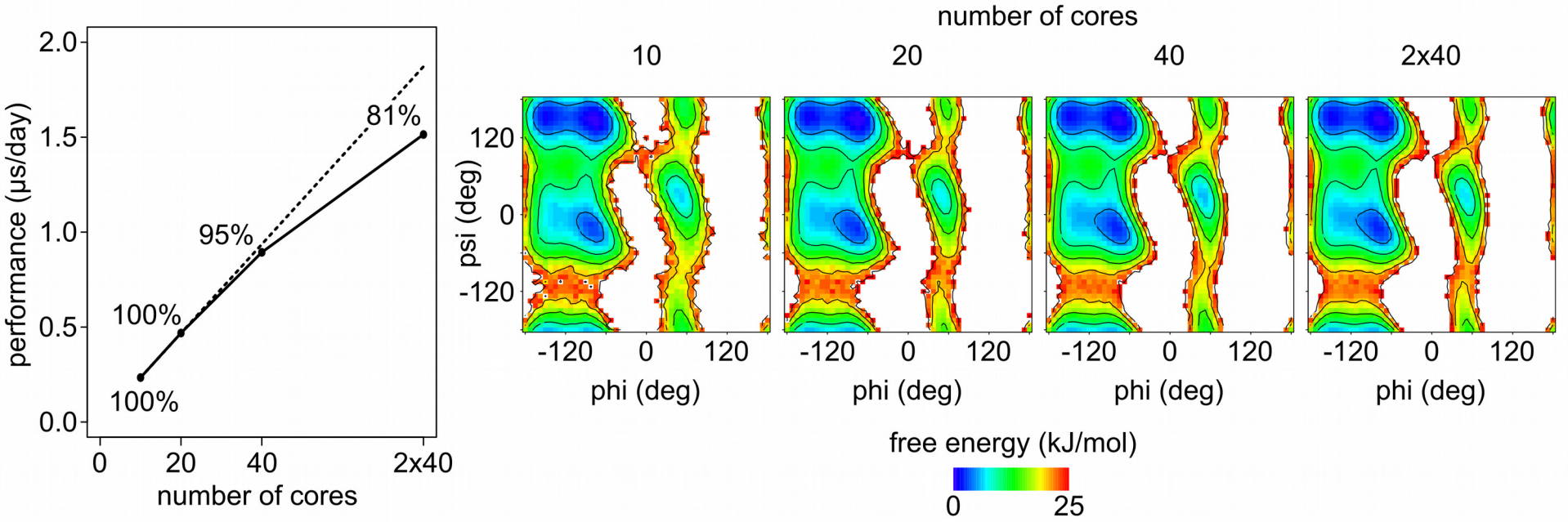
Disadvantages:

- it is necessary to parallelize

Flying Gaussian method

Advantages:

