

Rosetta集群安装与使用经验分享

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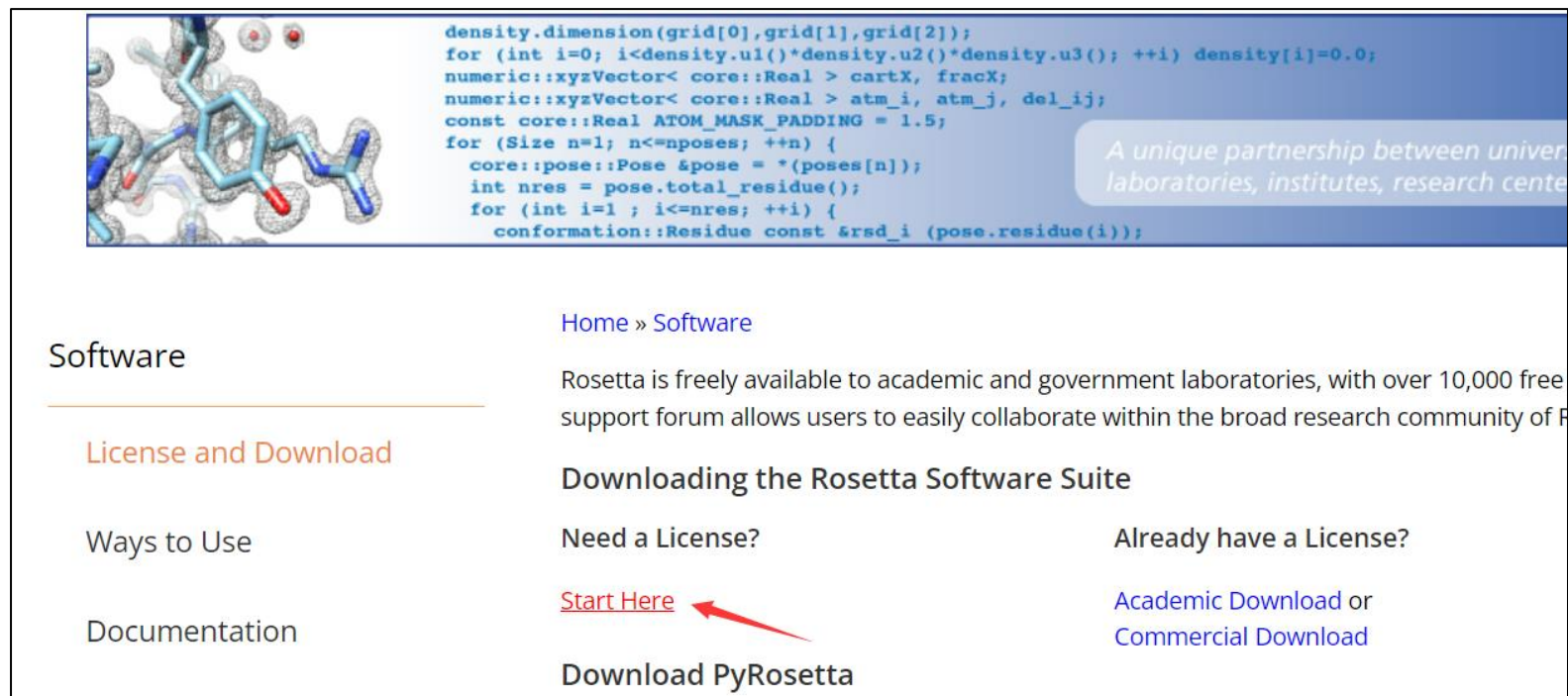
上海科技大学
ShanghaiTech University

高性能计算

Rosetta集群安装

一 获取Rosetta下载链接

1. 进入网址: <https://www.rosettacommons.org/software/license-and-download>
2. 选择start here, 之后会跳转链接到: <https://els2.comotion.uw.edu/>。注册用户并登录



