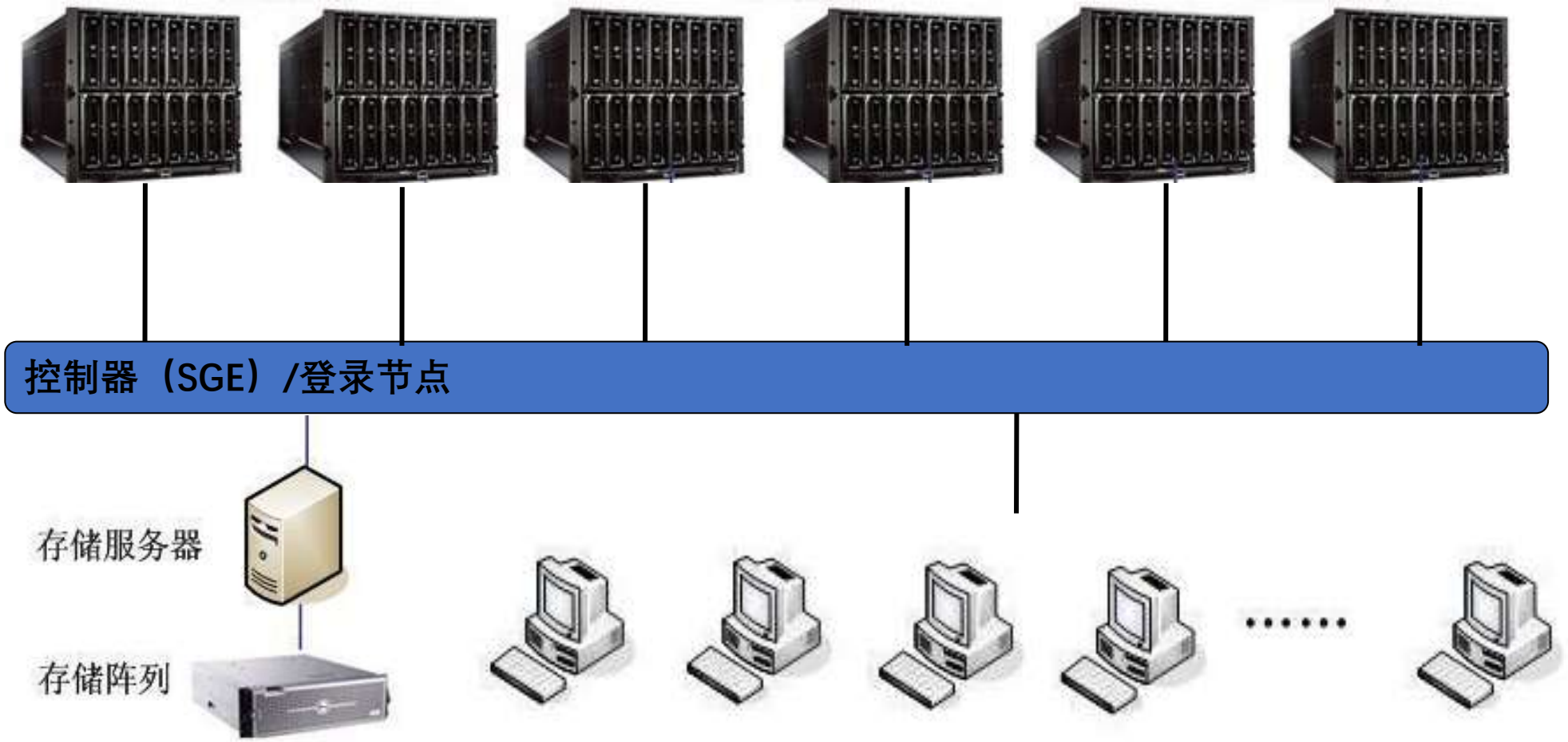
Linux 系统入门

生物信息学
助教-刘柯
助教-方明昊

目录

❖ 集群介绍

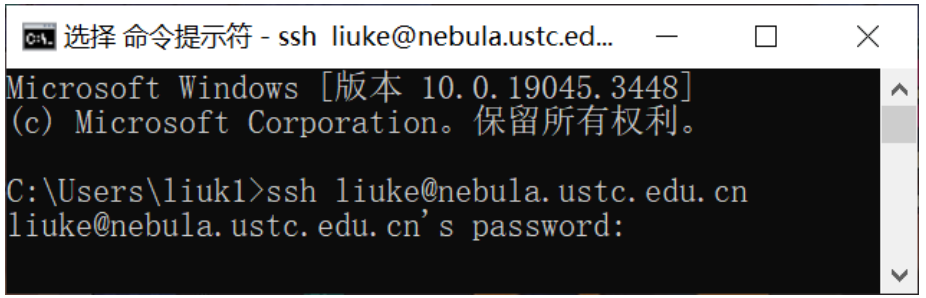
集群（cluster）就是一组计算机，它们作为一个整体向用户提供一组网络资源，这些单个的计算机系统就是集群的**节点**（node）。

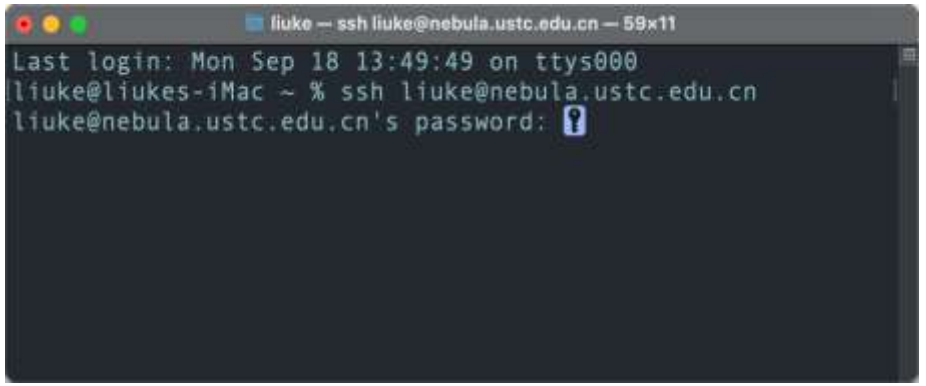


❖ 集群登录

在MacOS系统或者Linux系统下打开终端(Terminal)，Windows打开命令提示符

输入ssh <username>@nebula.ustc.edu.cn





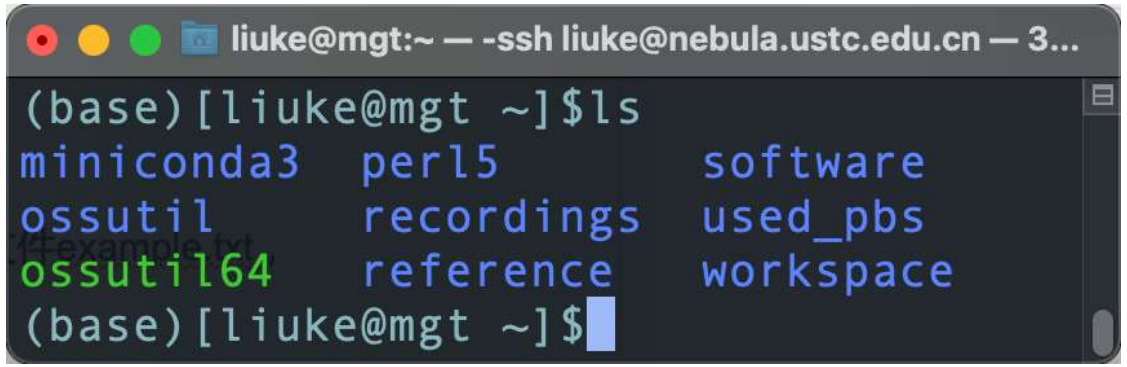
重要的事情说三遍：
不要在登录节点跑程序！！
不要在登录节点跑程序！！
不要在登录节点跑程序！！

注意：用户登陆机群之后，实际上位于登陆节点（资源很少）

❖ 常用linux命令

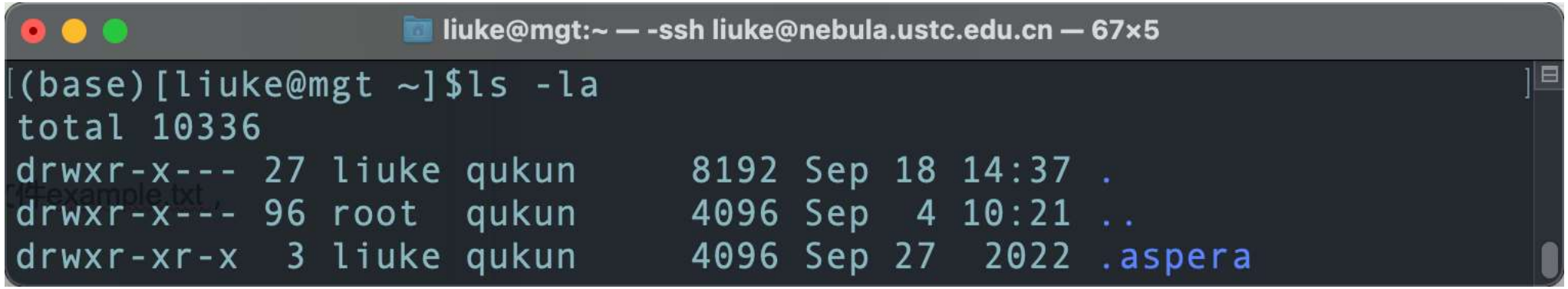
➢ 文件及目录管理

- **列出目录 ls**



相对路径和绝对路径:

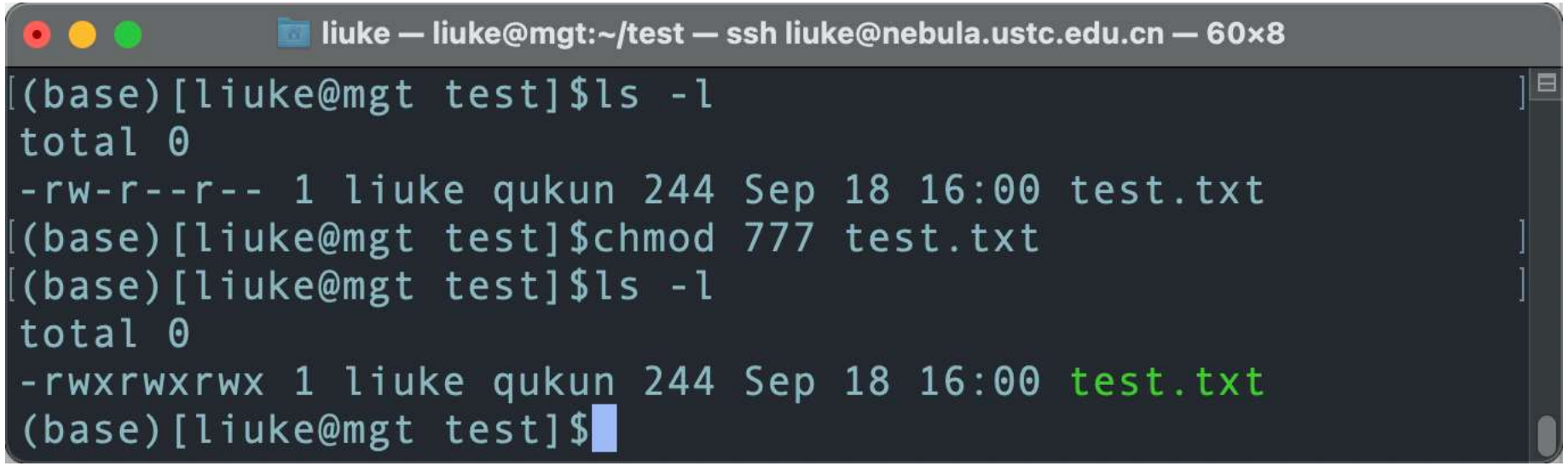
绝对路径 /home/qukun/liuke/workspace
相对路径 ./workspace ../liuke/workspace



➢ 文件及目录管理

文档属性:
[-] [rwx] [r-x] [r--]
[文档类别] [拥有者权限] [同群组权限] [其他使用者权限]

- 更改文档权限 chmod



可读取 r – 4
可写入 w – 2
可执行 x – 1

❖ 常用linux命令

➢ 文件及目录管理

- 创建目录 mkdir

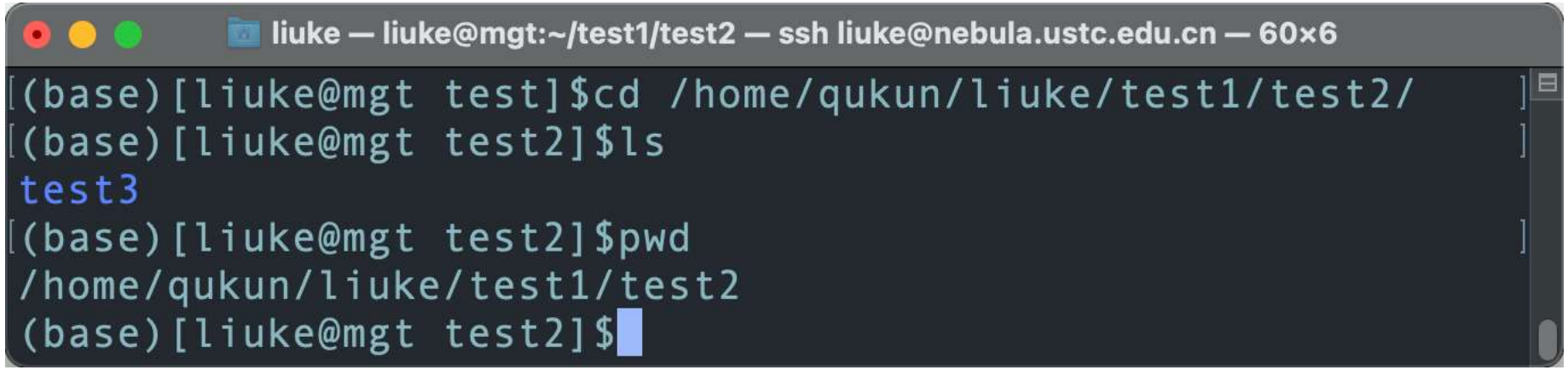
```
liuke — liuke@mgt:~ — ssh liuke@nebula.ustc.edu.cn — 60×6
(base)[liuke@mgt ~]$ls
miniconda3  ossutil64  recordings  software  workspace
ossutil     perl5      reference   used_pbs
(base)[liuke@mgt ~]$mkdir test
(base)[liuke@mgt ~]$mkdir -p test1/test2/test3
```

- 变换目录 cd

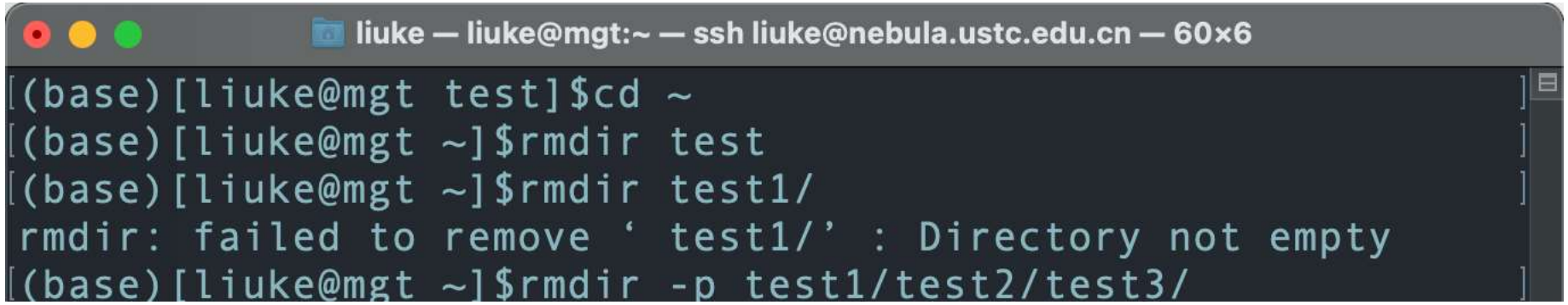
```
liuke — liuke@mgt:~/test — ssh liuke@nebula.ustc.edu.cn — 60×5
(base)[liuke@mgt ~]$cd /home/qukun/liuke/test1/test2/test3/
(base)[liuke@mgt test3]$cd ../../../test
```