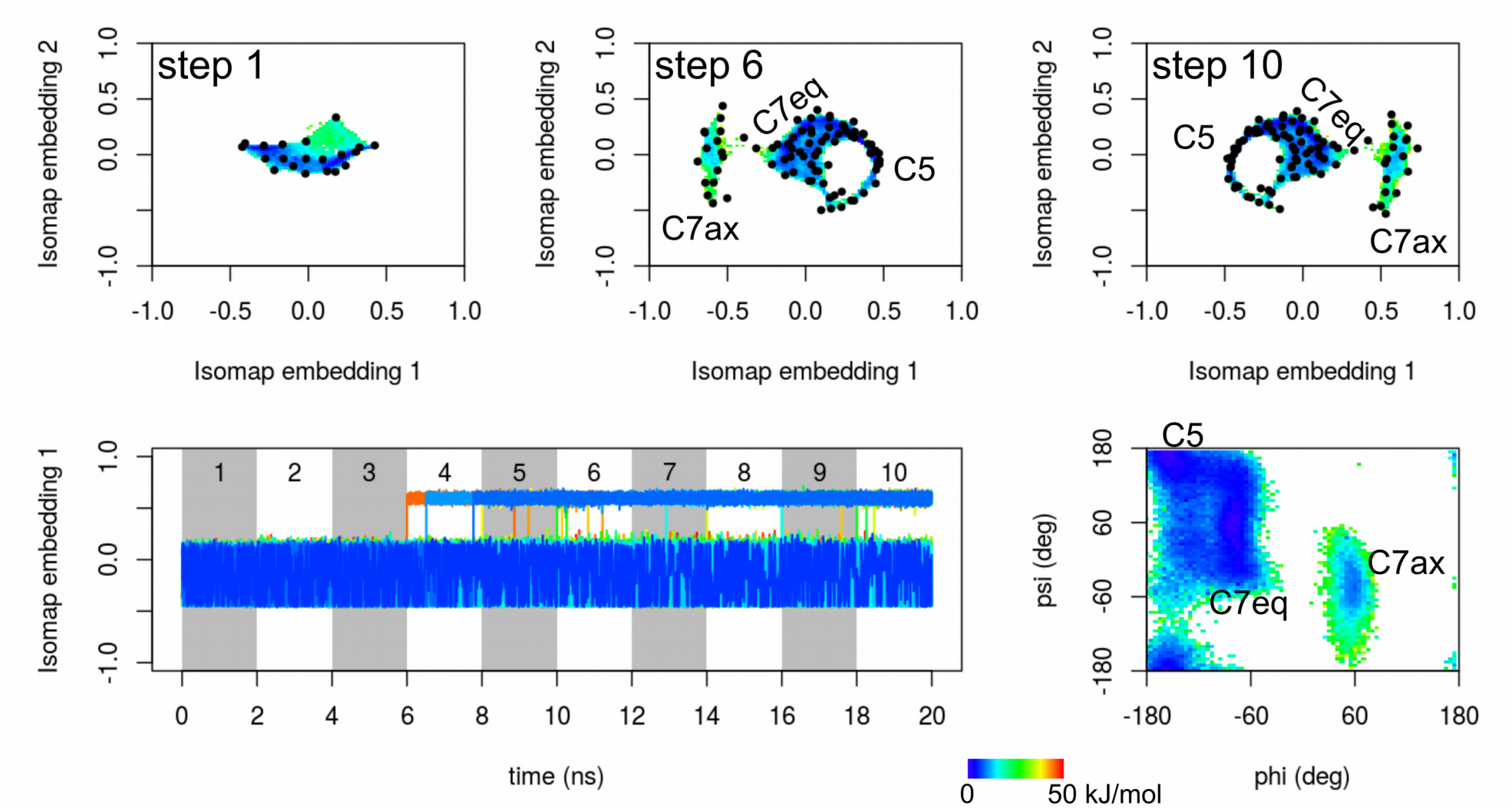
- easy to parallelize



Flying Gaussian method

Advantages:

- autonomous bias potential (CVs can be adaptive)



Flying Gaussian method

Disadvantages:

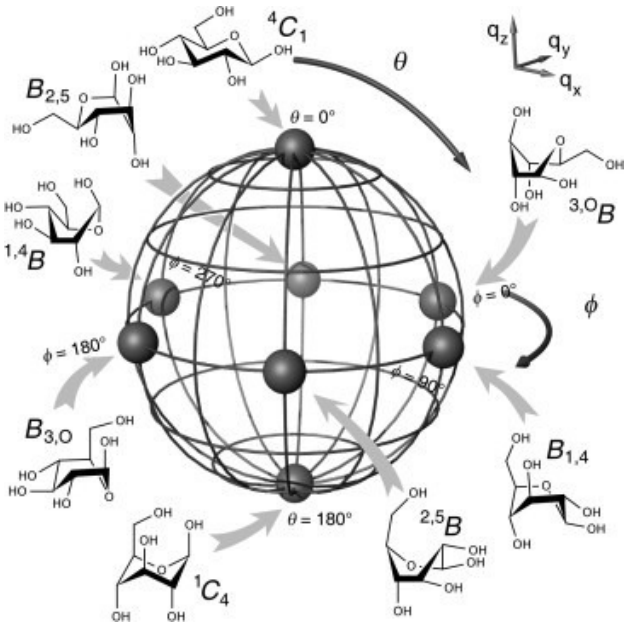
- it is necessary to parallelize

https://commons.wikimedia.org/wiki/File:ASDA_in_Keighley.jpg

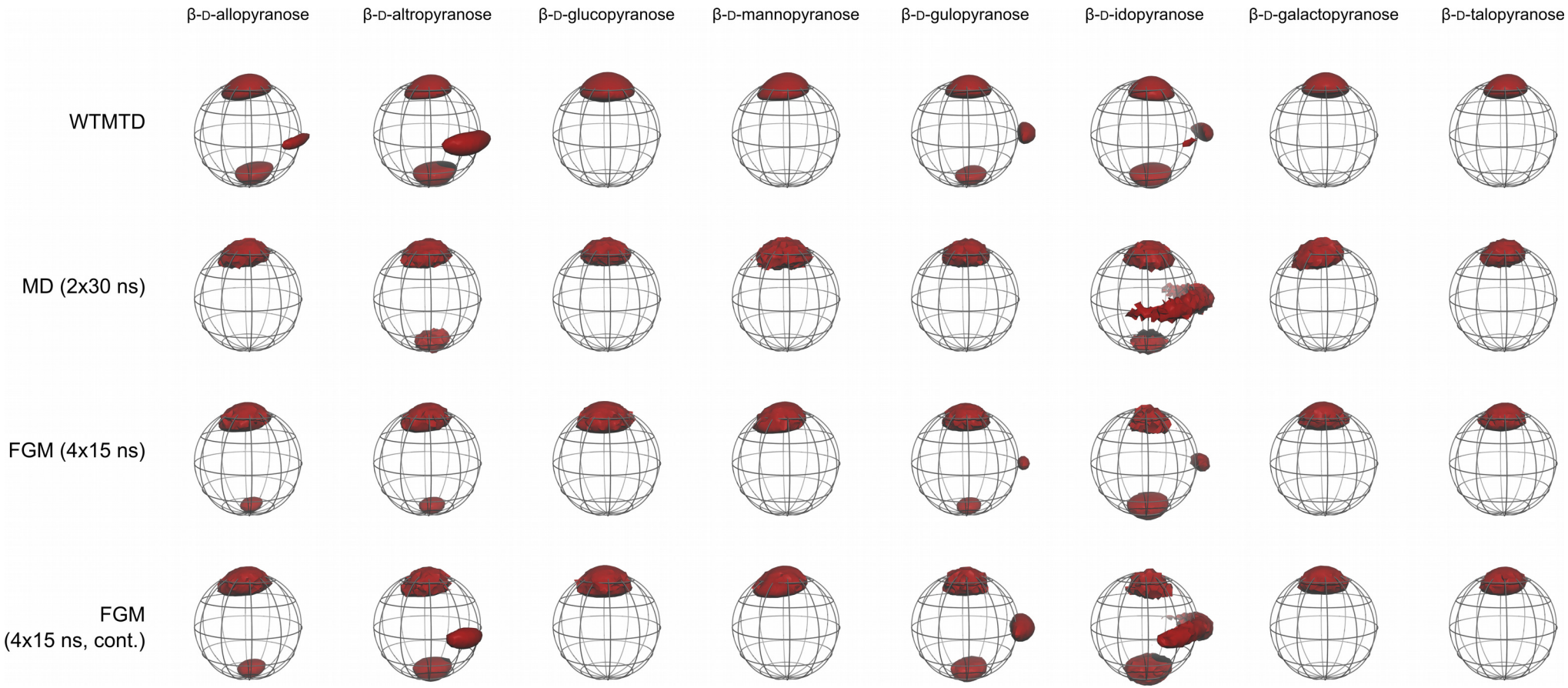
Flying Gaussian method

Disadvantages:

- it is necessary to parallelize



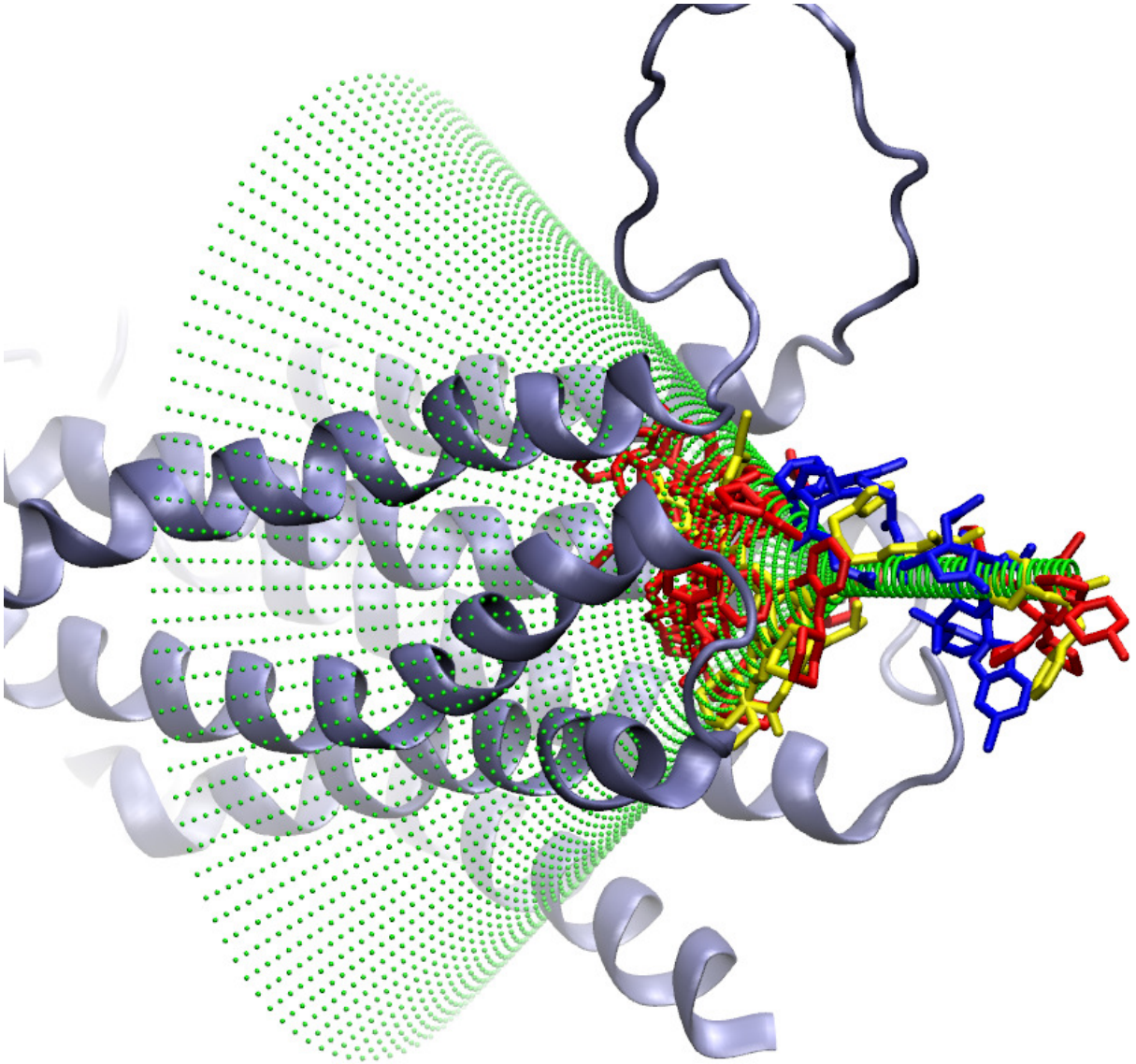
+20 kJ/mol



Flying Gaussian method

Disadvantages:

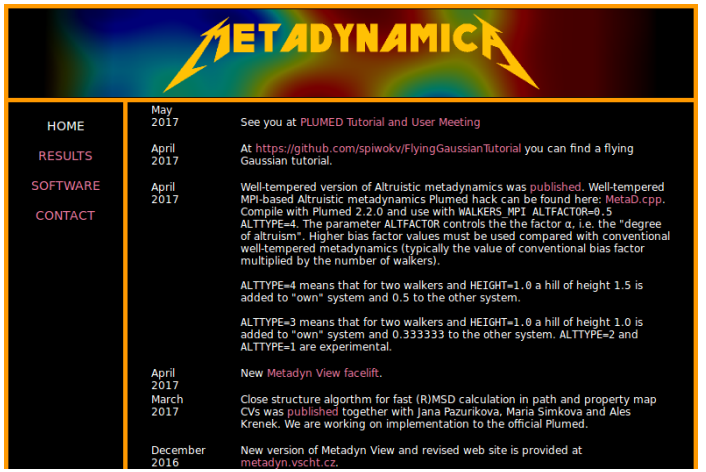
- it is necessary to parallelize



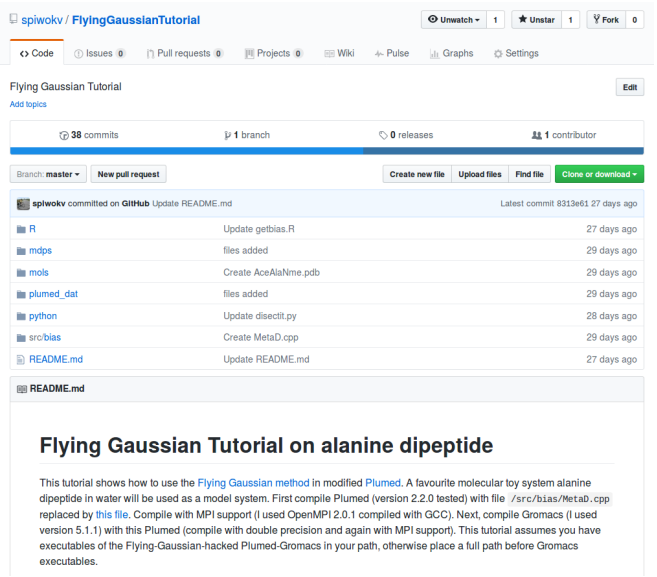
Flying Gaussian method

More info:
Z. Šućur & V. Spiwok: Sampling Enhancement and Free Energy Prediction by Flying Gaussian Method. *J Chem Theory Comput* **12**(9) 4644-4650 (2016).

