生物电镜平台电镜集群用户操作手册

- 一, 电镜集群用户计算资源配置
- 1, 管理/登录节点
 - ip: 10.15.56.103
 - 登录方法:

打开 terminal 终端软件, windows 电脑推荐使用 MobaXterm, mac 或 linux 电脑使用自带 terminal

- 通过云桌面登录: ssh 账号@10.15.56.103
- 通过校园网登录: ssh 账号@10.15.56.103-p 10086
- 注意事项:

管理节点上

- 允许:
 - 浏览/移动/拷贝/编辑 文件
 - 编辑作业脚本
 - 通过 Slurm 提交作业
 - 检查作业状态
- 不允许:
 - 运行作业
 - 多进程下载大量数据
- 2, 计算节点
 - CPU 节点: 80 个,

- 每节点两个 cpu,每节点含 28 个核
- 每 20 个节点分为一个队列,分别为 cpu-1, cpu-2, cpu-3, cpu-4
- GPU 节点: 8*4 卡 P100 节点 & 6*4 卡 P40 节点。
 - P100 卡的前 6 个节点为 GPU-A 队列,后两个节点分别为 cryosparc-1 与 cryosparc-2 队列。
 - P40 节点为 GPU-B 队列。
- FAT 节点: 一个,
 - 64 核,2TB 内存
 - 队列名 FAT

二, 修改账户密码的方法:

为了安全考虑,用户在集群上的账户在首次登陆之后应该及时修改密码,修改密码的方式:

■ 云桌面平台方式:

登录电镜平台云桌面,账户是默认的,密码是 Abc123!

进入云桌面系统后点击浏览器,并输入管理节点 ip: 10.15.56.103



点击 详细信息:



点击 继续转到网页,出现以下 CHESS 系统登录界面:

I CHESS	受录					
	名字	Usemame				
	密码	Password				
			爱爱	清除		
若这是你曾 书。	官次访问4	项,或者你访问	本页时见到词	书磬告,新	有限有此。中国	导入证

输入集群的用户账户以及密码,进入 chess 管理网页,在右上角账户下面选择修改密码,进行密码修改操作:



三, 用户提交作业方式

提交作业分为三种方式: CHESS 平台提交、终端文本提交、应用软件 UI 界面提交。首先无论以何种方式提交作业,应用软件必须先安装在集群 上。

下面针对三种方式进行详细描述:

■ CHESS 平台提交作业

1.1 使用云桌面打开浏览器,输入 https://10.15.56.103 进入登录页面, 输入账户名及密码

1.2 新建作业,点击"作业调度"—"作业"—"新建作业"

1.3 查看作业

1.4 删除作业

■终端文本提交

2.1 登录终端,使用 mobaxterm 选择 ssh 然后使用个人的账户登录集

群管理节点

2.2 编写提交脚本,脚本名称可以自定义,这里使用 1.slurm

脚本内容为:

#! /bin/basl	h	
#SBATCH	-J	test ###指定作业名称
#SBATCH	-p	GPU-A ### 指定队列名称
#SBATCH	-t	hh:mm:ss ### 指定本次作业运行的最大时长
#SBATCH	g	res=gpu:tesla:x ###指定使用 gpu 的个数,x 为数字
#SBATCH	-n	x ###指定使用的核数
#SBATCH	-N	x ###指定使用的节点数
#Command		
Mpirun -r	ר א	machinefile ./host.txt relion

2.3 提交作业

sbatch 1.slurm

输出信息为:

[reliontest@pre_mgmt01 ~]\$ sbatch 1 slurm Submitted batch job 134

2.4 查看作业,根据上面的输出查找对应的 jobID

squeue

2.5 查看作业详情

scontrol show job <job_id>

2.6 删除指定作业

scancel <job_id>

■应用软件 GUI 界面提交

需要根据软件特性做相应配置,具体见后面几种常用软件提交作业用 法。

四, relion 在集群中的使用方法

目前集群中安装的 relion 版本有: relion2.0, relion3.03, relion3.1-beta。

1, 登录集群,调用 relion 相应模块



2, 进入到数据所在的文件夹,调用 relion。注意:一定要 cd 到要计算的

数据所在文件夹后再调用 relion!

