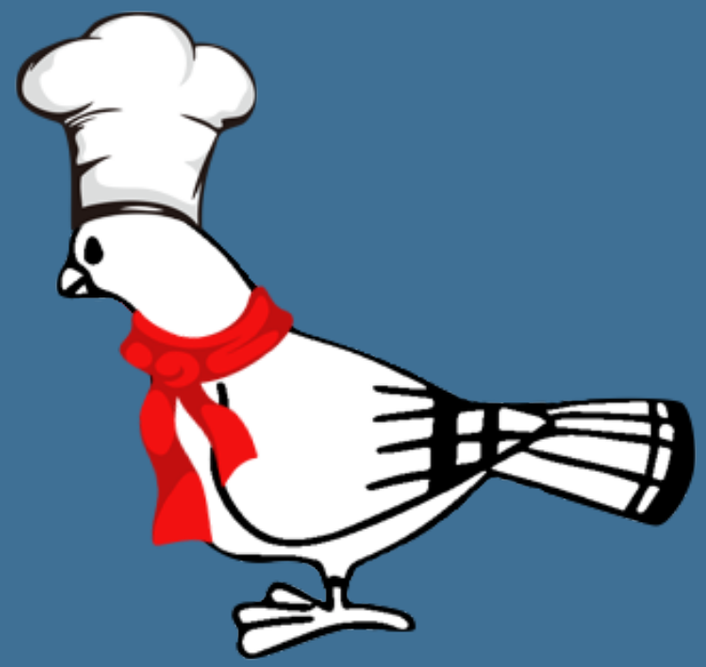
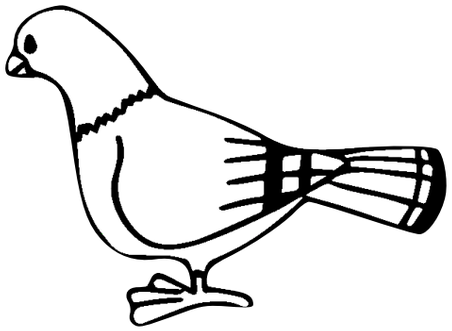


PLUMED Masterclass

21.1: PLUMED syntax and analysis

Max Bonomi
Institut Pasteur - CNRS
mbonomi@pasteur.fr



PLUMED

open-source
freely-available
C++ library

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

www.plumed.org

@plumed_org

Gareth Tribello

Max Bonomi

Carlo Camilloni

Giovanni Bussi

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

PLUMED functionalities

Collective Variables

- Distance, torsions, secondary structure,…
- “Material science” CVs
- PCA, Sketch-map
- Custom

Free energy / enhanced sampling methods

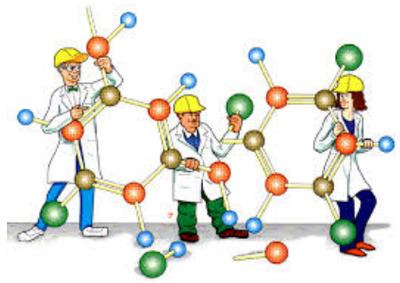
- Metadynamics
- Umbrella Sampling
- Stereed MD
- Combination with REM
- …

Analysis

- Calculate CVs on trajectories (via molfile/ xdrfile libraries)
- Postprocess MetaD, US
- Histograms / FES + errors

Interfaced with many popular MD codes

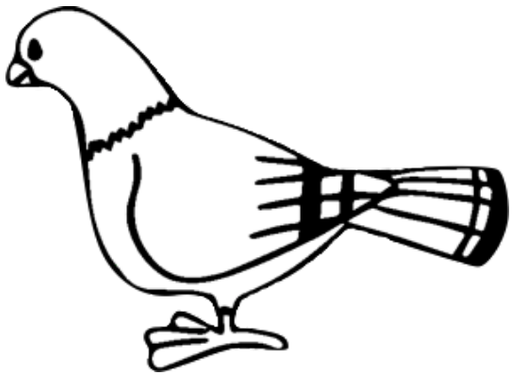
PINY-MD

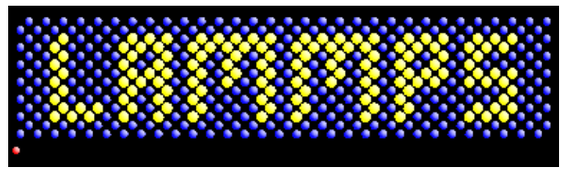


DL_POLY

GROMACS
FAST. FLEXIBLE. FREE.

