Notes on Firedrake

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目录

[1]:
```python
# for export pdf
import matplotlib.pyplot
import matplotlib_inline
matplotlib_inline.backend_inline.set_matplotlib_formats('png', 'pdf')
```

Notes on generate pdf:

```
jupyter nbconvert --to pdf 02_firedrake_notes.ipynb
```

Check for new version at https://github.com/lrtfm/notes-for-firedrake/blob/main/02_firedrake_notes.ipynb

Firedrake 是基于弱形式求解偏微分方程的工具：根据用户定义的有限元空间和变分形式，Firedrake 自动生

成代码组装线性或非线性方程组, 然后使用 PETSc 进行求解.

1 Solving Poisson equation

1.1 Dirichlet Problem

Considering the following Poisson equation

$$\begin{aligned} -\Delta u = f \qquad & \text{in} \quad \Omega, \\ u = g_D \qquad & \text{on} \quad \partial\Omega_D, \\ \frac{\partial u}{\partial n} = g_N \qquad & \text{on} \quad \partial\Omega_N, \end{aligned} \tag{1}$$

where $\partial\Omega_D \cap \partial\Omega_N = \partial\Omega$, and $\int_{\partial\Omega_D} \mathrm{d}s \neq 0$.

Define **trial** and **test** function space

$$\begin{aligned} H_E^1 &:= \{u \in H^1 \,|\, u = g_D \ \text{ on } \ \partial\Omega_D\}, \\ H_{E_0}^1 &:= \{u \in H^1 \,|\, u = 0 \ \text{ on } \ \partial\Omega_D\} \end{aligned} \tag{2}$$

The **variational form** is

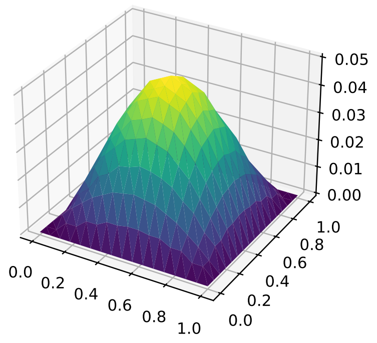
Find $u \in H_E^1$, such that

$$\int_\Omega \nabla u \cdot \nabla v = \int_\Omega fv + \int_{\partial\Omega_N} g_N v \qquad \forall v \in H_{E_0}^1. \tag{3}$$

1.1.1 A simple example

Now, we solve possion problem in domain $\Omega = (0,1) \times (0,1)$. Assume $\partial\Omega_N = \emptyset, \partial\Omega_D = \partial\Omega$ and $g_D = 0$ (homogeneous Dirichlet boundary condition). In addition, let the source term be $f = \sin(\pi x)\sin(\pi y)$.

[2]:
```python
from firedrake import *
import matplotlib.pyplot as plt

N = 8
test_mesh = RectangleMesh(nx=N, ny=N, Lx=1, Ly=1)   # Build mesh on the domain
x, y = SpatialCoordinate(test_mesh)
f = sin(pi*x)*sin(pi*y)
g = Constant(0)

V = FunctionSpace(test_mesh, 'CG', degree=1)        # define FE space

u, v = TrialFunction(V), TestFunction(V)            # define trial and test function
a = inner(grad(u), grad(v))*dx
L = inner(f, v)*dx                                  # or f*v*dx

bc = DirichletBC(V, g=g, sub_domain='on_boundary')

u_h = Function(V, name='u_h')
solve(a == L, u_h, bcs=bc)          # We will introduce other ways to code in the following.

fig, ax = plt.subplots(figsize=[4, 4], subplot_kw=dict(projection='3d'))
ts = trisurf(u_h, axes=ax)
```



1.1.2 Builtin meshes in Firedrake

[3]:
```python
from firedrake import utility_meshes
from pprint import pprint

print('List of builtin meshes:')
for i, name in enumerate(utility_meshes.__all__):
    print(f'  {name:<25s}', end='')
    if (i+1)%3 == 0:
        print('')
```

output
```
List of builtin meshes:
  IntervalMesh               UnitIntervalMesh           PeriodicIntervalMesh
  PeriodicUnitIntervalMesh   UnitTriangleMesh           RectangleMesh
  TensorRectangleMesh        SquareMesh                 UnitSquareMesh
  PeriodicRectangleMesh      PeriodicSquareMesh         PeriodicUnitSquareMesh
  CircleManifoldMesh         UnitDiskMesh               UnitBallMesh
  UnitTetrahedronMesh        BoxMesh                    CubeMesh
  UnitCubeMesh               PeriodicBoxMesh            PeriodicUnitCubeMesh
  IcosahedralSphereMesh      UnitIcosahedralSphereMesh  OctahedralSphereMesh
  UnitOctahedralSphereMesh   CubedSphereMesh            UnitCubedSphereMesh
  TorusMesh                  CylinderMesh
```

How to find the doc or help for functions/classes

1. ?<fun-name>
2. help(<fun-name>)

[4]:
```python
from firedrake import utility_meshes
help(utility_meshes.CubeMesh)
```

output
```
Help on cython_function_or_method in module firedrake.utility_meshes:

CubeMesh(nx, ny, nz, L, hexahedral=False, reorder=None,
distribution_parameters=None, comm=<mpi4py.MPI.Intracomm object at
0x7f9f97e9e8d0>, name='firedrake_default', distribution_name=None,
permutation_name=None)
    Generate a mesh of a cube

    :arg nx: The number of cells in the x direction
    :arg ny: The number of cells in the y direction
    :arg nz: The number of cells in the z direction
    :arg L: The extent in the x, y and z directions
    :kwarg hexahedral: (optional), creates hexahedral mesh, defaults to False
    :kwarg reorder: (optional), should the mesh be reordered?
    :kwarg comm: Optional communicator to build the mesh on (defaults to
        COMM_WORLD).
    :kwarg name: Optional name of the mesh.
    :kwarg distribution_name: the name of parallel distribution used
           when checkpointing; if `None`, the name is automatically
           generated.
    :kwarg permutation_name: the name of entity permutation (reordering) used
           when checkpointing; if `None`, the name is automatically
           generated.

    The boundary surfaces are numbered as follows:

    * 1: plane x == 0
    * 2: plane x == L
    * 3: plane y == 0
    * 4: plane y == L
    * 5: plane z == 0
    * 6: plane z == L
```

