

CentOS安装Materials studio

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安装yum源（如果yum源失效）

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2. 备份原文件
- 3.安装镜像库
- 4.清除缓存，载入新缓存

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设置自启动

安装yum源（如果yum源失效）

参考方法：【CentOS 7安装配置阿里云yum源】https://www.bilibili.com/video/BV1euMseUEZa/?share_source=copy_web&vd_source=d4a284ec36521608a5ed2b50d95a867c

1.使用root切换到指定文件

```
1 | cd /etc/yum.repos.d
```

2. 备份原文件

```
1 | mkdir yum.repos.d.backup
2 | mv *.repo yum.repos.d.backup/
```

3.安装镜像库

```
1 | curl -o /etc/yum.repos.d/CentOS-Base.repo
    http://mirrors.aliyun.com/repo/Centos-7.repo
```

4.清除缓存，载入新缓存

```
1 yum clean all
2 yum makecache
```

安装依赖库

安装依赖库方法：

```
1 yum install -y glibc* compat* libgcc* libstdc* redhatcsh* gcc gcc-c++ gcc-
  gfortran
```

安装依赖库需要root权限

关闭防火墙和SELINUX

```
1 systemctl disable firewalld
2 systemctl stop firewalld
3 sed -i 's/^SELINUX=.*$/SELINUX=disabled/' /etc/selinux/config
4 setenforce 0
```

上传安装包和许可文件

拖拽上传即可，不需要 root权限

安装过程不需要root

解压

退出root.快捷键ctrl+d

切换到安装包文件夹之后解压文件

```
1 [stuHc@node01 MaterialsStudio2020]$ tar -xvf MS2020.tar
```

更改破解文件

解压完成之后输入代码破解文件

```
1 [stuHc@node01 MaterialsStudio2020]$ chmod 777 -R MaterialsStudio2020/
```

运行解压文件中install文件进行安装

切换目录

```
1 [stuHc@node01 ms2020]$ cd MaterialsStudio2020/
```

运行文件：

```
1 | [stuHc@node01 MaterialsStudio2020]$ ./install
```

安装过程中一路全部默认，一直按回车即可

```
Copying 709 files to /home/stuHc/BIOVIA/BIOVIA_LicensePack/
Copying 1 files to /home/stuHc/BIOVIA/BIOVIA_LicensePack/
Completed installing License Pack 2020 at /home/stuHc/BIOVIA/BIOVIA_LicensePack/
Check log file [ /home/stuHc/BIOVIA/BIOVIA_LicensePack/Logs/Installer.log ] for more information.
Installation Complete.
Running installation ...
```

出现上面内容代表文件正在安装，注意，不推荐使用Root用户安装。

出现以下面内容代表安装成功，选择99退出安装

```
It works! ...

This is the simple cgi test output ...
Test succeeded, it appears!

1) Enter temporary license password
2) Set connection to license server
3) List command line license administration tools
99) Finished with license configuration

Choose one of the above options: 99
Exiting program
```

查看网关号码，安装过程中会弹出网关号

```
>>>[0]
Copying 709 files to /home/stuHc/BIOVIA/BIOVIA_LicensePack
Copying 1 files to /home/stuHc/BIOVIA/BIOVIA_LicensePack/Logs/Installer.log
Completed installing License Pack 2020 at /home/stuHc/BIOVIA/BIOVIA_LicensePack
Check log file [ /home/stuHc/BIOVIA/BIOVIA_LicensePack/Logs/Installer.log ] for more information.
Installation Complete.
Running installation ...
Running ConfigureMaterialsStudio.pl
Gateway configuration...
Port 18888 appears to be available right now...
Starting gateway at:
http://node01:18888/
/home/stuHc/BIOVIA/MaterialsStudio20.1/etc/Gateway/root_default/httpd/bin/apachectl start: httpd started
Gateway start succeeded - running as process 260311.
Testing gateway installation for script u/dsd_test.pl
Running GET for url http://node01:18888/dsd/commands/u/dsd_test.pl

It works! ...

This is the simple cgi test output ...
Test succeeded, it appears!
```

