Biskit

A python platform for structural bioinformatics (and design)

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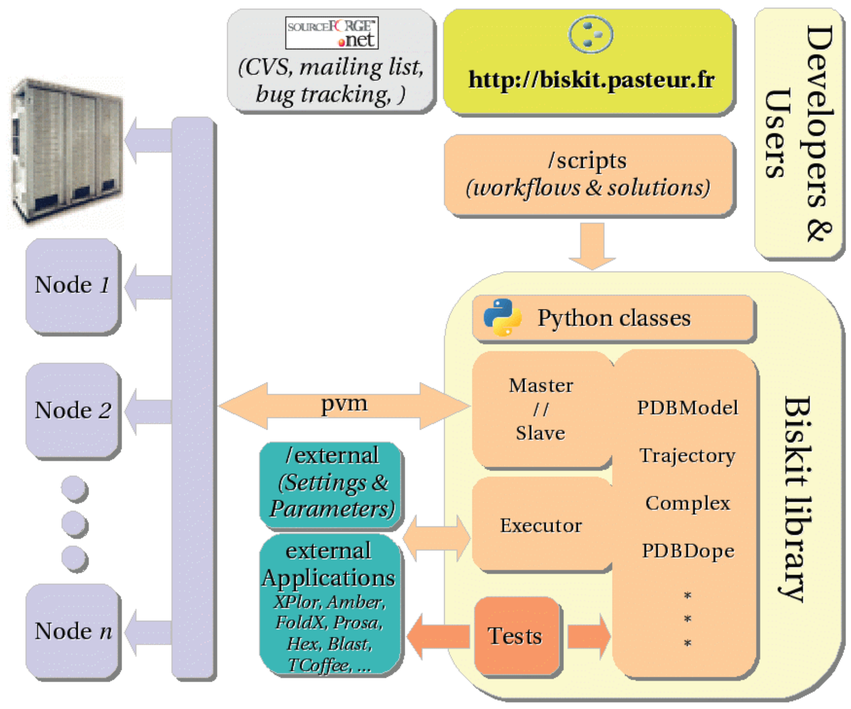
http://biskit.sourceforge.net

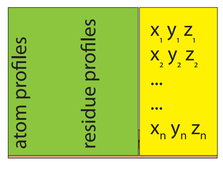
What is Biskit?

Biskit is a modular, object-oriented python library that provides intuitive classes for many typical tasks of structural bioinformatics research. It facilitates the manipulation and analysis of macromolecular structures, protein complexes, and molecular dynamics trajectories. At the same time, Biskit offers a software platform for the rapid integration of external programs and new algorithms into complex structural bioinformatics workflows. Calculations are thus often delegated to established programs like Xplor, Amber, Hex, Prosa, and Hmmer; interfaces to further software can be easily added. Moreover, Biskit simplifies the parallelization of time consuming calculations via PVM (Parallel Virtual Machine).

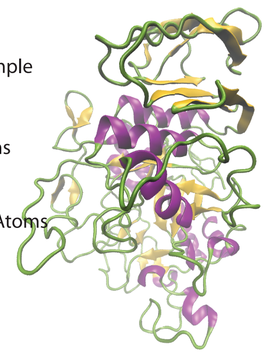


How is data handled?

PDBModel

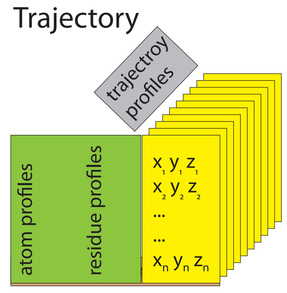


Some example functions:
- take
- takeChains
- concat
- fit / rms
- compareAtoms
...

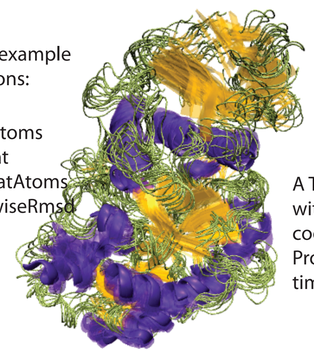


A PDBModel contains a coordinate matrix plus atom and residue profiles (arrays of values) with all the information from the PDB. New profiles with arbitrary additional data are easily added to atoms or residues.

