

Flying Gaussian method



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"Molecular" dynamics simulation



“Molecular” dynamics simulation

$$F(s) = -k T \log(P(s))$$



Metadynamics

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



Multiple walker metadynamics

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



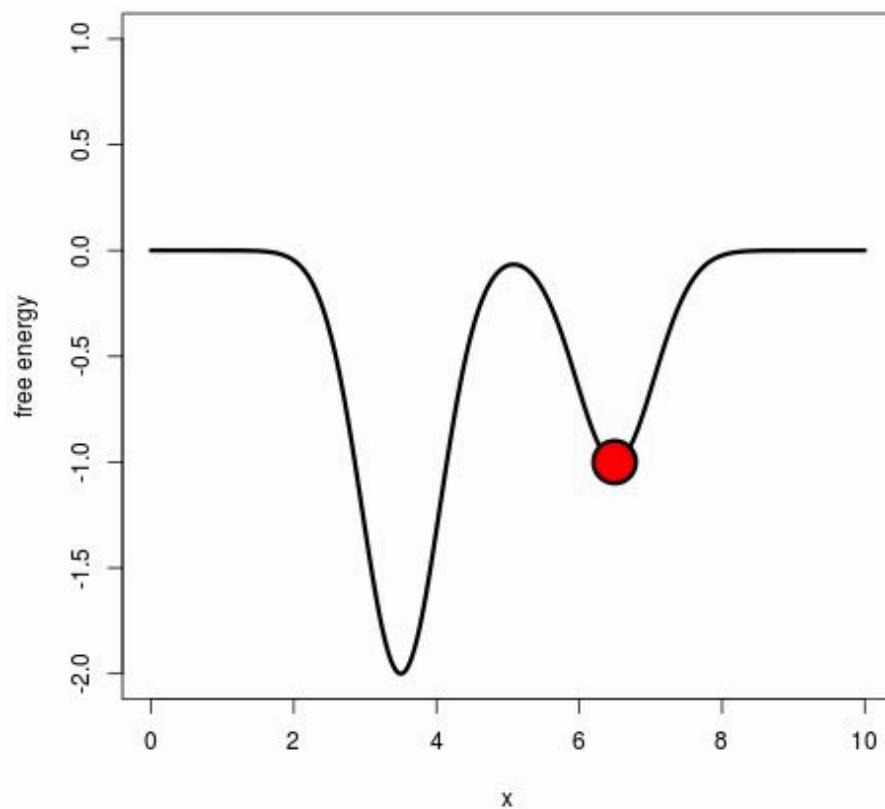
Flying Gaussian method

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

Flying Gaussian method

Model profile

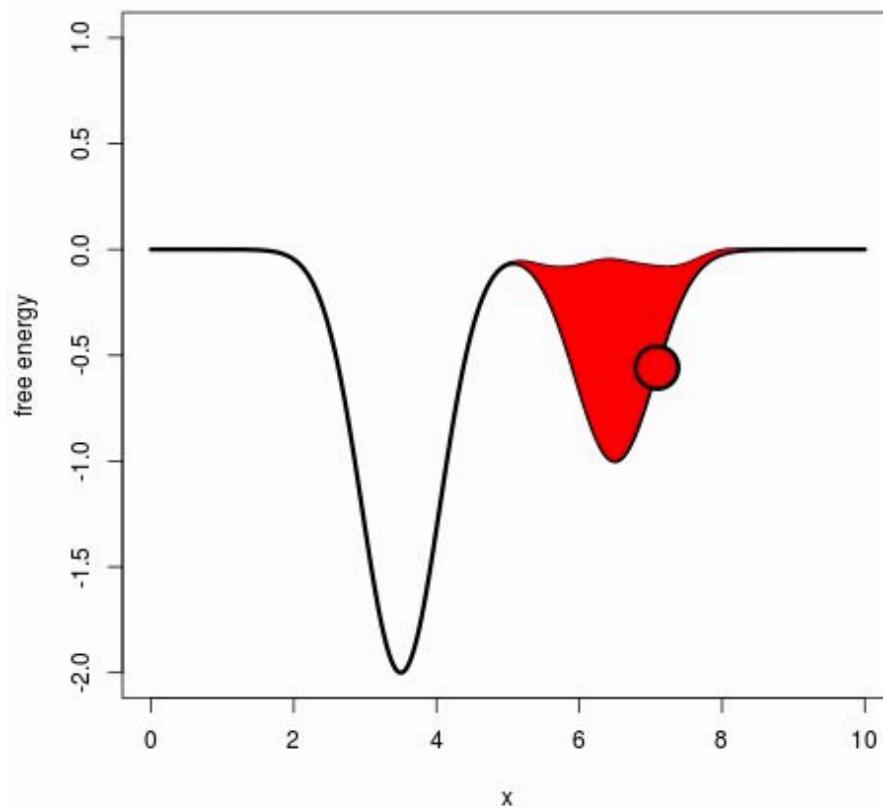
Unbiased MD



