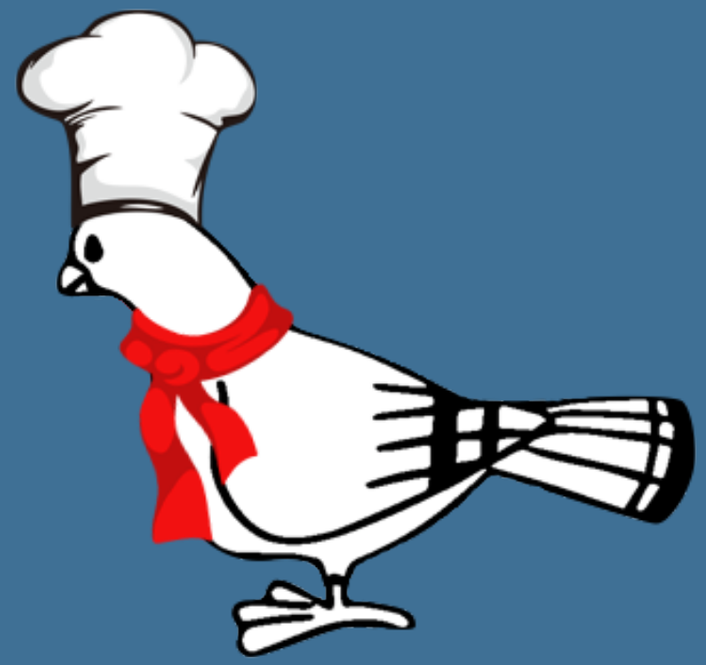

PLUMED Masterclass

21.2: PLUMED statistical errors in MD

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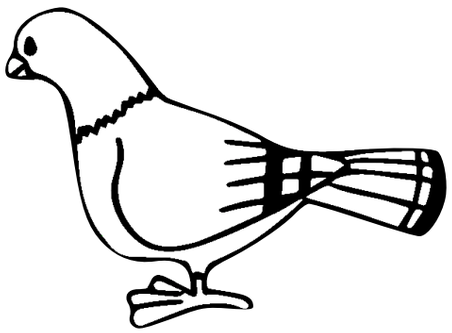


