

PLUMED Masterclass

21.1: PLUMED syntax and analysis

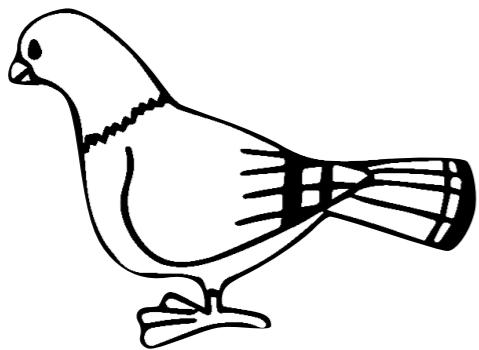
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 @BonomiMax





open-source
freely-available
C++ library

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



www.plumed.org



@plumed_org



PLUMED functionalities

Collective Variables

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

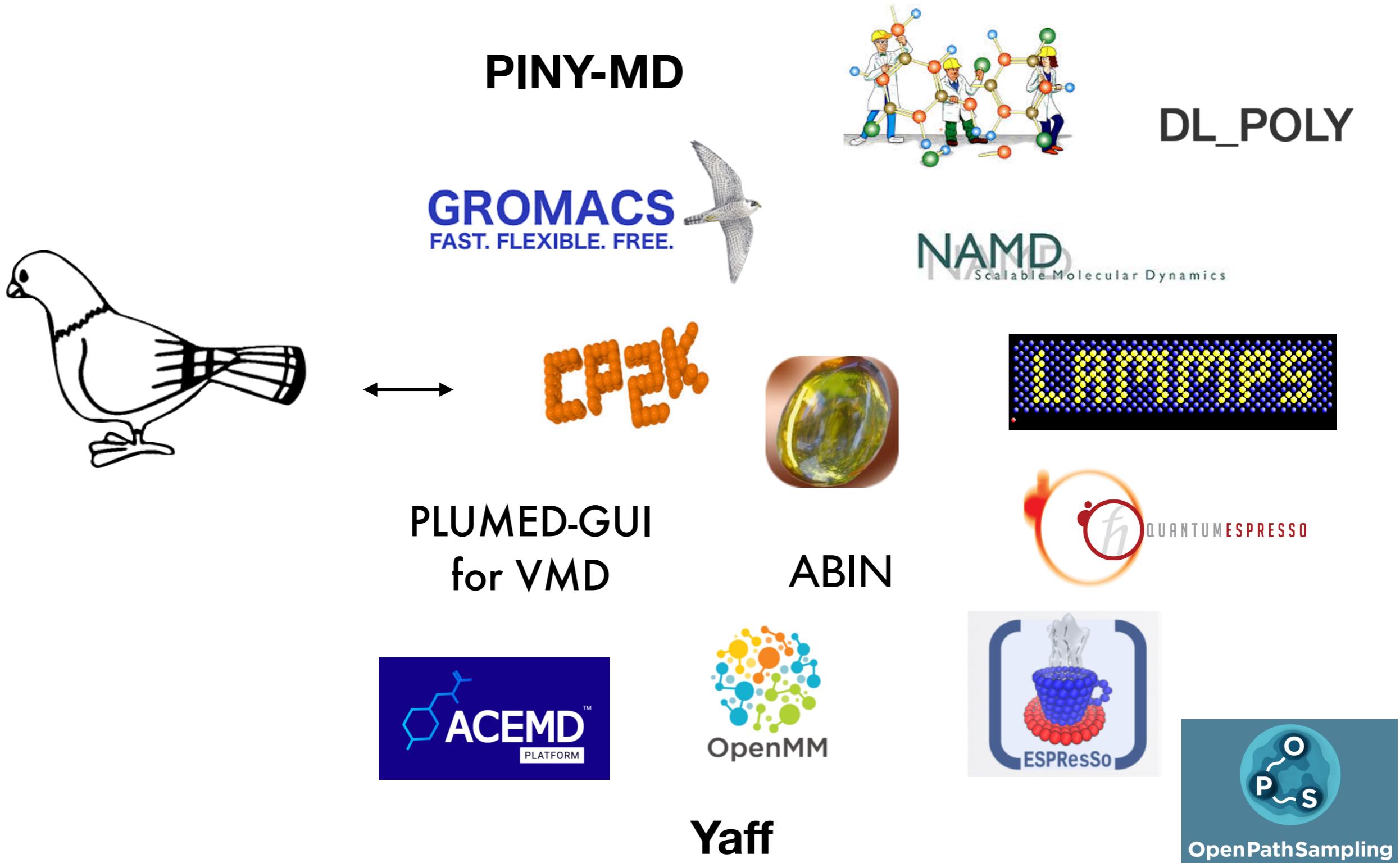
Free energy / enhanced sampling methods

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

Analysis

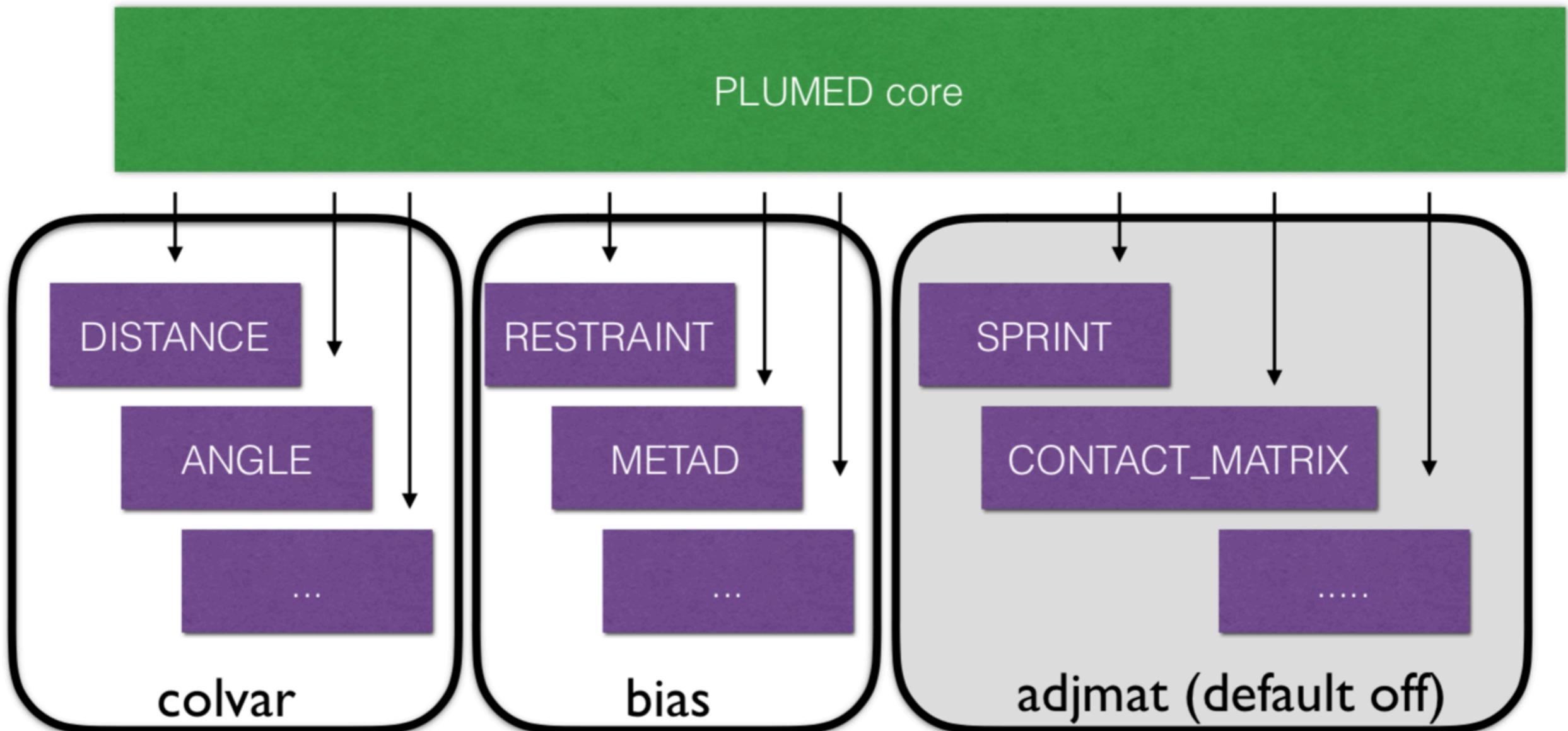
- Calculate CVs on trajectories (via molfile/xdrfile libraries)
- Postprocess MetaD, US
- Histograms / FES + errors