Flying Gaussian method

Model profile

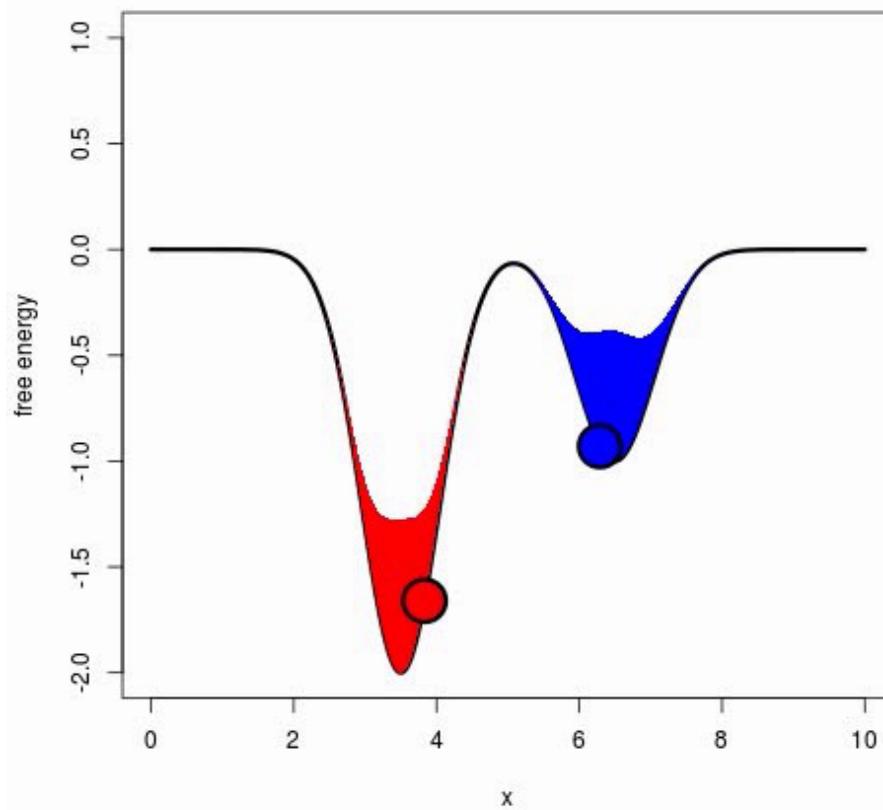
Metadynamics



Flying Gaussian method

Model profile

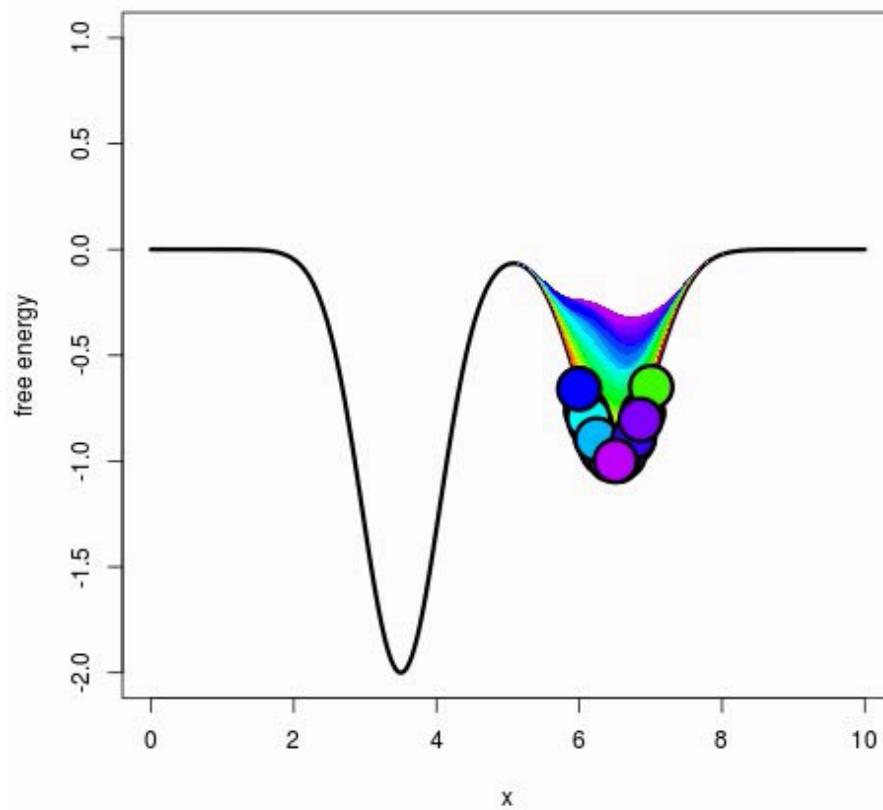
Multiple-walker metadynamics



Flying Gaussian method

Model profile

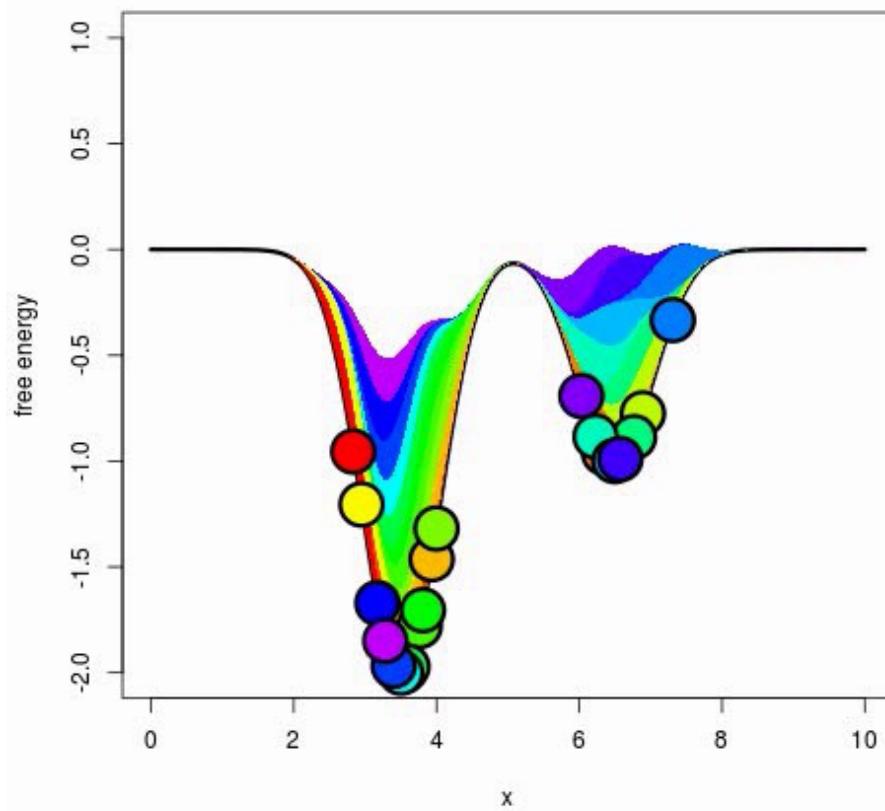
Flying Gaussian



Flying Gaussian method

Model profile

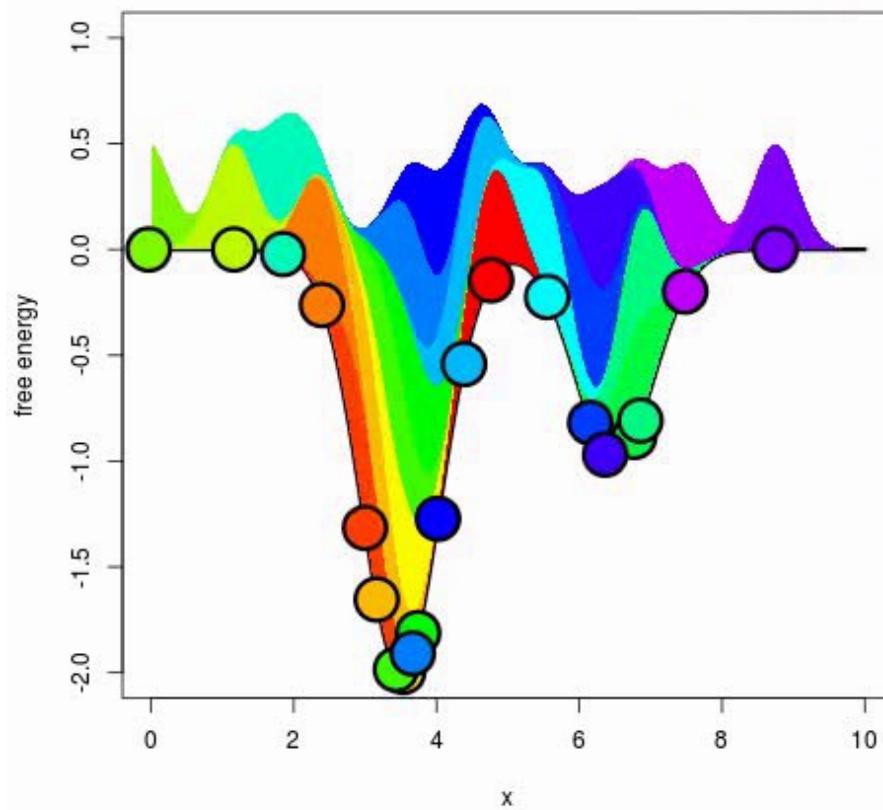
Flying Gaussian



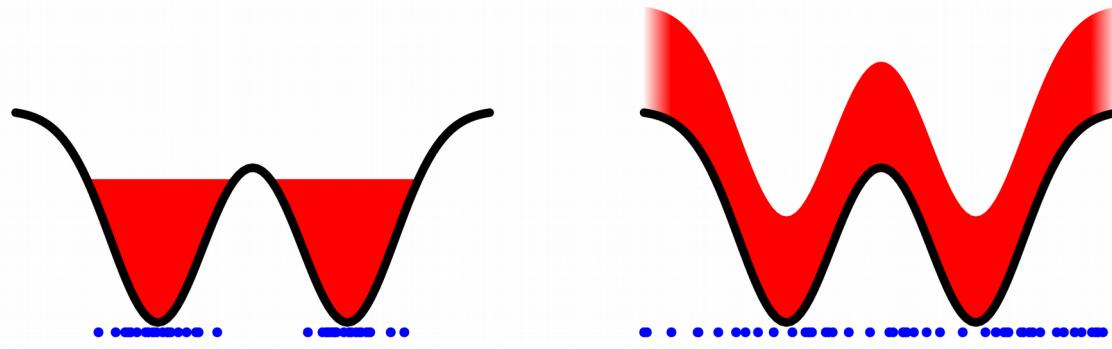
Flying Gaussian method

Model profile

Flying Gaussian



Flying Gaussian method



Free energy estimate:

On-the-fly reweighing:

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

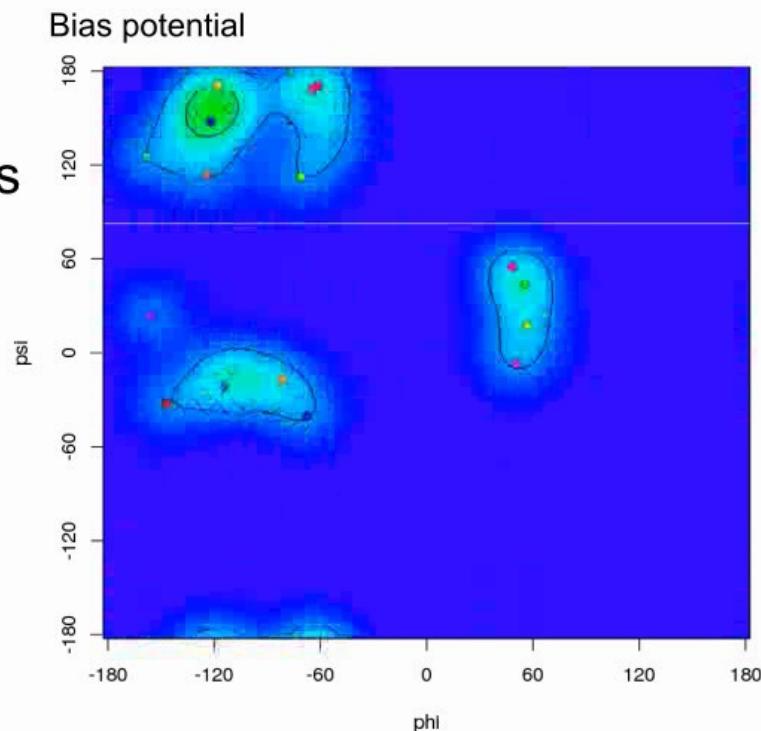
Weighted histogram analysis method

Flying Gaussian method

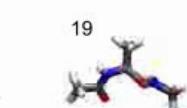
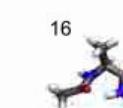
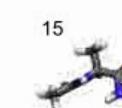
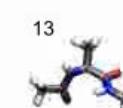
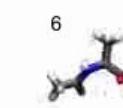
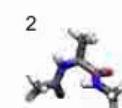
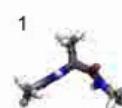
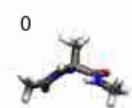
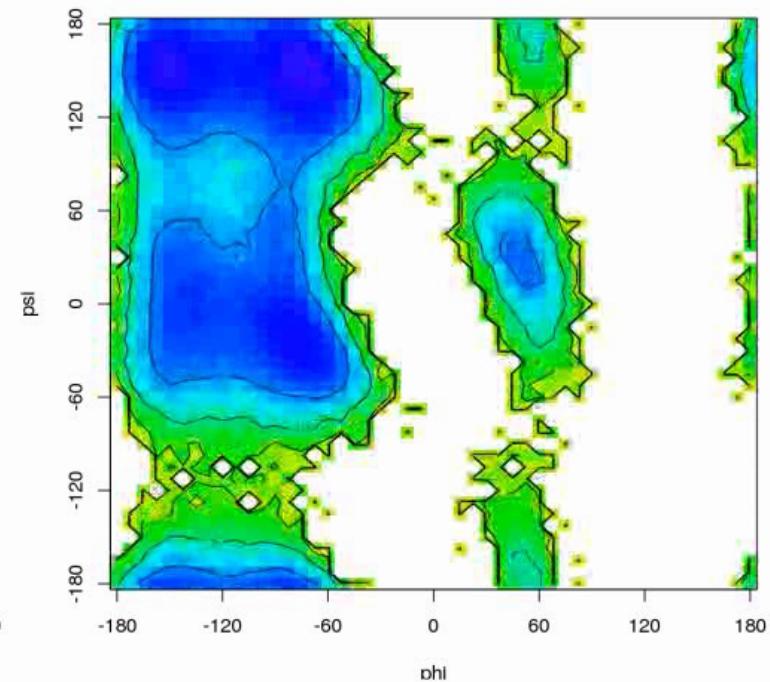
Ace-Ala-Nme in water, 20 walkers