Trajectory

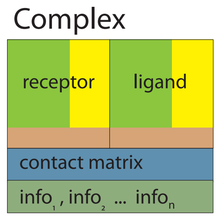


Some example functions:
-take
-takeAtoms
-concat
- concatAtoms
- pairwiseRmsd
- fit
...

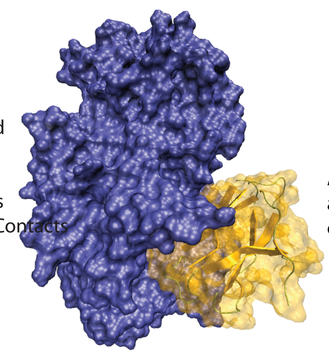


A Trajectory is most easily described as a PDBModel with an additional time dimension. Hence, the 2D coordinate array of PDBModel turns into a 3D array. Profiles of arbitrary data can be assigned to the new time axis.

Complex



Some example functions:
-contactsShared
-rmsInterface
-foldXEnergy
-compareAtoms
-fractionNativeContacts
-interfaceArea
...



A Complex is basically two PDBModels with an associated rotation/translation matrix and a contact matrix for intramolecular contacts.

Biskit Modules

Biskit
- PDBModel.py
- PCRModel.py
- ChainSeparator.py
- PDBCleaner.py
- ChainCleaner.py
- ChainWriter.py
- Pymoler.py
- FuzzyCluster.py
- PDBDope.py
- Hmmer.py
- Fold_X.py
- DSSP.py
- SurfaceRacer.py
- surfaceRacerTools.py
- Prosa2003.py
- WhatIf.py
- msms.py
- IcmCad.py
- rmsFit.py
- Xplorer.py
- XplorInput.py
- ProfileCollection.py
- Trajectory.py
- EnsembleTraj.py
- TrajCluster.py
- TrajFlexMaster.py
- TrajFlexSlave.py
- AmberCrdEntropist.py
- AmberCrdParser.py
- AmberEntropist.py
- AmberEntropyMaster.py
- AmberEntropySlave.py
- AmberParmBuilder.py
- AmberRstParser.py
- tools.py
- BisList.py
- Blast2Seq.py
- ColorSpectrum.py
- molTools.py
- molUtils.py
- decorators.py
- hosts.py
- default_hosts.py
- settings_default.py
- SettingsManager.py
- settings.py
- DictList.py
- ModelList.py
- ErrorHandler.py
- Errors.py
- Executor.py
- ExeConfigCache.py
- ExeConfig.py
- gnuplot.py
- hist.py
- LocalPath.py
- LogFile.py
- match2seq.py
- mathUtils.py
- MatrixPlot.py
- plotUtils.py
- QualSlave.py
- Ramachandran.py
- ReduceCoordinates.py
- SparseArray.py
- StructureSlave.py

Biskit/Dock
- Analyzer.py
- ComplexEvolvingList.py
- ComplexEvolving.py
- ComplexList.py
- ComplexModelRegistry.py
- Complex.py
- ComplexRandomizer.py
- ComplexTraj.py
- ContactMaster.py
- ContactSlave.py
- Docker.py
- FixedList.py
- HexParser.py
- hexTools.py
- settings_default.py
- settings.py