➢ 文件及目录管理

- 查看绝对路径 pwd



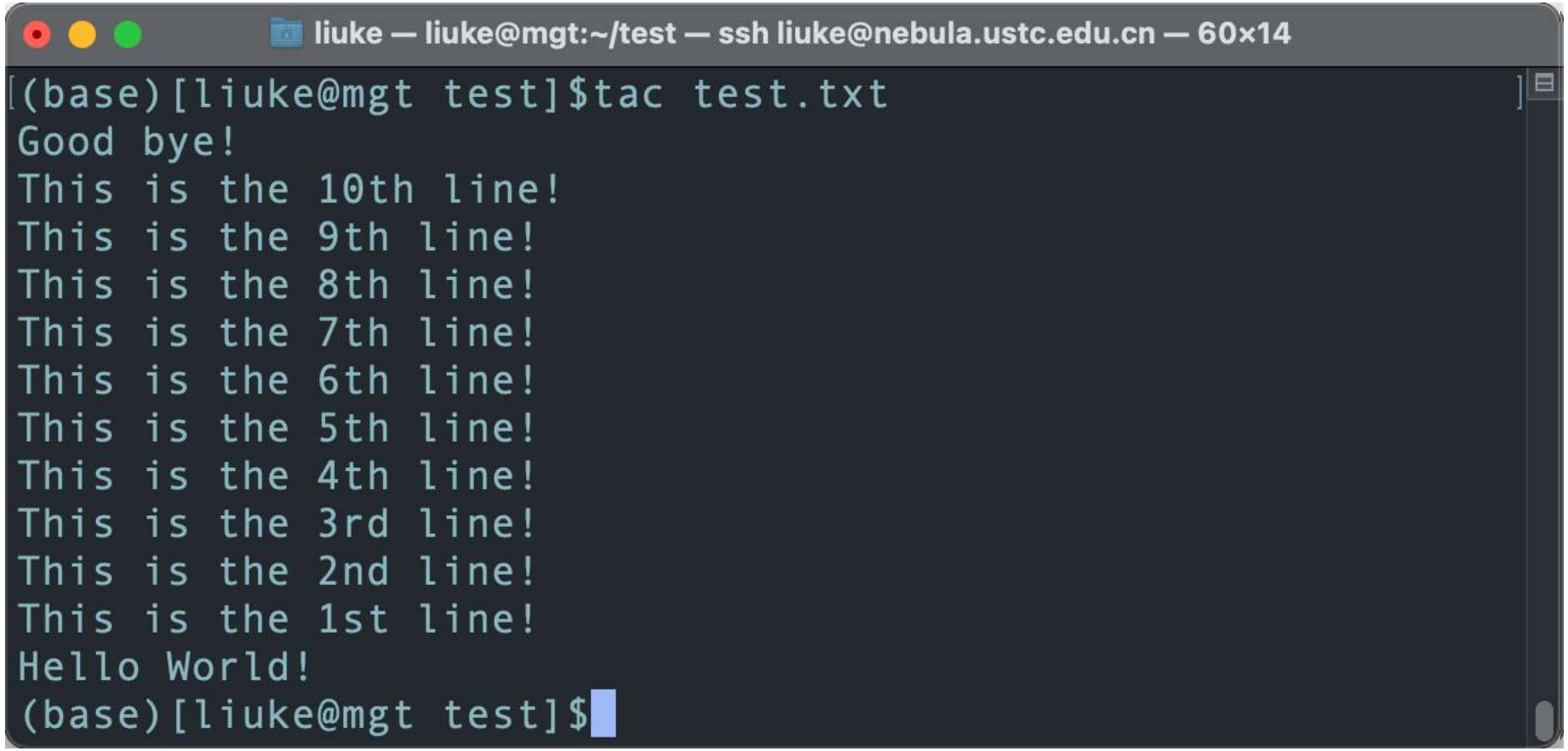
- 删除目录 rmdir



❖ 常用linux命令

➢ 文档查看及管理

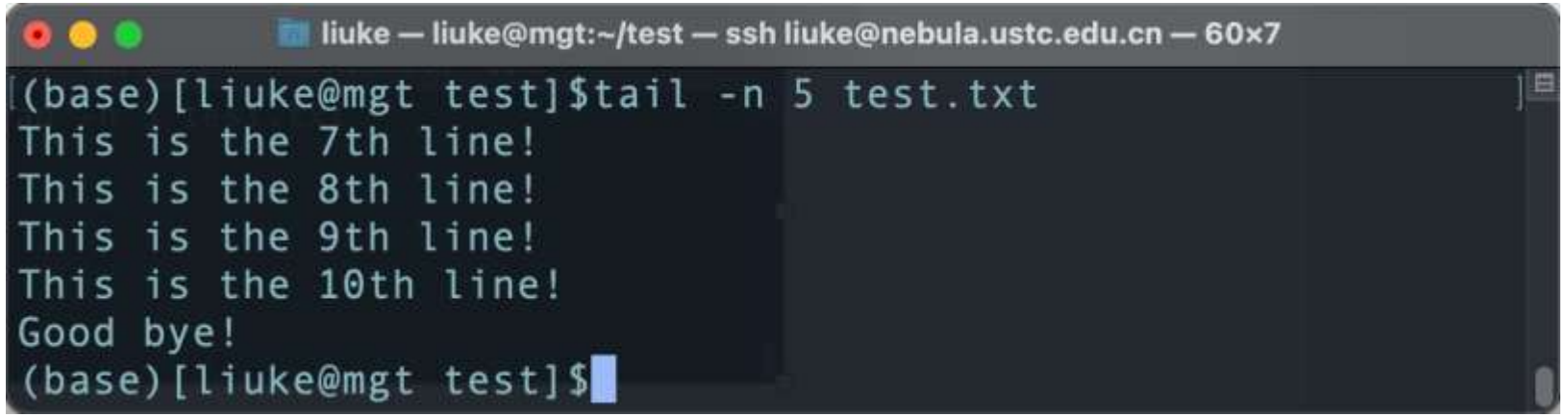
- cat和tac



➢ 文档查看及管理

- head

- tail



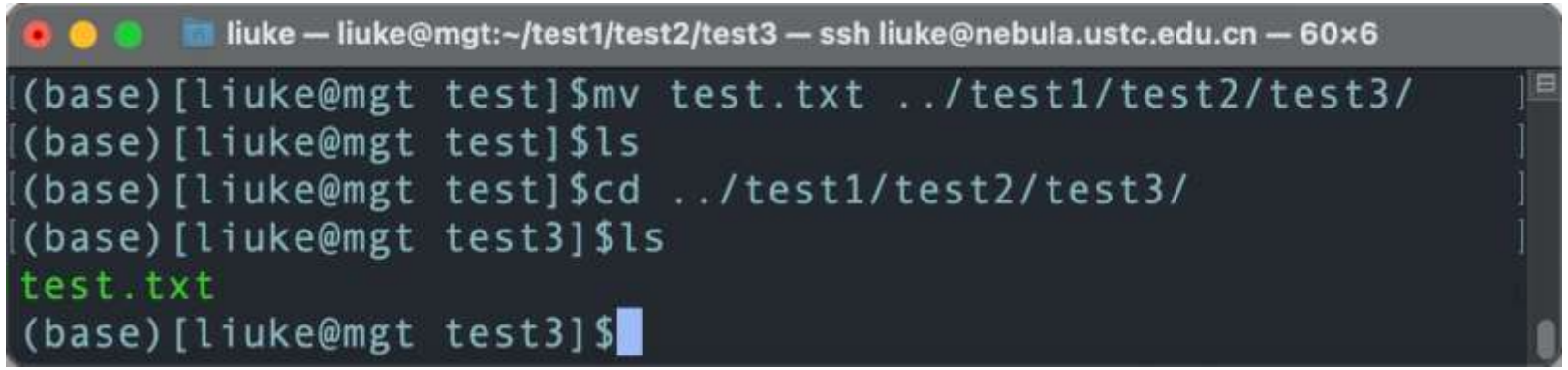
➢ 文档查看及管理

- more

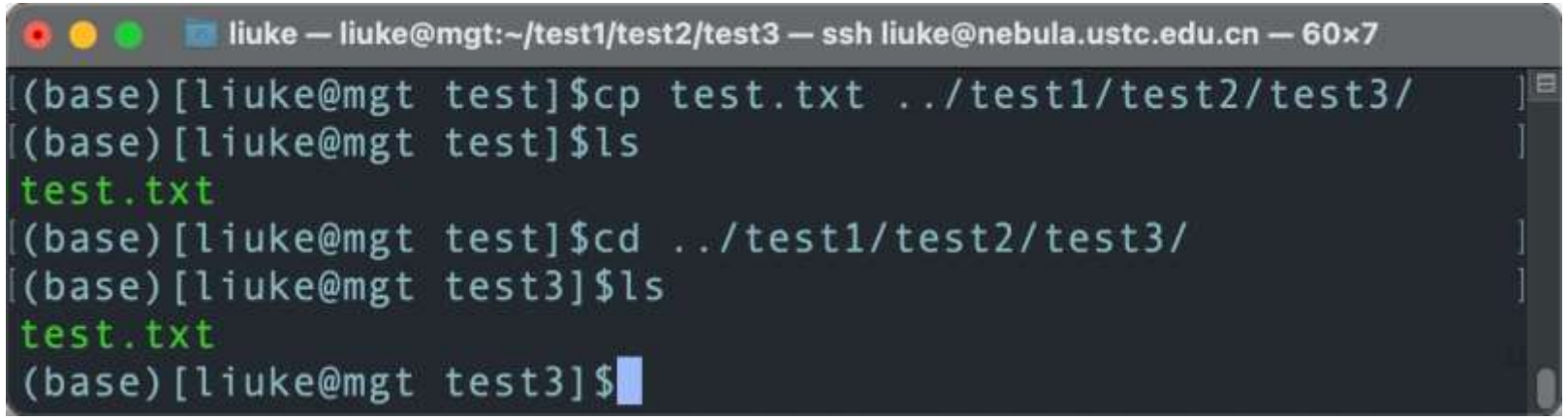
- less

➢ 文档查看及管理

- 移动mv

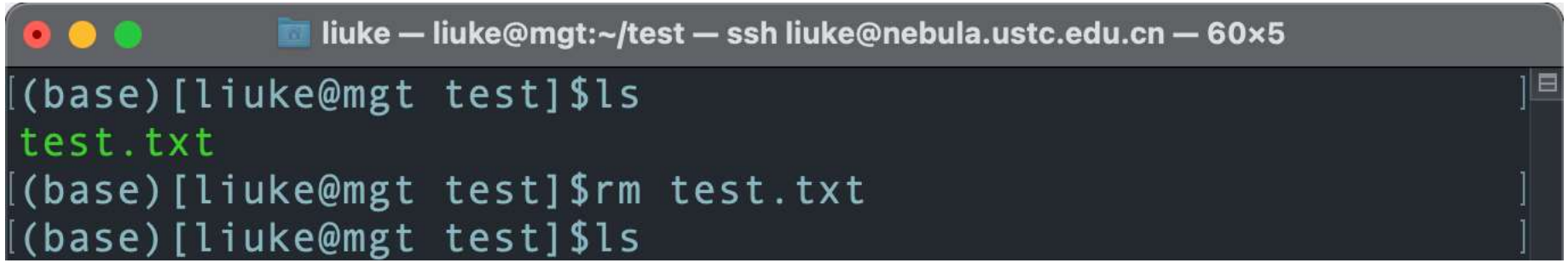


- 复制 cp



➢ 文档查看及管理

- 删除 rm



重要的事情说三遍：

慎用rm！！！！

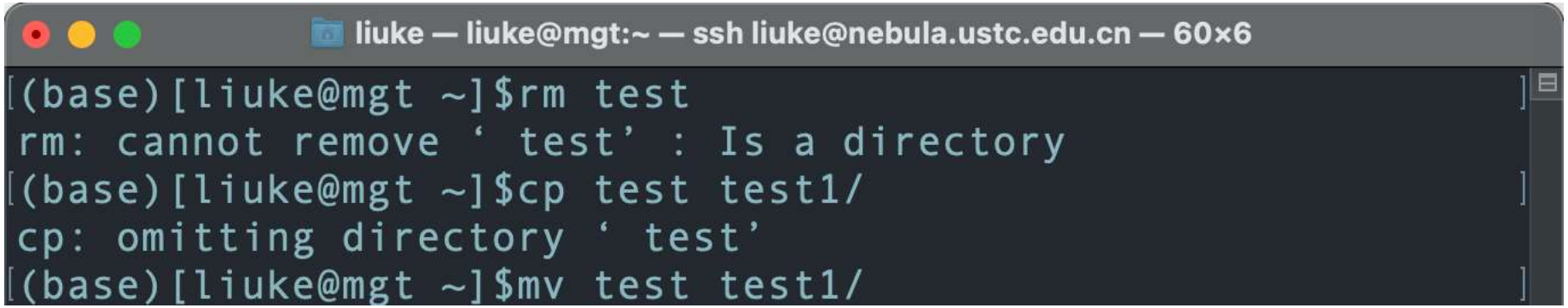
慎用rm！！！！

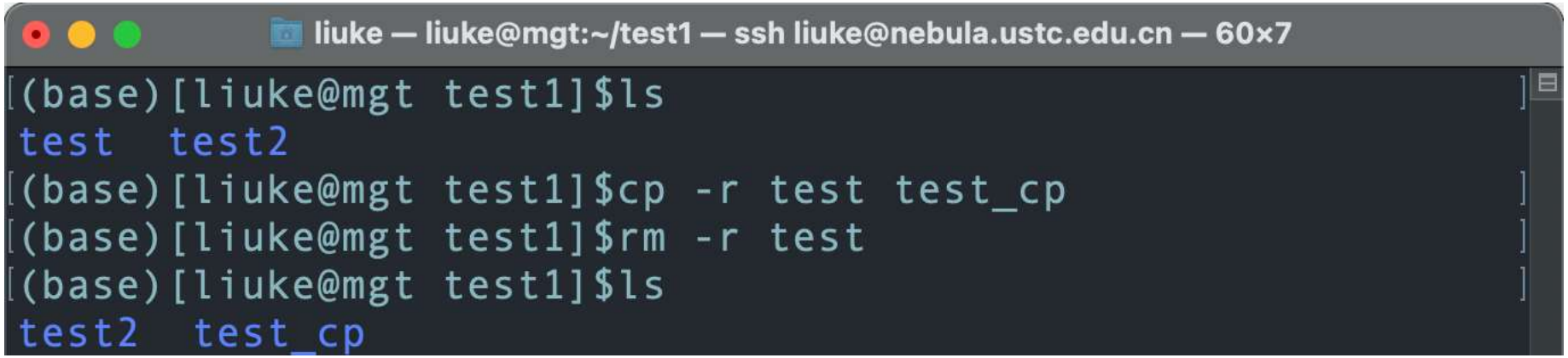
慎用rm！！！！

❖ 常用linux命令

➢ 文档查看及管理

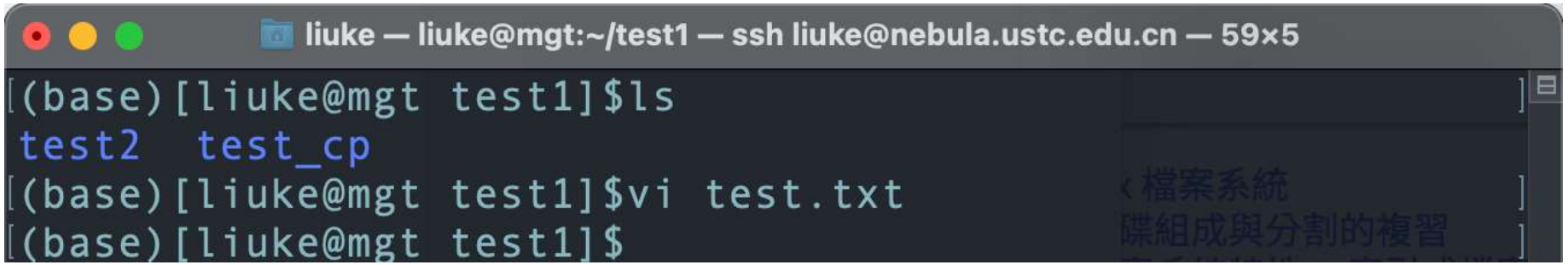
mv可以直接处理文件夹
cp和rm需要使用-r





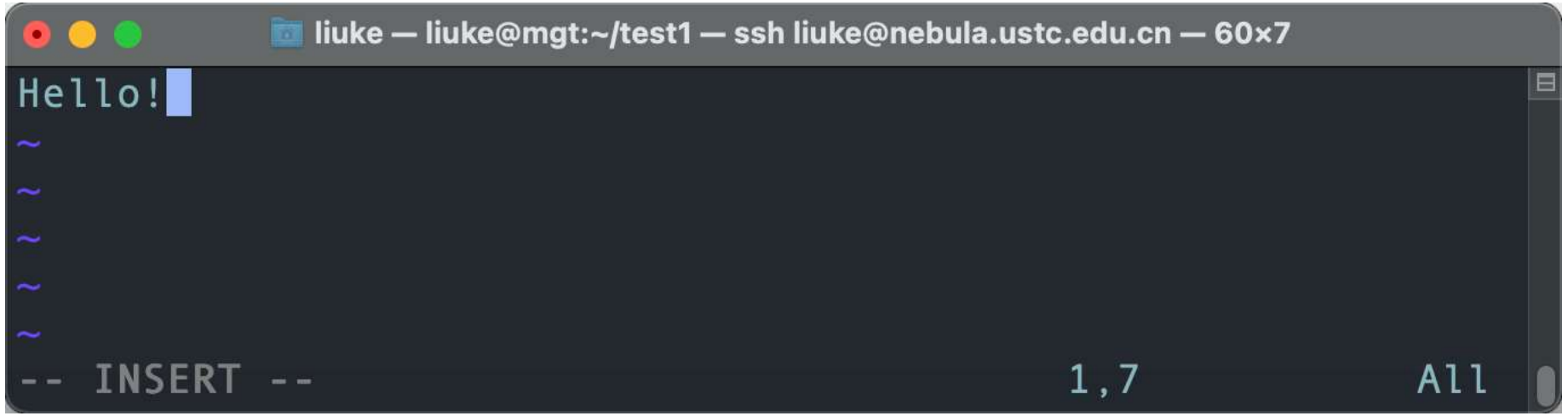
❖ 常用linux命令

➢ vim编辑器



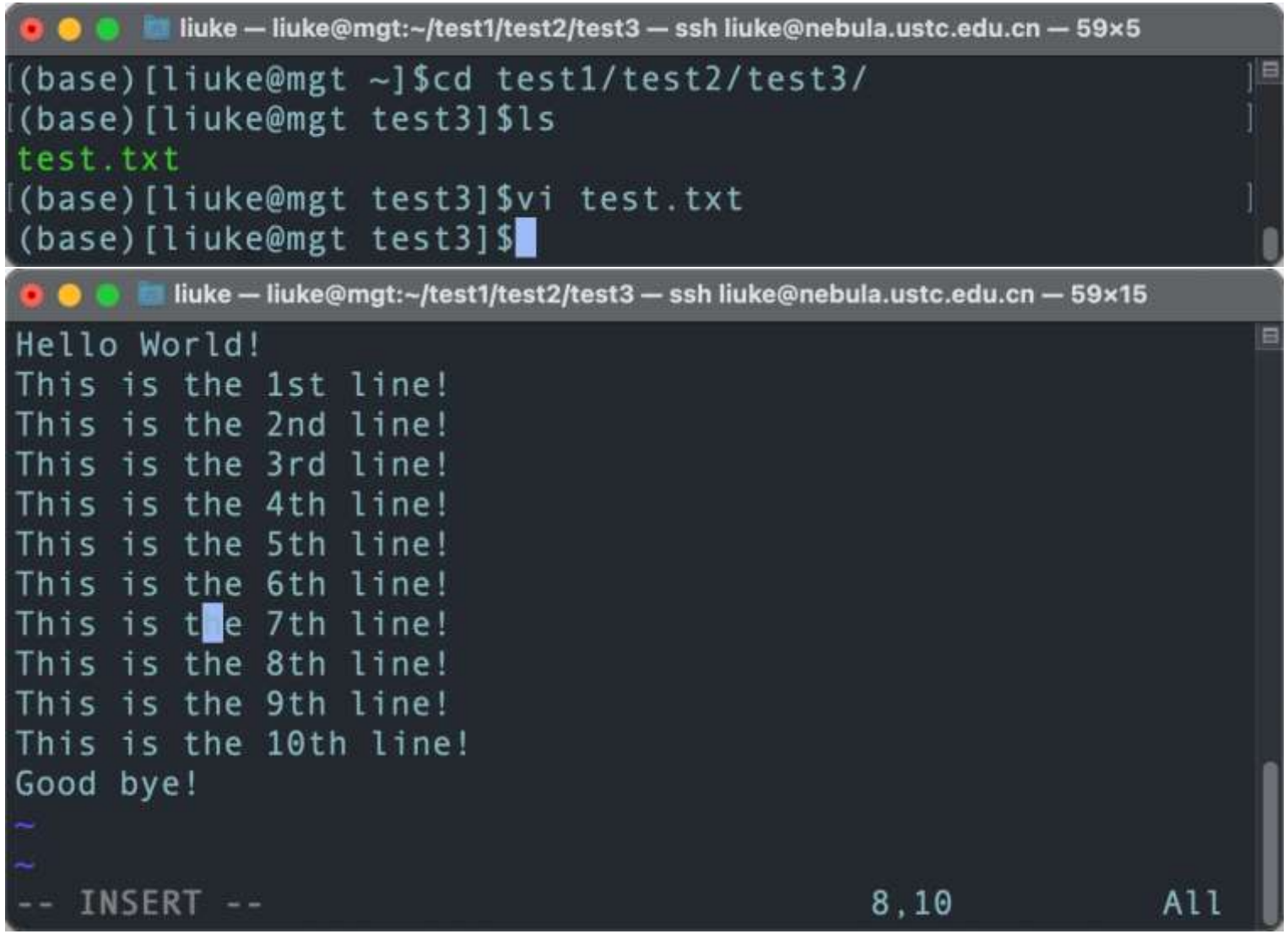
❖ 常用linux命令

➢ vim编辑器



❖ 常用linux命令

➢ vim编辑器



❖ PBS脚本

➢ PBS脚本的基本介绍

liuke — liuke@mgt:~/used_pbs/01_shell/00_jupyter — ssh liuke@nebula.ustc.edu.cn — 63×15

```
#!/bin/sh
#An example for serial job.
#DO NOT RUN THIS SCRIPT DIRECTLY,
#PLEASE RUN THIS SCRIPT WITH qsub: qsub serial_job.pbs
#
#PBS -N test                          任务名称
#PBS -o test.log                      任务输出文件
#PBS -e test.err                      任务错误文件
#PBS -q batch                         节点类型：fat，gpu，batch
#PBS -l walltime=360:00:00            任务时间：时：分：秒
#PBS -l nodes=comput10:ppn=20         节点及线程

echo Start time: `date`
cd /home/qukun/liuke
                                                    1,1           Top
```

➢ PBS脚本的基本介绍

- **pestat查看节点信息**

liuke — liuke@mgt:~/test1 — ssh liuke@nebula.ustc.edu.cn — 126×11