1.1.3 UFL 表达式

算 子 DOC: https://fenics.readthedocs.io/projects/ufl/en/latest/manual/form_language.html#tensor-algebra-operators)

1. `dot`

   张量缩并, `dot(u, v)` 对 `u` 的最后一个维度和 `v` 的第一个维度做缩并.

2. `inner`

   张量内积 (分量对应乘积之和). 对第二个张量取复共轭.

3. `grad` and `nabla_grad`

   1. `grad`

      对张量求导, 新加维度为最后一个维度.

      1. scalar

         $$\mathrm{grad}(u) = \nabla u = \frac{\partial u}{\partial x_i}\mathbf{e}_i$$

      2. vector

         $$\mathrm{grad}(\mathbf{v}) = \nabla \mathbf{v} = \frac{\partial v_i}{\partial x_j}\mathbf{e}_i \otimes \mathbf{e}_j$$

      3. tensor

         设 $\mathbf{T}$ 为秩为 r 的张量, 那么

         $$\mathrm{grad}(\mathbf{T}) = \nabla \mathbf{T} = \frac{\partial \mathbf{T}_\ell}{\partial x_i}\mathbf{e}_{\ell_1} \otimes \cdots \otimes \mathbf{e}_{\ell_r} \otimes \mathbf{e}_i$$

         其中 ℓ 是长度为 r 的多指标 (multi-index).

2. `nabla_grad`

   类似 `grad`, 不过新加维度为第一个维度

   1. scalar (same with `grad`)
   $$\text{nabla\_grad}(u) = \nabla u = \frac{\partial u}{\partial x_i}\mathbf{e}_i$$
   2. vector
   $$\text{nabla\_grad}(\mathbf{v}) = (\nabla \mathbf{v})^T = \frac{\partial v_j}{\partial x_i}\mathbf{e}_i \otimes \mathbf{e}_j$$
   3. tensor

      设 $\mathbf{T}$ 为秩为 r 的张量, 那么
   $$\text{nabla\_grad}(\mathbf{T}) = \frac{\partial \mathbf{T}_\ell}{\partial x_i}\mathbf{e}_i \otimes \mathbf{e}_{\ell_1} \otimes \cdots \otimes \mathbf{e}_{\ell_r}$$

4. `div` and `nabla_div`

   1. `div`

      对最后一个维度的偏导数进行缩并.

      设 $\mathbf{T}$ 为秩为 r 的张量, 那么
   $$\text{div}(\mathbf{T}) = \sum_i \frac{\partial \mathbf{T}_{\ell_1\ell_2\cdots\ell_{r-1}i}}{\partial x_i}\mathbf{e}_{\ell_1} \otimes \cdots \otimes \mathbf{e}_{\ell_{r-1}}$$
   2. `nabla_div`

      类似 `div`, 不过对第一个维度的偏导数进行缩并.

5. 两个表达式:

   1. $(u \cdot \nabla)v \to$ `dot(u, nabla_grad(v))` or `dot(grad(v), u)`
   2. $\Delta u \to$ `div(grad(u))`

非线性函数 Ref: https://fenics.readthedocs.io/projects/ufl/en/latest/manual/form_language.html#basic-nonlinear-functions

- `abs`, `sign`
- `pow`, `sqrt`
- `exp`, `ln`
- `cos`, `sin`, …
- …

Measures

1. `dx`: the interior of the domain Ω (`dx`, cell integral);
2. `ds`: the boundary $\partial\Omega$ of Ω (`ds`, exterior facet integral);
3. `dS`: the set of interior facets Γ (`dS`, interior facet integral).

在区域内部的边界上积分时, 需要使用 dS 并使用限制算子 + 或 -, 如:

```
a = u('+')*v('+')*dS
```

Check UFL form

[5]:
```
from firedrake import *
import ufl

N = 8
test_mesh = RectangleMesh(nx=N, ny=N, Lx=1, Ly=1)
V = FunctionSpace(test_mesh, 'CG', degree=1)
u, v = TrialFunction(V), TestFunction(V)
a = inner(grad(u), grad(v))*dx + inner(Constant(0), v)*dx

print(ufl.formatting.printing.tree_format(a))
```

output
```
Form:
    Integral:
        integral type: cell
        subdomain id: everywhere
        integrand:
            Conj
                Inner
                (
                    Grad
Argument(WithGeometry(FunctionSpace(<firedrake.mesh.MeshTopology object at
0x7f9f80207400>, FiniteElement('Lagrange', triangle, 1), name=None),
Mesh(VectorElement(FiniteElement('Lagrange', triangle, 1), dim=2), 7)), 0, None)
                    Grad
Argument(WithGeometry(FunctionSpace(<firedrake.mesh.MeshTopology object at
0x7f9f80207400>, FiniteElement('Lagrange', triangle, 1), name=None),
Mesh(VectorElement(FiniteElement('Lagrange', triangle, 1), dim=2), 7)), 1, None)
                )
    Integral:
        integral type: cell
        subdomain id: everywhere
        integrand:
            Product
            (
                Constant(FiniteElement('Real', None, 0), 12)
                Conj
Argument(WithGeometry(FunctionSpace(<firedrake.mesh.MeshTopology object at
0x7f9f80207400>, FiniteElement('Lagrange', triangle, 1), name=None),
Mesh(VectorElement(FiniteElement('Lagrange', triangle, 1), dim=2), 7)), 0, None)
            )
```