记住这个网管号码“18888”，一般情况下默认即是18888

修改许可文件

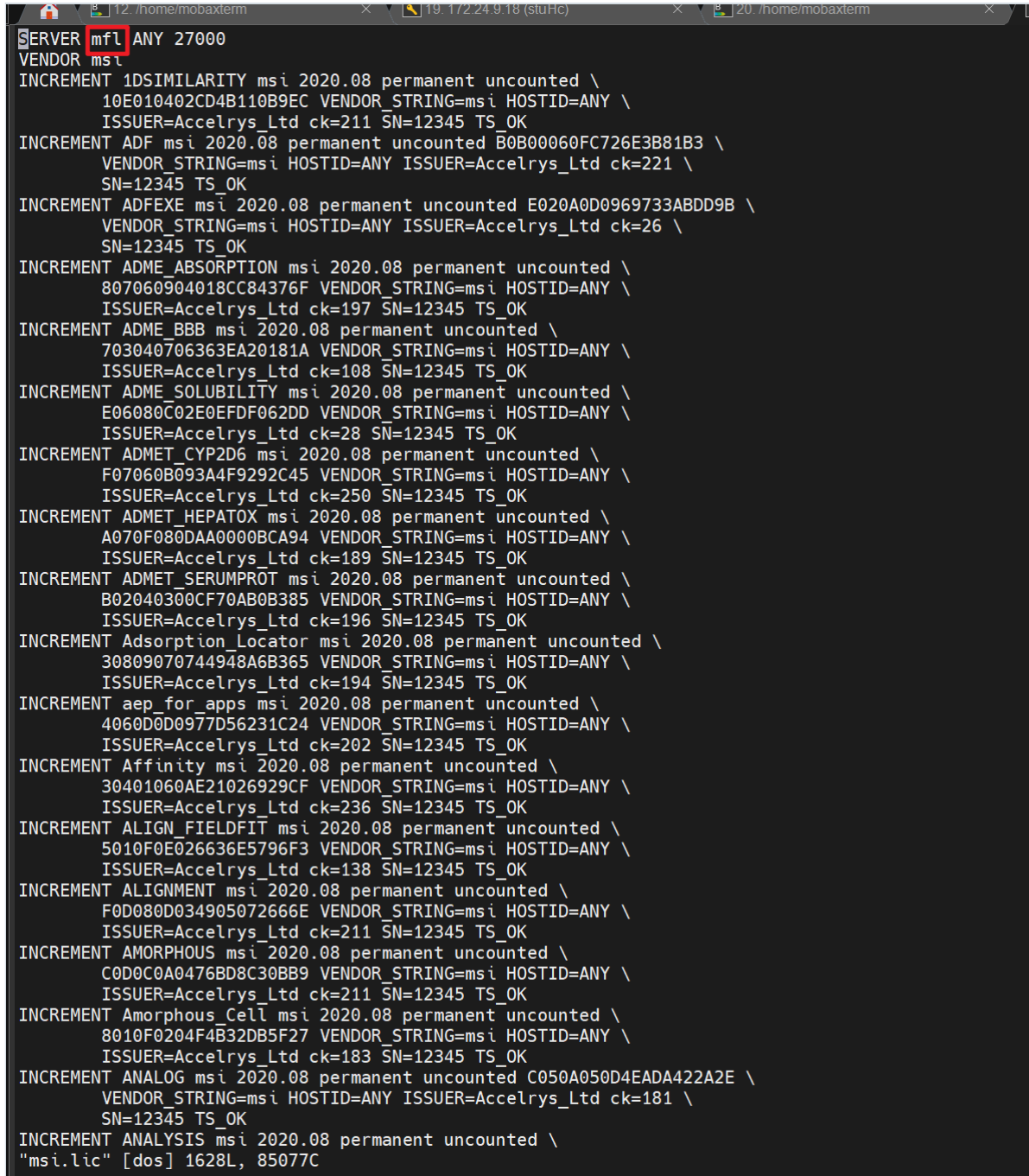
1.查看主机名称

```
1 | [stuHc@node01 MaterialsStudio2020]$ hostname
```

2.修改上传的文件

```
1 %切换到上一级文件
2 [stuHc@node01 MaterialsStudio2020]$ cd ..
3 %编辑msi.lic
4 [stuHc@node01 ms2020]$ vim msi.lic
```

