How to install Firedrake

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目录

1 Firedraka 安装

需要计算机网络环境正常, 否则请参考 无网络安装

1.1 Ubuntu

下载安装脚本 `firedrake-install` 然后运行即可

```
curl -O https://raw.githubusercontent.com/firedrakeproject/firedrake/master/scripts/firedrake-install
python3 firedrake-install
```

查看安装帮助

```
python3 firedrake-install -h
```

注: 有时安装会出现 pip 源不能访问的问题, 类似错误信息如下:

```
Starting new HTTPS connection (6): pypi.org:443
Could not fetch URL https://pypi.org/simple/pulp/: connection error: HTTPSConnectionPool(host='pypi.org', port=443
Skipping link: not a file: https://pypi.org/simple/pulp/
Given no hashes to check 0 links for project 'pulp': discarding no candidates
ERROR: Could not find a version that satisfies the requirement PuLP (from versions: none)
ERROR: No matching distribution found for PuLP
```

可以通过设置 pip 的源解决, 如更改为 中科大的源:

```
mkdir -p $HOME/.pip && \
cat > $HOME/.pip/pip.conf <<EOF
[global]
index-url = https://pypi.mirrors.ustc.edu.cn/simple
[install]
trusted-host=pypi.mirrors.ustc.edu.cn
EOF
```

1.1.1 Real Int32

```
python3 firedrake-install --slepc --disable-ssh --documentation-dependencies --remove-build-files
```

1.1.2 Complex Int64

```
PETSC_CONFIGURE_OPTIONS='--download-scalapack --download-mumps' \
    python3 firedrake-install --petsc-int-type int64 --complex --slepc \
    --disable-ssh --documentation-dependencies --remove-build-files
```

1.1.3 测试

```
source firedrake/bin/activate
cd $VIRTUAL_ENV/src/firedrake
pytest tests/regression/ -k "poisson_strong or stokes_mini or dg_advection"
```

1.2 Windows

安装 WSL (适用于 Linux 的 Windows 子系统, Windows Subsystem for Linux). 默认情况下，安装的系统为 Ubuntu.

1.2.1 WSL 安装

https://docs.microsoft.com/zh-cn/windows/wsl/install

1.2.2 Firedrake 安装

按照 Ubuntu 安装方式

1.3 Mac

先安装 Homebrew (https://brew.sh/), 然后使用 Homebrew 安装 python3, 之后类似于 Ubuntu 直接安装 firedrake

1.4 Linux Server

若服务器不能访问网络, 请参考下节: 无网络安装.

1.4.1 Spack I

Firedrake 团队提供了基于 Spack (HPC 上的包管理器) 安装的方式.

详见: https://github.com/firedrakeproject/firedrake-spack

1.4.2 Spack II

使用 spack 安装依赖包, 然后类似于 Ubuntu 方式安装 (需要禁用包管理器: `--no-package-manager`)

可参考如下脚本:

https://raw.githubusercontent.com/lrtfm/notes-for-firedrake/main/scripts/spack-firedrake.py

1.4.3 Docker

可以使用 Firedrake 团队构建的镜像

https://hub.docker.com/u/firedrakeproject.

2 无网络安装

若需在无网络访问的工作站上安装 firedrake, 需要使用 spack 的镜像功能.

假设本地可以 `git` 访问 github. 下面我们以安装软件在 `$HOME/opt` 目录为例.

注: 下面多行命令块中各行之间使用了 `&& \` 连接, 直接拷贝多行到终端输入回车即可.

Reference:

1. spack install:
   - https://spack.readthedocs.io/en/latest/getting_started.html#installation
2. spack mirror:
   - https://spack.readthedocs.io/en/latest/mirrors.html#mirror-environment
   - https://spack.readthedocs.io/en/latest/mirrors.html#mirror-files
3. firedrake spack:
   - https://github.com/firedrakeproject/firedrake-spack
   - https://hackmd.io/@TzVnFeL0TMCb3FaAi9qYBA/ByaRskMQ5

2.1 本地

2.1.1 创建安装目录

```
mkdir $HOME/opt
```

2.1.2 下载安装 spack

```
cd $HOME/opt && \
git clone -c feature.manyFiles=true https://github.com/spack/spack.git && \
source $HOME/opt/spack/share/spack/setup-env.sh
```

