

- 图形
  - 启动脚本示例
  - 图形计算设置
    - 算例设置
      - 导入算例文件
      - 导入setup
    - 并行设置
      - 界面参数设置
      - 并行配置文件
      - 求解计算

## 图形

### 启动脚本示例

```
#!/bin/bash
#SBATCH -p kshcnormal
#SBATCH -N 2
#SBATCH --ntasks-per-node=30
#SBATCH --exclusive

# module加载
module purge
module load compiler/intel/2021.3.0 mpi/intelmpi/2021.3.0

# 图形启动参数
export DISPLAY=vncserver01:17
export QT_OPENGL=software
export MESA_GL_VERSION_OVERRIDE=3.3

# 软件启动环境
export RLM_LICENSE=50531@10.15.200.4
SCRIPTDIR=/public/home/jsyadmin/apprepo/converge/4.1.2-none
export PATH=$PATH:$SCRIPTDIR/app/Convergent_Science/CONVERGE_CFD/4.1.2/CONVERGE_Studio/x64/bin/
export PROGLIST=$SCRIPTDIR/app/Convergent_Science/CONVERGE_CFD/4.1.2/CONVERGE_Studio/x64/bin/
export LD_LIBRARY_PATH=$SCRIPTDIR/app/Convergent_Science/CONVERGE_CFD/4.1.2/CONVERGE/x64/lib64

# 图形启动
$PROGLIST -o
```

## ! Tip

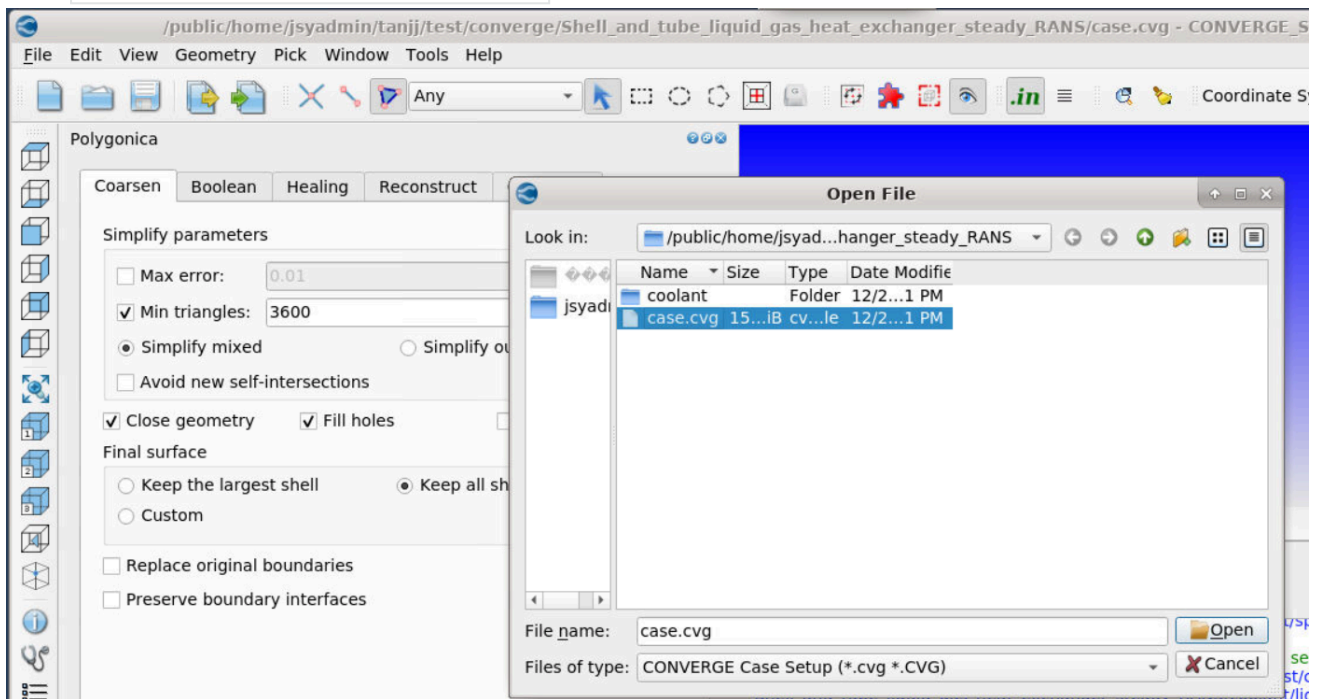
1. 图形脚本里 `module load compiler/intel/2020.1.217 mpi/intelmpi/2020.1.217` 走图形计算并不会识别相关环境参数要在 `/Path-to/Convergent_Science/CONVERGE_CFD/4.1.2/environment/x64/scripts/CONVERGE/CONVERGE-INTEL/4.1.2.sh` 配置
2. 图形闪退的话启动参数加上 `-o`

