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Phenix User Workshop, July 29 2022

Introduction

Dorothee Liebschner
Lawrence Berkeley Laboratory
Phenix - a Structural Biology Hub

We have nucleated the development of new computational methods for structural biology.
What is *Phenix*?

- Package for **automated structure solution**
- Modern programming concepts and new algorithm development
- Designed to be used by **both novices and experienced users**
- Long-term development and **support**
- Why is it called *Phenix*?

  **Python Hierarchical ENvironment for Integrated Xtallography**
Key Features

• **Python**
  - Easy scripting of repetitive tasks
  - Enables rapid prototyping and development

• **Advanced algorithms**
  - Experimental phasing
  - Molecular replacement
  - Automated model building and rebuilding
  - Structure refinement and validation
  - Ligand coordinate and restraint generation

• **Rapid development and bug fixing**
Tools for Crystallography

Image of a diagram showing tools for crystallography, including:
- AutoSol
- Xtriage
- LABELIT
- Experimental phasing
- Density modification
- Molecular replacement
- AutoBuild
- Phaser
- Model (Re)building
- MolProbity
- LigandFit
- eLBOW
- Ligand fitting
- Resolve
- phenix.refine
- Refinement
- Deposition
- Table one
  - Prepare PDB deposition
  - Get PDB validation report

References:
Tools for Cryo-EM

Map quality assessment
- Mtriage

Map improvement
- Density Modification
- Auto-sharpen

Map symmetry
- Map-symmetry
- Map-box
- Extract-unique

Model building
- Dock-in-map
- Map-to-model

Docking
- Dock-in-map

Refinement
- Real-space-refine

Validation

Deposition
- Rebuild-predicted-model
- MolProbity
- Mtriage

Phenix GUI

Central GUI to view job control and launch new jobs
Coot/PyMOL integration

• Most results can be opened directly in graphics apps

![Open in Coot and Open in PyMOL]

• Any PDB file listed in GUI can also be opened

• AutoSol, AutoBuild, and phenix.refine will update Coot continuously while running

• Coot must have Python support (default on Mac)

• Specific paths to executables usually required on Linux

Preferences → Graphics → Full path to Coot [...PyMOL]
Command Line Tools

Run on the terminal

- phenix.mtriage
- my_model.pdb, my_map.map
- resolution=4

Run in a python script

```python
try:
    easy_run.call("phenix.mtriage\my_model.pdb\my_map.map")
except Exception as e:
    msg = traceback.format_exc()
    print(msg)
```
**Phenix Availability**

Phenix-online.org

**Supported on:**
- Linux (RedHat, Fedora)
- Mac OSX
- Windows

**Extensive documentation**
(online and via GUI)

**Nightly builds**

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<td>ci, intel-linux-2.6-x86_64-centos6, mac-intel-osx-x86_64, intel-windows-x86_64</td>
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Accurate predicted models

**AlphaFold: a solution to a 50-year-old grand challenge in biology**

Sequence
Multiple sequence alignment

3D prediction
New tools for predicted models in Phenix

- Process predicted model
- Dock_predicted_model
- Rebuild predicted model
# Acknowledgements

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Garib Murshudov & Alexi Vagin
Paul Emsley, Bernhard Lohkamp, Kevin Cowtan
David Abrahams
Phenix Testers & Users

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- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory
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