The screenshot shows the Rosetta Commons website. At the top, there is a banner with a molecular structure on the left and C++ code on the right. Below the banner, the page is divided into a left sidebar and a main content area. The sidebar contains links for 'Software', 'License and Download', 'Ways to Use', and 'Documentation'. The main content area has a breadcrumb 'Home » Software' and a paragraph about Rosetta's availability. Below this, there are three columns of links: 'Downloading the Rosetta Software Suite', 'Need a License?', and 'Already have a License?'. The 'Need a License?' column contains a red link 'Start Here' with a red arrow pointing to it. The 'Already have a License?' column contains links for 'Academic Download or Commercial Download' and 'Download PyRosetta'.

```
density.dimension(grid[0],grid[1],grid[2]);
for (int i=0; i<density.u1()*density.u2()*density.u3(); ++i) density[i]=0.0;
numeric::xyzVector< core::Real > cartX, fracX;
numeric::xyzVector< core::Real > atm_i, atm_j, del_ij;
const core::Real ATOM_MASK_PADDING = 1.5;
for (Size n=1; n<=nposes; ++n) {
  core::pose::Pose &pose = *(poses[n]);
  int nres = pose.total_residue();
  for (int i=1 ; i<=nres; ++i) {
    conformation::Residue const &rsd_i (pose.residue(i));
```

Home » Software

Rosetta is freely available to academic and government laboratories, with over 10,000 free support forum allows users to easily collaborate within the broad research community of F

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The screenshot shows the WCOMOTION website header. The logo 'WCOMOTION' is on the left, with the tagline 'Your Innovation Partner'. On the right, there are icons for a shopping cart, a user profile, and a plus sign, followed by the text 'Sign-in' and 'Register'. A red arrow points to the 'Register' link. Below the header, there is a navigation bar with 'HOME' and 'PRODUCTS' links. At the bottom, there is a banner with the text 'WELCOME TO EXPRESS DIGITAL' and a partial image of a person's face.

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HOME PRODUCTS

WELCOME TO EXPRESS DIGITAL

HOME PRODUCTS

Home > All products

Search by keyword

rosetta

PyRosetta Rosetta™

Home > All products > Software > Other > Rosetta™

Rosetta™

Rosetta™ is a molecular modeling software package for understanding protein structures, protein design, protein docking, protein-DNA and protein-protein interactions. The Rosetta software contains multiple functional modules, including RosettaAbinitio, RosettaDesign, RosettaDock, RosettaAntibody, RosettaFragments, RosettaNMR, RosettaDNA, RosettaRNA, RosettaLigand, RosettaSymmetry, and more. For a list of current features, see current release notes.

PyRosetta can be found here.

For more information: <http://www.rosettacommons.org/>

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Technical Support: <https://www.rosettacommons.org/support>

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Rosetta™

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Total: \$0.00

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CANCEL ORDER

Downloads

RosettaCommons encourages use of weekly releases, but we will regularly attach version numbers to norm resource environment encourages less frequent versioning.

Last Numbered Release

- Rosetta 3.13

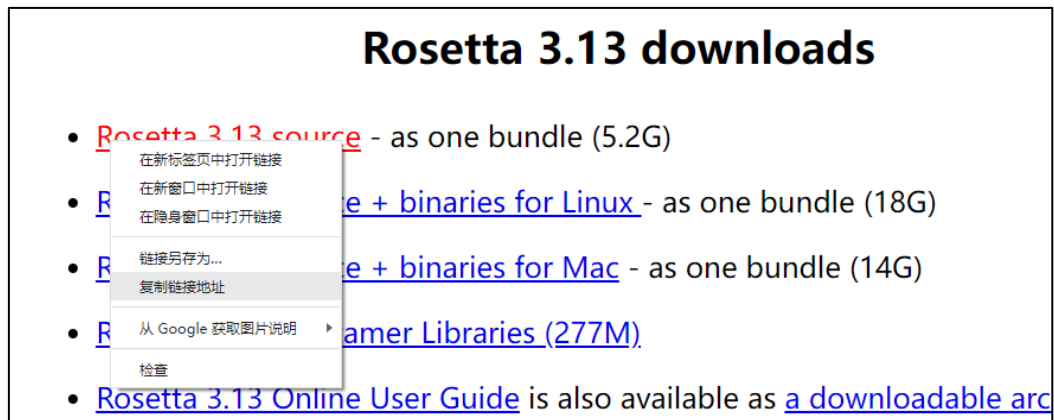
Release date:
Tuesday, June 1, 2021

[Download Rosetta 3.13](#)

Weekly Releases

- Rosetta 2022.11

复制链接地址



从集群下载：

```
wget https://www.rosettacommons.org/download.php?token=a64t4Q78m&file=rosetta\_src\_3.13\_bundle.tgz
```

也可直接下载到本地再上传至集群。

安装及编译： 以下载rosetta_src_3.13_bundle.tgz为例

1、解压

```
gunzip rosetta_src_3.13_bundle.tgz, 将tgz文件转为tar文件  
tar -xvf rosetta_src_3.13_bundle.tar 解压
```