PLUMED

open-source
freely-available
C++ library

- enhanced-sampling methods
- free-energy methods
- analysis MD data

www.plumed.org

@plumed_org

Bonomi *et al.* CPC 2009
Tribello *et al.* CPC 2014

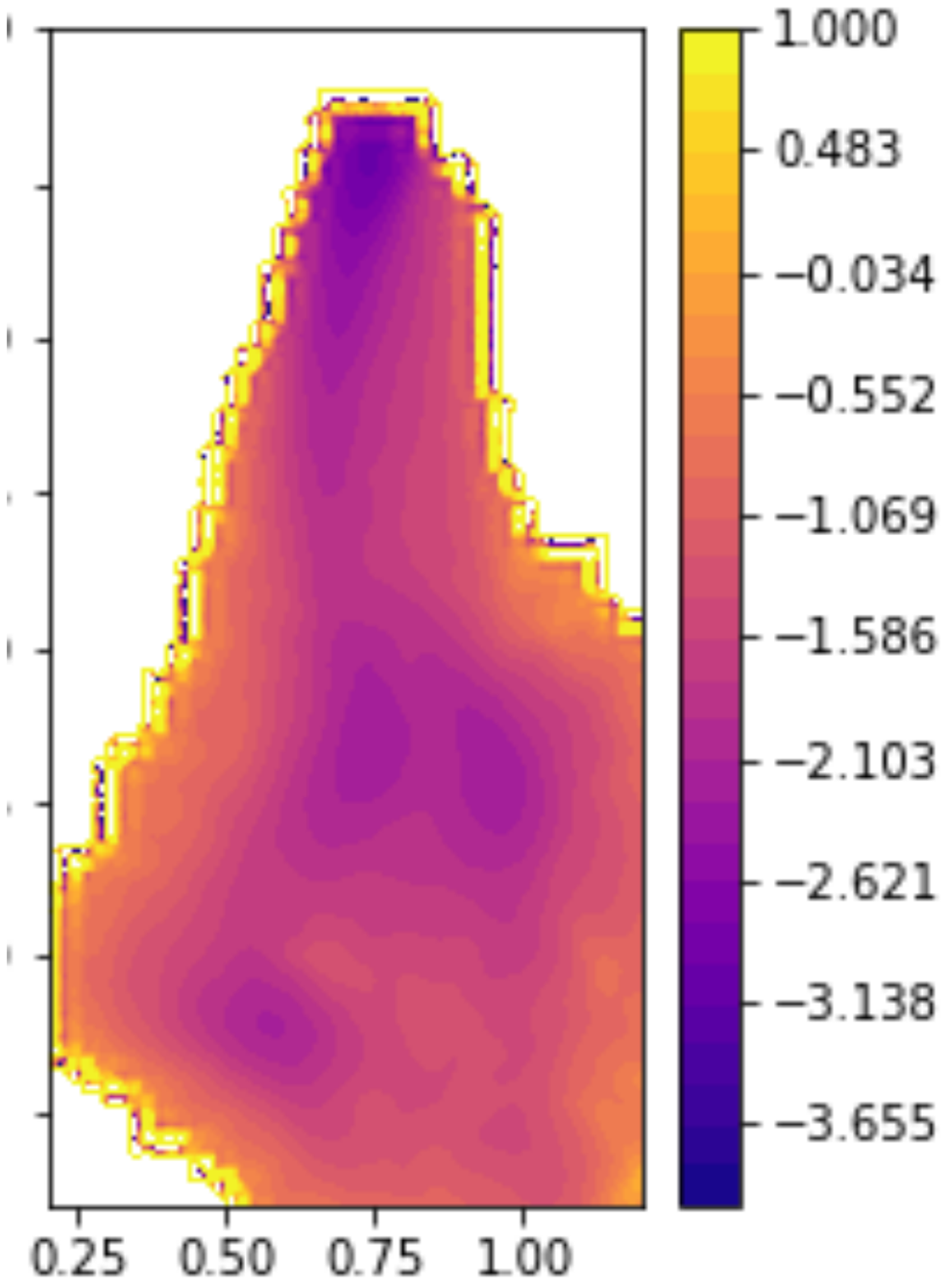
Gareth Tribello

Max Bonomi

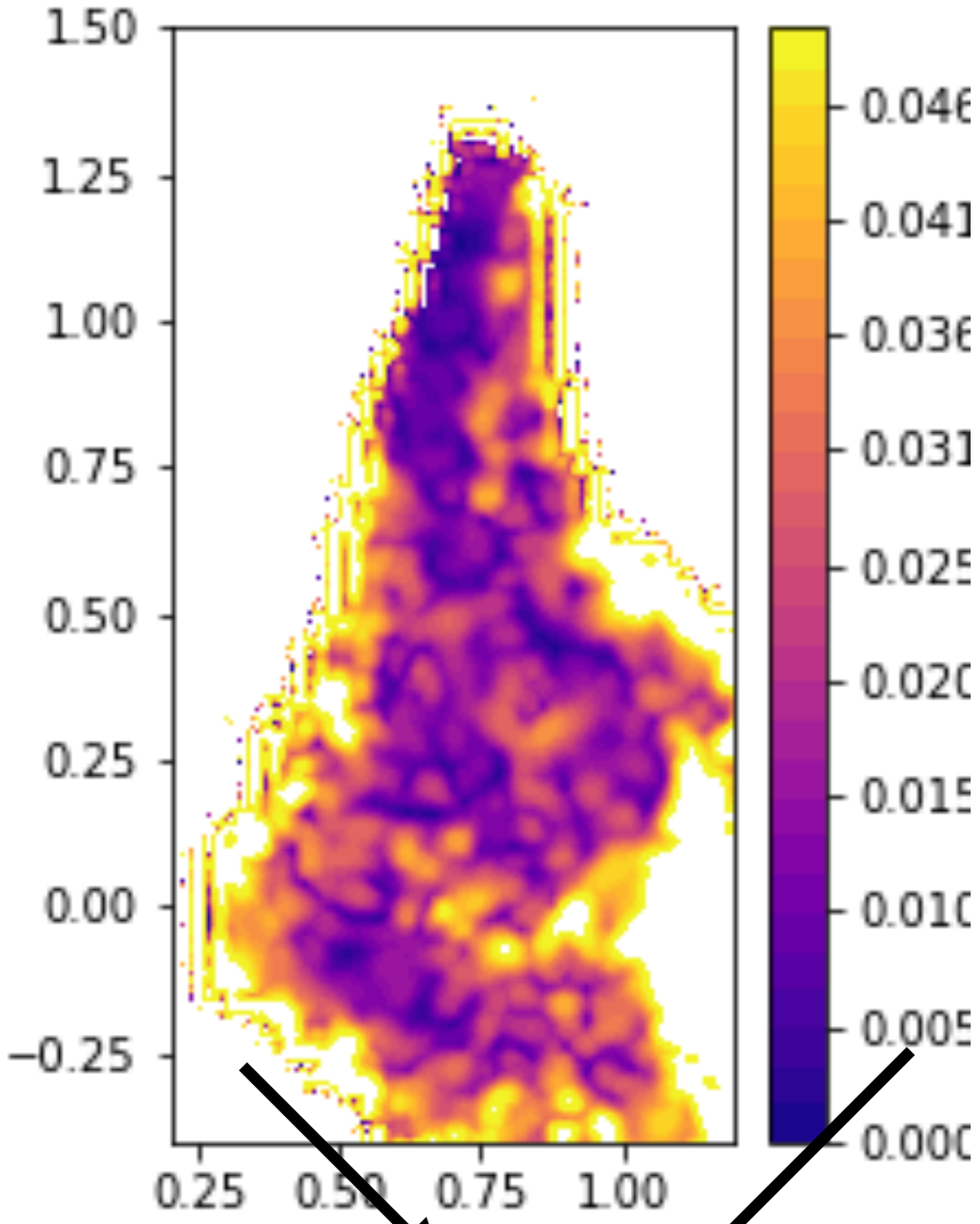