1.1.4 函数空间创建

- FunctionSpace 标量函数空间
- VectorFunctionSpace 向量函数空间
- MixedFunctionSpace 混合空间

支持的单元类型: CG, DG, RT, BDM, …

Reference: https://firedrakeproject.org/variational-problems.html#supported-finite-elements

1.1.5 线性方程组参数设置

三种求解方程组 Coding 方式 仍然以上述 Poisson 方程为例: Possion Example

可以使用 `%load` 加载文件内容到 notebook 中

`%load py/possion_example1.py`

[6]:
```
# %load py/possion_example1.py
from firedrake import *
from firedrake.petsc import PETSc

methods = ['solve',
           'assemble',
           'LinearVariationalSolver']

# Get commandline args
opts = PETSc.Options()
case_index = opts.getInt('case_index', default=0)
if case_index < 0 or case_index > 2:
    raise Exception('Case index must be in [0, 2]')

case = methods[case_index]

N = 8
test_mesh = RectangleMesh(nx=N, ny=N, Lx=1, Ly=1)
x, y = SpatialCoordinate(test_mesh)
f = sin(pi*x)*sin(pi*y)
g = Constant(0)

V = FunctionSpace(test_mesh, 'CG', degree=1)

u, v = TrialFunction(V), TestFunction(V)

a = inner(grad(u), grad(v))*dx
L = inner(f, v)*dx                    # or f*v*dx

bc = DirichletBC(V, g=g, sub_domain='on_boundary')

u_h = Function(V, name='u_h')

if case == 'solve':
    PETSc.Sys.Print('Case: solve')
    # solve(a == L, u_h, bcs=bc)
    solve(a == L, u_h, bcs=bc,
          solver_parameters={           # 设置方程组求解算法
              # 'ksp_view': None,
              'ksp_type': 'preonly',
              'pc_type': 'lu',
              'pc_factor_mat_solver_type': 'mumps'
          },
          options_prefix='test'         # 命令行参数前缀
         )


elif case == 'assemble':
    PETSc.Sys.Print('Case: assemble')
    A = assemble(a, bcs=bc)
    b = assemble(L, bcs=bc)
    solve(A, u_h, b,
          options_prefix='test'
         )

elif case == 'LinearVariationalSolver':
    PETSc.Sys.Print('Case: LinearVariationalSolver')
    problem = LinearVariationalProblem(a, L, u_h, bcs=bc)
    solver = LinearVariationalSolver(problem,
                                     solver_parameters={
                                         # 'ksp_view': None,
                                         'ksp_monitor': None,
                                         'ksp_converged_reason': None,
                                         'ksp_type': 'cg',
                                         'pc_type': 'none'
                                     },
                                     options_prefix='test')

    solver.solve()
else:
    raise Exception(f'Unknow case: {case}')

File('pvd/poisson_example.pvd').write(u_h)
```

output

```
Case: solve
```

- KSP (Krylov subspace solver with preconditioner)
  - https://petsc.org/main/manualpages/KSP/index.html

  参数: https://petsc.org/main/manual/ksp/#tab-kspdefaults

  关于检查 KSP 的收敛结果请参考下面 4.2 节 KSP.

- PC

  参数: https://petsc.org/main/manual/ksp/#tab-pcdefaults

  - 外部包 pc 参数: https://petsc.org/main/manual/ksp/#tab-externaloptions

命令行参数 Reference:

1. https://petsc.org/main/manualpages/KSP/KSPSetErrorIfNotConverged/

参数说明

1. `mat_type`: `aij` 或 `matfree`
2. `ksp_type`: 设置迭代法
3. `pc_type`: 设置预处理方式
4. `pc_factor_mat_solver_type`: 设置使用做矩阵分解的包
5. `ksp_monitor`: 输出每步迭代的残差
6. `ksp_view`: 迭代完成后输出 ksp 的设置等内容
7. `ksp_converged_reason`: 输出收敛或不收敛的原因
8. `ksp_error_if_not_converged`: 不收敛时, 输出错误信息, 并停止.

LU 分解参数设置

Ref:

1. https://petsc.org/main/src/dm/impls/stag/tutorials/ex4.c.html
2. https://petsc.org/main/manualpages/Mat/MatSolverType/

`-ksp_type preonly -pc_type lu -pc_factor_mat_solver_type mumps`

选项 `pc_factor_mat_solver_type` 用于设置 LU 分解使用的 package, 如 petsc, umfpack, superlu, mkl_pardiso, mumps, superlu_dist, mkl_cpardiso 等.