```
(base)[liuke@mgt test1]$pestat
   node         state  load     phymem   ncpus   allmem resi    usrs     tasks   jobidlist
   comput10     excl   8.42*    257679      28   321679 61617   37/7     28       12103675 lshouzhe2 12103424 liuke 12104753
richardo 12105087 migene 12105155 yanpingsun5
   comput11     free   24.08*   257679      28   321679 29214   7/5      8        12105072 cuiting 12105147 yanpingsun5 12105
178 ws174012
   comput12     free   0.02*    257679      28   321679 27442   15/4     26       12104899 ljy090609 12105090 pyh234 12105101
 hai_li
   comput13     busy*  41.61*   257679      28   321679 56166   11/5     23       12104823 migene 12104952 yexin0616 12104953
 yexin0616 12105076 ws174012
   comput14     free   10.27*   257679      28   321679 78662   24/8     25       12104264 zl0517 12104636 zfh 12104989 gchua
```

- **qstat –u <username>查看自己的任务**

liuke — liuke@mgt:~/test1 — ssh liuke@nebula.ustc.edu.cn — 126×11

```
(base)[liuke@mgt test1]$qsub test.pbs
12105184.mgt
(base)[liuke@mgt test1]$qstat -u liuke

mgt:
                                                                  Req'd    Req'd       Elap
Job ID                  Username    Queue           Jobname         SessID  NDS   TSK   Memory   Time    S   Time
----------------------- ----------- --------------- --------------- ------ ----- ------ ------ --------- - ---------
12103424.mgt            liuke       batch           lab1              1237     1     20    --   360:00:00 R 211:39:14