Carlo Camilloni

Giovanni Bussi

The objective

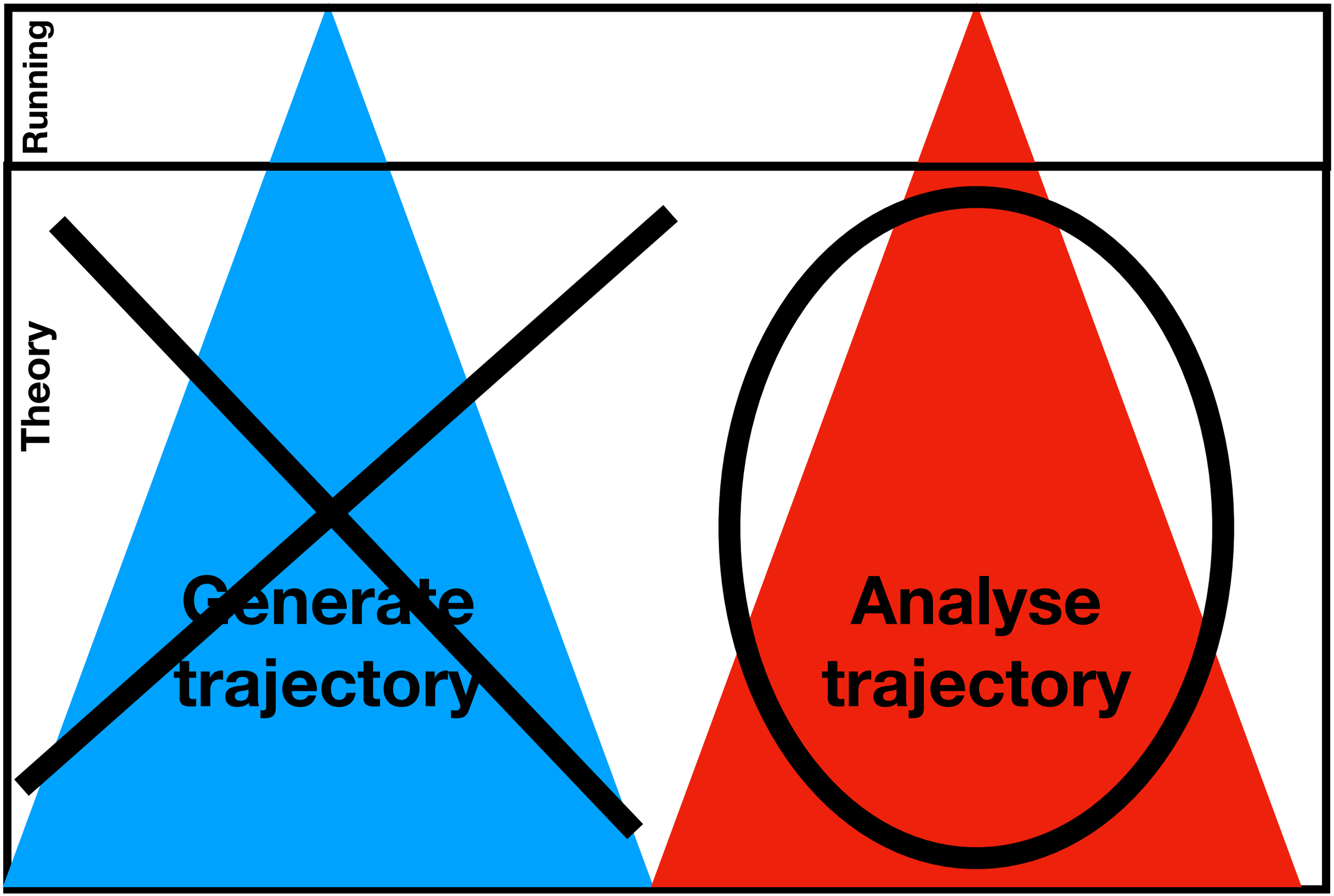


Free energy surface
from metadynamics

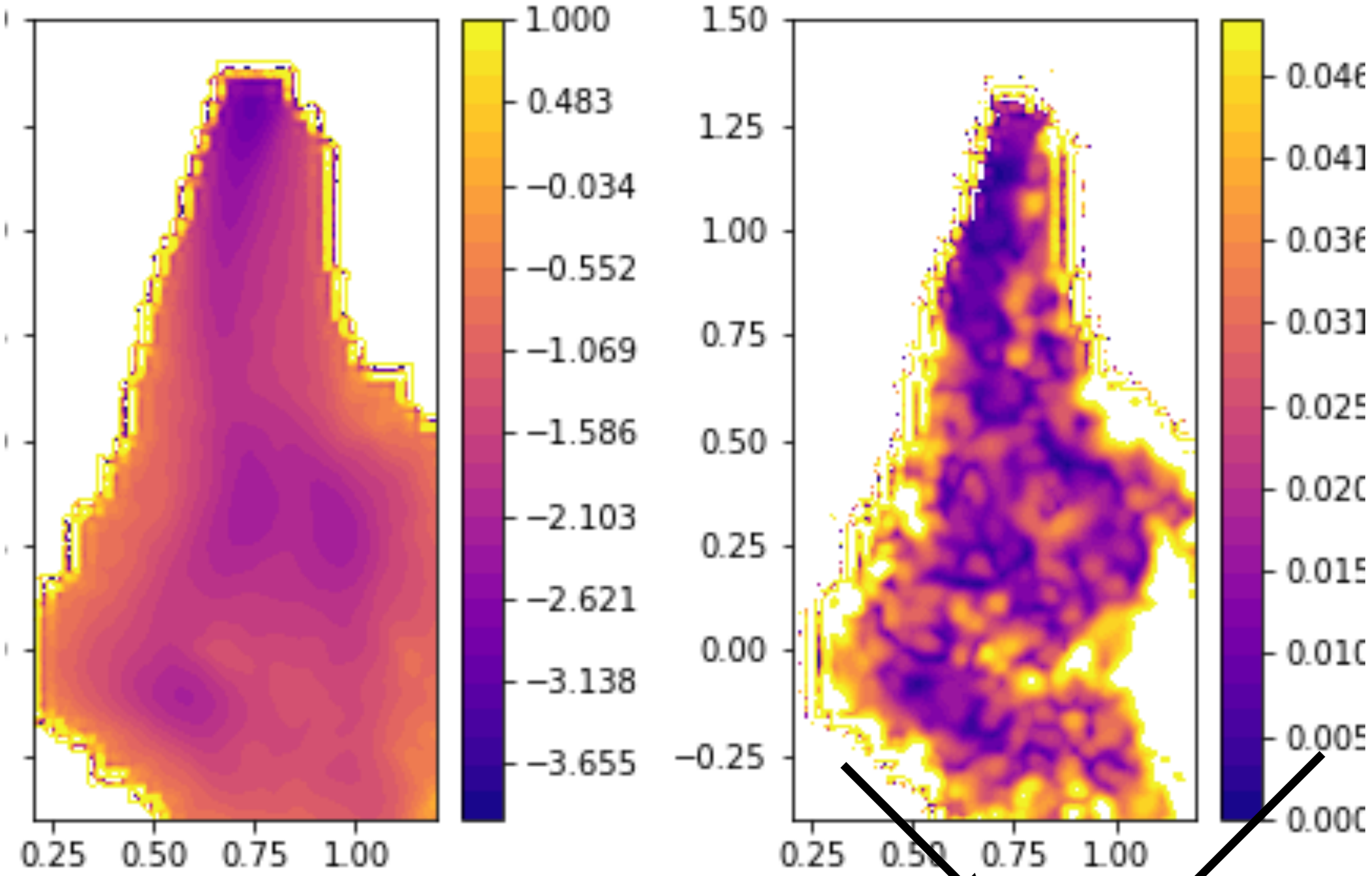


Error on **estimate** of
free energy surface

The objective continued



Why is the free energy we get from metadynamics an estimate?