多重网格

https://nbviewer.org/github/firedrakeproject/firedrake/blob/master/docs/notebooks/07-geometric-multigrid.ipynb

终端演示: 设置命令行参数控制线性方程组的求解

```
python py/possion_example1.py -case solve \
    -ksp_monitor -ksp_converged_reason \
    -ksp_type cg -pc_type jacobi

python py/possion_example1.py -case assemble \
    -ksp_monitor -ksp_converged_reason \
    -ksp_type gmres -pc_type none

python py/possion_example1.py -case LinearVariationalSolver \
    -ksp_monitor -ksp_converged_reason \
    -ksp_type minres -pc_type none
```

1.1.6 数值积分公式

查看数值积分公式

[7]:
```python
import FIAT
import finat
from pprint import pprint

ref_cell = FIAT.reference_element.UFCTriangle()

ret = {}
for i in range(0, 4):
    qrule = finat.quadrature.make_quadrature(ref_cell, i)
    ret[i] = {'points': qrule.point_set.points, 'weights': qrule.weights}

pprint(ret)
```

output

```
{0: {'points': array([[0.33333333, 0.33333333]]), 'weights': array([0.5])},
 1: {'points': array([[0.33333333, 0.33333333]]), 'weights': array([0.5])},
 2: {'points': array([[0.16666667, 0.16666667],
       [0.16666667, 0.66666667],
       [0.66666667, 0.16666667]]),
     'weights': array([0.16666667, 0.16666667, 0.16666667])},
 3: {'points': array([[0.65902762, 0.23193337],
       [0.65902762, 0.10903901],
       [0.23193337, 0.65902762],
       [0.23193337, 0.10903901],
       [0.10903901, 0.65902762],
       [0.10903901, 0.23193337]]),
     'weights': array([0.08333333, 0.08333333, 0.08333333, 0.08333333,
0.08333333,
       0.08333333])}}
```

显示选择积分公式

[8]:
```
import logging

# Disable warnings. If we do not do this, there will be warnings:
#     UFL:WARNING Applying str() to a metadata value of type QuadratureRule, don't know if this␣
 ↪is safe.
level = logging.getLogger().level
set_log_level(CRITICAL) # Disable warnings


mesh = RectangleMesh(nx=8, ny=8, Lx=1, Ly=1)
V = FunctionSpace(mesh, 'CG', 1)
cell = V.finat_element.cell

x, y = SpatialCoordinate(mesh)
f = x**3 + y**4 + x**2*y**2

for i in range(0, 5):
    qrule = finat.quadrature.make_quadrature(ref_cell, i)
    ret[i] = {'points': qrule.point_set.points, 'weights': qrule.weights}
    v = assemble(f*dx(scheme=qrule))
    print(f'degree={i}, v = {v}', )

print('Default:  v =', assemble(f*dx(scheme=None)))

# restore the log level
set_log_level(level) # restore log level
```

output

```
degree=0, v = 0.5579329125675148
degree=1, v = 0.5579329125675148
degree=2, v = 0.5611099431544168
degree=3, v = 0.5611100938585061
degree=4, v = 0.5611111111111102
Default:  v = 0.5611111111111102
```

output

```
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
```

```
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
```

自定义数值积分

[9]:
```python
from firedrake import *
import FIAT
import finat
import numpy as np

ref_cell = FIAT.reference_element.UFCTriangle()
print('vertices:', ref_cell.vertices)

point_set = finat.quadrature.PointSet(ref_cell.vertices)
weights = [1/6, 1/6, 1/6]

qrule = finat.quadrature.QuadratureRule(point_set, weights)

print("points: ", qrule.point_set.points)
print("weights: ", qrule.weights)

mesh = RectangleMesh(nx=8, ny=8, Lx=1, Ly=1)
x = SpatialCoordinate(mesh)
print("integral of x[0] on domain by default scheme: ", assemble(x[0]*dx))
print("integral of x[0] on domain by new defined-scheme: ", assemble(x[0]*dx(scheme=qrule)))
```

output
```
vertices: ((0.0, 0.0), (1.0, 0.0), (0.0, 1.0))
points:  [[0. 0.]
 [1. 0.]
 [0. 1.]]
weights:  [0.16666667 0.16666667 0.16666667]
integral of x[0] on domain by default scheme:  0.49999999999999994
integral of x[0] on domain by new defined-scheme:  0.4999999999999957
```

output
```
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
```

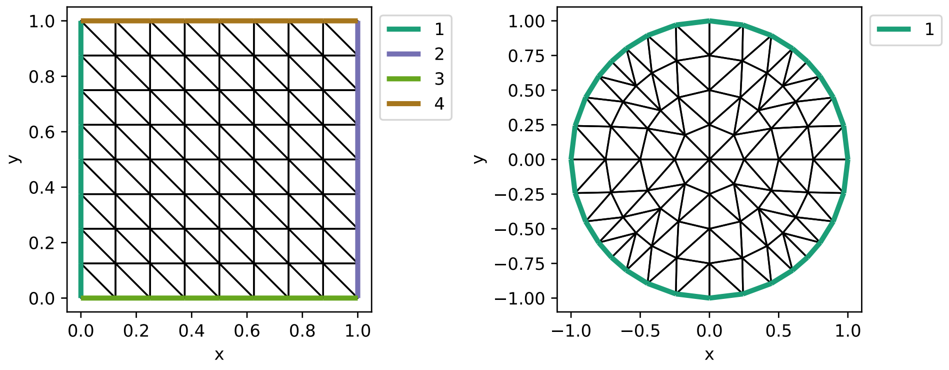
1.1.7 Dirichlet bounary conditions

Tags of the boundaries of builtin meshes `RectangleMesh`:

- 1: plane x == 0
- 2: plane x == Lx
- 3: plane y == 0
- 4: plane y == Ly

[10]:
```python
from firedrake import *
import matplotlib.pyplot as plt
from py.intro_utils import plot_mesh_with_label
```

```
N = 8
rect_mesh = RectangleMesh(nx=N, ny=N, Lx=1, Ly=1)
circ_mesh = UnitDiskMesh(2)

fig, ax = plt.subplots(1, 2, figsize=[8, 4])
plot_mesh_with_label(rect_mesh, axes=ax[0])
plot_mesh_with_label(circ_mesh, axes=ax[1])
fig.tight_layout()
```