12105184.mgt            liuke       batch           test               --      1     20    --   360:00:00 Q       --
(base)[liuke@mgt test1]$
```

➢ PBS脚本的基本介绍

- showq查看排队信息

liuke — liuke@mgt:~/test1 — ssh liuke@nebula.ustc.edu.cn — 118×11

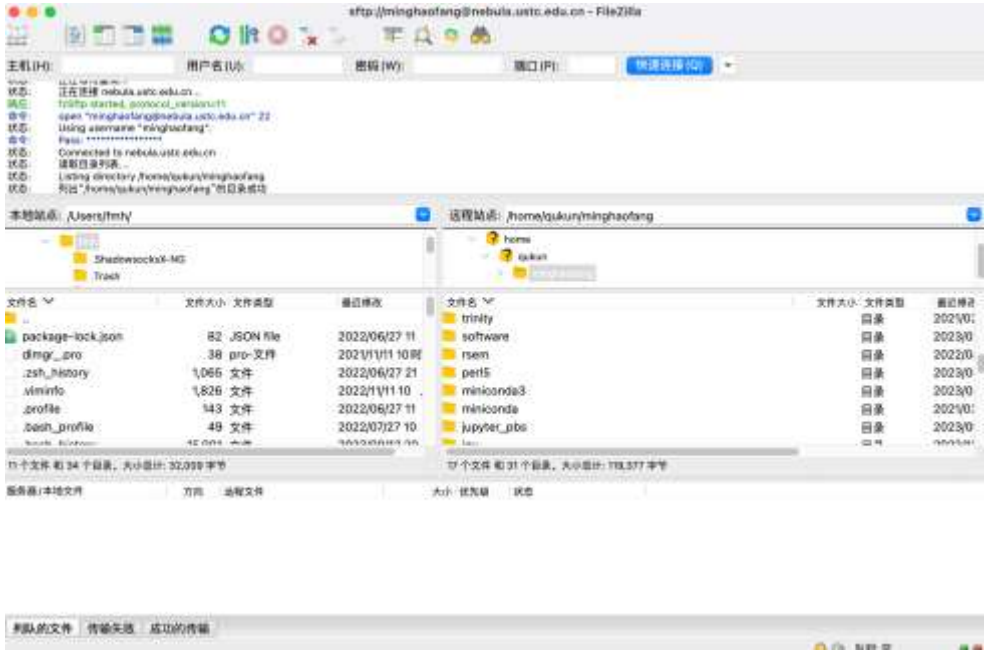
```
(base)[liuke@mgt test1]$showq
ACTIVE JOBS--------------------
JOBNAME            USERNAME      STATE  PROC   REMAINING            STARTTIME

12100798           lshouzhe2     Running     1   -INFINITY  Sat Aug 12 12:18:22
12102949              za666      Running     3    00:05:38  Sun Sep  3 17:01:40
12103980           hx120892214     Running     1    10:17:01  Sun Sep 10 19:13:03
12104018            dengwt9      Running    10    15:01:06  Sun Sep 10 23:57:08
12105059           yanpingsun523     Running     5    17:47:05  Sun Sep 17 22:43:07
12105144           ws174012      Running     1    21:58:15  Mon Sep 18 14:54:17
12103075            dengwt9      Running     4    22:45:43  Mon Sep  4 15:41:45
```

liuke — liuke@mgt:~/test1 — ssh liuke@nebula.ustc.edu.cn — 118×11

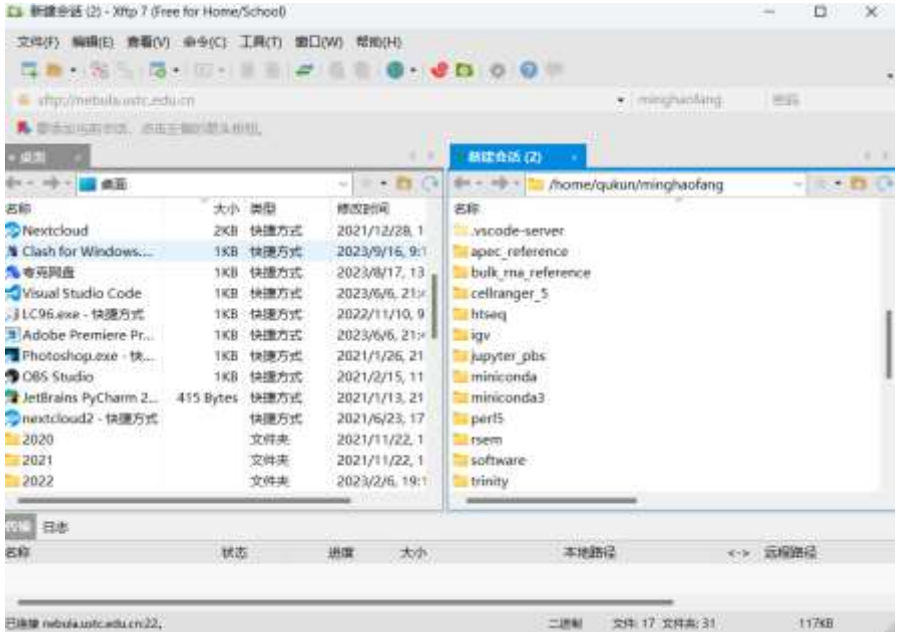
```
IDLE JOBS----------------------
JOBNAME            USERNAME      STATE  PROC     WCLIMIT            QUEUETIME

12105185           ws174012       Idle     8  3:00:00:00  Mon Sep 18 16:56:01
12105184              liuke       Idle    20 15:00:00:00  Mon Sep 18 16:52:22

2 Idle Jobs

BLOCKED JOBS-----------------
JOBNAME            USERNAME      STATE  PROC     WCLIMIT            QUEUETIME
```