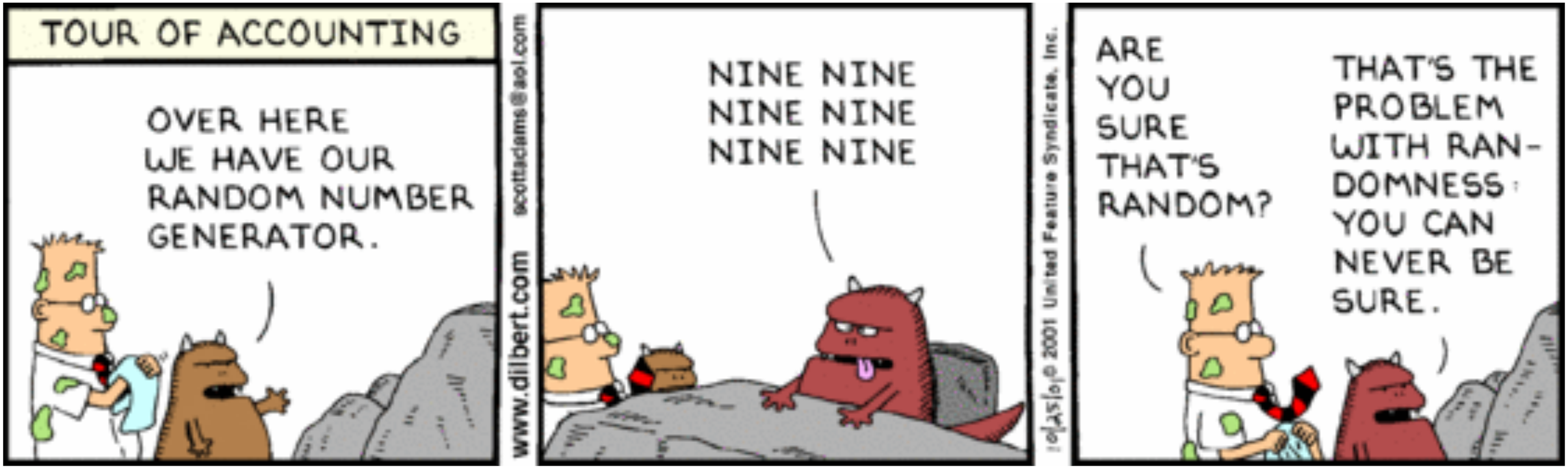


Error on **estimate** of free energy surface

$s(t)$

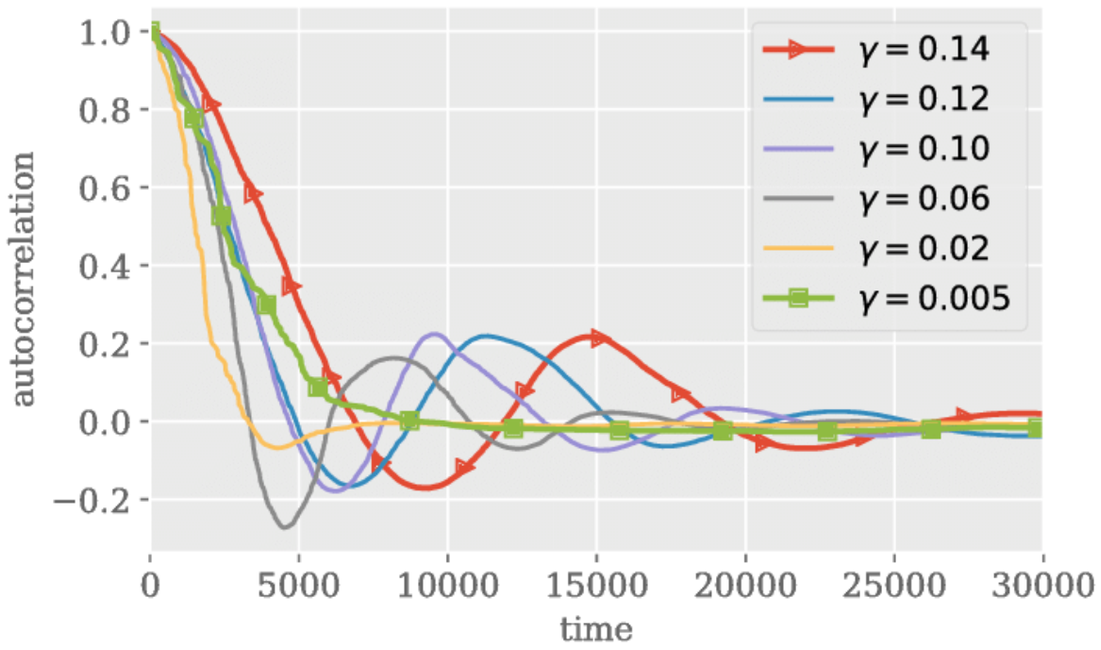
We treat the CV values during the trajectory as samples from a probability distribution