## 图形计算设置

### 算例设置

### 导入算例文件

点击 `File --> Open project --> 选择*.cvg`

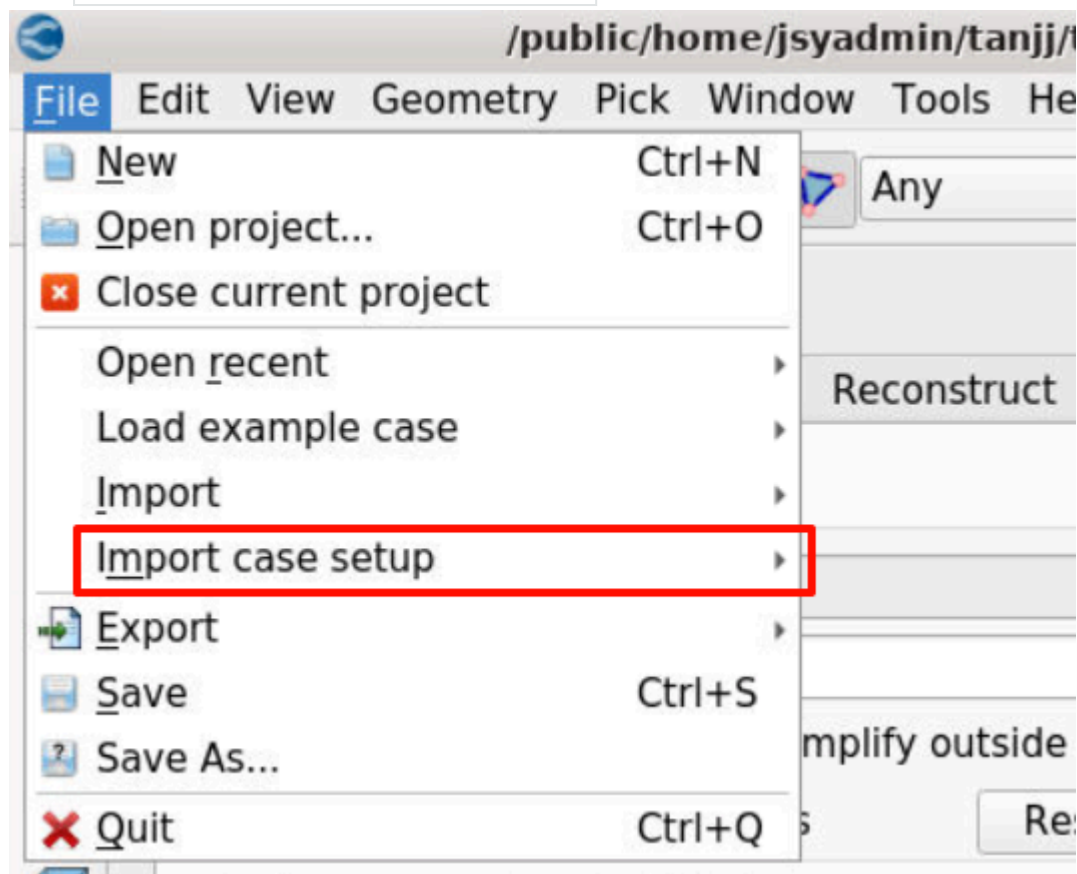


## ! Tip

- `*cvg` 是保存的图形配置文件
- `*.in *.dat` 是输入文件
- `*.echo、*.out、outputs_original` 等是输出文件