❖ Linux 系统文件传输

FileZilla



XFTP



MAC

Windows

1.Top –u $user 命令查看进程和内存占用
2.禁止在登录节点直接运行程序(需通过pbs运行)
3.登录节点可以运行基本装包和访问文件等命令

目录

❖ Conda&Jupyter 安装(linux)

CSDN

环境配置

JupyterLab 配置远程python、R环境(与Jupyter兼容)

python pip修改安装镜像源

linux 环境下配置ftp服务器

linux 环境下安装和配置mysql数据库以及远程登录

linux 环境下配置python虚拟环境

windows环境下python 虚拟环境的创建和使用（virtualenvwrapper）

Linux环境下 安装python3

ANACONDA®

jupyter

https://blog.csdn.net/jeffery0207/article/details/103440598

❖ Conda&Jupyter 安装(linux)

Anaconda 个人版

Anaconda 个人版是一个免费、易于安装的包管理器、环境管理器和 Python 发行版，包含 1,500 多个开源包，并提供 免费社区支持。Anaconda 与平台无关，因此无论您在 Windows、macOS 还是 Linux 上都可以使用它。

查看Anaconda 个人版文档。

一、什么是Jupyter Notebook?

1. 简介

> Jupyter Notebook是基于网页的用于交互计算的应用程序。其可被应用于全过程计算：开发、文档编写、运行代码和展示结果。——Jupyter Notebook官方介绍

简而言之，Jupyter Notebook是以网页的形式打开，可以在网页页面中**直接编写代码**和**运行代码**，代码的**运行结果**也会直接在代码块下显示的程序。如在编程过程中需要编写说明文档，可在同一个页面中直接编写，便于作及时的说明和解释。

❖ Conda&Jupyter 安装(linux)

安装Anaconda

删繁就简就是我的个人原则，所以安装Anaconda, 我选择Miniconda, 它是Anaconda的最小化版本，只包含conda、python以及一些必须的包。进入Miniconda选择适合你的版本即可下载安装:

```
# 以下所有安装演示均在terminal中进行
$ wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
$ /bin/bash Miniconda3-latest-Linux-x86_64.sh  # 启动安装，接下来按照提示完成即可

Do you wish the installer to initialize Miniconda3
by running conda init? [yes|no]
[no] >>> no  # 建议不init，其他yes就好
```

接下来在`.bashrc`中添加环境变量，并加载环境变量:

```
echo 'export PATH="~/miniconda3/bin:$PATH"' >> ~/.bashrc
source ~/.bashrc

conda info --envs  # 测试以下conda
```

❖ Conda&Jupyter 安装(linux)

安装配置jupyter lab

它的安装很简单啦，官网列出了很多安装方式，但是以我的经验和踩坑经历，大多数的时候，尽量别在base环境下安装包，更加明智的选择是按照你的工作类型、项目创建不同的虚拟环境，以免一个环境被破坏，全盘奔溃。所以这里我们先创建一个虚拟环境，再进行各种包的安装以及环境配置。

```
1 conda create --name common python=3.6.8
2 source activate common
3 pip install jupyterlab # 推荐在conda中使用pip安装各种包
```

conda list　　查看对应环境所安装的包
conda env list　　查看已创建虚拟环境
conda activate $env_name　　激活特定虚拟环境

❖ Conda&Jupyter 安装(linux)

下面先生成密钥，然后再在 `~/.jupyter/jupyter_notebook_config.py` 中修改配置文件即可：

```
jupyter lab --generate-config  # 生成默认配置文件 ~/.jupyter/jupyter_notebook_c
ipython
# ------------------------------------------------
In [1]: from notebook.auth import passwd
In [2]: passwd()
Enter password:
Verify password:
Out[2]: 'sha1:c2d56265c773:e06ef2b97c94bbb014f65bd2975d43c7da12520e'
```

update logs (2021.01.07) ==> jupyterlab 3.0近期发布， 配置文件为: `jupyter_lab_config.py`

修改配置文件中的以下项：

```
c.NotebookApp.ip='*'
# c.NotebookApp.allow_remote_access = True
c.NotebookApp.password = u'sha1:c2d56265c773:e06ef2b97c94bbb014f65bd2975d43c
c.NotebookApp.open_browser = False
c.NotebookApp.port =8989 #可自行指定一个端口， 访问时使用该端口
```

update logs (2021.01.07) ==> jupyterlab 3.0近期发布， 配置文件中的信息有所改变， `c.NotebookApp.*` 变成了 `c.ServerApp.*`，另外，如安装jupyter插件可以设置 `c.ExtensionApp.open_browser = False`

❖ Conda&Jupyter 安装(linux)

远程连接jupyter lab

首先我们在远程服务器开启jupyter lab，下面代码中，`nohup`可以使代码进入后台运行，关于更多linux命令后台运行，请参考Linux 后台运行程序方法总结

```
source activate common
nohup jupyter lab &
```

然后在本地使用ssh和服务器建立连接，其中`-N`：SSH没有命令要被远程执行；`-f`：SSH在后台执行；`-L`：指定port forwarding的配置：

服务器

```
ssh -p port -N -f -L localhost:8989:localhost:8989 username@ip
```

最后在本地浏览器中访问：http://localhost:8989/lab 就可以啦

ssh –p 22 –N –f –L localhost:8989:wks1:8989 minghaofang@nebula.ustc.edu.cn

❖ Conda&Jupyter 安装(linux)

R语言

默认jupyter lab使用的应该是系统的R，我们一般使用自己虚拟环境中创建的R环境，这样不需要管理员权限就可以方便地管理自己的packages:

```
conda install r==3.6
which R
```

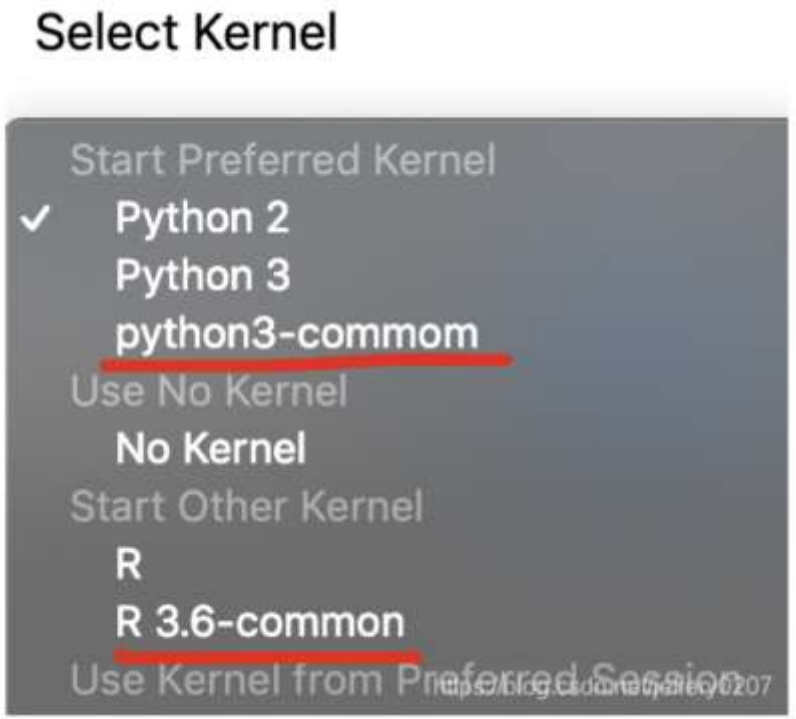
在R语言中安装相关package:

```
> install.packages("devtools")
> devtools::install_github('IRkernel/IRkernel')
> IRkernel::installspec(name = 'ir36-common', displayname = 'R 3.6-common')
[InstallKernelSpec] Installed kernelspec ir36-common in ~/.local/share/jupyt
```

Python

类似R语言，首先需要安装一个ipykernel，然后再安装一个kernel到`~/.local/share/jupyter/kernels`目录下，原理一模一样:

```
pip install ipykernel
python -m ipykernel install --user --name python3-commom
```