[test@mgmt01 ~]\$ ls
ncin.sh relion_benchmark slum.txt
<pre>[test@mgmt01 ~]\$ cd relion_benchmark/</pre>
<pre>[test@mgmt01 relion benchmark]\$ relion</pre>



- 3, 提交作业方法:
 - a) 实例一: 以其中一个 3D classification 任务为例,以下参数设置方法 是使用 GPU-A 队列中的两个节点,并且申请所有的八张 GPU 卡。

RELION-3.0.3: /home/test/r	elion_benchmark@mgmt01.chess	- 🗆 🗙
File Jobs Autorun	I/O Reference CTF Optimisation Sampling Helix Compute	Running
Import Motion correction CTF estimation Manual picking Auto-picking Particle extraction Particle extraction 2D classification 3D auto-refine 3D auto-refine 3D auto-refine 3D multi-body CTF refinement Bayesian polishing Mask creation Join star files Particle subtraction Post-processing	Use parallel disc I/O? [Yes Number of pooled particles: 100	
Local resolution Job actions Curren	Print command Sched	fule Continue!
Finished jobs 009: Class3D/job009/ 008: Class3D/job008/	Running jobs Input to this jobs 001: Class3D/job001/ Input to this jobs 003: Class3D/job003/ Input to this jobs 005: Class3D/job005/ Input to this jobs Scheduled jobs Output from to the set of the set o	b his job
TranslationalSampling= 1 Expectation iteration 25 of 1.03/1.03 min Maximization 49/ 49 sec GPU_A_node01.chess.203 GPU_A_node01.chess.203	VrTranslations= 84 25	

,		
le Jobs Autorun	I/O Reference CTF Optimisation Auto-sampling Helix Compute Running	RELION-3.0.3: /home/test/relion
Import Motion correction CTF estimation Manual picking Auto-picking Particle extraction Particle sorting Subset selection 2D classification 3D initial model 3D classification 8D auto-refine 3D multi-body CTF refinement Bayesian polishing Mask creation Join star files Particle subtraction Post-processing Local resolution	Number of MPI procs: 5 7 Number of threads: 6 7 Submit to queue? Yes 7 Queue name: GPU_A 7 Queue submit command: sbatch -N 1 7 Max number of hours in queue 72 7 slurm other command -gres=gpu:tesla:4 7 Standard submission script: 0_beta/bin/relion_template.sh 7 Minimum dedicated cores per node: 1 7 Additional arguments: 7	File Jobs Autorun Import Motion correction CTF estimation Manual picking Auto-picking Particle extraction Particle extraction Particle sorting Subset selection 2D classification 3D initial model 3D classification 3D auto-refine 3D multi-body CTF refinement Bayesian polishing Mask creation Join star files Particle subtraction Post-processing Local resolution
Job actions Current	iob: 151: Refine3D/job151/ Display:	Job actions Current jo
		Finished jobs 009: Class3D/job009/ 008: Class3D/job008/

TranslationalSampling= 1 NrT Expectation iteration 25 of 25 1.03/1.03 min Maximization ... 49/49 sec

GPU_A_node01.chess.20345P GPU_A_node01.chess.20346P GPU_A_node01.chess.20347P

关键参数:

Submit to queue? 一定要选 Yes, 如此该任务才会提交到计算节点上运

行,否则会在管理节点运行。

如果申请一个 GPU 节点,相应参数改为:

File Jobs Autorun	I/O Reference CTF Optimisation Sampling Helix Compute Running
Import Motion correction CTF estimation Manual picking Auto-picking Particle extraction Particle sorting Subset selection 2D classification 3D initial model 3D classification 3D auto-refine 3D multi-body CTF refinement Bayesian polisbing	Use parallel disc I/O? Yes ? Number of pooled particles: 3 ? Skip padding? No ? Pre-read all particles into RAM? No ? Copy particles to scratch directory: ? Combine iterations through disc? No ? Use GPU acceleration? Yes ? Which GPUs to use: 0:1:2:3 ?