Interfaced with many popular MD codes



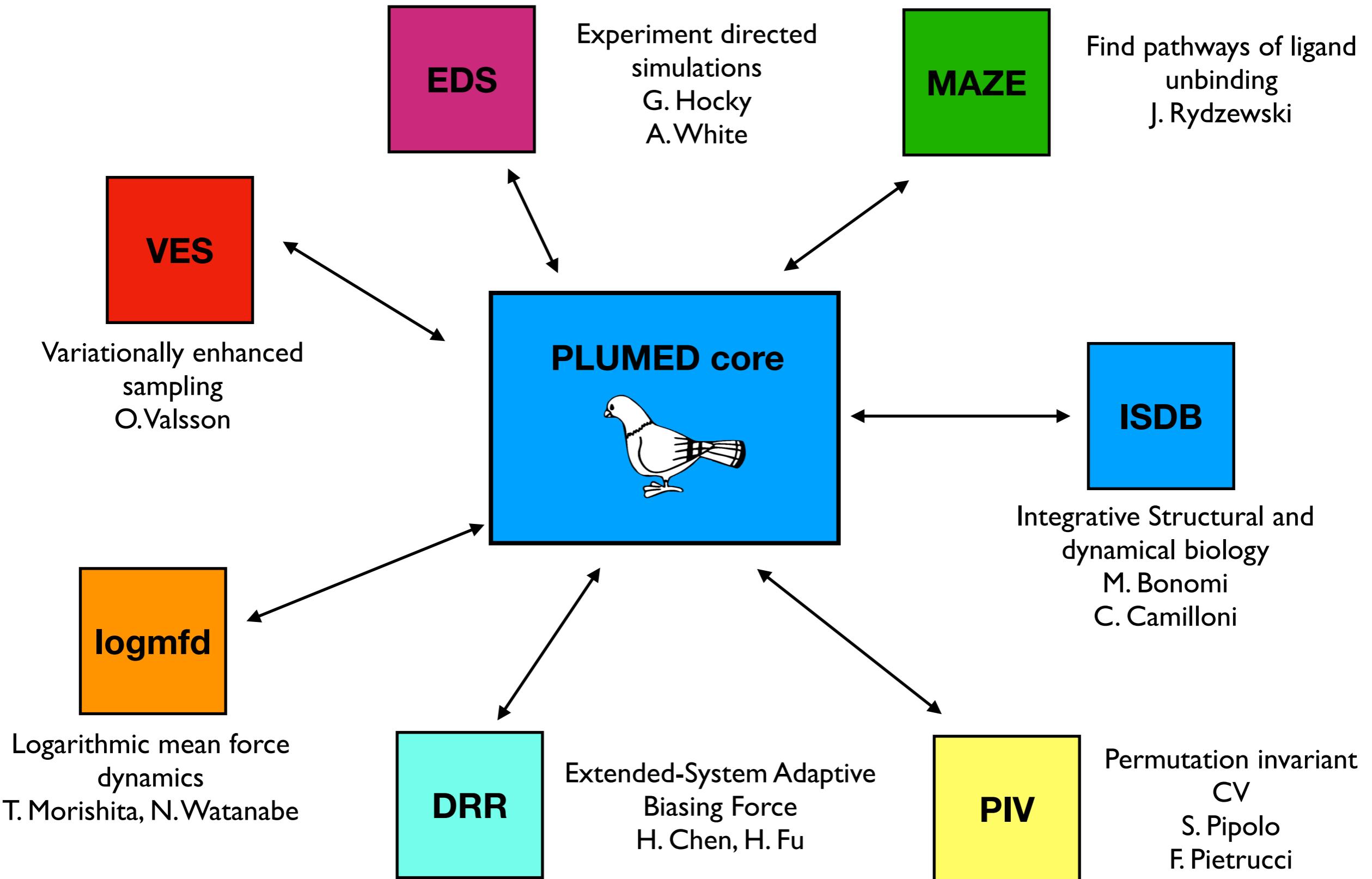
A new modular structure...

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



Instructions



PLUMED
The community-developed PLUGin for MolEcular Dynamics

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Cite NEST **Masterclass** Funding

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](#)