完成后得到一个名为rosetta_src_2021.16.61629_bundle的目录
获取绝对路径：

```
readlink -f 文件名/文件夹名
```

2、编译：使用mpi进行编译

1) 先查看集群中的mpi模块：`module avail mpi`

```
[hpc_train@hpc-login-gpu01 ~]$ module avail mpi

----- /public/software/modules/ -----
mpi/intelmpi/2017                mpi/intelmpi/5.1.3.223          mpi/openmpi/2.1.6/gnu/7.4.0    mpi/openmpi/4.0.0/gnu/7.4.0
mpi/intelmpi/2017.4.239         mpi/openmpi/1.6.5/intel         mpi/openmpi/2.1.6/gnu/8.3.0    mpi/openmpi/4.0.0/intel
mpi/intelmpi/2019.1.144        mpi/openmpi/1.8.7/intel         mpi/openmpi/2.1.6/intel        mpi/openmpi/4.0.1/gnu/8.3.0
mpi/intelmpi/2019.7            mpi/openmpi/2.0.0/gnu           mpi/openmpi/3.1.3/6/gnu        mpi/openmpi/4.1.1
mpi/intelmpi/2020.1.217        mpi/openmpi/2.0.0/intel         mpi/openmpi/3.1.3/6/intel      mpi/openmpi/gnu/4.0.3
mpi/intelmpi/2021.3.0          mpi/openmpi/2.0.2/gnu           mpi/openmpi/3.1.3/7/gnu        mpi/openmpi/intel/4.0.3
mpi/intelmpi/5.0.2.044         mpi/openmpi/2.1.1/gnu           mpi/openmpi/3.1.3/7/intel

----- /public/spst/software/modules/ -----
mpi/intelmpi/2017.4.239  mpi/openmpi/intel/2.1.2
```

选择版本，推荐mpi/openmpi/2.0.0/gnu

2) pbs脚本编译

```
#!/bin/bash
#PBS -N intall_rosetta 任务名
#PBS -l nodes=1:ppn=32 调用资源 (1节点, 32核)
#PBS -q amdnode        所用队列
#####

cd $PBS_O_WORKDIR

source /hpc/data/XXX/XXX...../XXXXXXXX/XXX/rosetta/rosetta_src_2021.16.61629_bundle/main/source/2022_mpi_env.sh
module load mpi/openmpi/2.0.0/gnu

python ./scons.py -j64 mode=release bin extras=mpi
```

Rosetta环境

2022_mpi_env.sh

```
export ROSETTA=/hpc/data/XXX/XXX...../XXXXXXXX/XXX/XXXX/software/rosetta_src_2021.16.61629_bundle
export ROSETTA3_DB=$ROSETTA/main/database
export ROSETTA_BIN=$ROSETTA/main/source/bin
export PATH=$PATH:$ROSETTA_BIN
```

提交命令，开始编译：

```
qsub install.pbs
```

查看状态：

```
qstat
```

```
drwxr-xr-x  2 hpc_train hpc_lab 4.0K Oct 24 22:44 bin
-rw-----  1 hpc_train hpc_lab  767 Oct 24 23:23 intall_rosetta.e5944569
-rw-----  1 hpc_train hpc_lab 5.4M Oct 24 23:23 intall_rosetta.o5944569
```

intall_rosetta.e5944569: 报错error/警告warning文件

intall_rosetta.o5944569: 输出文件

Rosetta集群使用

摘要：

input文件

output文件夹

xml程序文件——主程序

flags参数文件——IO等参数设置

pbs提交脚本——将作业提交至后台

pbs提交脚本

/hpc/data/home/XXX/XXX...../XXXX/XXXX/examples/GeneralizedKIC/exercise1/exercise1_3gbn.pbs

```
#!/bin/bash
#PBS -N GeneralizedKIC_exercise1 任务名
#PBS -l nodes=1:ppn=14          调用资源 (1节点, 14核)
#PBS -q pub_jx                  所用队列
#####

cd $PBS_O_WORKDIR

source /hpc/data/XXX/XXX...../XXXXXXXX/XXX/XXX/software/rosetta_src_2021.16.61629_bundle/main/source/2022_mpi_env.sh
module load mpi/openmpi/2.0.0/gnu

Rosetta环境

主命令: 用rosetta_3gbn.flags中的参数运行rosetta_scripts.mpi.linuxgccrelease程序
rosetta_scripts.mpi.linuxgccrelease @inputs/rosetta_3gbn.flags
```