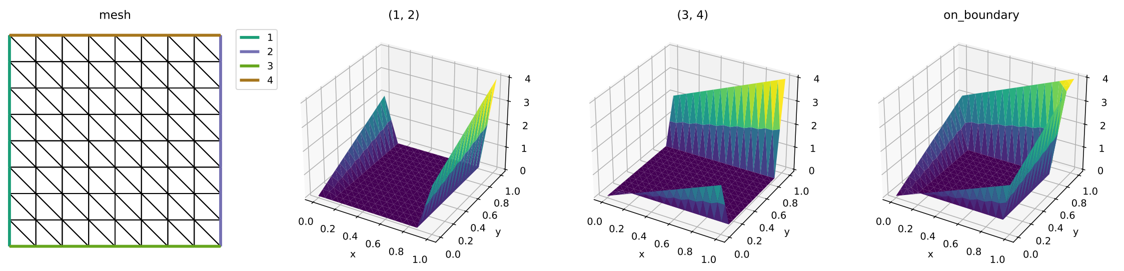


Set Dirichlet boundary conditions

[11]:
```
N = 8
test_mesh = RectangleMesh(nx=N, ny=N, Lx=1, Ly=1)
x, y = SpatialCoordinate(test_mesh)

g = x*2 + y*2
V = FunctionSpace(test_mesh, 'CG', degree=1)


def trisurf_bdy_condition(V, g, sub_domain, axes=None):
    bc = DirichletBC(V, g=g, sub_domain=sub_domain)
    g = Function(V)
    bc.apply(g)

    trisurf(g, axes=axes)
    if axes:
        axes.set_xlabel('x')
        axes.set_ylabel('y')
        axes.set_title(sub_domain)
```

[12]:
```
# plot the mesh and boundry conditons
fig, ax = plt.subplots(1, 4, figsize=[16, 4], subplot_kw=dict(projection='3d'))
ax = ax.flat

ax[0].remove()
ax[0] = fig.add_subplot(1, 4, 1)
plot_mesh_with_label(test_mesh, ax[0])
ax[0].set_title('mesh')
ax[0].axis('off')

sub_domains = [(1, 2), (3, 4), 'on_boundary']
for i in range(3):
    trisurf_bdy_condition(V, g=g, sub_domain=sub_domains[i], axes=ax[i+1])
```

```
fig.tight_layout()
```



sub_domain of DirichletBC The following comments are copy from `firedrake/bcs.py`

```
# Define facet, edge, vertex using tuples:
# Ex in 3D:
#           user input                                         returned keys
# facet  = ((1, ), )              ->     ((2, ((1, ), )), (1, ()),         (0, ()))
# edge   = ((1, 2), )             ->     ((2, ()),        (1, ((1, 2), )), (0, ()))
# vertex = ((1, 2, 4), )          ->     ((2, ()),        (1, ()),         (0, ((1, 2, 4),
↪  ))
#
# Multiple facets:
# (1, 2, 4) := ((1, ), (2, ), (4,))   ->     ((2, ((1, ), (2, ), (4, ))), (1, ()), (0, ()))
#
# One facet and two edges:
# ((1,), (1, 3), (1, 4))              ->     ((2, ((1,),)), (1, ((1,3), (1, 4))), (0, ()))
```

1.1.8 Gmsh 网格边界设置

需要在 gmsh 中给相应的边界加上标签 (Physical Tag)

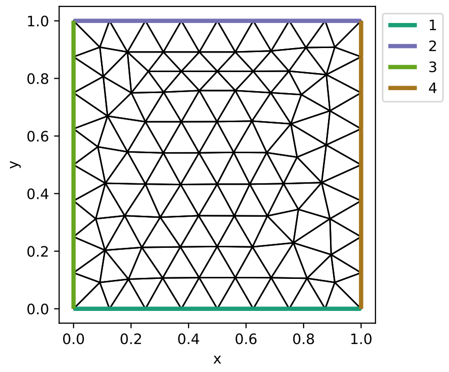
gmsh gui 演示: 生成如下 `geo` 文件和 `msh` 文件

File: `gmsh/rectangle.geo`

```
// Gmsh project created on Tue Sep 30 15:09:53 2022
SetFactory("OpenCASCADE");
//+
Rectangle(1) = {0, 0, 0, 1, 1, 0};
//+
Physical Curve("lower", 1) = {1};
//+
Physical Curve("upper", 2) = {3};
//+
Physical Curve("left", 3) = {4};
//+
Physical Curve("right", 4) = {2};
//+
Physical Surface("domain", 1) = {1};
```

Gmsh file: `gmsh/rectangle.msh`

[13]:
```
from firedrake import *
from firedrake.petsc import PETSc
from py.intro_utils import plot_mesh_with_label

# opts = PETSc.Options()
# opts.insertString('-dm_plex_gmsh_mark_vertices True')

gmsh_mesh = Mesh('gmsh/rectangle.msh')
plot_mesh_with_label(gmsh_mesh)
```

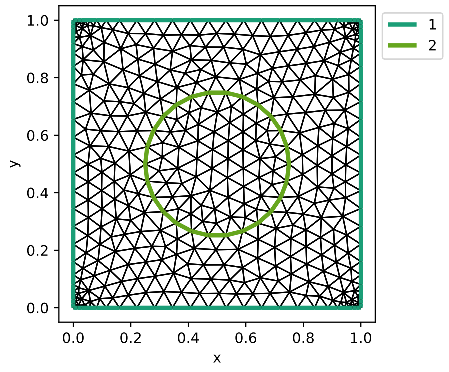


使用 *gmsh* 的 *python SDK*: gmsh 或者 pygmsh

example: `py/make_mesh_circle_in_rect.py`

[14]:
```
from firedrake import *
from py.intro_utils import plot_mesh_with_label
from py.make_mesh_circle_in_rect import make_circle_in_rect

h = 1/16
filename = 'gmsh/circle_in_rect.msh'
make_circle_in_rect(h, filename, p=3, gui=False)

cr_mesh = Mesh(filename)
plot_mesh_with_label(cr_mesh)
```

output
```
Info    : Writing 'gmsh/circle_in_rect.msh'…
Info    : Done writing 'gmsh/circle_in_rect.msh'
```