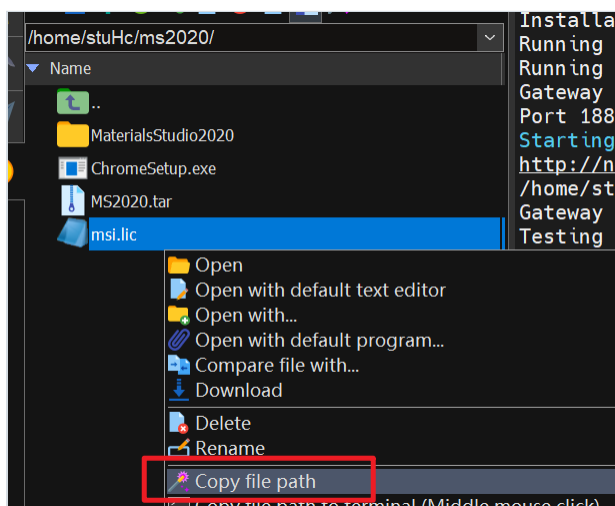
打开之后按i进入编辑模式，将下图中红框位置切换为刚刚查到的hostname。修改完成之后按Esc退出编辑模式，再按shift+;, 输入wq保存并推出。



```
SERVER mfl ANY 27000
VENDOR msi
INCREMENT 1DSIMILARITY msi 2020.08 permanent uncoun ted \
    10E010402CD4B110B9EC VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=211 SN=12345 TS_OK
INCREMENT ADF msi 2020.08 permanent uncoun ted B0B00060FC726E3B81B3 \
    VENDOR_STRING=msi HOSTID=ANY ISSUER=Accelrys_Ltd ck=221 \
    SN=12345 TS_OK
INCREMENT ADFEXE msi 2020.08 permanent uncoun ted E020A0D0969733ABDD9B \
    VENDOR_STRING=msi HOSTID=ANY ISSUER=Accelrys_Ltd ck=26 \
    SN=12345 TS_OK
INCREMENT ADME_ABSORPTION msi 2020.08 permanent uncoun ted \
    807060904018CC84376F VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=197 SN=12345 TS_OK
INCREMENT ADME_BBB msi 2020.08 permanent uncoun ted \
    703040706363EA20181A VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=108 SN=12345 TS_OK
INCREMENT ADME_SOLUBILITY msi 2020.08 permanent uncoun ted \
    E06080C02E0EFD062DD VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=28 SN=12345 TS_OK
INCREMENT ADMET_CYP2D6 msi 2020.08 permanent uncoun ted \
    F07060B093A4F9292C45 VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=250 SN=12345 TS_OK
INCREMENT ADMET_HEPATOX msi 2020.08 permanent uncoun ted \
    A070F080DAA0000BCA94 VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=189 SN=12345 TS_OK
INCREMENT ADMET_SERUMPROT msi 2020.08 permanent uncoun ted \
    B02040300CF70AB0B385 VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=196 SN=12345 TS_OK
INCREMENT Adsorption_Locator msi 2020.08 permanent uncoun ted \
    30809070744948A6B365 VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=194 SN=12345 TS_OK
INCREMENT aep_for_apps msi 2020.08 permanent uncoun ted \
    4060D0D0977D56231C24 VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=202 SN=12345 TS_OK
INCREMENT Affinity msi 2020.08 permanent uncoun ted \
    30401060AE21026929CF VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=236 SN=12345 TS_OK
INCREMENT ALIGN_FIELDFIT msi 2020.08 permanent uncoun ted \
    5010F0E026636E5796F3 VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=138 SN=12345 TS_OK
INCREMENT ALIGNMENT msi 2020.08 permanent uncoun ted \
    F0D080D034905072666E VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=211 SN=12345 TS_OK
INCREMENT AMORPHOUS msi 2020.08 permanent uncoun ted \
    C0D0C0A0476BD8C30BB9 VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=211 SN=12345 TS_OK
INCREMENT Amorphous_Cell msi 2020.08 permanent uncoun ted \
    8010F0204F4B32DB5F27 VENDOR_STRING=msi HOSTID=ANY \
    ISSUER=Accelrys_Ltd ck=183 SN=12345 TS_OK
INCREMENT ANALOG msi 2020.08 permanent uncoun ted C050A050D4EADA422A2E \
    VENDOR_STRING=msi HOSTID=ANY ISSUER=Accelrys_Ltd ck=181 \
    SN=12345 TS_OK
INCREMENT ANALYSIS msi 2020.08 permanent uncoun ted \
    "msi.lic" [dos] 1628L, 85077C
```