2022_mpi_env.sh

```
export ROSETTA=/hpc/data/XXX/XXX...../XXXXXXXX/XXX/XXXXXXXX/software/rosetta_src_2021.16.61629_bundle
export ROSETTA3_DB=$ROSETTA/main/database
export ROSETTA_BIN=$ROSETTA/main/source/bin
export PATH=$PATH:$ROSETTA_BIN
```

flag参数文件

```
-nstruct 5
-in:file:s ./inputs/3gbn_A.pdb
-in:file:fullatom
-parser:protocol ./xml/exercise1_3gbn.xml
-out:path:all ./outputs/3gbn/
```

输出数量：设置为5

Input文件的路径：一般为处理好的pdb结构

Input文件的类型

主程序路径：xml文件

output文件的路径：输出为pdb结构，按0001、、编号

```
[hpc_train@hpc-login-gpu01 exercise1]$ l
total 52K
-rw----- 1 hpc_train hpc_lab 24K Nov 3 20:50 GeneralizedKIC_exercise1.o6048107
-rw----- 1 hpc_train hpc_lab 747 Nov 3 20:50 GeneralizedKIC_exercise1.e6048107
-rw-r--r-- 1 hpc_train hpc_lab 176 Nov 3 20:50 GeneralizedKIC_exercise1.timelog
drwxr-xr-x 4 hpc_train hpc_lab 4.0K Nov 3 20:55 outputs
drwxr-xr-x 2 hpc_train hpc_lab 4.0K Nov 3 20:57 xml
-rw-r--r-- 1 hpc_train hpc_lab 602 Nov 3 20:57 exercise1_2ND2.pbs
-rw-r--r-- 1 hpc_train hpc_lab 597 Nov 3 22:59 exercise1_3gbn.pbs
drwxr-xr-x 2 hpc_train hpc_lab 4.0K Nov 3 23:04 inputs
```

input文件

output文件夹

```
[hpc_train@hpc-login-gpu01 exercise1]$ l inputs/
total 132K
-rw-r--r-- 1 hpc_train hpc_lab 25K Oct 31 21:28 2ND2_state1_glyonly.pdb
-rw-r--r-- 1 hpc_train hpc_lab 22K Oct 31 21:28 2ND2_state1_glyonly_loop_removed.pdb
-rw-r--r-- 1 hpc_train hpc_lab 33K Nov 3 20:41 3gbn.pdb
-rw-r--r-- 1 hpc_train hpc_lab 32K Nov 3 20:42 3gbn_A.pdb
-rw-r--r-- 1 hpc_train hpc_lab 57 Nov 3 20:42 3gbn_A.fasta
-rw-r--r-- 1 hpc_train hpc_lab 159 Nov 3 20:56 rosetta_2ND2.flags
-rw-r--r-- 1 hpc_train hpc_lab 133 Nov 3 22:59 rosetta_3gbn.flags
```

xml程序文件

flags参数文件

pbs提交脚本

xml文件

定义区

程序区

```
<ROSETTASCRIPTS>
  <SCOREFXNS>
</SCOREFXNS>
  <RESIDUE_SELECTORS>
</RESIDUE_SELECTORS>
  <TASKOPERATIONS>
</TASKOPERATIONS>
  <SIMPLE_METRICS>
</SIMPLE_METRICS>
  <FILTERS>
</FILTERS>
  <MOVERS>
</MOVERS>
  <PROTOCOLS>
</PROTOCOLS>
  <OUTPUT />
</ROSETTASCRIPTS>
```

打分函数

选择残基

操作限制

xml脚本主体

程序主体

```
<ScoreFunction name="bb_only" weights="empty.wts" >
  <Reweight scoretype="fa_rep" weight="0.1" />
  <Reweight scoretype="fa_atr" weight="0.2" />
</ScoreFunction>
```

```
<RESIDUE_SELECTORS>
  <Chain name="chA" chains="A"/>
  <Index name="res1to10" resnums="1-10"/>
</RESIDUE_SELECTORS>
```

```
<TASKOPERATIONS>
  <OperateOnResidueSubset name="helice_unchange" selector="a1">
    <PreventRepackingRLT/>
  </OperateOnResidueSubset>
</TASKOPERATIONS>
```

```
<MOVERS>
  <PeptideStubMover name="add_loop_residues" >
    <Insert anchor_rsd="28" resname="ALA" />
    <Prepend anchor_rsd="32" resname="ALA" />
  </PeptideStubMover>
</MOVERS>
```

```
<PROTOCOLS>
  <Add mover="add_loop_residues" />
  <Add mover="new_bond" />
</PROTOCOLS>
```