注: 添加下面命令到文件 `$HOME/.bashrc` 中, 用于添加 spack 的 shell 支持, 使得每次开启终端都可以使用 spack.

```
source $HOME/opt/spack/share/spack/setup-env.sh
```

2.1.3 打包 spack 文件, 用于服务器安装

```
tar -czvf spack.tar.gz spack
```

2.1.4 下载 firedrake-spack 仓库

```
cd $HOME/opt && \
git clone https://github.com/lrtfm/firedrake-spack.git && \
git checkout tmp-fix-petsc-ptscotch
```

2.1.5 打包 firedrake-spack 文件, 用于服务器安装

```
tar -czvf firedrake-spack.tar.gz firedrake-spack
```

2.1.6 添加该仓库到 spack

```
spack repo add firedrake-spack
```

2.1.7 检查 spack 安装情况

现在运行 `spack info py-firedrake` 查看 firedrake-spack 仓库是否添加成功

```
$ spack info py-firedrake
PythonPackage:   py-firedrake

Description:
    Firedrake is an automated system for the portable solution of partial
    differential equations using the finite element method (FEM)

Homepage: https://firedrakeproject.org

Preferred version:
    develop    [git] https://github.com/firedrakeproject/firedrake.git on branch master

Safe versions:
    develop    [git] https://github.com/firedrakeproject/firedrake.git on branch master

Deprecated versions:
    None

Variants:
    Name [Default]               When    Allowed values    Description
    ========================    ====    ==============    ============================================

    64-bit-indices [off]         --      on, off           Install PETSc using 64bit indices
    build_system [python_pip]    --      python_pip        Build systems supported by the package
    complex [off]                --      on, off           Install Firedrake in complex mode
    minimal-petsc [off]          --      on, off           Build PETSc with minimal packages for Firedrake
    slepc [off]                  --      on, off           Install SLEPc and slepc4py

Build Dependencies:
    eigen            mpi            py-cython  py-h5py        py-mpi4py    py-pip        py-pyadjoint  py-scipy
    libspatialindex  petsc          py-fiat    py-islpy       py-numpy     py-pkgconfig  py-pyop2      py-setuptoo
    libsupermesh     py-cachetools  py-finat   py-matplotlib  py-petsc4py  py-progress   py-requests   py-slepc4py

Link Dependencies:
    eigen  libspatialindex  libsupermesh  mpi  petsc  python  slepc

Run Dependencies:
    eigen            petsc          py-finat       py-mpi4py    py-pip        py-pyop2        py-scipy       py-t
```

```
    libspatialindex  py-cachetools  py-h5py        py-nbval     py-pkgconfig  py-pytest        py-setuptools  py-u
    libsupermesh     py-cython      py-islpy       py-numpy     py-progress   py-pytest-xdist  py-slepc4py    py-v
    mpi              py-fiat        py-matplotlib  py-petsc4py  py-pyadjoint  py-requests      py-sympy       pyth
```

当前 $HOME/opt 目录文件如下:

```
$ ls -lha
total 214M
drwxrwxr-x  4 z2yang z2yang  112 Oct 30 15:17 .
drwxrwxr-x  3 z2yang z2yang   47 Oct 30 15:02 ..
drwxrwxr-x  5 z2yang z2yang  204 Oct 30 15:16 firedrake-spack
-rw-rw-r--  1 z2yang z2yang 211K Oct 30 15:17 firedrake-spack.tar.gz
drwxrwxr-x 10 z2yang z2yang 4.0K Oct 30 15:17 spack
-rw-rw-r--  1 z2yang z2yang 214M Oct 30 15:15 spack.tar.gz
```

2.2 工作站

2.2.1 创建安装目录

```
mkdir $HOME/opt
```

2.2.2 上传文件

使用 ftp 等工具上传本地的 firedrake-spack.gz 和 spack.tar.gz 到服务器的 $HOME/opt 目录.