1.2 纯 Neumann 边界条件

求解如下 Poisson 方程

$$\begin{aligned} -\Delta u &= f && \text{in} \quad \Omega, \\ \frac{\partial u}{\partial n} &= g_N && \text{on} \quad \partial\Omega, \end{aligned} \tag{4}$$

变分问题

求 $u \in H^1$, 且 $\int_\Omega u = 0$ 使得

$$\int_\Omega \nabla u \cdot \nabla v = \int_\Omega f v + \int_{\partial\Omega} g_N v \qquad \forall v \in H^1. \tag{5}$$

兼容性条件

$$\int_\Omega f v + \int_{\partial\Omega} g_N v = 0$$

1.2.1 Use nullspace of solve

通过 nullspace 求出的解 `u_h` 并不满足积分为 0, 而是其对应的解向量的范数最小, 所以我们需要做后处理得到积分为 0 的解:

```
s = assemble(u_h*dx)/assemble(Constant(1)*dx(domain=mesh)
u_h.assign(u_h - s)
```

Reference:

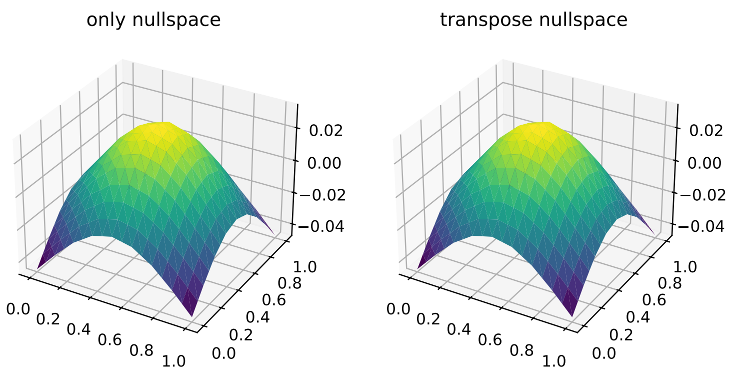
1. https://petsc.org/main/manual/ksp/#solving-singular-systems
2. https://petsc.org/main/manualpages/KSP/KSPSolve/
3. https://petsc.org/main/manualpages/Mat/MatSetNullSpace/

[15]:
```
from firedrake import *

N = 8
test_mesh = RectangleMesh(nx=N, ny=N, Lx=1, Ly=1)
x, y = SpatialCoordinate(test_mesh)
f = sin(pi*x)*sin(pi*y)

subdomain_id = None # None for all boundray, 或者单个编号 如 1, 或者使用 list 或 tuple 如: (1, 2)

if False:
    # 不满足兼容性条件
    g = Constant(1)
else:
    # 满足兼容性条件
    length = assemble(1*ds(domain=test_mesh, subdomain_id=subdomain_id))
    g = Constant(-assemble(f*dx)/length)
    # g = Constant(-1/pi**2)

V = FunctionSpace(test_mesh, 'CG', degree=1)
u, v = TrialFunction(V), TestFunction(V)
a = inner(grad(u), grad(v))*dx
L = inner(f, v)*dx + inner(g, v)*ds(subdomain_id=subdomain_id)
```

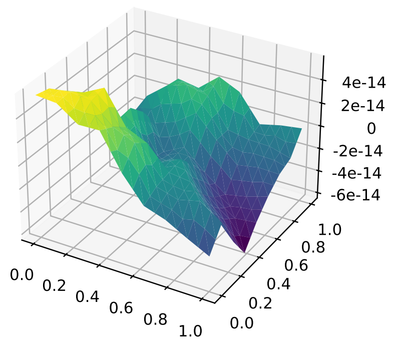
```python
u1_h = Function(V, name='u1_h')

nullspace = VectorSpaceBasis(constant=True, comm=test_mesh.comm)

solve(a == L, u1_h,
      solver_parameters={
          # 'ksp_view': None,
          'ksp_monitor': None,
      },
      options_prefix='test1',
      nullspace=nullspace,
      transpose_nullspace=None)

u2_h = Function(V, name='u2_h')
solve(a == L, u2_h,
      solver_parameters={
          # 'ksp_view': None,
          'ksp_monitor': None,
      },
      options_prefix='test2',
      nullspace=nullspace,
      transpose_nullspace=nullspace)

# 通过 nullspace 求出的解并不满足积分为 0, 需要做后处理
omega = assemble(Constant(1)*dx(domain=test_mesh))
s1 = assemble(u1_h*dx)/omega
u1_h.dat.data_with_halos[:] = u1_h.dat.data_ro_with_halos[:] - s1

s2 = assemble(u2_h*dx)/omega
u2_h.dat.data_with_halos[:] = u2_h.dat.data_ro_with_halos[:] - s2

fig, ax = plt.subplots(1, 2, figsize=[8, 4], subplot_kw=dict(projection='3d'))
ts1 = trisurf(u1_h, axes=ax[0])
title1 = ax[0].set_title('only nullspace')
ts2 = trisurf(u2_h, axes=ax[1])
title2 = ax[1].set_title('transpose nullspace')
```

output

```
Residual norms for test1_ solve.
0 KSP Residual norm 9.134205437239e-02
1 KSP Residual norm 2.635631193496e-13
Residual norms for test2_ solve.
0 KSP Residual norm 9.134205437239e-02
1 KSP Residual norm 1.416258567001e-16
```



```
[16]: fig, ax = plt.subplots(figsize=[4, 4], subplot_kw=dict(projection='3d'))
err = Function(u1_h).assign(u1_h - u2_h)
trisurf(err, axes=ax)

# The z ticklabel do not show properly, when the values are small.
# we set the major formatter to make it show correctly
fmt = lambda x, pos: f'{x:10g}'
ax.zaxis.set_major_formatter(fmt)

# ax.ticklabel_format(axis='z', style='plain') # may work for not too small values
```