### 导入setup

点击 `File-->Import case setup-->算例所在目录`



### Tip

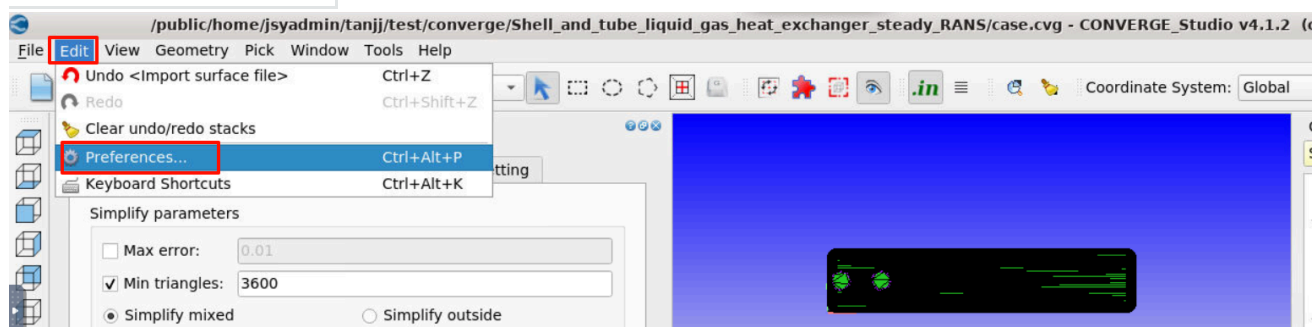
选中的目录文件所在位置，不是任何文件，软件会自动识别目录下的配置文件

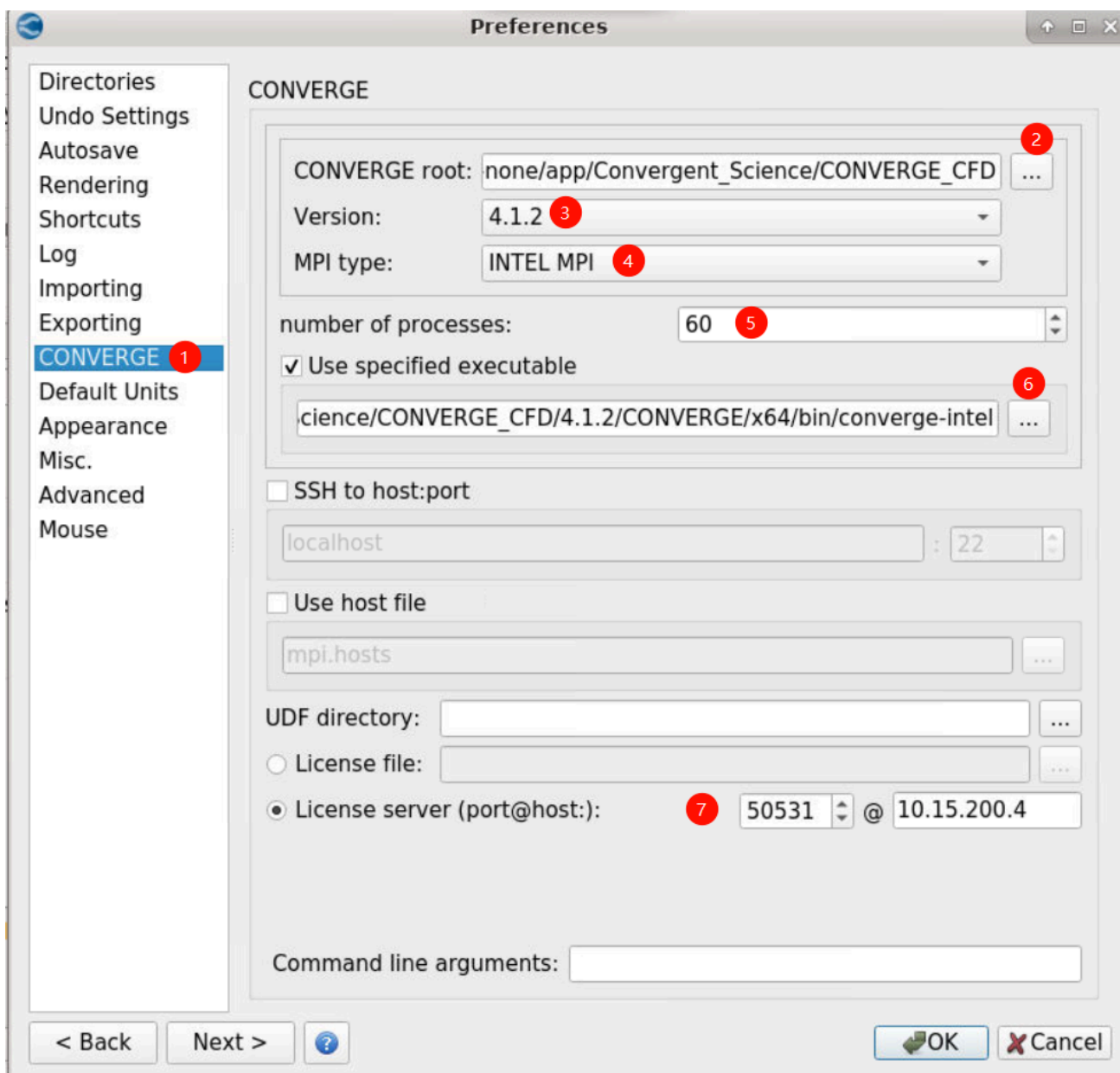
## 并行设置

### 界面参数设置

以 `CONVERGE 4.1.2` 版本为例，其余版本可能会有些差异，但大同小异，点击 `Edit -->`

`Preferences --> CONVERGE`





- **CONVERGE root** 设置为 `/PATH-TO/Convergent_Science/CONVERGE_CFD`
- **MPI** 版本类型设置为 **INTEL MPI** 即可
- **number of processes** 设置为申请资源的核数, **hostfile** 不用设置, **mpirun** 会自动识别
- **License** 根据实际版本设置浮动许可或者本地授权文件

