

SCHRODINGER在集群的安装与使用示例

薛定谔简介

Schrodinger（薛定谔）是药物发现的完整软件包，包括：基于受体和配体结构的诱导契合和柔性对接模式；基于受体结构及配体极性的对接模式；基于受体结构及溶液环境性质的对接模式；组合化学库设计及基于组合库的对接模式；基于配体结构的药物设计，药效团和3D-QSAR；生物分子结构模拟，蛋白、糖、核酸、小肽等；基于靶点的药物设计；ADME性质预测。

在集群上安装薛定谔

软件下载地址：

<https://www.schrodinger.com/downloads/releases>

1.下载完成后，解压：

```
[root@hpc2 Schrodinger]# ls
Schrodinger_Suites_2017-4_Linux-x86_64.tar
[root@hpc2 Schrodinger]# tar -xvf Schrodinger_Suites_2017-4_Linux-x86_64.tar
Schrodinger_Suites_2017-4_Linux-x86_64/combiglide-v4.7-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/aacq-v2.2-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/canvas-v3.4-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/mcpro-v4.8-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/EULA_standard.rtf
Schrodinger_Suites_2017-4_Linux-x86_64/psp-v5.0-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/phase-v5.3-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/glide-v7.7-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/epik-v4.2-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/jaguar-v9.8-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/impact-v7.7-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/bioluminate-v2.9-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/desmond-v5.2-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/psp-hmmerpfamdb-thirdparty-database.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/mmshare-v4.0-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/knime-v4.0-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/INSTALL
Schrodinger_Suites_2017-4_Linux-x86_64/macromodel-v11.8-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/SchrodingerKNIMEFreeUpdateSite_4.0.11.201711131631.zip
Schrodinger_Suites_2017-4_Linux-x86_64/qikprop-v5.4-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/SchrodingerKNIMEUpdateSite_4.0.11.201711131631.zip
Schrodinger_Suites_2017-4_Linux-x86_64/alldocs-v4.0-docs.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/maestro-v11.4-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/psp-blastwebdb-thirdparty-database.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/pldb-v4.0-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/psp-hmmerpfam-thirdparty-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/psp-blast-thirdparty-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/CHECKSUM.md5
```

2.进入至解压目录，运行命令./INSTALL

```
aacg-v2.2-Linux-x86_64.tar.gz      impact-v7.7-Linux-x86_64.tar.gz      psp-blast-thirdparty-Linux-x86_64.tar.gz
alldocs-v4.0-docs.tar.gz          INSTALL                               psp-blastwebdb-thirdparty-database.tar.gz
bioluminate-v2.9-Linux-x86_64.tar.gz  jaguar-v9.8-Linux-x86_64.tar.gz      psp-hmmerpfamdb-thirdparty-database.tar.gz
canvas-v3.4-Linux-x86_64.tar.gz      knime-v4.0-Linux-x86_64.tar.gz       psp-hmmerpfam-thirdparty-Linux-x86_64.tar.gz
CHECKSUM.md5                       macromodel-v11.8-Linux-x86_64.tar.gz  psp-v5.0-Linux-x86_64.tar.gz
coombiglide-v4.7-Linux-x86_64.tar.gz  maestro-v11.4-Linux-x86_64.tar.gz    qikprop-v5.4-Linux-x86_64.tar.gz
desmond-v5.2-Linux-x86_64.tar.gz     ocpro-v4.0-Linux-x86_64.tar.gz       SchrodingerKNIMEFreeUpdateSite_4.0.11.201711131631.zip
epik-v4.2-Linux-x86_64.tar.gz        mshare-v4.0-Linux-x86_64.tar.gz     SchrodingerKNIMEUpdateSite_4.0.11.201711131631.zip
EULA_standard.rtf                  phase-v9.3-Linux-x86_64.tar.gz
glide-v7.7-Linux-x86_64.tar.gz       pldb-v4.0-Linux-x86_64.tar.gz
[root@hpc2 Schrodinger_Suites_2017-4_Linux-x86_64]# ./INSTALL
```

3.按Enter以继续

```

Schrodinger Software Installer

Please respond to each question by entering the appropriate response
or pressing ENTER to accept the default (shown in parentheses).

You will be given a chance to review all of your installation choices
before any files are actually installed.

You can quit the installation at any time by pressing CTRL+C.

For more information, see the Installation Guide, which is in the file
"install_guide.pdf", in the same directory as this INSTALL script.

Proceed to Schrodinger Suite2017-4 installation...

[Press ENTER to continue]
█
```

4.此处需要输入安装的路径：以/share/install/Schrodinger（安装目录）为例

```
1) SCHRODINGER directory

Select the directory where you want to install this software.

This directory will hold a script to launch each installed product,
a subdirectory for each release of each product, and documentation.
To run the software, you must set the SCHRODINGER variable to this
directory.

It is necessary to install the software for each major release in
a separate SCHRODINGER directory. If you are installing additional
products for a release, or upgrading a product to a new version with
the same major version number, you can install into the same
SCHRODINGER as the existing software from that release, but software
from different major releases should never be mixed.

Current SCHRODINGER directory: /share/install/schrodinger2017-4
SCHRODINGER directory: (/share/install/schrodinger2017-4) /share/install/Schrodinger█
```