3.移动修改之后的文件到指定目录

将修改之后的文件复制到安装文件中，如果不是以root用户安装的，安装文件位置一般都在用户文件下的BIOVIA文件。首先复制刚刚修改的文件路径。



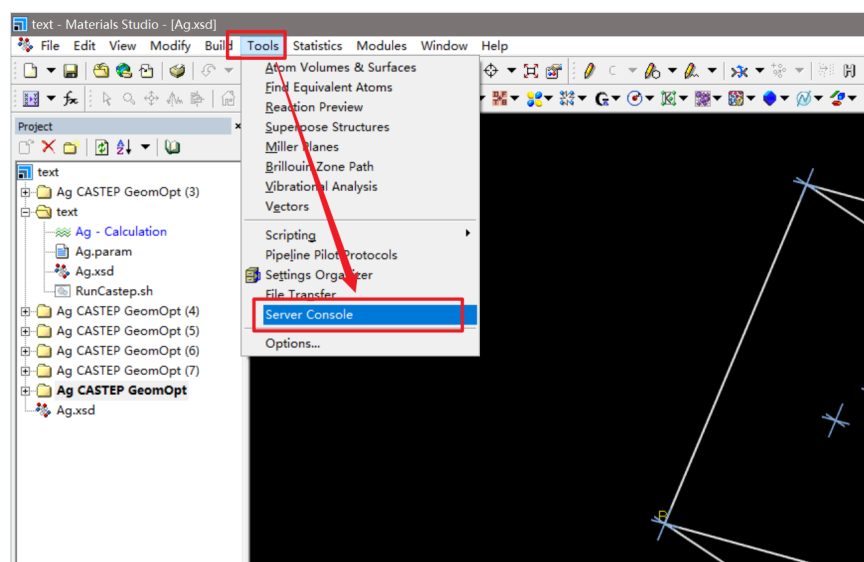
```
1 %%切换到安装文件中的/BIOVIA/BIOVIA_LicensePack/Licenses/文件路径，具体路径自己找
2 [stuHc@node01 ms2020]$ cd "/home/stuHc/BIOVIA/BIOVIA_LicensePack/Licenses/"
3 %%复制文件到指定文件夹
4 [stuHc@node01 Licenses]$ cp "/home/stuHc/ms2020/msi.lic" .
5 %%查看是否复制成功
6 [stuHc@node01 Licenses]$ ll
7 %%如果列表中有msi.lic文件即复制成功
```