NAMD
Scalable Molecular Dynamics



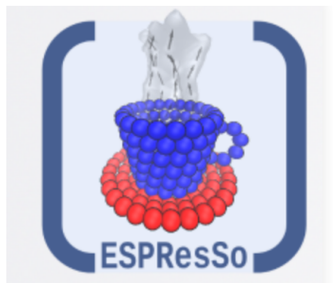


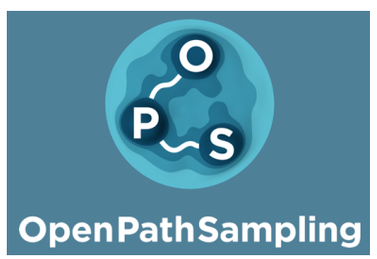
PLUMED-GUI
for VMD

ABIN

ACEMD
PLATFORM

OpenMM

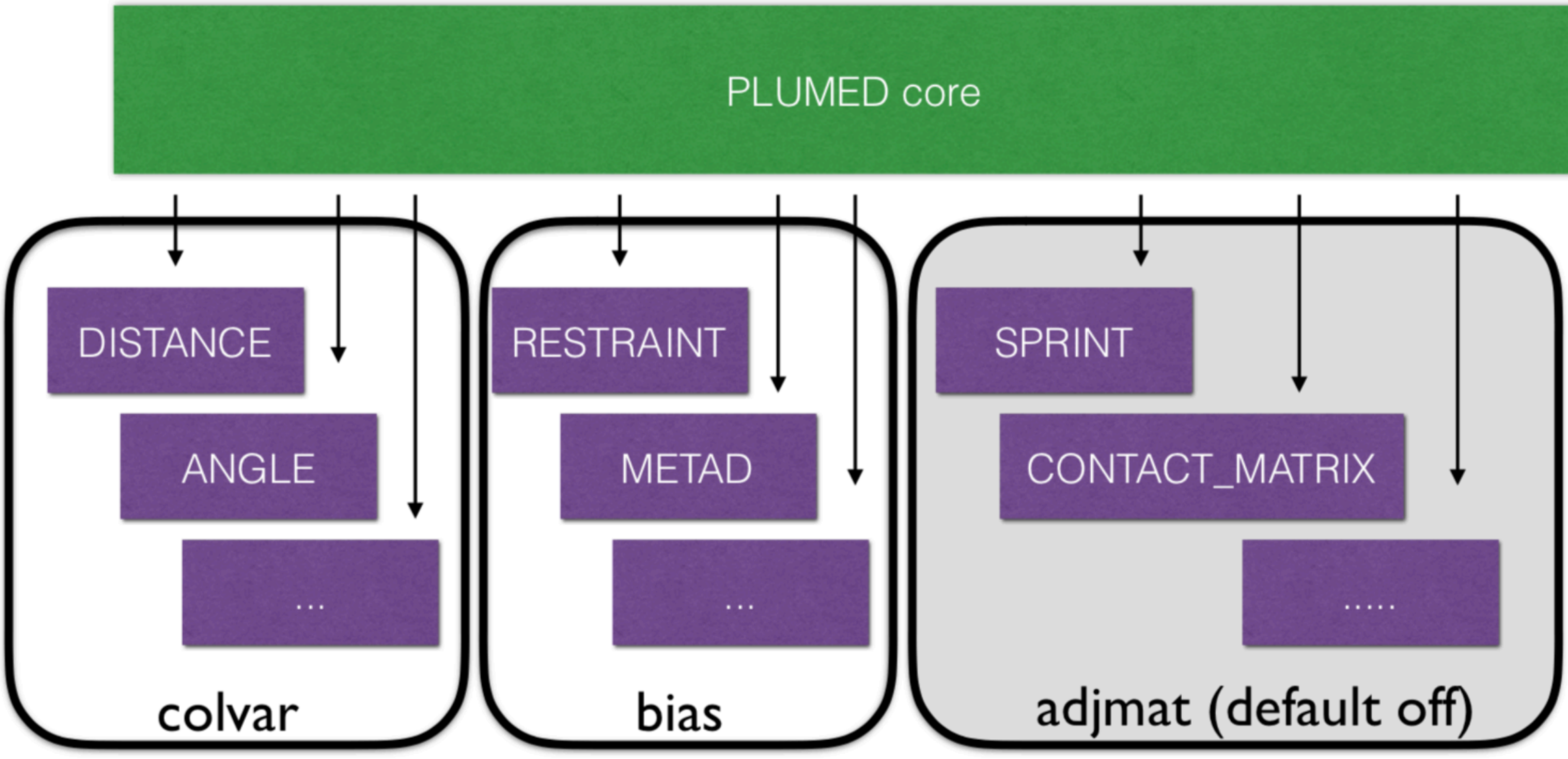




Yaff

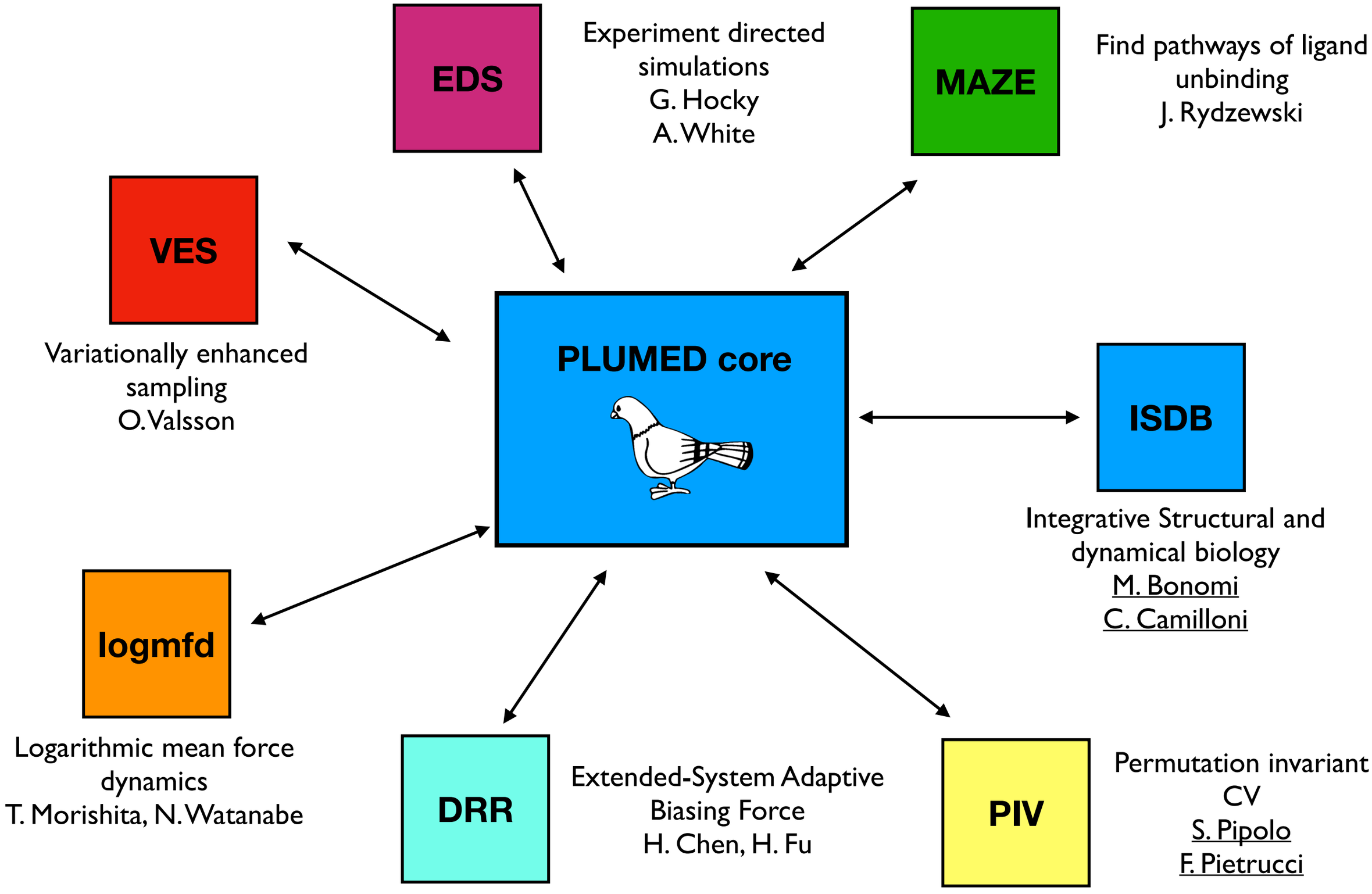
A new modular structure…

Tribello, Bonomi, Branduardi, Camilloni, Bussi CPC 2014



A modular architecture made to grow with users contributions!

…that enables external contributions



On the WEB

Website: http://www.plumed.org/

Github: http://github.com/plumed/plumed2

Twitter: @plumed_org

User & developer mailing lists

User & developer manuals + tutorials (mostly from cecam schools)

Webinars: SBGrid CONSORTIUM bioexcel

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 21.1
4. 1 week to complete the exercises
5. Questions/discussions on Slack channel masterclass-21-1
6. Lecture I and II available on YouTube