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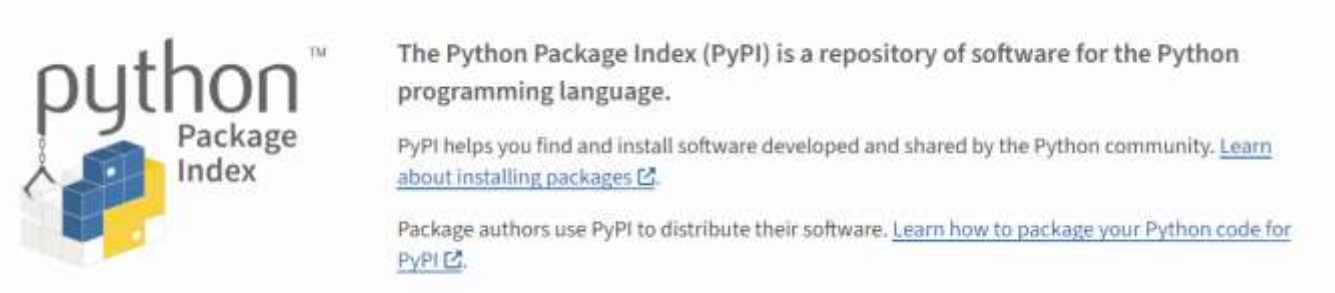
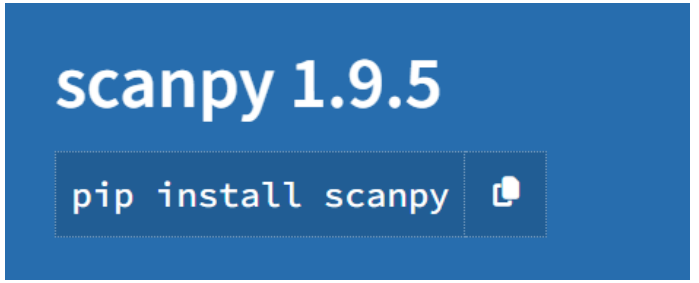
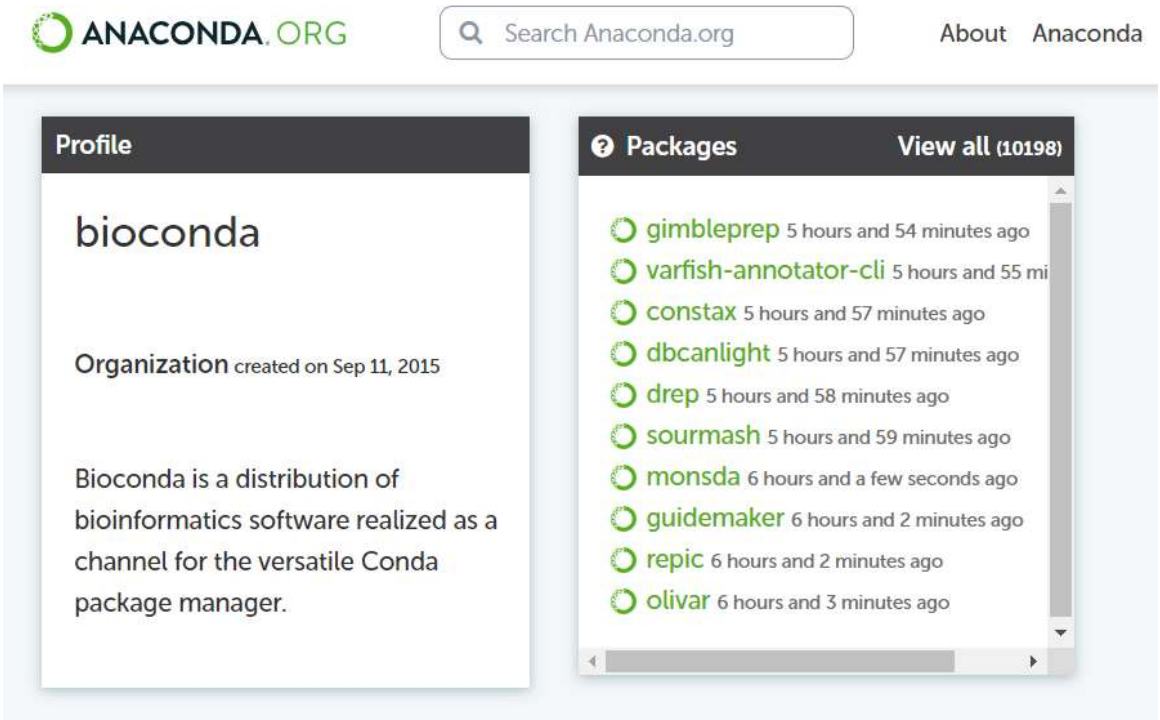
- ❖Linux 基本操作
- ❖Conda&Jupyter 安装(可视化分段编程)
- ❖简要环境安装

❖ 简要环境安装

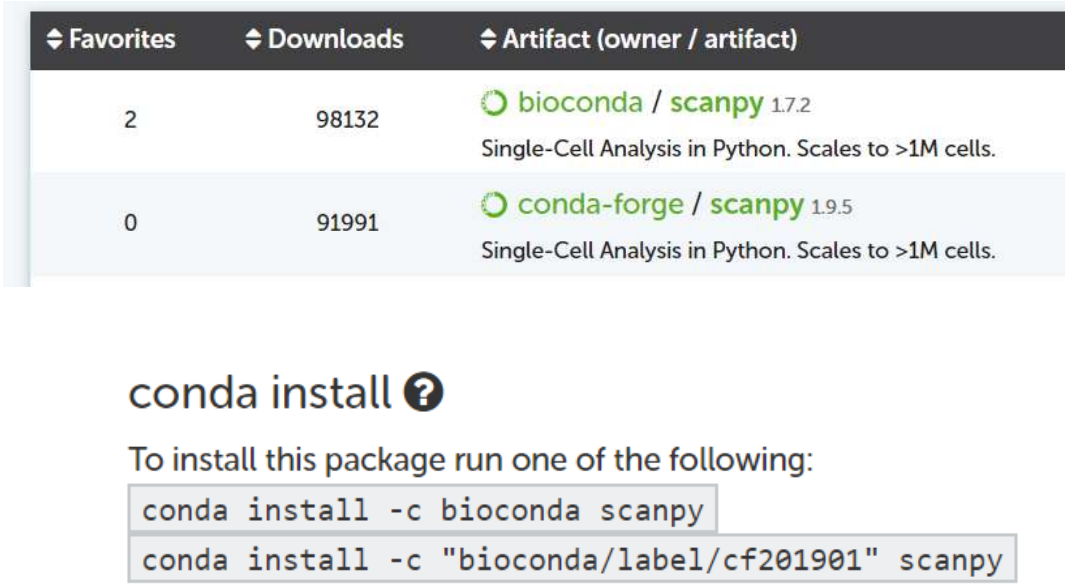


https://pypi.org/

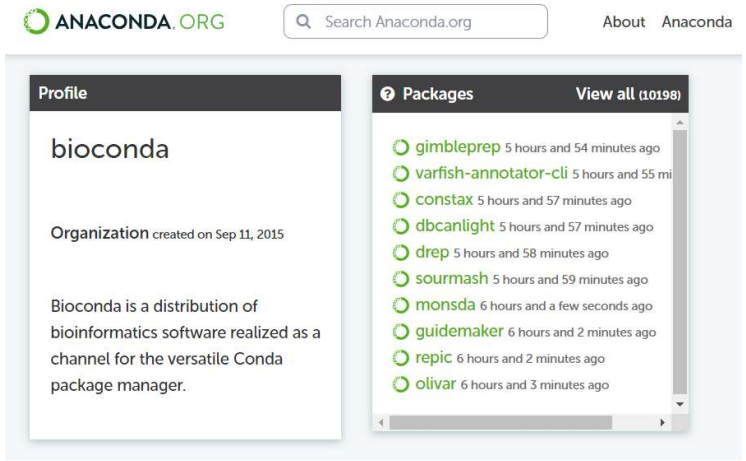




https://anaconda.org/bioconda/



❖ 简要环境安装



To install this package run one of the following:

```
conda install -c bioconda bioconductor-deseq2
conda install -c "bioconda/label/broken" bioconductor-deseq2
conda install -c "bioconda/label/cf201901" bioconductor-deseq2
conda install -c "bioconda/label/gcc7" bioconductor-deseq2
```

Bioconductor
OPEN SOURCE SOFTWARE FOR BIOINFORMATICS

https://bioconductor.org/

Installation

To install this package, start R (version "4.3") and enter:

```
if (!require("BiocManager", quietly = TRUE))
    install.packages("BiocManager")

BiocManager::install("DESeq2")
```

For older versions of R, please refer to the appropriate Bioconductor release.