## Tip

1. **MPI type** 选中后未出现, 点击ok后再打开一下
2. **MPI type** 无法切换, 可以删下配置文件 `rm -fr ~/.config/Convergent\ Science\ Inc./CONVERGE_Studio.conf`, 后重新打开软件

## 并行配置文件

以选中 **INTEL MPI** 为例, 图形计算的环境激活文件为 `/PATH-`

`TO/Convergent_Science/CONVERGE_CFD/4.1.2/environment/x64/scripts/CONVERGE/CONVERGE-INTEL/4.1.2.sh`

```
export installroot=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science
export env_scripts=$installroot/CONVERGE_CFD/4.1.2/environment/x64/scripts
source $env_scripts/CONVERGE/CONVERGE-INTEL/cvg/4.1.2.sh
source $env_scripts/CONVERGE/CONVERGE-INTEL/mpi/4.1.2.sh
source $env_scripts/CONVERGE/CONVERGE-INTEL/utilities/4.1.2.sh
source $env_scripts/CONVERGE/CONVERGE-INTEL/udf/4.1.2.sh

# When ParaView is installed
if [[ -d $installroot/ParaView/5.11.0 ]]; then
    source $env_scripts/paraview/INTEL/5.11.0.sh
```

可见会涉及到目录下 `mpi`、`cvg`、`tilities`、`udf`、`paraview` 等配置文件

- `mpi/4.1.2.sh` 中将集群的加载的调试环境填入，原先的环境均可以注释，`mpi` 的实际影响环境文件可以在此脚本中调试配置

```
module purge
module load compiler/intel/2021.3.0 mpi/intelmpi/2021.3.0
export I_MPI_SHM_HEAP_VSIZE=512
export UCX_TLS=all
export UCX_MEM_EVENTS=n
```

- `cvg/4.1.2.sh` 中注释掉原先的 `I_MPI_ROOT` 变量

```
export installroot=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Scienc
export cvgdir=$installroot/CONVERGE_CFD/4.1.2/CONVERGE
#export I_MPI_ROOT=$cvgdir/x64/bin/mpi/INTEL
export PATH=$cvgdir/x64/bin:$PATH
export LD_LIBRARY_PATH=$cvgdir/x64/lib64:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$cvgdir/x64/lib64/INTEL:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=.:$LD_LIBRARY_PATH
export CONVERGE_ROOT=$installroot
```