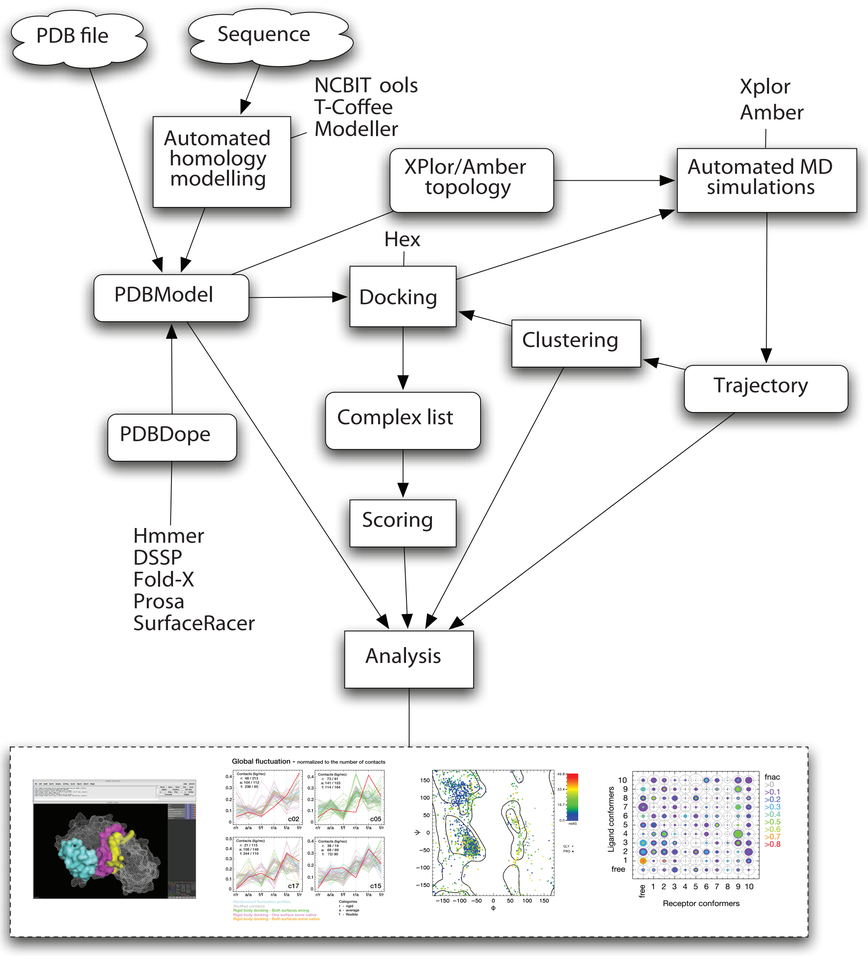
Biskit/Mod
- AlignerMaster.py
- Aligner.py
- AlignerSlave.py
- Analyse.py
- Benchmark.py
- CheckIdentities.py
- Modeller.py
- ModelMaster.py
- ModelSlave.py
- modUtils.py
- SequenceSearcher.py
- settings_default.py
- settings.py
- TemplateCleaner.py
- TemplateSearcher.py
- ValidationSetup.py

Biskit/PVM
- dispatcher.py
- pvm.py
- PVMThread.py
- pvmTools.py
- Status.py
- TrackingJobMaster.py