5.确认安装 (y)

```
Your installation choices were:

SCHRODINGER directory:      /share/install/Schrodinger
SCHRODINGER_THIRDPARTY directory: /share/install/Schrodinger/thirdparty
Scratch directory:          /usr/tmp

product      version  platform      status      compatible  action
-----
glide        7.7     Linux-x86_64  NEW         yes         INSTALL
pldb         4.0     Linux-x86_64  NEW         yes         INSTALL
bioluminate  2.9     Linux-x86_64  NEW         yes         INSTALL
aacg        2.2     Linux-x86_64  NEW         yes         INSTALL
hmmerpfamdb <database> NEW         yes         INSTALL
blastwebdb  <database> NEW         yes         INSTALL
alldocs     4.0     <docs>        NEW         yes         INSTALL
canvas      3.4     Linux-x86_64  NEW         yes         INSTALL
desmond     5.2     Linux-x86_64  NEW         yes         INSTALL
mcpro       4.8     Linux-x86_64  NEW         yes         INSTALL
psp         5.0     Linux-x86_64  NEW         yes         INSTALL
blast       Linux-x86_64 NEW         yes         INSTALL
hmmerpfam   Linux-x86_64 NEW         yes         INSTALL
impact      7.7     Linux-x86_64  NEW         yes         INSTALL
jaguar      9.8     Linux-x86_64  NEW         yes         INSTALL
macromodel  11.8    Linux-x86_64  NEW         yes         INSTALL
maestro     11.4    Linux-x86_64  NEW         yes         INSTALL
qikprop     5.4     Linux-x86_64  NEW         yes         INSTALL
combiglide  4.7     Linux-x86_64  NEW         yes         INSTALL
phase       5.3     Linux-x86_64  NEW         yes         INSTALL
epik        4.2     Linux-x86_64  NEW         yes         INSTALL
knime       4.0     Linux-x86_64  NEW         yes         INSTALL
mmshare     4.0     Linux-x86_64  NEW         yes         INSTALL

Note: The mmshare module provides common resources for all products.
      It is installed automatically when necessary.

Are these choices correct? [y/n] ( ) █
```

6.完成安装

```
*) Configuring your installation

If you need to request licenses, install or transfer licenses, or configure
remote machines for calculations, run the the Schrodinger software
configuration tool on a machine with a display.

The tool can be launched directly via $SCHRODINGER/utilities/configure
or by choosing the Configure Software item under the Help menu in Maestro.
If the current machine has a display, you can also launch it from this screen.

Launch the configuration GUI now? [y/n] ( ) n

***** Schrodinger software installation is complete. *****

[root@hpc2 Schrodinger_Suites_2017-4_Linux-x86_64]# █
```

7.待完成安装后, 在命令行中输入vi ~/.bashrc

导入软件的安装路径（此处为/share/install/Schrodinger）及license授权，将下面三行输入.bashrc文件中，保存并退出。安装完成。

```
export PATH=/share/install/Schrodinger:/share/install/Schrodinger/utilities:$PATH
export LM_LICENSE_FILE=27008@compbio.shanghai.edu.cn
export SCHRODINGER=/share/install/Schrodinger
```

安装完成后，需要修改Hosts文件才可以在计算集群上使用（如果只是在本地计算机上使用CPU的话可以忽视，要在本地使用GPU的话需要添加gpgpu信息），具体修改的文件为安装目录下的schrodinger.host文件。即，在Host文件中添加属于集群作业管理系统的信息：

本地添加GPU：

```
name: localhost
tmpdir: 自定义临时文件路径
gpgpu: 0, Tesla V100 (你的显卡型号)
```

对于CPU队列（分子对接、同源建模、结构优化、量子化学任务）：

```
name: HPC_CPU (名字可以随便起)
host: hpc-login-gpu01 (登录节点的hostname)
user: 用户名
queue: Torque (根据作业管理系统的类型更换)
qargs: -q 队列名 -l nodes=1:ppn=%NPROC%
schrodinger: 自己的薛定谔安装路径
processors: 240
processors_per_node: 28
tmpdir: 自定义临时文件路径
```

对于GPU队列（分子动力学模拟、机器学习任务）：

```
name: HPC_GPU (名字可以随便起)
host: hpc-login-gpu01 (登录节点)
user: 用户名
queue: Torque (根据作业管理系统的类型更换)
qargs: -q 队列名 -l nodes=1:ppn=%NPROC%:gpus=%NPROC%
```

schrodinger:自己的薛定谔安装路径

processors: 16

processors_per_node: 4

tmpdir: 自定义临时文件路径

(显卡类型和数量要跟随你使用的GPU节点来更换)