Bias potential

1.52 ns

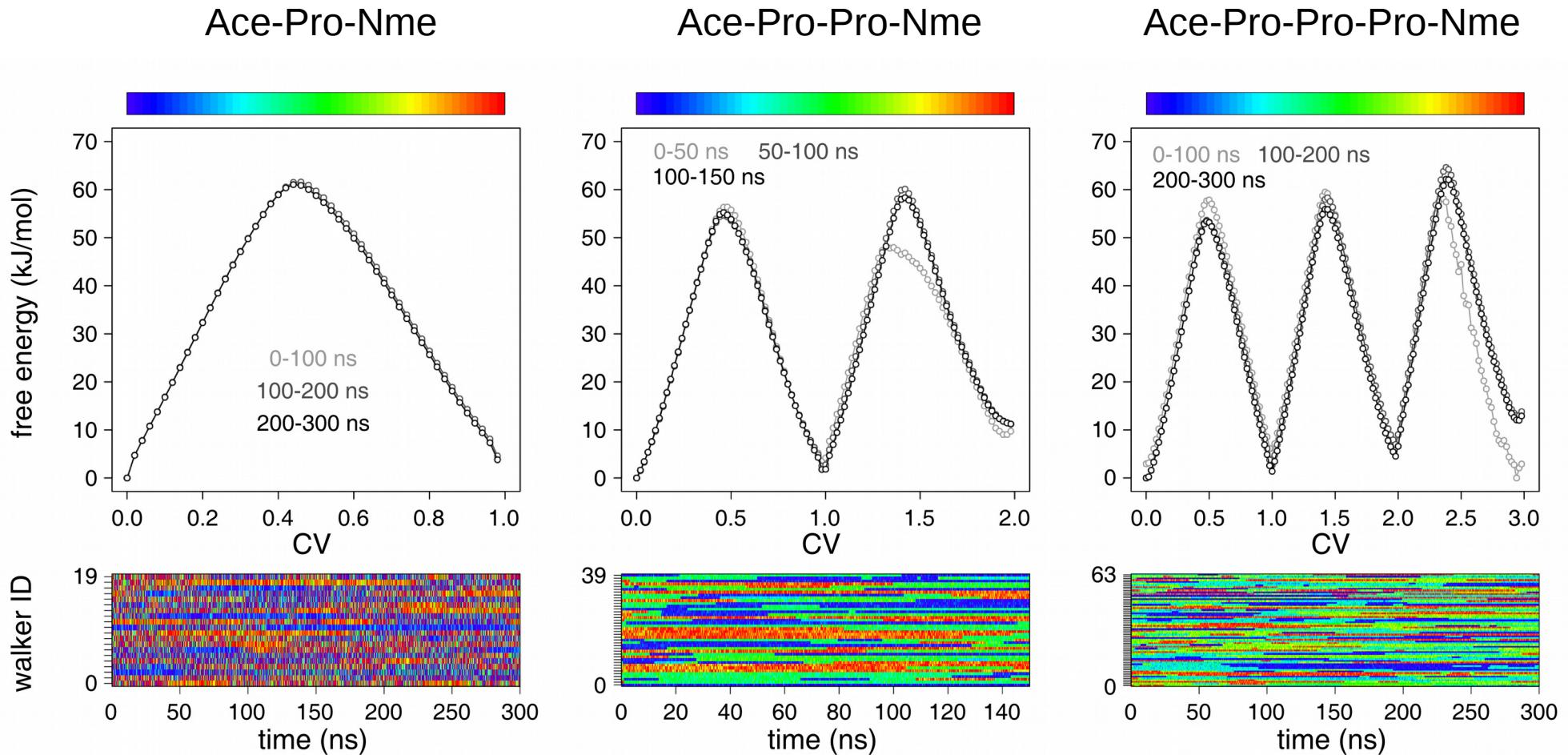


Free energy surface



Flying Gaussian method

Ace-(Pro) n -Nme in vacuum



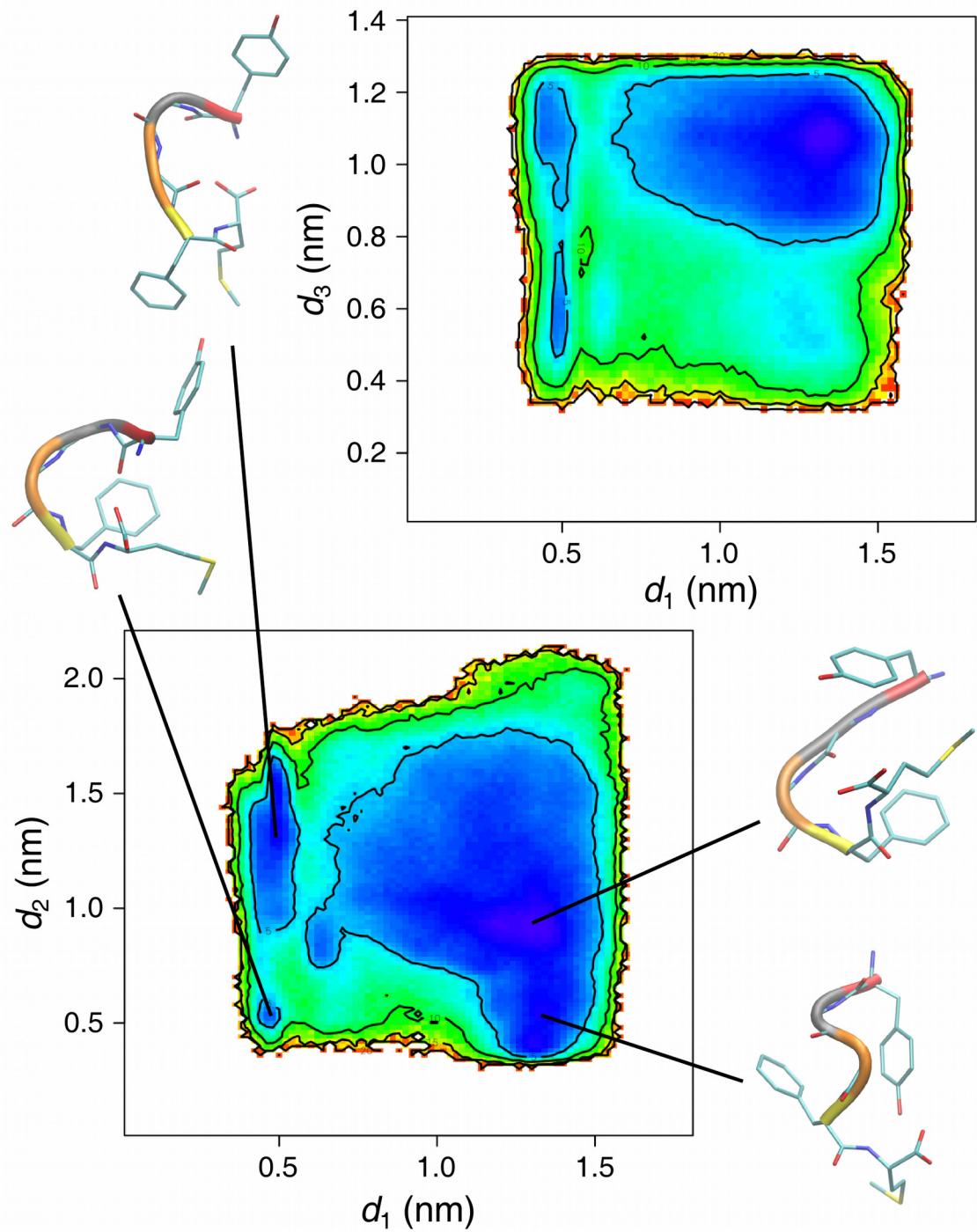
$$CV = \sum_{i=1}^n \cos^2(\omega_i/2)$$

