



UMR3528



Department of Structural Biology
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Introduction to PLUMED NEST

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What is PLUMED NEST



PLUMED-NEST

The public repository of the PLUMED consortium

- A public repository
- Data needed to reproduce PLUMED-enhanced simulations
- PLUMED input files tested for compatibility
- Text highlight and link to documentation to learn from real-life examples
- Promote scientific reproducibility - create educational material

Our manifesto

Promoting transparency and reproducibility in enhanced molecular simulations

The PLUMED consortium unifies developers and contributors to PLUMED, an open-source library for enhanced-sampling, free-energy calculations and the analysis of molecular dynamics simulations. Here, we outline our efforts to promote transparency and reproducibility by disseminating protocols for enhanced-sampling molecular simulations.

The PLUMED consortium

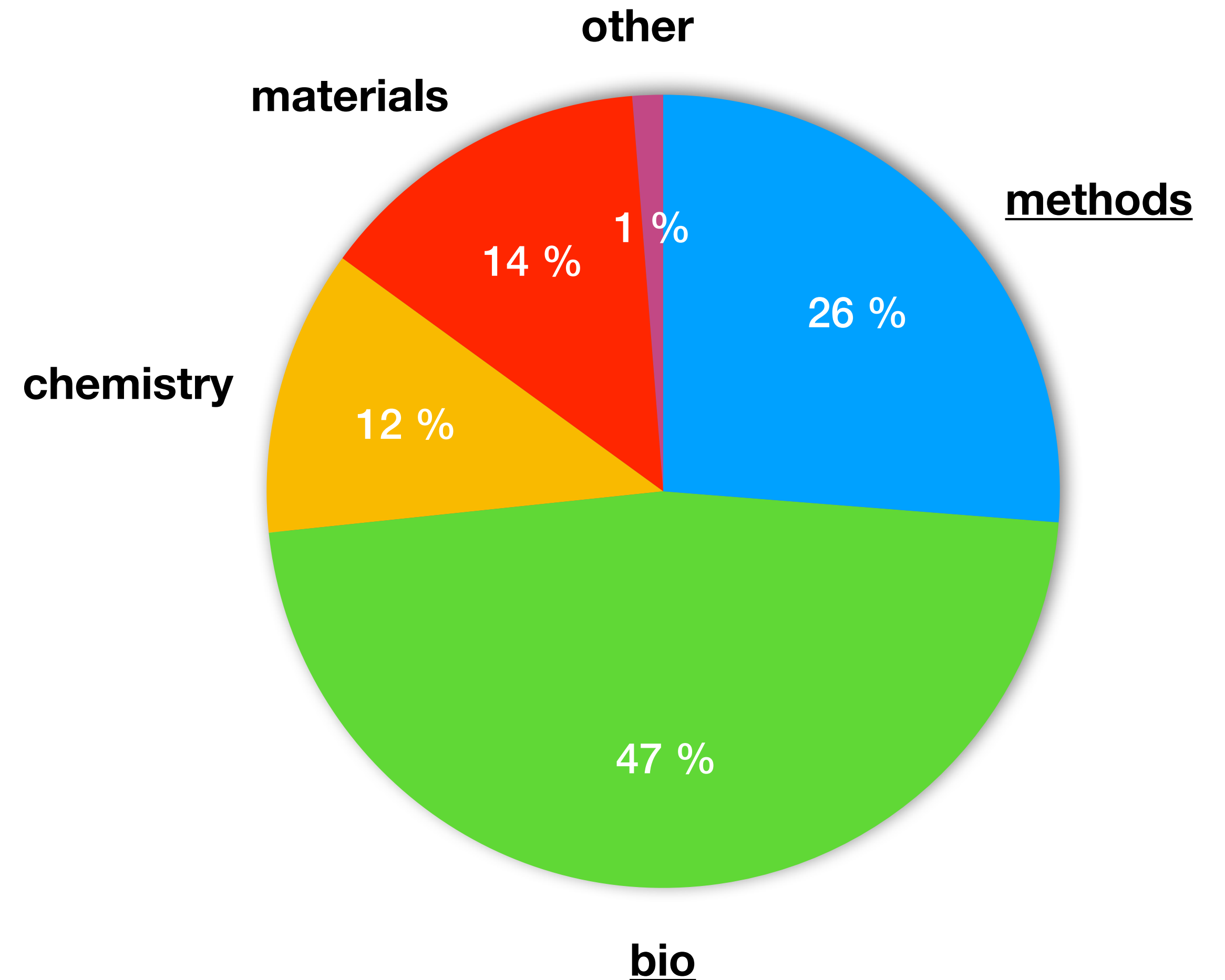
NATURE METHODS | VOL 16 | AUGUST 2019 | 667-673 | www.nature.com/naturemethods

DEMO: Overview of the database

www.plumed-nest.org

A few numbers

- First egg deposited in April 2019
- 241 eggs deposited so far
- 100 unique contributors
- ~1500 PLUMED protocols
- Multidisciplinary



DEMO: How to submit an egg

www.plumed-nest.org

Which data should I provide?