Rosetta集群使用案例

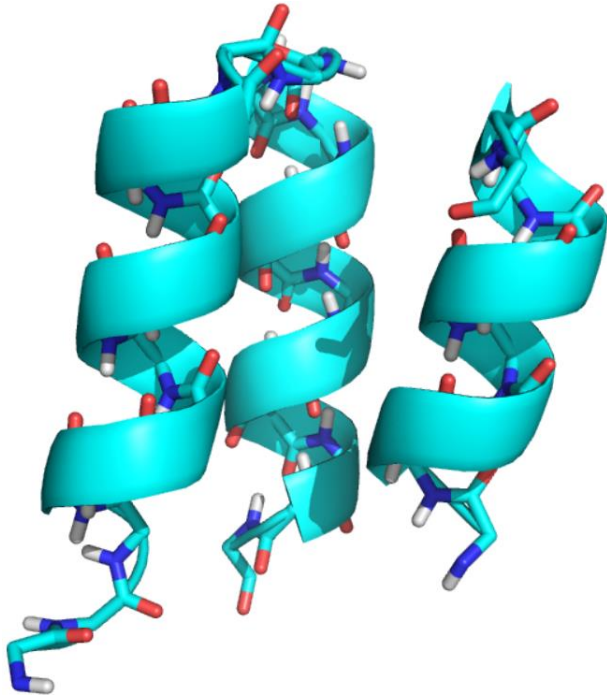
Loop modeling(GeneralizedKIC)

Fastdesign

Docking

Loop modeling(GeneralizedKIC)

Examples:

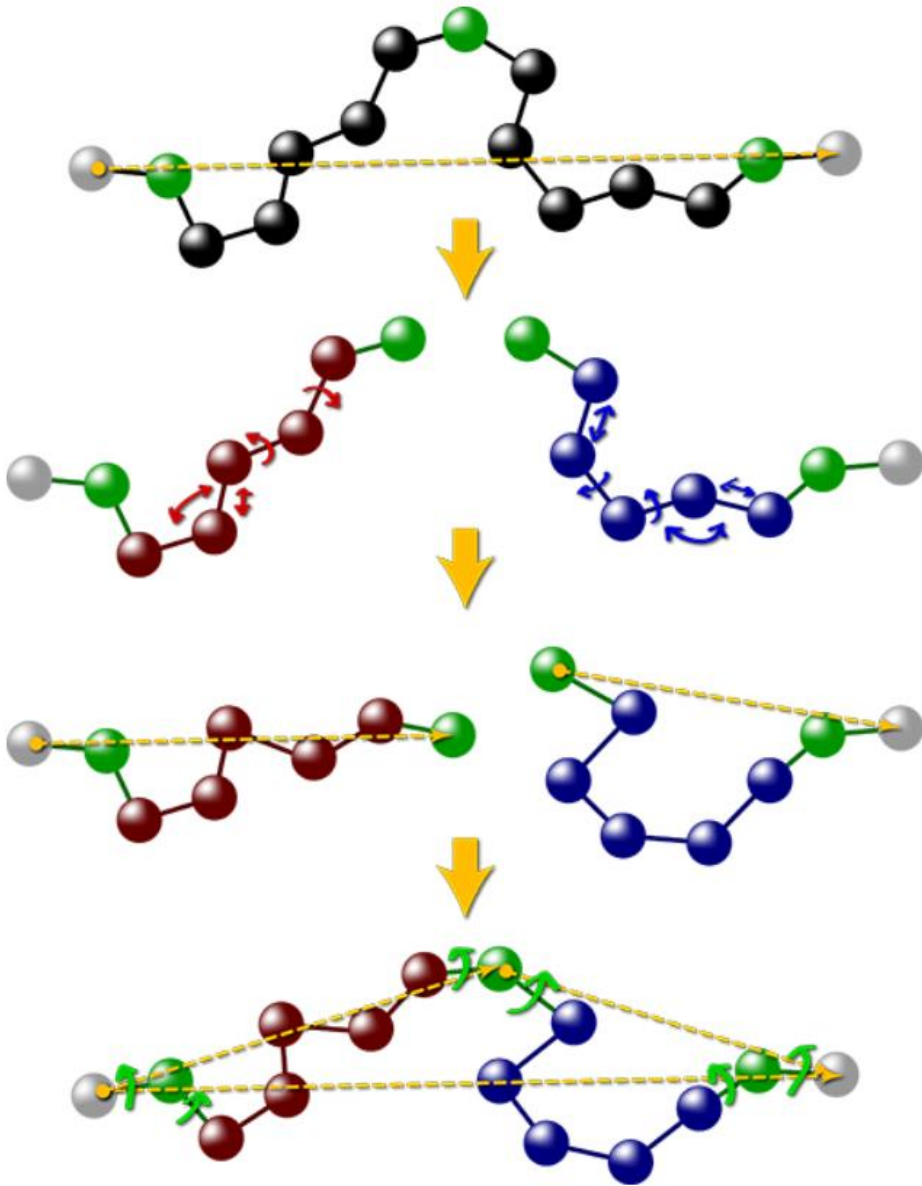


2ND2



3gbn

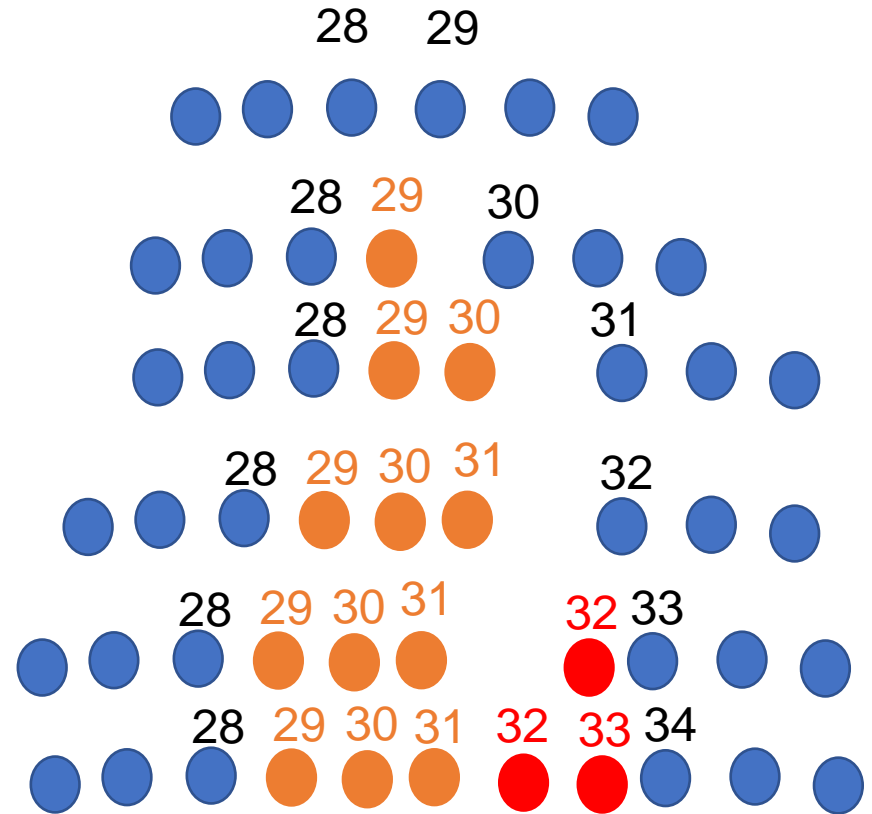
Loop modeling (GeneralizedKIC)



1. Compute and store rigid-body transformation from start of loop to end (gold). Divide loop into two segments using three pivots (green).

2. Perturb degrees of freedom (torsions, bond angles, bond lengths) within each segment in user-defined ways (red and blue arrows).