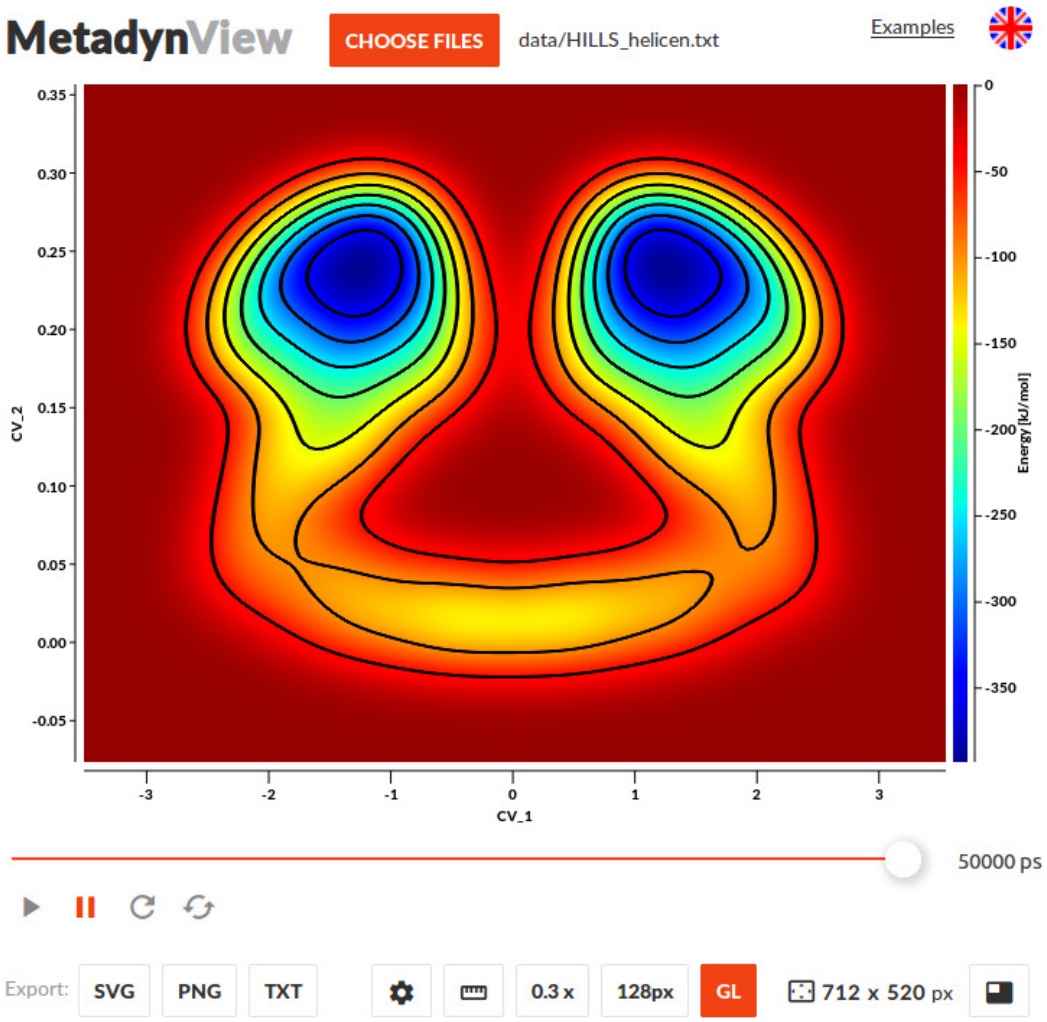
http://www.metadynamics.cz



https://github.com/spiwokv/FlyingGaussianTutorial



http://metadyn.vscht.cz



Acknowledgments:

UCT Prague: Petr Hošek, Pavel Kříž, Václav Mareška, Daniela Toulcová, Dalibor Trapl

MU Brno: Jana Pazúriková, Aleš Křenek

HPC resources:

Metacentrum CERIT-SC IT4I

Money:

Czech Science Foundation (15-17269S)

COST (Glisten, LD14133)