gpgpu: 0, Tesla V100

gpgpu: 1, Tesla V100

gpgpu: 2, Tesla V100

gpgpu: 3, Tesla V100

```
# Guide for a description of the settings that can be made here.
#
##### NOTE #####
# The 'localhost' entry is special:
# * Settings in the 'localhost' entry are implicitly included in
#   every other host entry as well, so settings common to all entries
#   can be placed in the localhost entry.
# * The 'schrodinger:', 'host:' and 'queue:' fields may not be used in
#   the localhost entry.
#####

#
name: localhost
tmpdir: /public/home/.../tmp

# HPC CPU
name: HPC_CPU
host: hpc-login-gpu01
user: ...
queue: Torque
qargs: -q ... -l nodes=1:ppn=%NPROC%
schrodinger: /public/home/.../Desktop/Software/MS21
processors: 240
processors_per_node: 28
tmpdir: /public/home/.../tmp

#
name: HPC_CPU
host: HPC-login
user: ...
queue: Torque
qargs: -q ... -l nodes=1:ppn=%NPROC%
schrodinger: /public/home/.../Software/MS21
processors: 240
processors_per_node: 28
tmpdir: /public/home/.../tmp

name: HPC_GPU
host: hpc-login-gpu01
user: ...
queue: Torque
qargs: -q ... nodes=1:ppn=%NPROC%:gpus=%NPROC%:v100
schrodinger: /public/home/.../Software/MS21
processors: 16
processors_per_node: 4
tmpdir: /public/home/.../tmp
gpgpu: 0, Tesla V100
gpgpu: 1, Tesla V100
gpgpu: 2, Tesla V100
gpgpu: 3, Tesla V100
```

最终示例Host文件:

队列名

用户名

登录节点

安装路径

当使用v100系列节点

知乎 @啮大侠

最终修改完的host文件如上图所示。

linux集群上的SCHRODINGER 使用实例-Ligpred

Glide作为广为人知的分子对接软件, 提供了非常方便的各类型对接工作, 接下来介绍如何方便的在无图形化界面的linux集群中进行分子对接前的配体准备

(Ligpred)

```
$SCHRODINGER/ligprep -isd my_2D_cts.sd -omae my_3D_cts.mae -HOST  
HPC_CPU
```

其中，`-i***` 是输入的文件格式(sd格式写成 `-isd`)，一般输出文件格式选 `-omae`，并指定输出文件名，`-HOST` 指定为`.hosts`文件中的name，例如上述的 `HPC_CPU`

我该怎么学习薛定谔

薛定谔的在线入门资源有很多，尤其是官方文档（英文），内容非常详尽，是软件使用方面的最好选择；其次，薛定谔有一系列在线的讲座（中英文都有）和培训，是入门的最佳选择。

- 讲座和会议：[Upcoming Scientific Events](#)
- 中文在线讲座：[Chinese Life Sciences Webinar Series, Online](#)
- 官方培训：[Training | Schrödinger](#)
- 软件使用教程：每一个Panel（面板）的右下角的问号，打开可查看程序的使用手册
- 官方脚本介绍：[Scripts | Schrödinger](#)
- 官方Python API文档：[Python API | Schrödinger](#)
- 官方文档：[Documentation | Schrödinger](#)

以2021-3版本为例，官方文档中包含如下内容：

Getting Help

Maestro Quick Reference Guide

▶ Academy Tutorials

▶ Quick Start Guides

▶ Best Practices

▶ Help

▶ User Manuals

▶ Command References

▶ Quick Reference

▶ Installation and Jobs

Third Party Legal Notices

Getting Help

Welcome to the Maestro Help System! We have a variety of materials

To get started with Maestro, you can use our [Online Workshop Series](#) or the [Maestro Quick Reference Guide](#) to quickly familiarize yourself with

For the latest documentation, go to the [Documentation page](#) on our website.

Inside Maestro you will find information in a number of places.

遇到报错如何解决？

- 点击右上角的Monitor工具，双击查看任务的log，尤其是每个任务的子log，通常薛定谔的log文件会给出来比较详细的错误原因，如果找到了最深一层的报错还是不知道怎么办，可以在社区论坛求助；
- 比较常见的问题是没有做Protein Preparation和LigPrep，请注意一般导入外部文件后均需要进行预处理。

各个模块的内容如下：

- **Academy Tutorials** 包含了一些典型计算生物学任务的详尽教程，如 Generating and Visualizing Ligand Conformations, Covalent Docking for Virtual Screening and Pose Prediction, Cross-Docking with IFD-MD等；
- Quick Start Guide 是介绍各个程序使用方法的简单教程；
- **Best Practices** 是原理、应用场景与使用方法兼备的高级教程；
- Help 包含了软件中具体应用程序的使用方法
- **User Manual** 是各个应用程序原理、应用场景的介绍，着重介绍了当我们运行任务时，软件究竟在干什么，这将帮助我们了解出现了问题应该如何排查原因；
- Command References 是各种应用程序在命令行模式下的使用方法；

如果实在不喜欢英文教程，可以在B站和微信公众号搜索其他入门级中文教程。

参考学习资料

- [Schrödinger\(薛定谔\)入门级Q&A - 知乎 \(zhihu.com\)](#)
- [Schrodinger \(shanghaitech.edu.cn\)](#)
- 流程化虚拟筛选和分子动力学模拟 [Schrödinger脚本库：在Linux集群上轻松运行计算生物学任务 - 知乎 \(zhihu.com\)](#)

特别致谢

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