2.2.3 解压安装 spack

```
cd $HOME/opt && \
tar -zxf spack.tar.gz && \
source $HOME/opt/spack/share/spack/setup-env.sh
```

注 1: 添加下面命令到文件 $HOME/.bashrc 中, 用于添加 spack 的 shell 支持, 使得每次开启终端都可以使用 spack.

```
source $HOME/opt/spack/share/spack/setup-env.sh
```

注 2: 某些工作站上 /tmp 目录内容没有执行权限, 需要更改 spack 的构建目录配置如下:

```
mkdir -p $HOME/.spack && \
cat > $HOME/.spack/config.yaml <<EOF
config:
  build_stage:
    - \$user_cache_path/stage
EOF
```

2.2.4 解压安装 firedrake-spack 仓库

```
cd $HOME/opt && \
tar -zxf firedrake-spack.tar.gz && \
spack repo add firedrake-spack
```

2.2.5 准备 firedrake 安装环境

1. 创建环境

```
FIREDRAKE_ENV_NAME=firedrake-complex-int64 && \
spack env create -d $FIREDRAKE_ENV_NAME && \
spack env activate -p $FIREDRAKE_ENV_NAME && \
spack -e $SPACK_ENV config add concretizer:unify:true
```

2. 添加软件包 (可根据需要添加或删减)

```
spack add python py-firedrake@develop%gcc +64-bit-indices+complex ^mpich ^openblas \
    ^petsc+mumps+scalapack+int64+complex+libyaml+parmmg+mmg \
    ^hypre+complex+int64+superlu-dist && \
spack add py-pygmsh py-meshio py-tqdm py-pyyaml
```

注: 需要显式添加 python, 不然 `view` 中 `python` 是链接而不是拷贝, 会导致 `firedrake` 找不到 `spatialindex`: https://github.com/spack/spack/issues/32456

3. 运行 `concretize` (spack 计算软件依赖关系)

```
spack concretize -f 2>&1 | tee $SPACK_ENV/spack-firedrake-concretize.log
```

4. 查看 `$SPACK_ENV` 目录, 有如下内容

```
$ ls -la $SPACK_ENV
total 620
drwxrwxr-x 3 z2yang z2yang    118 Oct 30 16:01 .
drwxrwxr-x 5 z2yang z2yang    147 Oct 30 15:33 ..
drwxrwxr-x 4 z2yang z2yang     89 Oct 30 16:01 .spack-env
-rw-rw-r-- 1 z2yang z2yang  54343 Oct 30 16:01 spack-firedrake-concretize.log
-rw-rw-r-- 1 z2yang z2yang 572917 Oct 30 16:01 spack.lock
-rw-rw-r-- 1 z2yang z2yang    457 Oct 30 16:01 spack.yaml
```

2.2.6 本地创建镜像文件上传服务器

通过 `spack.lock` 文件在本地创建 firedrake 环境, 构建镜像, 并上传服务器.

1. 下载 `spack.lock` 文件到本地.

2. (本地) 运行如下命令创建镜像 (创建镜像需要 10min 左右)

```
cd $HOME/opt && \
spack env create -d firedrake-mirror-env spack.lock && \
spack env activate -p ./firedrake-mirror-env && \
time spack mirror create -a -d spack-firedrake-mirror 2>&1 | tee creat-mirror.logs
```

结束后会有如下输出

```
==> Summary for mirror in file:///home/z2yang/z2yang/local/opt/spack-firedrake-mirror
==> Archive stats:
    0    already present
    244  added
    0    failed to fetch.

real    10m56.048s
```

```
user    1m1.559s
sys     0m13.604s
```

如果有失败的, 需要先删除缓存, 重新创建镜像:

```
spack clean -ds && \
time spack mirror create -a -d spack-firedrake-mirror 2>&1 | tee creat-mirror.logs
```

3. (本地) 打包镜像

```
tar -czvf spack-firedrake-mirror.tar.gz spack-firedrake-mirror
```

4. 上传镜像

   使用 ftp 工具上传 `spack-firedrake-mirror.tar.gz` 到服务器上 `$HOME/opt` 目录

5. (服务器) 解压镜像

```
tar -xzvf spack-firedrake-mirror.tar.gz
```

6. (服务器) 添加镜像路径到 spack

```
cat > $HOME/.spack/mirrors.yaml <<EOF
mirrors:
  local_filesystem: file://$HOME/opt/spack-firedrake-mirror
EOF
```