Flying Gaussian method

Met-enkephalin (YGGFM) in water

CVs:

- d1: N[Tyr1]-C α [Met5]
- d2: C ζ [Tyr1]-C ζ [Phe4]
- d3: C ζ [Phe4]-S δ [Met5]



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Flying Gaussian method

Advantages:

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

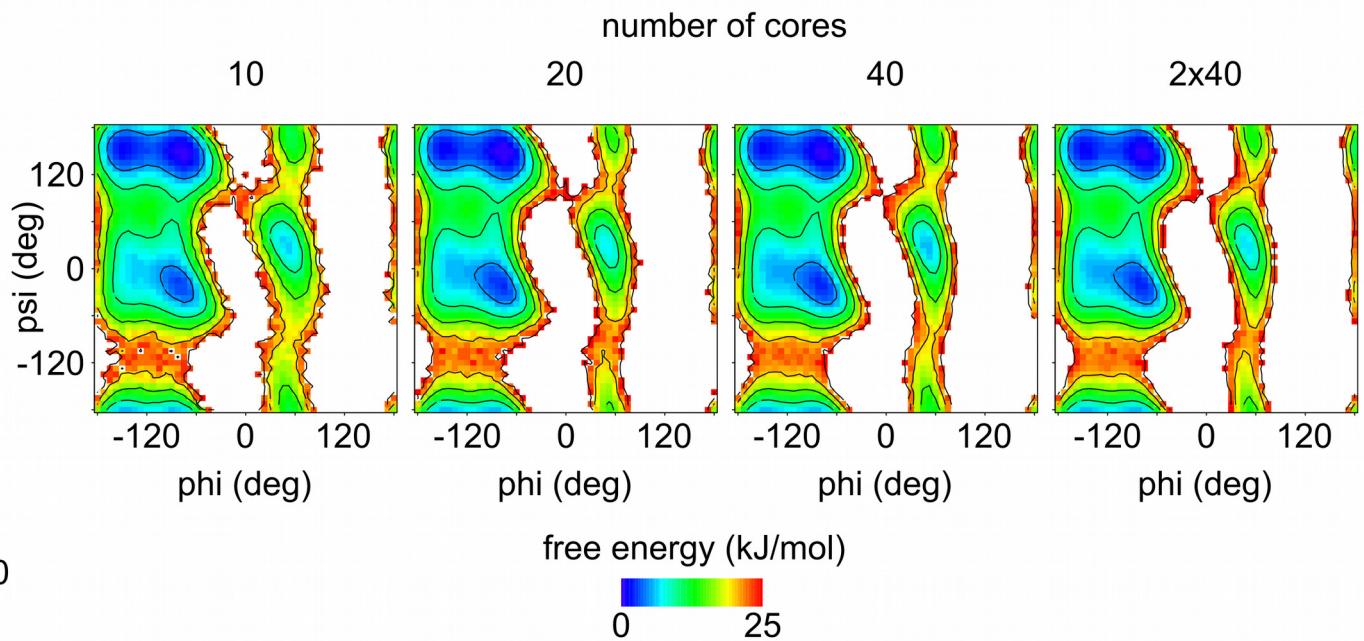
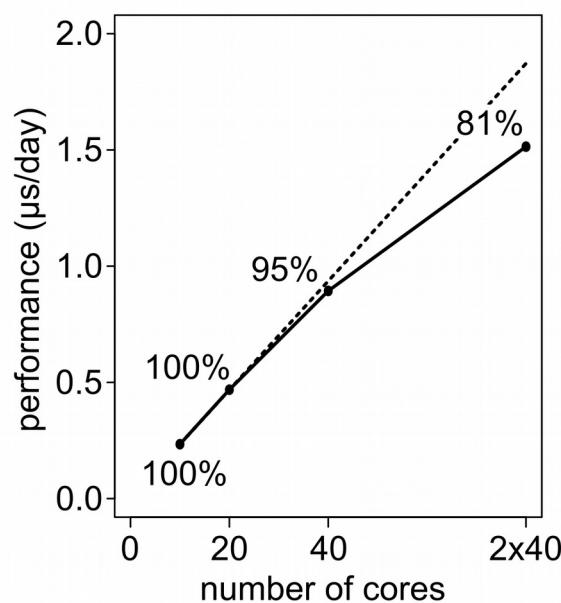
Disadvantages:

- it is necessary to parallelize

Flying Gaussian method

Advantages:

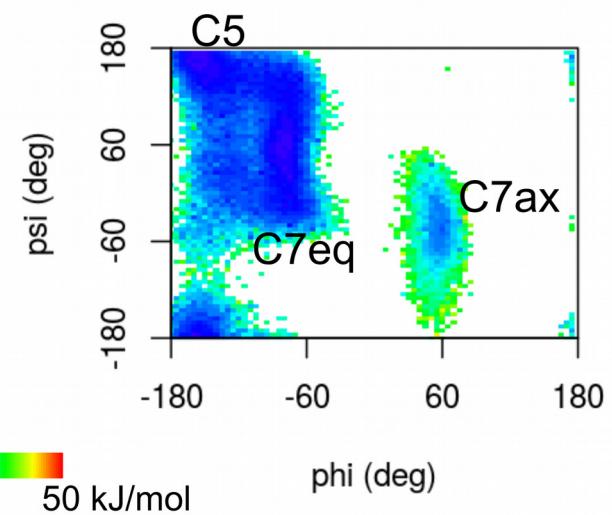
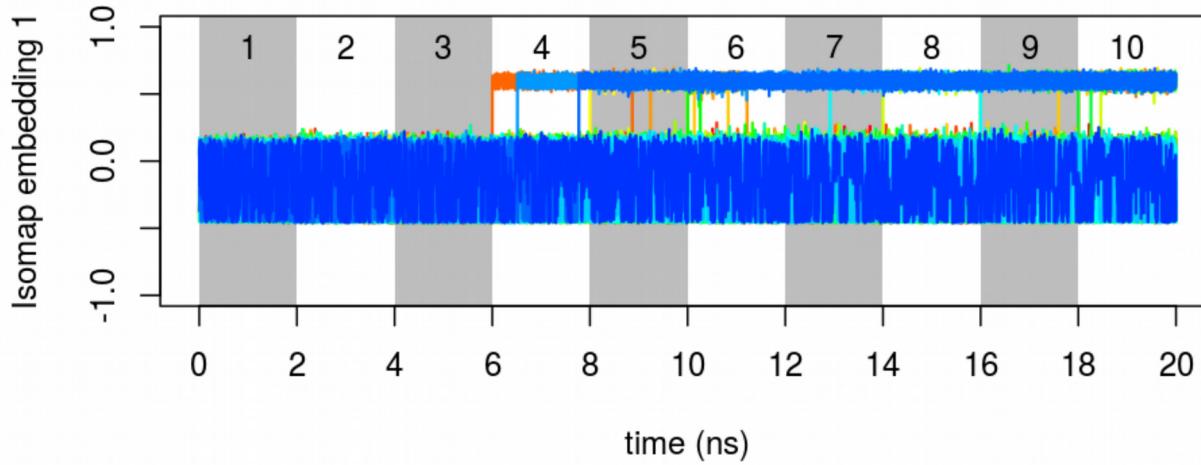
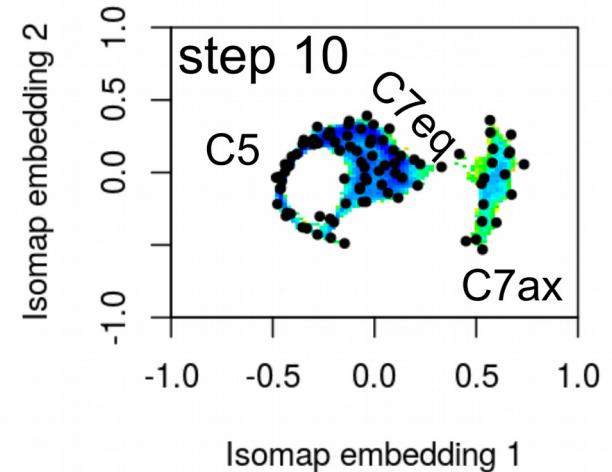
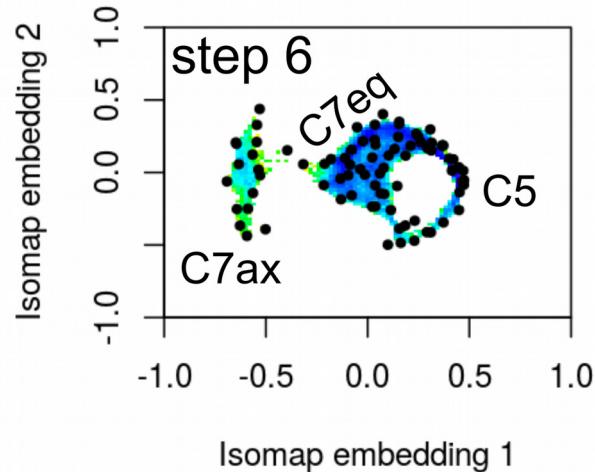
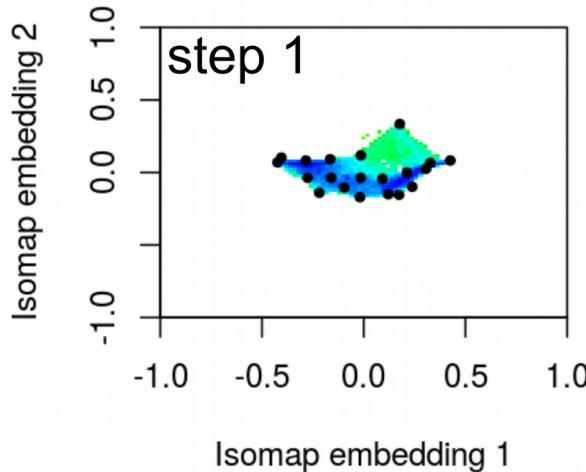
- easy to parallelize



Flying Gaussian method

Advantages:

- autonomous bias potential (CVs can be adaptive)



0
50 kJ/mol

Flying Gaussian method

Disadvantages:

- it is necessary to parallelize

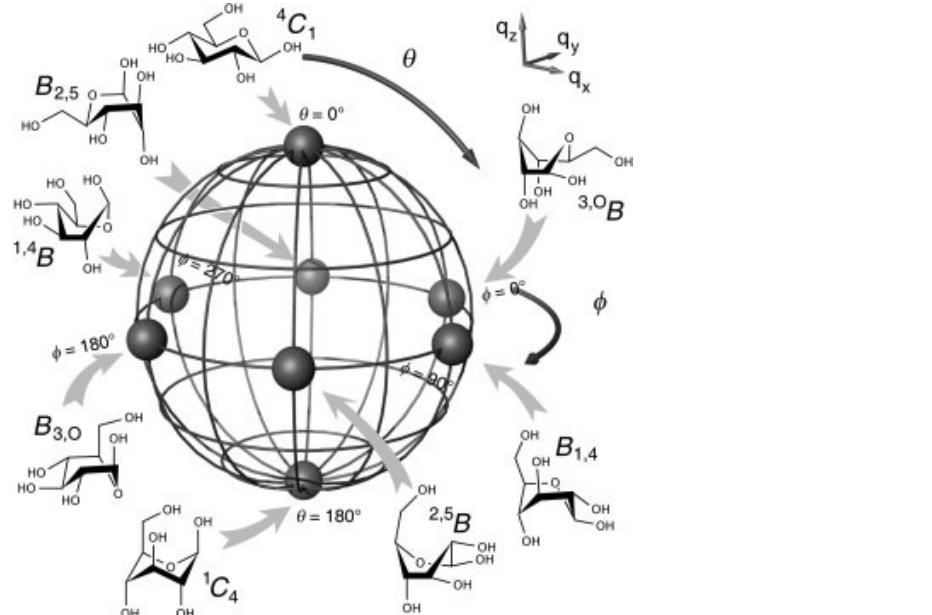
https://commons.wikimedia.org/wiki/File:ASDA_in_Keighley.jpg