到此安装成功，使用Windows上MS软件测试网关

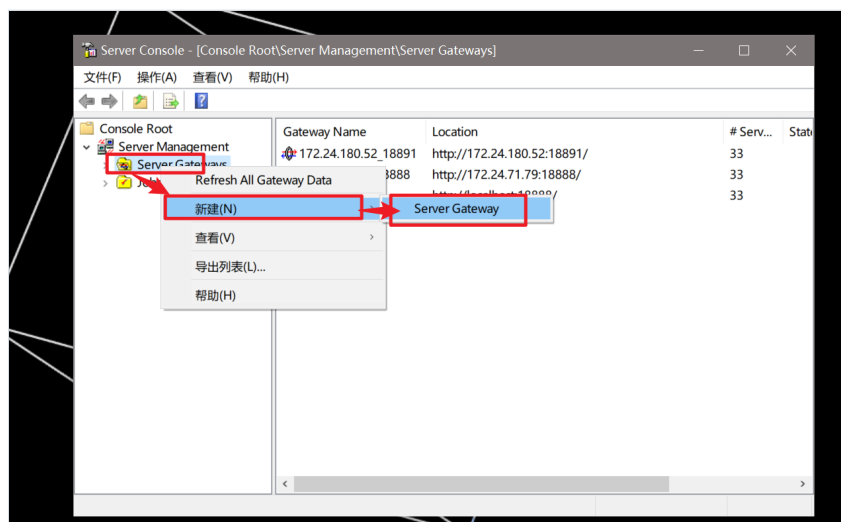
测试网关

创建网关

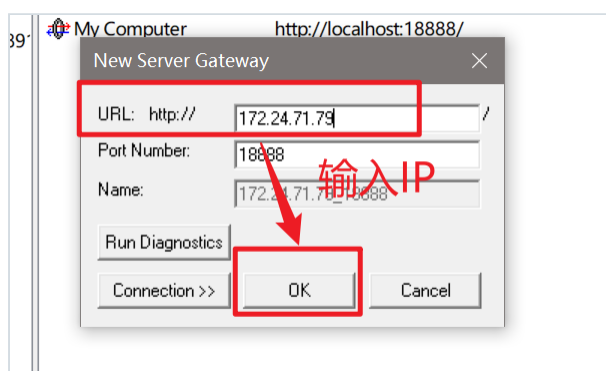
这里我以我自己电脑链接为例子



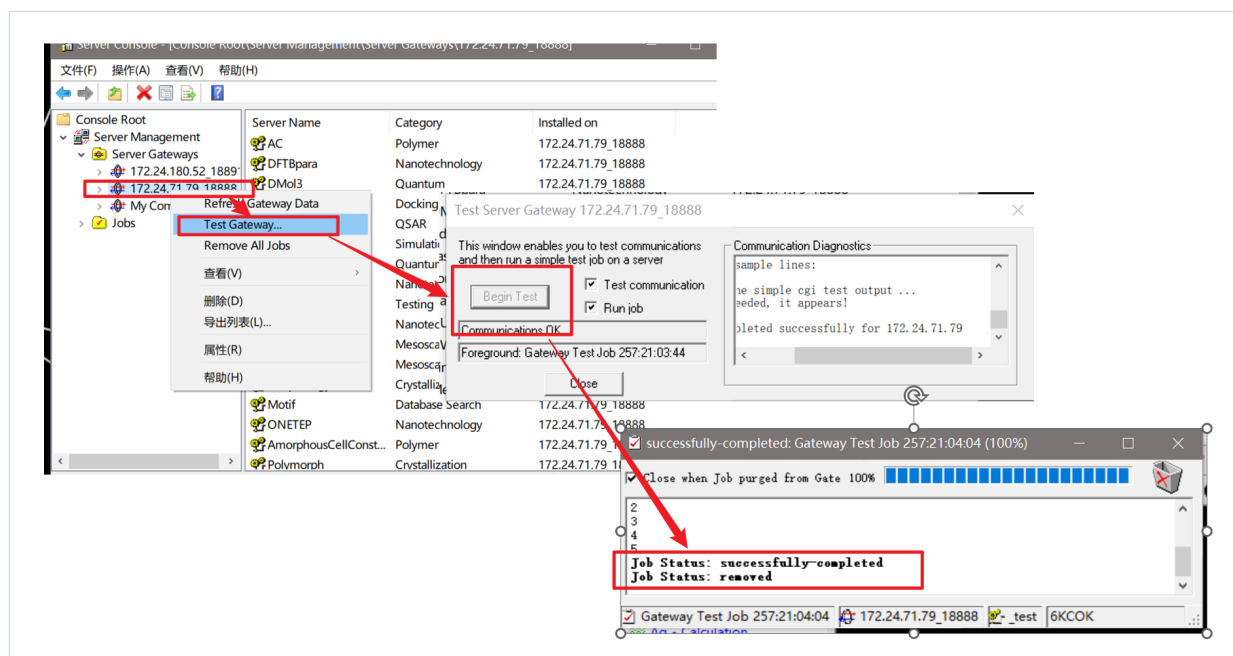
点开之后创建新网关:



输入IP地址, 下面的Port Number对于谢宜龙老师工作站Node07 IP: 172.24.71.79是18888,其他工作站有可能不一样,后面我再整理更新

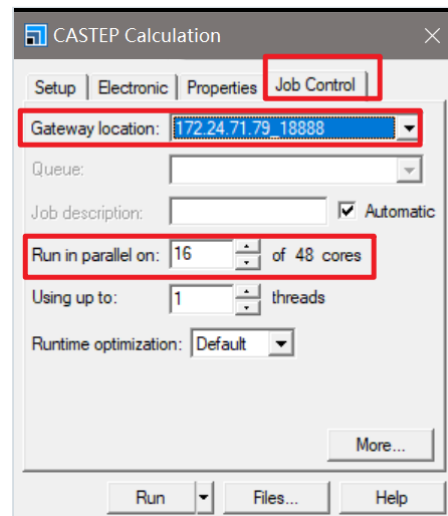


测试



运行

在配置完成参数之后, 选择Job Control,选择刚刚添加到网关,配置核心数目,最后运算,运算结果会自动下载到本机电脑上.



设置开机自启动

找到gateway文件

```
1 | cd /home/stuHc/BIOVIA/MaterialsStudio20.1/etc/Gateway
```

设置自启动

需要root权限

```
1 | //复制文件到目录
2 | cp msgateway_control_18888 /etc/rc.d/init.d/
3 | chkconfig --add msgateway_control_18888
4 | //重启一下查看状态是否正常
```