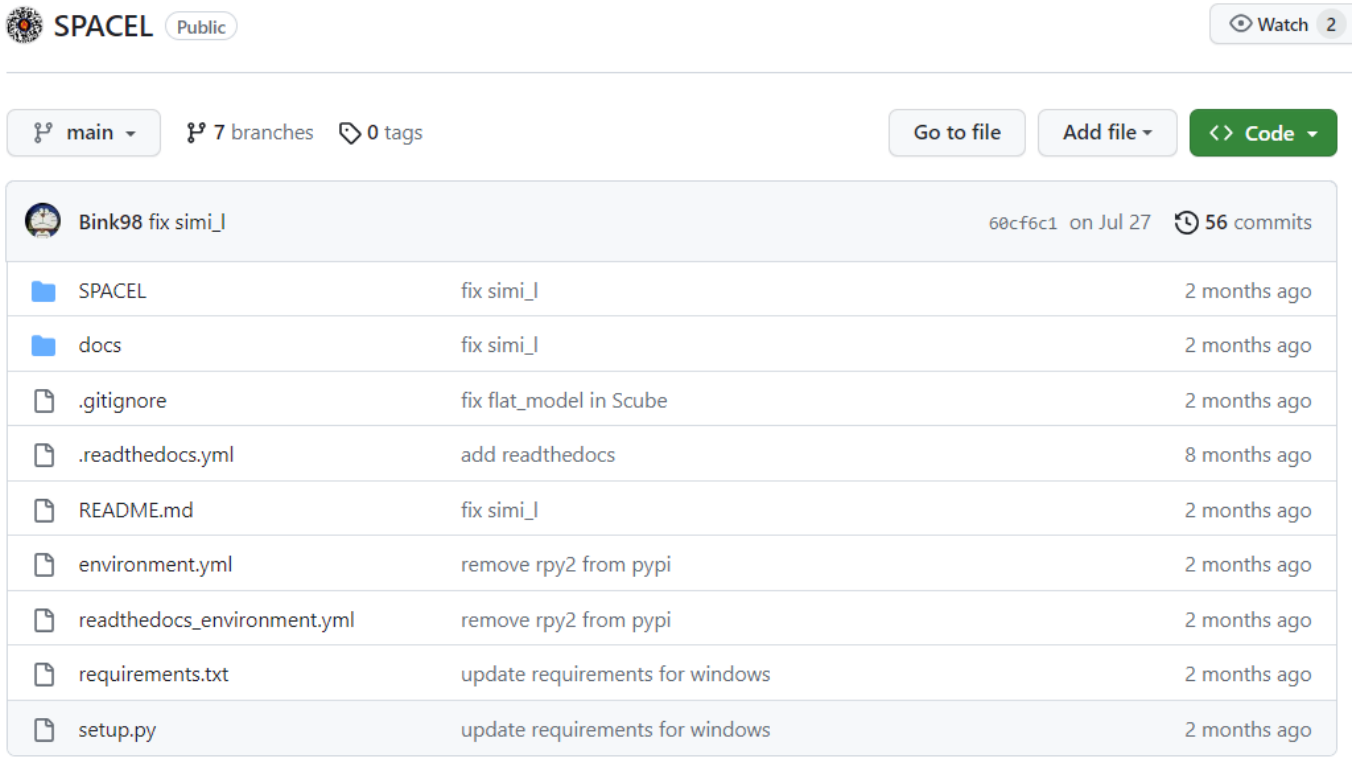
Documentation

To view documentation for the version of this package installed in your system, start R and enter:

```
browseVignettes("DESeq2")
```

HTML	R Script	Analyzing RNA-seq data with DESeq2
PDF		Reference Manual
Text		NEWS

❖ 简要环境安装



SPACEL Public

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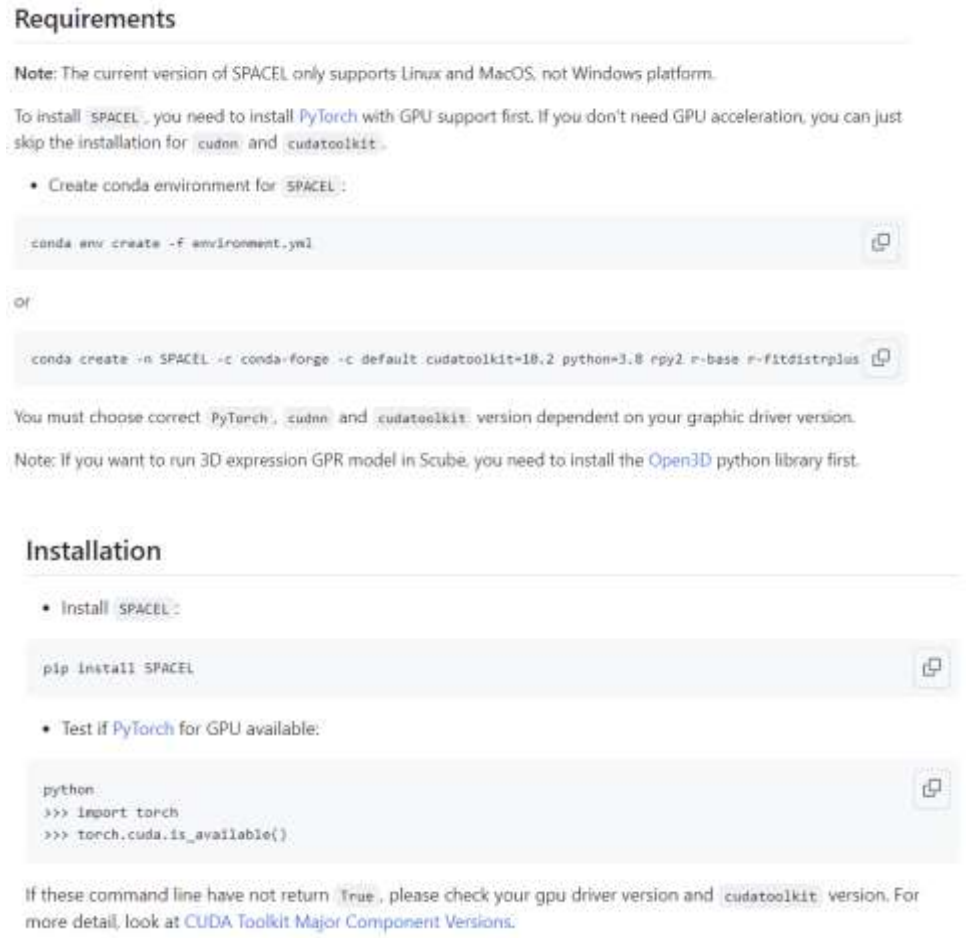
Bink98 fix simi_l — 60cf6c1 on Jul 27 — 56 commits

SPACEL	fix simi_l	2 months ago
docs	fix simi_l	2 months ago
.gitignore	fix flat_model in Scube	2 months ago
.readthedocs.yml	add readthedocs	8 months ago
README.md	fix simi_l	2 months ago
environment.yml	remove rpy2 from pypi	2 months ago
readthedocs_environment.yml	remove rpy2 from pypi	2 months ago
requirements.txt	update requirements for windows	2 months ago
setup.py	update requirements for windows	2 months ago

https://github.com/QuKunLab/SPACEL



Requirements

Note: The current version of SPACEL only supports Linux and MacOS, not Windows platform.

To install `SPACEL`, you need to install PyTorch with GPU support first. If you don't need GPU acceleration, you can just skip the installation for `cudnn` and `cudatoolkit`.

- Create conda environment for `SPACEL`:

```
conda env create -f environment.yml
```

or

```
conda create -n SPACEL -c conda-forge -c default cudatoolkit=10.2 python=3.8 rpy2 r-base r-fitdistrplus
```

You must choose correct `PyTorch`, `cudnn` and `cudatoolkit` version dependent on your graphic driver version.

Note: If you want to run 3D expression GPR model in Scube, you need to install the Open3D python library first.

Installation

- Install `SPACEL`:

```
pip install SPACEL
```

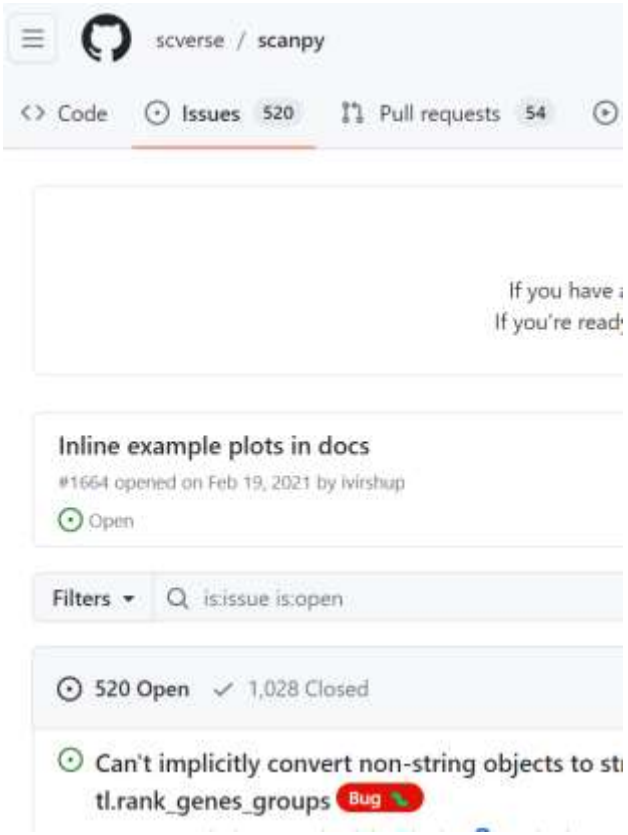
- Test if PyTorch for GPU available:

```
python
>>> import torch
>>> torch.cuda.is_available()
```

If these command line have not return `True`, please check your gpu driver version and `cudatoolkit` version. For more detail, look at CUDA Toolkit Major Component Versions.

❖ 简要环境安装


GitHub


scverse / scanpy
Code
Issues 520
Pull requests 54
If you have
If you're read
Inline example plots in docs
#1664 opened on Feb 19, 2021 by ivirshup
Open
Filters
is:issue is:open
520 Open
1,028 Closed
Can't implicitly convert non-string objects to st
tl.rank_genes_groups
Bug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