b) 实例 2: 以 motion correction 任务为例,以下任务申请两个 GPU 节



五, cisTEM 在集群中的使用方法

■ 登陆 管理节点 10.15.56.103,并运行:

module load cistem

cisTEM

```
[lenovo.LAPTOP-GDLAE9T3] > ssh sunqq@10.15.56.103 -p 10086
Last login: Wed Jan 15 16:14:04 2020 from 10.20.70.161
[sunqq@mgmt01 ~]$ module load cistem
[sunqq@mgmt01 ~]$ cisTEM
```

之后打开已有 project 或者新建 project, 点击 左栏的 settings:

Project Help			
	Pun Profiles		
Overview	Default Local Add	Total Number of Processes : 25 Manager Command -	
-97	Rename	/home/software/cistem-1.0.0/\$command	
Assets	Remove		
	Duplicate	Controller Address : Automatic	Auto Specify Auto
Actions	Export	Command	No. Copies Launch Delay (ms)
æ ;;		/home/software/cistem-1.0.0/\$command	25 10
Results			
Settings			
		Add Edit Remove	Save

■ 在打开的 Gui 窗口里设置 settings:

1, 在左边窗口处点击 rename, 将当前 profile 名字改为 slurm-sbatch (也可选用其他名字)

2,点击右边窗口的 Specify 按钮,分别将 GUI Address 与 Controller Address 改为登陆节点 IP: 10.15.56.103

3,双击 Command 下面的蓝条,可以进入编辑命令状态

sisTEM - [cs286]@mgmt01.chess			- 0 ×
Project Help Overview Overview Assets Assets Actions Results Social S	Add Rename Remove Duplicate Import Export	Total Number of Processes : 4 Manager Command :- /home/software/cistem-1.0.0/\$command Gui Address : 10.15.56.103 Controller Address : 10.15.56.103 Command : sbatch n5 c 1 p cpu-2wrap==home/softwa sbatch No. Copies : 4 Delay (ms) : 100 OK Cancel	Auto Specify Auto Specify No. Copies Launch Delay (ms) 4 100
		Add Edit Remove	Save

编辑完命令,点击 OK, GUI 窗口内容此时如下:

💐 cisTEM - [cs286]@mgmt01.chess		×
Project Help			
	Run Profiles		
Overview	Image: Command :- Image: Command :-		
	Add	Manager Command :-	
	Rename	/home/software/cistem-1.0.0/\$command	
Assets	Remove		
	Duplicate	Gui Address : 10.15.56.103	Auto Specify
	Import	Controller Address : 10.15.56.103	Auto Specify
Actions			
(گ) ا	Export	Command sbatch n 5 c 1 p cpu-2wrap="home/software/cistem-1.0.0/\$command"	No. Copies Launch Delay (ms) 4 100
Results			
Č.			
Settings			
		Add Edit Remove	Save

4,此时点击右下角 save 保存。切记一定要保存,尤其首次使用 cisTEM 时, 否则就会在管理节点上跑任务。

后续每次调整该提交命令中的参数之后都需点击 save。

● 提交作业命令示例 1:

sbatch –n 5 –c 1 –p cpu-2 --wrap="home/software/cistem-1.0.0/\$command"

No copies 为 4

命令含义: 5个任务,每个任务使用 1 个核,在 cpu-2 队列上执行。 并复制 4 个提交命令,也即产生 4 个作业,有 4 个不同的 jobid。

使用如下命令可以查看队列 cpu-2 上的使用核的情况 sinfo --format="%12P %.10n %.5T %.14C" |grep 'cpu-2' 显示:

CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2 CPU_2	CPU_nodel1 CPU_nodel2 CPU_nodel3 CPU_nodel3 CPU_nodel5 CPU_nodel6 CPU_nodel7 CPU_node19 CPU_node19 CPU_node21	Info1 mixed idle idle idle idle idle idle idle id	Ormat="%12P %.10n 20/8/0/28 0/28/0/28 0/28/0/28 0/28/0/28 0/28/0/28 0/28/0/28 0/28/0/28 0/28/0/28 0/28/0/28 0/28/0/28 0/28/0/28	\$.5T \$.14C* grep) 'СРU_2' Т
--	--	--	--	--------------------	----------------

● 提交作业命令 多节点示例 2:

将提交作业的命令改为

sbatch -n 5 -c 2 -p cpu-2 --wrap="home/software/cistem-1.0.0/\$command"

No copies 为 4

命令含义: 5个任务, 每个任务使用 2个核, 在队列 cpu-2 上执行。

产生四个 jobid

每个作业使用 10 个核。4 个作业使用 40 个核,因为每个节点 28 个核,所 以提交任务后 squeue 显示分配 2 节点。

同样使用命令查看 cpu-2 上的使用核的情况

sinfo --format="%12P %.10n %.5T %.14C" |grep 'cpu-2'

显示:

CPU_2	CPU nodell mixed	20/8/0/20 *.101 %.51 %.14C " grep 'CPU_2'
CPU_2	CPU_node12 mixed	20/8/0/28
CPU_2	CPU_nodel3 idle	0/28/0/28
CPU_2	CPU_node14 idle	0/28/0/28
CPU_2	CPU_node15 idle	0/28/0/28
CPU_2	CPU_node16 idle	0/28/0/28
CPU_2	CPU_node17 idle	0/28/0/28
CPU_2	CPU_node18 idle	0/28/0/28
CPU_2	CPU_node19 idle	0/28/0/28
CPU_2	CPU_node20_ idle	0/28/0/28

六, cryoSPARC 在集群中的使用方法

目前集群中有专门的两个节点 gpu-a-node07.chess 与 gpu-a-node08.chess 分别作为队列 cryosparc-1 与 cryosparc-2 运行用户的 cryoSPARC 作业。

使用 cryoSPARC 前,用户需要先向集群管理员申请账号,并向管理员说 明处理数据所在位置,由管理员修改文件夹权限,增加 cryoSPARC 管理员读 写权限。

₩ Log In cryoSPARC v2 × +		- 🗆 ×
← → C ① 不安全 10.15.56.106:39000/login?redirect	t=%2F	☆ ⊶ \varTheta :
	cryoSPARC v2 R Email Password Forgat password	

1, 使用浏览器(推荐 google chrome)登录 10.15.56.106: 39000

使用申请到的账号密码登录之后,显示如下:

CryoSPARC Projects Workspaces Image: CryoSPARC Statistics Charge Log This week This month Total Projects 2 38 Image: CryoSPARC Image: CryoSPARC Vorkspaces 5 13 79 Jobs 243 611 2929 Completed 9.1 c.o. 796 Jobs 2.1 0.00 Defence: Vorkspaces 5 13 79 Jobs 2.1 c.o. 796 Jobs 2.1 c.o. 796 Jobs 2.1 c.o. 796 Jobs 2.1 c.o. 796 Jobs Defence: Defence: Dornalition relations and substration of the proving the	豢 Dashboard cryoSPARC	v2 × +				- • ×
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This week This month Total Projects 2 38 Workspaces 5 13 79 Jobs 243 611 2929 Completed 241 603 2767 Delight of the point of the	Statistics				Links	DETAILS 38 79 2929 Projects Workspaces Jobs
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2,点击 Projects-Add

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 ← → C ▲ 不安全 10.15.56.1 ☆ cryoSPARC ● Projects P5 11 Created 4 months ago 	106-39000/projects	Add Import New Project Trite test Directory in which to create new pr Proses select a project directory that Select a location where the project directory c should be readable and writable. Description	Oldisi1	RECENT PROJECTS
🕜 Dashboard 👼 Projects 🕴	Resource Manager	lew update available: v2.14.2		👤 liuyh2

新建 project。

3 提交作业

		- o ×
← → C ▲ 不安全 10.15.56.106:39000/projects/P51		☆ or 🕒 :
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		D Raw pixel size (A) :
	Cancel	
		D Accelerating Voltage (kV) :
		D Spherical Abberation (mm) :
		D Total exposure dose (e/A*2) :
		NONE
	Clearing intermediate results for all jobs in P25 ×	Cancel Queue
Dashboard Projects H Resource Manager	New update available: v2.14.2	👤 liuyh2

目前集群有两个单节点队列作为 cryoSPARC 专门队列,提交作业时点击右下 角的 queue 按钮,出现选择队列的对话框,用户可以根据队列的忙闲程度 选择,之后点击 Create 按钮。