1.2.2 Using Lagrange multiplier

变分问题

求 $u \in H^1, \mu \in R$ 使得

$$\begin{aligned}&\int_\Omega \nabla u \cdot \nabla v + \mu \int_\Omega v - \int_\Omega f v - \int_{\partial\Omega} g_N v = 0, \quad \forall \in H^1\\ &\eta \int_\Omega u = 0, \quad \forall \eta \in \mathbb{R}\end{aligned} \tag{6}$$

```
[17]: # %load possion_neumann_lagrange.py
from firedrake import *
from firedrake.petsc import PETSc

opts = PETSc.Options()
N = opts.getInt('N', default=8)
test_mesh = RectangleMesh(nx=N, ny=N, Lx=1, Ly=1)

x, y = SpatialCoordinate(test_mesh)
f = sin(pi*x)*sin(pi*y)

subdomain_id = None
length = assemble(1*ds(domain=test_mesh, subdomain_id=subdomain_id))
g = Constant(-assemble(f*dx)/length)
# g = Constant(-1/pi**2)

V = FunctionSpace(test_mesh, 'CG', degree=1)
R = FunctionSpace(test_mesh, 'R', 0)

W = MixedFunctionSpace([V, R]) # or W = V*R
```

```
u, mu = TrialFunction(W)
v, eta = TestFunction(W)

a = inner(grad(u), grad(v))*dx + inner(mu, v)*dx + inner(u, eta)*dx
L = inner(f, v)*dx + inner(g, v)*ds(subdomain_id=subdomain_id)

w_h = Function(W)
solve(a == L, w_h,
      solver_parameters={
          # 'mat_type': 'nest',
          # 'ksp_view': None,
          # 'pc_type': 'fieldsplit',
          # 'ksp_monitor': None,
      },
      options_prefix='test')

u_h, mu_h  = w_h.subfunctions

filename = 'pvd/u_h_neumann.pvd'
PETSc.Sys.Print(f'Write pvd file: {filename}')
File(filename).write(u_h)
```

output

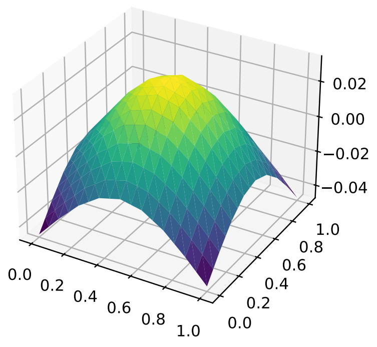
```
firedrake:WARNING Real block detected, generating Schur complement elimination
PC
```

output

```
Write pvd file: pvd/u_h_neumann.pvd
```

[18]:

```
fig, ax = plt.subplots(figsize=[4, 4], subplot_kw=dict(projection='3d'))
ts = trisurf(u_h, axes=ax)
```



终端演示

```
$ python possion_neumann_lagrange.py -test_ksp_monitor -test_ksp_converged_reason -N 64
Number of Dofs: 4226
firedrake:WARNING Real block detected, generating Schur complement elimination PC
    Residual norms for test_ solve.
    0 KSP Residual norm 2.501422711621e-01
    1 KSP Residual norm 1.747929427611e-01
    2 KSP Residual norm 1.071502741145e-14
  Linear test_ solve converged due to CONVERGED_RTOL iterations 2
Write pvd file: pvd/u_h_neumann.pvd

$ mpiexec -n 2 python possion_neumann_lagrange.py \
    -test_ksp_monitor -test_ksp_converged_reason -N 64
```

```
Number of Dofs: 4226
firedrake:WARNING Real block detected, generating Schur complement elimination PC
    Residual norms for test_ solve.
    0 KSP Residual norm 2.501422711621e-01
    1 KSP Residual norm 2.085403806063e-02
    2 KSP Residual norm 9.317076546546e-16
  Linear test_ solve converged due to CONVERGED_RTOL iterations 2
Write pvd file: pvd/u_h_neumann.pvd
```

