





Docker


<https://git.nju.edu.cn/escience/singularity-example>

-  root 
- 
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Singularity

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 Conda 
 Python Numpy 

☐ Dockerfile ☐ Docker ☐

FROM continuumio/miniconda3:22.11.1

```
# 创建 conda 环境
COPY .condarc /root/.condarc

# 运行
RUN conda create -n my-env python=3.10 numpy

# 设置 shell
SHELL ["/bin/bash", "--login", "-c"]
RUN conda init bash
RUN echo "source activate my-env" > ~/.bashrc
ENV PATH /opt/conda/envs/my-env/bin:$PATH
```

创建 .condarc 文件

numpy

安装 Python 环境

安装 Docker 环境

docker 环境

```
docker build -t escience/conda-numpy .
```

“ Docker 环境 Docker 环境 docker.nju.edu.cn ”

运行 Docker 环境

```
docker run -i escience/conda-numpy python < test.py
```

CI/CD

CI/CD 环境 git.nju.edu.cn 环境

.gitlab-ci.yml 环境

CI/CD

运行 CI/CD 环境

CI/CD 环境 gcr.nju.edu.cn 环境

```
# 运行
stages:
```

```
- build
- test

# [ ] [ ] [ ] [ ] [ ] [ ]

build:
  stage: build
  image:
    name: gcr.nju.edu.cn/kaniko-project/executor:debug # [ ] [ ] gcr[ ] [ ] [ ]
    entrypoint: ["" ]
  script:
    - /kaniko/executor
    - --context "${CI_PROJECT_DIR}"
    - --dockerfile "${CI_PROJECT_DIR}/Dockerfile"
    - --destination "${CI_REGISTRY_IMAGE}:${CI_COMMIT_TAG}"
  rules: # [ ] [ ] [ ] [ ] [ ] [ ] [ ] [ ]
    - if: $CI_COMMIT_TAG

# [ ] [ ] [ ] [ ] [ ] [ ]

test:
  stage: test
  image:
    name: ${CI_REGISTRY_IMAGE}:${CI_COMMIT_TAG}
  script:
    - python "${CI_PROJECT_DIR}/test.py"
  rules:
    - if: $CI_COMMIT_TAG
```

test

“

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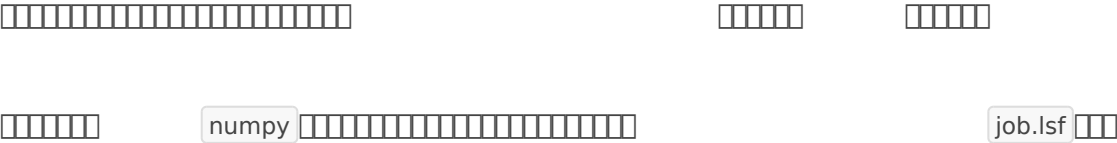
 ” “

--	--	--	--	--	--	--	--

 ”

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```
INFO: Starting build...
Getting image source signatures
Copying blob 3389e9eb8624 done
Copying blob 3f4ca61aafcd done
Copying blob baee49be4542 done
Copying blob 7b4354700ca4 done
Copying blob 69a5d9e1ecd6 done
Copying blob 8a7a15cee421 done
Copying blob 5f4e24b7e321 done
Copying config 51871566f8 done
Writing manifest to image destination
Storing signatures
2023/08/29 21:46:55 info unpack layer: sha256:3f4ca61aafcd4fc07267a105067db35c0f0ac630e1970f3cd0c7bf552780e985
2023/08/29 21:46:57 info unpack layer: sha256:69a5d9e1ecd6566da53d0978004bdf37dddfaba1d8a6117966f397b41cbbc529
2023/08/29 21:46:59 info unpack layer: sha256:7b4354700ca480732ead22a553cc45916dc5466709ca64d964c4647b5b9343e9
2023/08/29 21:47:02 info unpack layer: sha256:baee49be454261f20f9770566da694b7e7845cf7d279cc2421c6b3eed68c012c
2023/08/29 21:47:02 info unpack layer: sha256:8a7a15cee4219b244df17b401664119dfd5b7e52a5659107f1ee3ec210722373
2023/08/29 21:47:20 info unpack layer: sha256:3389e9eb8624f21330c272ba23defc59ba31d46273e38cde475e7256edea80cb
2023/08/29 21:47:20 info unpack layer: sha256:5f4e24b7e32113995e0417eb5c4de5cbef9be70a4a3841a19cdb2fa1f3f12a34
INFO: Creating SIF file...
INFO: Build complete: conda-numpy.sif
```



```
#BSUB -q 6140ib
#BSUB -n 1

module load singularity/latest

SINGULARITY="singularity run --env MKL_NUM_THREADS=$LSB_DJOB_NUMPROC conda-numpy.sif"
${SINGULARITY} python test.py
```

```
bsub < job.lsf
```



CI/CD Docker HPC eScience



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- CI/CD[] [git.nju.edu.cn] [reg.nju.edu.cn]
- [] [hpc.nju.edu.cn]

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