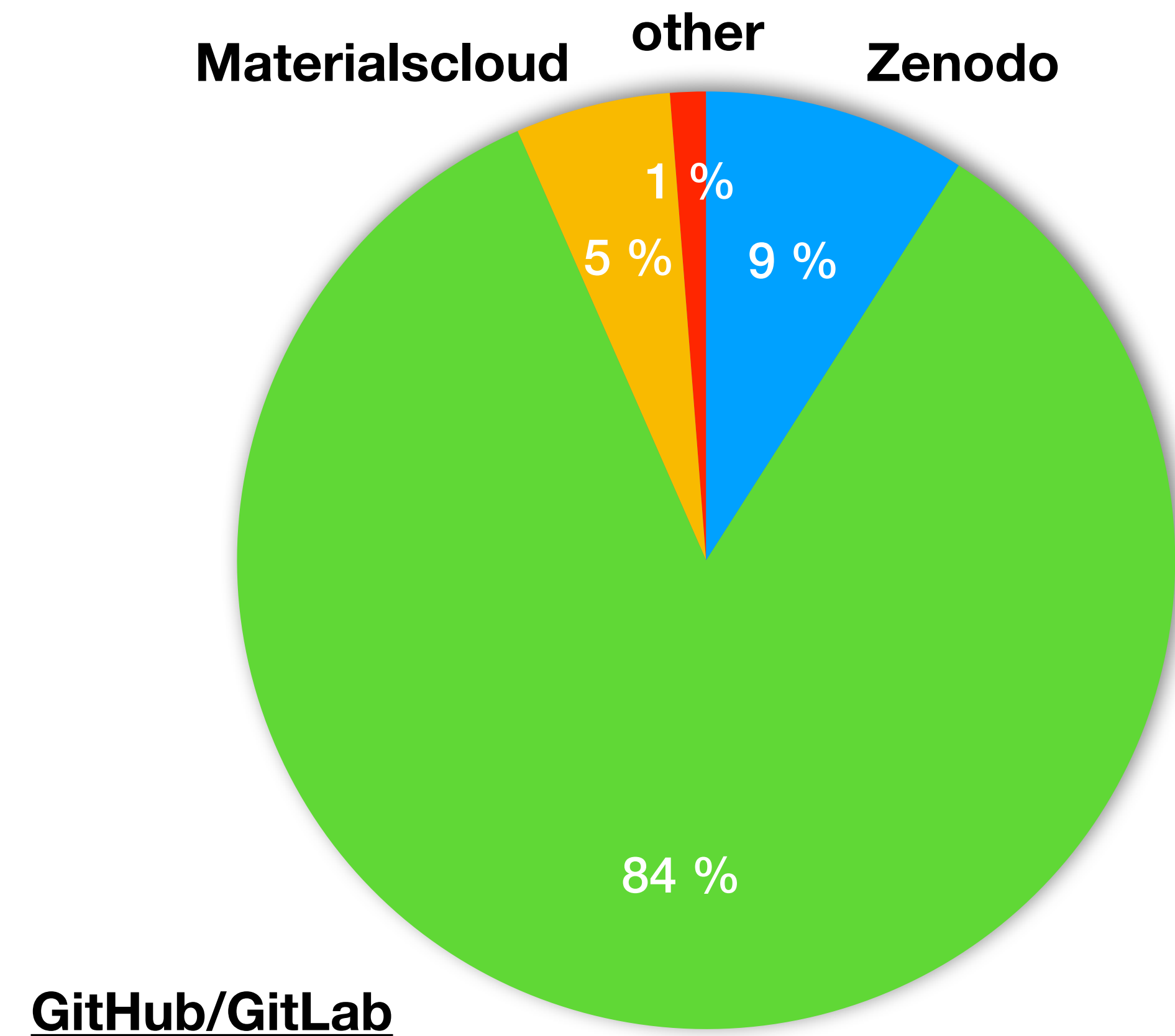
- Input files for your MD simulation: initial structure, topology, “control” file, i.e. GROMACS mdp files
- PLUMED input files and related files
- Analysis scripts
- A README file with instructions/protocol
- Please, do not upload trajectory files
- Try to keep the zip file ~100/200 MB

Where to store your data

Frequently used repositories:

- GitHub/GitLab
- Zenodo
- Materialscloud
-

Watch out for MDDB!



Common issues when submitting eggs

- The URL is not accessible, often GitHub private repository
- The archive is not in zip format (tar, tar.gz, etc etc)
- Files are missing, typically PDB or cpp file, or paths not correct
- Errors in PLUMED input file
- Requires special PLUMED version/fork

How to make sure your input files are correct?

```
plumed driver --natoms 100000 --parse-only --kt 2.49 --plumed plumed.dat
```

DEMO: How to debug errors

www.plumed-nest.org

Take home messages

- Share, share, share
- Document what you did as clearly as possible
- Check PLUMED files before submitting an egg
- Monitor compatibility with future PLUMED versions