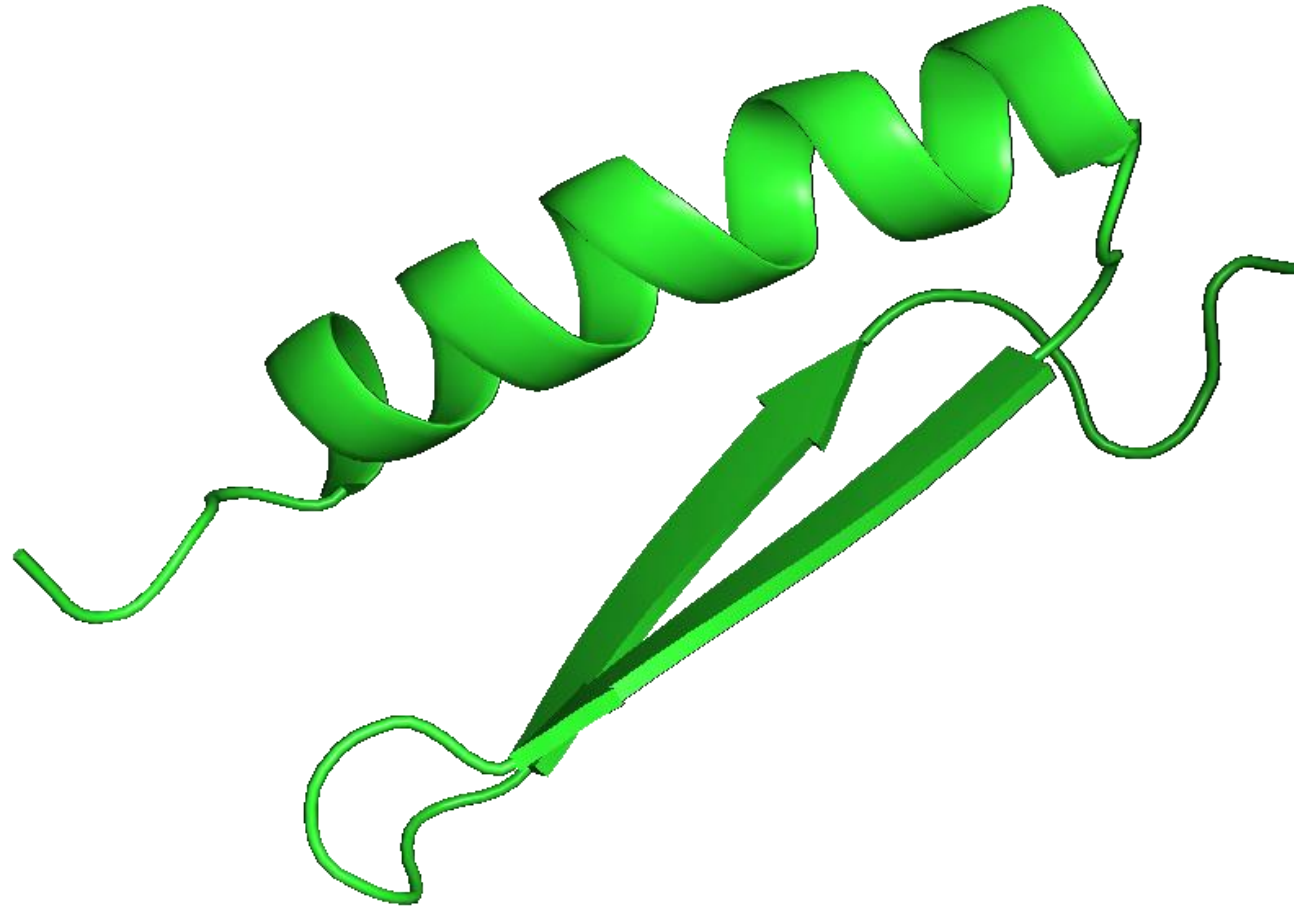
3. Calculate and set pivot torsion values (green arrows) to orient each rigid segment so that the original rigid-body transform between the loop ends is preserved.



```
<PeptideStubMover name="add_loop_residues" >
  <Insert anchor_rsd="28" resname="ALA" />
  <Insert anchor_rsd="29" resname="GLY" />
  <Insert anchor_rsd="30" resname="ALA" />
  <Prepend anchor_rsd="32" resname="ALA" />
  <Prepend anchor_rsd="32" resname="ALA" />
</PeptideStubMover>
```