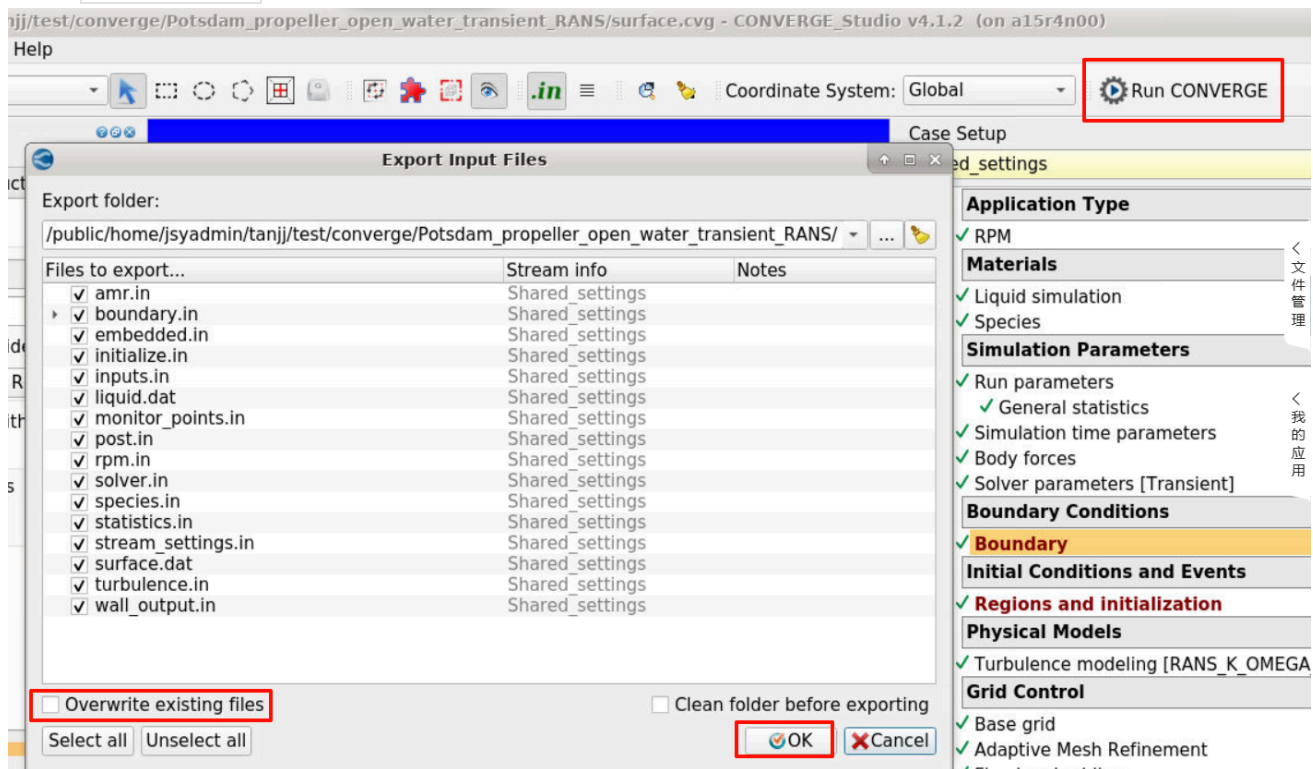
- `udf/4.1.2.sh`、`utilities/4.1.2.sh`、`paraview/INTEL/5.11.0.sh` 中可默认不改

## ⚠ Warning

所有配置文件注意修改 `$installroot` 变量，商城安装的还是原来的安装路径

## 求解计算

点击 Run CONVERGE



## Tip

如果算例配置文件已经设置好，尽量不要 overwrite



计算日志会在该界面打印出来，往前翻就可以看到前期加载的配置文件，设置的环境等，出现运行问题也可在此根据日志 debug



```
+ source /public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science/CONVERGE_CFD/4.1.2/environment/
x64/scripts/CONVERGE/CONVERGE-INTEL/4.1.2.sh
++ export installroot=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science
++ installroot=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science
++ export env_scripts=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science/CONVERGE_CFD/4.1.2/
environment/x64/scripts
++ env_scripts=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science/CONVERGE_CFD/4.1.2/
environment/x64/scripts
++ source /public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science/CONVERGE_CFD/4.1.2/environment/
x64/scripts/CONVERGE/CONVERGE-INTEL/cvg/4.1.2.sh
+++ export installroot=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science
+++ installroot=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science
+++ export cvgdir=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science/CONVERGE_CFD/4.1.2/
CONVERGE
+++ cvgdir=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science/CONVERGE_CFD/4.1.2/CONVERGE
+++ export PATH=/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science/CONVERGE_CFD/4.1.2/
CONVERGE/x64/bin:/public/software/compiler/intel/intel-2020/compilers_and_libraries_2020.1.217/mpi/intel64/bin:/
public/software/compiler/intel/intel-2020/compilers_and_libraries_2020.1.217/mpi/intel64/libfabric/bin:/public/
software/compiler/intel/intel-2020/compilers_and_libraries_2020.1.217/bin/intel64:/public/home/jsyadmin/apprepo/
vaspkit/1.5.1-none/source/bin:/opt/gridview/pmix/bin:/opt/gridview/pmix/sbin:/usr/local/bin:/opt/notify/bin:/opt/
gridview/slurm/bin:/opt/gridview/slurm/sbin:/opt/gridview/munge/bin:/opt/gridview/munge/sbin:/public/home/jsyadmin/
apprepo/vaspkit/1.5.1-none/source/bin:/usr/lib64/qt-3.3/bin:/opt/gridview/pmix/bin:/opt/gridview/pmix/sbin:/public/
home/jsyadmin/perl5/bin:/usr/local/bin:/opt/notify/bin:/opt/gridview/slurm/bin:/opt/gridview/slurm/sbin:/opt/
gridview/munge/bin:/opt/gridview/munge/sbin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/public/home/jsyadmin/
bin:/public/home/jsyadmin/apprepo/converge/4.1.2-none/app/Convergent_Science/CONVERGE_CFD/4.1.2/CONVERGE_Studio/x64/
```



Forced Termination

Log file location: [/public/home/jsyadmin/... original/converge.log](#)

Normal Stop

Hide

Clear text