Biskit/Statistics
- Density.py
- lognormal.py
- pstat.py
- stats.py

Many workflows are possible

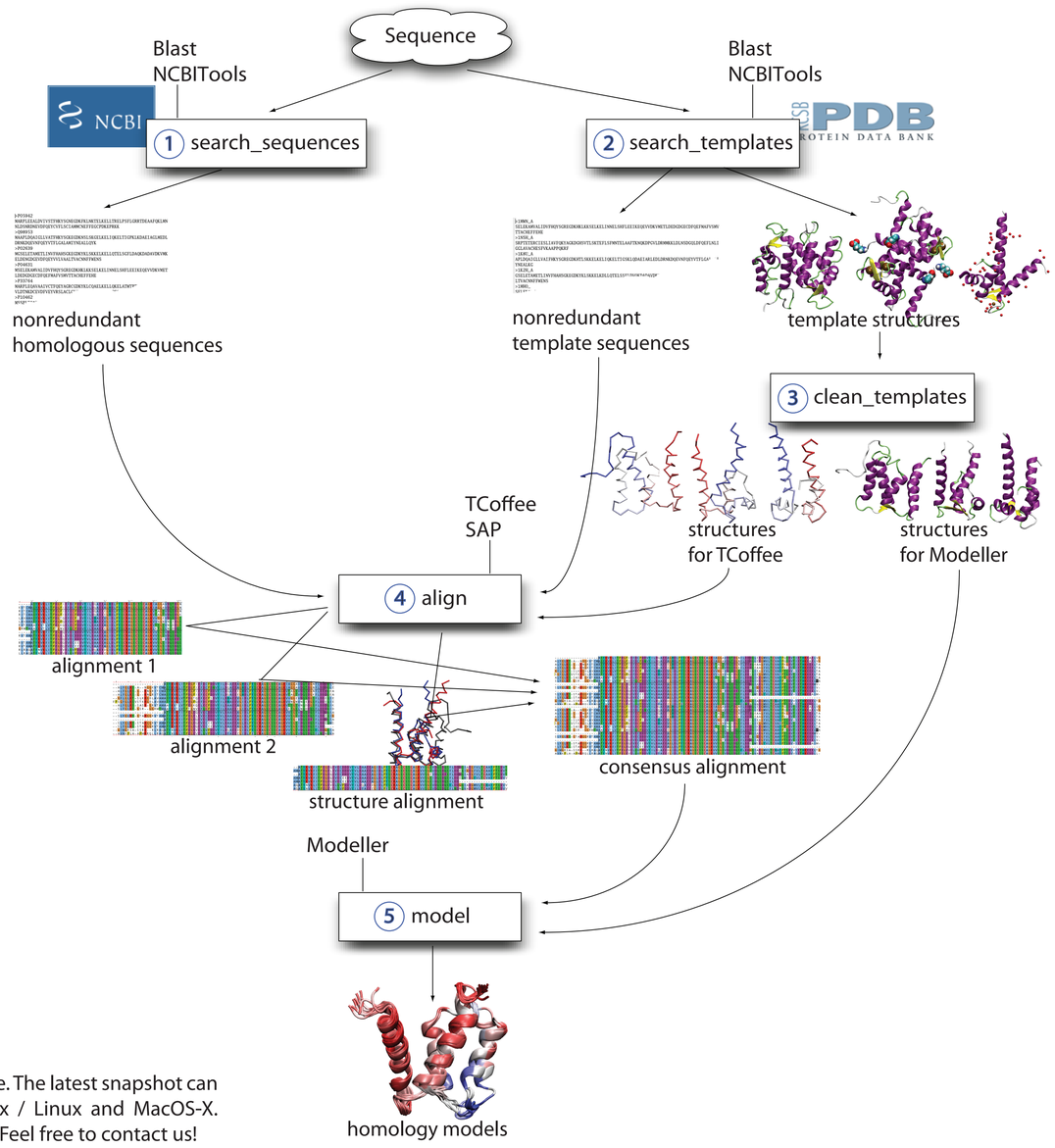
See: http://biskit.pasteur.fr/use !



Example: automatted homology modelling

See: http://biskit.pasteur.fr/use/workflows/homology-modelling !

The first step of structural bioinformatics is getting a structure. We have implemented a Biskit workflow that builds a homology model in 5 fully automatted steps. Despite the automatization, intermediate data (alignments, template selections, parameters, ...) can also be optimized manually in between the different steps.



Next step:
Tools for modular protein design

Proteins are complex three-dimensional systems with intricate dynamics. Even though there is a great deal of modularity, the engineering of synthetic protein circuits will certainly have to deal with this complexity. The successful design of swappable protein devices will ultimately depend on the combination of systems biology tools with structural modelling and molecular simulations. We are now further extending Biskit to aid the construction and simulation of multi-domain proteins and assemblies. Our goal are tools and strategies for the routine design and in-silico optimization of modular protein devices with defined dynamic behaviour.

License and availability

Biskit is freely available under the terms of the GNU General Public License. The latest snapshot can be downloaded from the sourceforge project site. Biskit runs on Unix / Linux and MacOS-X. Windows installations are also possible but are currently not well tested. Feel free to contact us!

References

Grünberg R, Nilges M, Leckner J. (2007) "Biskit--a software platform for structural bioinformatics." Bioinformatics 23, 769-70

1. Grünberg R, Nilges M & Leckner J (2006) "Flexibility and conformational entropy in protein-protein binding." Structure 14, 683-93
2. Grünberg R, Leckner J & Nilges M (2004) "Complementarity of structure ensembles in protein-protein binding." Structure 12, 2125-36
3. Johansson T, Pedersen A, Leckner J & Karlsson B. G. (2006) "Structure Determination of a Transient Complex by NMR using Paramagnetic Distance Restraints - the Complex of the Soluble Domains of Escherichia coli Transhydrogenase" submitted manuscript

Questions?

Have a biskit!

If you have read this far - you deserve a biscuit!