Fastdesign

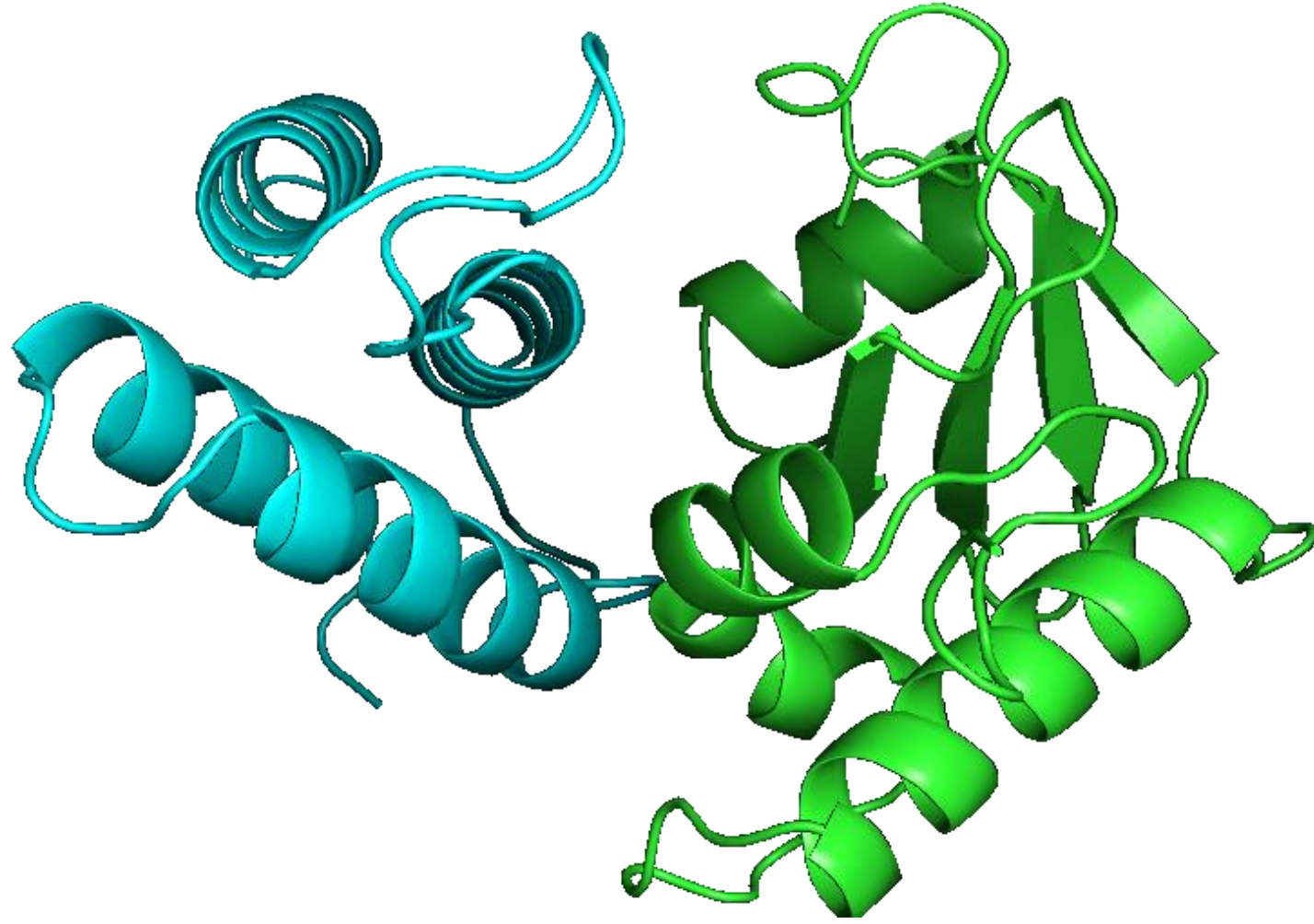
Example



1FR6

Docking

Example



1V74

Rosetta参考资料

<https://www.rosettacommons.org/demos/latest/Home#tutorials>

https://new.rosettacommons.org/docs/latest/application_documentation/Apps

https://new.rosettacommons.org/docs/latest/application_documentation/Application-Documentation

```
[hpc_train@hpc-login-gpu01 main]$ l
total 44K
-rw-r--r--  1 hpc_train hpc_lab 1.6K Apr 21  2021 README.md
-rw-r--r--  1 hpc_train hpc_lab 4.0K Apr 21  2021 LICENSE.md
drwxr-xr-x 17 hpc_train hpc_lab 4.0K Apr 21  2021 database
drwxr-xr-x  9 hpc_train hpc_lab 4.0K Apr 21  2021 tests
drwxr-xr-x 42 hpc_train hpc_lab 4.0K Apr 21  2021 tools
drwxr-xr-x  4 hpc_train hpc_lab 4.0K Apr 21  2021 rosetta_scripts_scripts
drwxr-xr-x  8 hpc_train hpc_lab 4.0K Apr 21  2021 pyrosetta_scripts
drwxr-xr-x  5 hpc_train hpc_lab 4.0K Apr 21  2021 PyRosetta.notebooks
drwxr-xr-x 16 hpc_train hpc_lab 4.0K Apr 21  2021 documentation
drwxr-xr-x  8 hpc_train hpc_lab 4.0K Apr 21  2021 demos
drwxr-xr-x 19 hpc_train hpc_lab 4.0K Nov  3 17:19 source
```

谢谢观看