7. (工作站) 查看镜像是否添加成功, 运行 `spack mirror lsit` 应该有如下信息

```
$ spack mirror list
local_filesystem    file://<your-home-path>/opt/spack-firedrake-mirror
spack-public        https://mirror.spack.io
```

2.2.7 安装 Firedrake

1. 运行 develop 命令以避免一些错误

```
spack develop py-firedrake@develop && \
spack develop libsupermesh@develop && \
spack develop petsc@develop && \
spack develop chaco@petsc && \
spack develop py-fiat@develop && \
spack develop py-finat@develop && \
spack develop py-islpy@develop && \
spack develop py-petsc4py@develop && \
spack develop py-pyadjoint@develop && \
spack develop py-pyop2@develop && \
spack develop py-coffee@develop && \
spack develop py-loopy@develop && \
spack develop py-cgen@develop && \
spack develop py-codepy@develop && \
spack develop py-genpy@develop && \
spack develop py-tsfc@develop && \
spack develop py-ufl@develop
```

2. 安装

   在服务器端运行下面命令安装 (第一次安装需要等待一段时间 1-2hour, 中间可能会失败, goog luck!)

```
spack concretize -f 2>&1 | tee $SPACK_ENV/spack-firedrake-develop.log && \
time spack install --fail-fast --show-log-on-error \
    --log-file $SPACK_ENV/spack-firedrake-install.log
```

   最后几行输出如下:

```
[+] /home/z2yang/z2yang/server2/opt/spack/opt/spack/linux-ubuntu22.04-cascadelake/gcc-11.3.0/py-firedrake-dev
==> Updating view at /home/z2yang/z2yang/server2/opt/firedrake-complex-int64/.spack-env/view

real    184m44.242s
user    836m56.348s
sys     97m42.901s
```

3. 取消激活环境

```
despacktivate
```

   会有如下 Warning 忽略即可

```
$ despacktivate
==> Warning: Skipping reversal of unreversable operation<class 'spack.util.environment.UnsetEnv'> PETSC_ARCH
==> Warning: Skipping reversal of unreversable operation<class 'spack.util.environment.UnsetEnv'> PETSC_ARCH
==> Warning: Skipping reversal of unreversable operation<class 'spack.util.environment.UnsetEnv'> PETSC_ARCH
==> Warning: Skipping reversal of unreversable operation<class 'spack.util.environment.UnsetEnv'> PETSC_ARCH
```

2.2.8 使用

1. 激活环境

```
cd $HOME/opt && \
spack env activate -p $FIREDRAKE_ENV_NAME
```

2. 测试

```
cd $SPACK_ENV/py-firedrake && \
pytest tests/regression/ -k "poisson_strong or stokes_mini or dg_advection"
```

3 Colab 上尝试 Firedrake

Colab 是 Colaboratory 的简称, (可以看作是在线版 Jupyter, 浏览器中编写和执行 Python 代码)

FEM on Colab 支持在 Colab 上安装 FEniCS, FEniCSx, Firedrake, NGSolve, gmsh

3.1 导入 Package

3.1.1 Firedrake

大概 3 分钟

```
try:
    import firedrake
except ImportError:
    !wget "https://fem-on-colab.github.io/releases/firedrake-install-real.sh" \
        -O "/tmp/firedrake-install.sh" && bash "/tmp/firedrake-install.sh"
    import firedrake
```

3.1.2 Gmsh

```
try:
    import gmsh
except ImportError:
    !wget "https://fem-on-colab.github.io/releases/gmsh-install.sh" \
        -O "/tmp/gmsh-install.sh" && bash "/tmp/gmsh-install.sh"
    import gmsh
```

3.2 示例

https://colab.research.google.com/drive/1gM3zMWTskH7XyDi1yJL76BPFnOJjSdYh?usp=sharing

4 问题求助

官方文档:

- https://www.firedrakeproject.org/documentation.html

Github 仓库 (issues and discussions):

- https://github.com/firedrakeproject/firedrake
- https://github.com/firedrakeproject/firedrake/issues
- https://github.com/firedrakeproject/firedrake/discussions

Slack 讨论组:

- https://firedrakeproject.herokuapp.com/

邮件列表:

- https://mailman.ic.ac.uk/mailman/listinfo/firedrake

5 其他有限元工具

- FEniCSx
- NgSolve
- deal.II
- libMesh

- FreeFEM
- Dune