$P(s) \propto e^{-\beta F(s)}$ ← **Free energy**



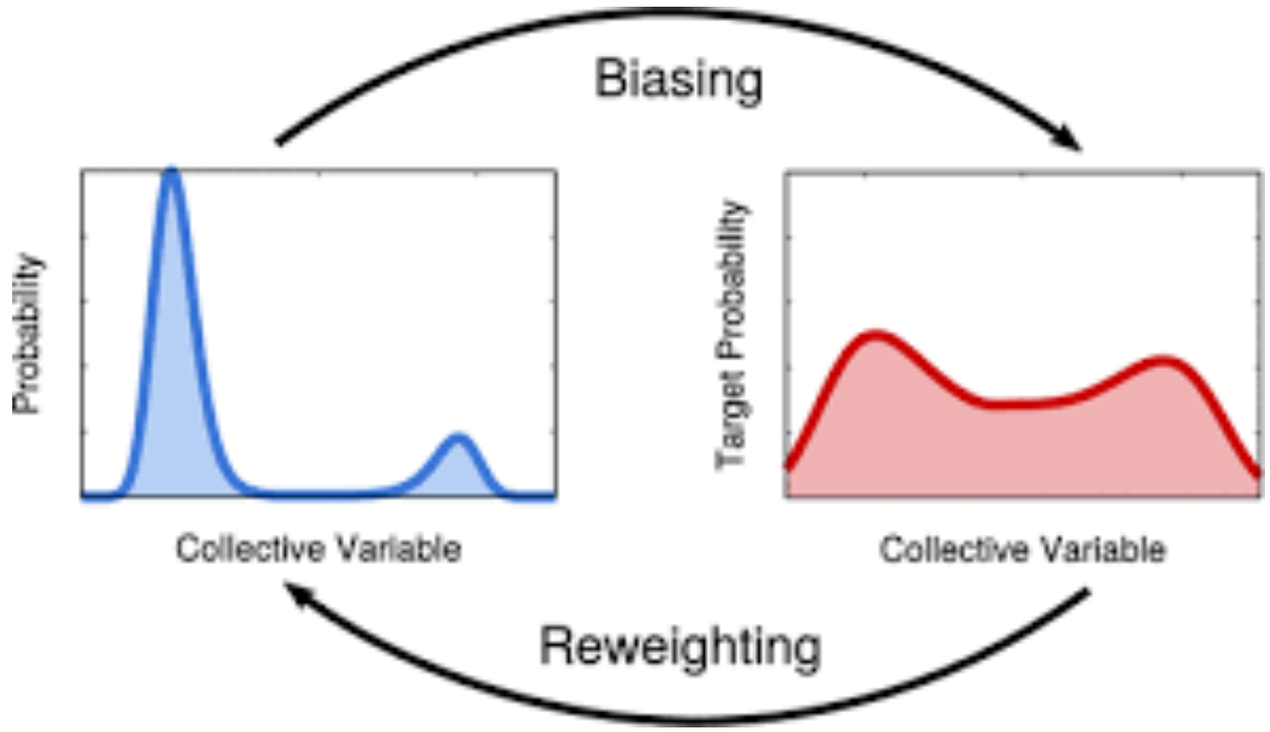
You can find many good explanations of basic statistics online or in elementary textbooks

The basic treatment of statistics in these books doesn’t work for metadynamics for two big reasons



There are correlations between the values the CV takes at different times during the simulation

We need to reweight the frames in order to undo the effect of the bias



Instructions

Class	Topic	Lecture I	Lecture II	Instructor
21.1	PLUMED syntax and analysis	January 18, 2021	January 25, 2021	M. Bonomi
21.2	Statistical errors in MD	February 1, 2021	February 8, 2021	G. Tribello
21.3	Umbrella sampling	February 15, 2021	February 22, 2021	G. Bussi
21.4	Metadynamics	March 1, 2021	March 8, 2021	M. Bonomi
21.5	Replica exchange methods	March 15, 2021	March 22, 2021	G. Bussi
21.6	Dimensionality reduction	April 12, 2021	April 19, 2021	G. Tribello
21.7	Performance optimization	April 26, 2021	May 3, 2021	M. Bonomi
21.8	Poster session	May 10, 2021		

1. Go to www.plumed.org
2. Click on the Masterclass tab
3. Click on the Topic of class 21.2
4. 1 week to complete the exercises
5. Questions/discussions on Slack channel masterclass-21-2
6. Lecture I and II available on YouTube