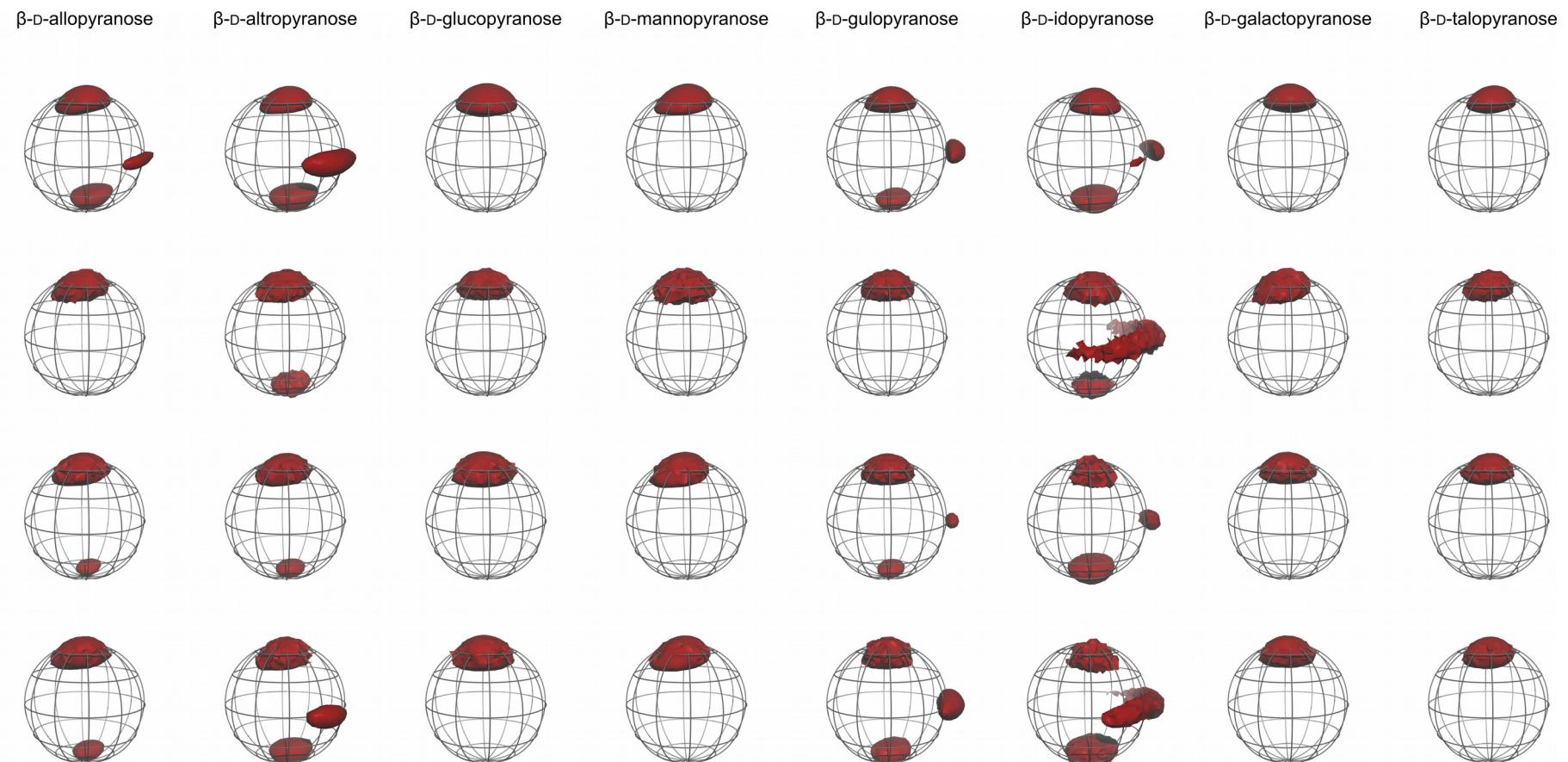
Flying Gaussian method

Disadvantages:

- it is necessary to parallelize



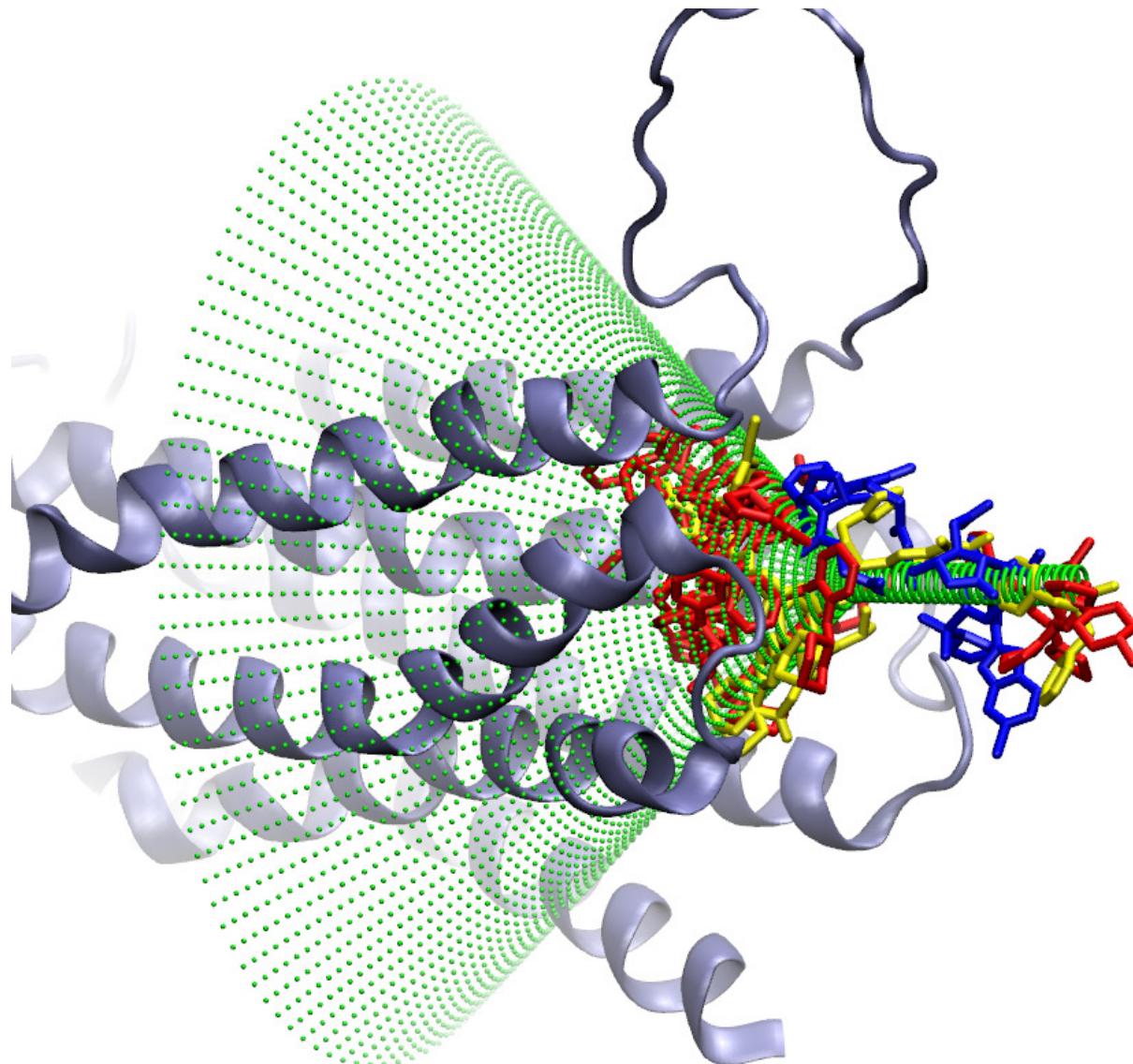
+20 kJ/mol



Flying Gaussian method

Disadvantages:

- it is necessary to parallelize

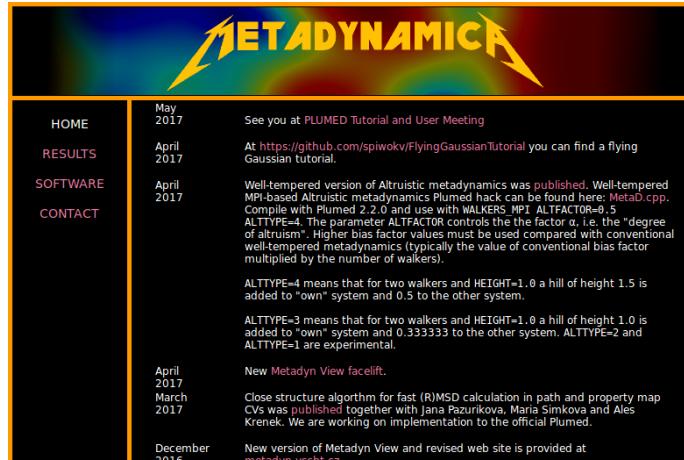


Flying Gaussian method

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).

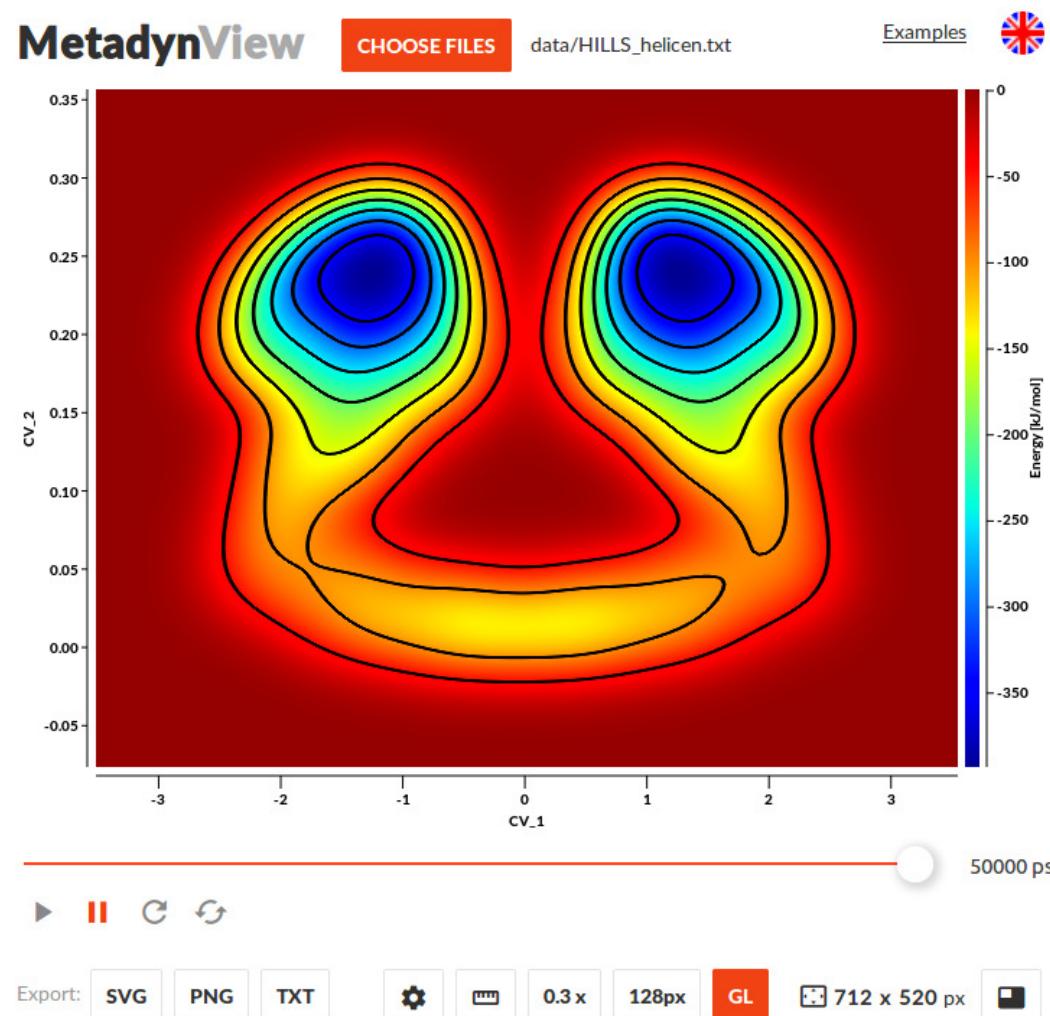
<http://www.metadynamics.cz>



<https://github.com/spiwokv/FlyingGaussianTutorial>

A screenshot of a GitHub repository page for "Flying Gaussian Tutorial". The page shows basic repository statistics: 38 commits, 1 branch, 0 releases, and 1 contributor. It lists recent commits from the "master" branch, all made by "spiwokv". The commits include updates to files like README.md, R, mdps, mols, plumed_dat, python, and src_bias. Below the repository stats is a section titled "Flying Gaussian Tutorial on alanine dipeptide" which provides a brief overview of the tutorial's purpose and setup.

<http://metadyn.vscht.cz>



Acknowledgments:

UCT Prague: Petr Hošek, Pavel Kříž, Václav Mareška, Daniela Toulcová,
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MU Brno: Jana Pazúriková, Aleš Křenek

HPC resources:

Metacentrum



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