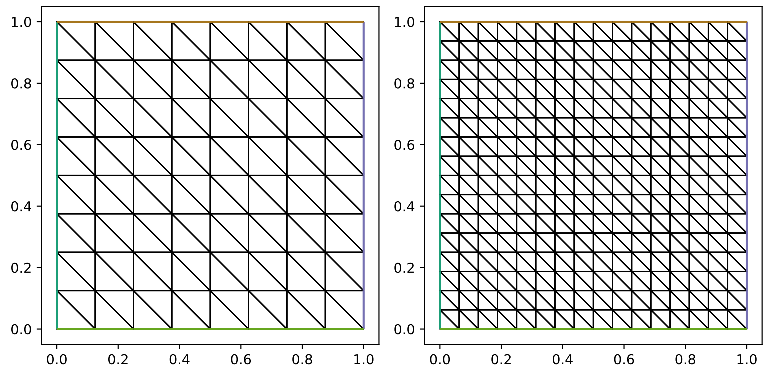
1.3 计算收敛阶

- 和真解对比
- 和参考解对比
- 相邻三层之间对比 (Cauchy 序列): py/possion_convergence.py

1.3.1 生成网格序列

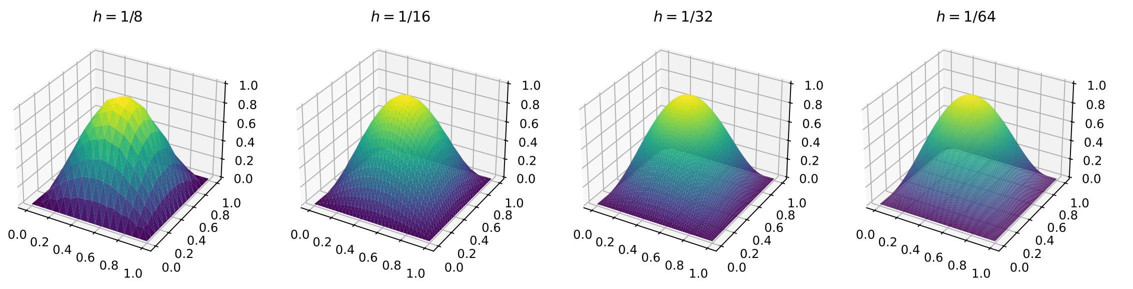
```
base = RectangleMesh(N, N, 1, 1)
meshes = MeshHierarchy(test_mesh, refinement_levels=4)
```

[19]:
```python
from firedrake import *
import matplotlib.pyplot as plt

N = 8
base = RectangleMesh(N, N, 1, 1)
meshes = MeshHierarchy(base, refinement_levels=3)

n = len(meshes)
m = min(2, n)
fig, ax = plt.subplots(1, m, figsize=[4*m, 4])
for i in range(m):
    triplot(meshes[i], axes=ax[i])
fig.tight_layout()
```



[20]:
```python
us = []
for mesh in meshes:
    x, y = SpatialCoordinate(mesh)
    f = sin(pi*x)*sin(pi*y)
    V = FunctionSpace(mesh, 'CG', degree=1)
    u = Function(V).interpolate(f)
    us.append(u)
```

```
m = min(4, n)
fig, ax = plt.subplots(1, 4, figsize=[4*4, 4], subplot_kw=dict(projection='3d'))
ax = ax.flat
for i in range(n):
    trisurf(us[i], axes=ax[i])
    ax[i].set_title(f'$h=1/{N*2**i}$')
```



1.3.2 投影到细网格上的空间中

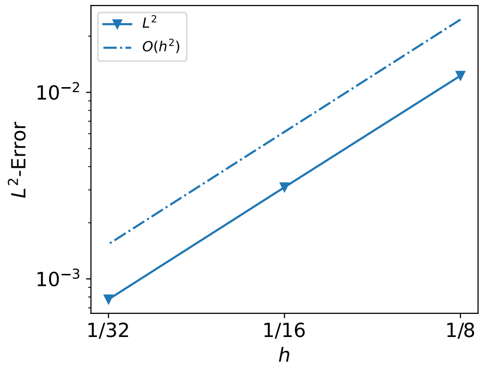
目前 Firedrake 只能投影函数到相邻层的网格上 (由 MeshHierarchy 生成的网格), 和最密网格比较时可以多次投影, 直至最密网格, 然后比较结果.

下面我们仅比较相邻层的误差

[21]:
```
errors = []
hs = []
for i, u in enumerate(us[:-1]):
    u_ref = us[i+1]
    u_inter = project(u, u_ref.function_space())
    error = errornorm(u_ref, u_inter)
    errors.append(error)
    hs.append(1/(N*2**i))

hs, errors
```

[21]:
```
([0.125, 0.0625, 0.03125],
 [0.012284003199971312, 0.003100763810085326, 0.000777061416610528])
```

[22]:
```
from py.intro_utils import plot_errors
plot_errors(hs, errors, expect_order=2)
```

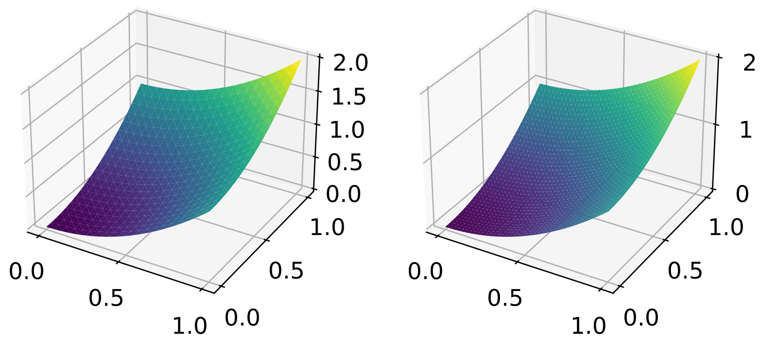


1.3.3 插值到细网格上的空间中

- VertexOnlyMesh
- PointCloud: https://github.com/lrtfm/fdutils

Example of `PointCloud` Interpolate function `f1` on mesh `m1` to function `f2` on mesh `m2`

[23]:
```python
import firedrake as fd
from fdutils import PointCloud
from fdutils.tools import get_nodes_coords
import matplotlib.pyplot as plt

m1 = fd.RectangleMesh(10, 10, 1, 1)
V1 = fd.FunctionSpace(m1, 'CG', 2)
x, y = fd.SpatialCoordinate(m1)
f1 = fd.Function(V1).interpolate(x**2 + y**2)

m2 = fd.RectangleMesh(20, 20, 1, 1)
V2 = fd.FunctionSpace(m2, 'CG', 3)
f2 = fd.Function(V2)

points = get_nodes_coords(f2)
pc = PointCloud(m1, points, tolerance=1e-12)
f2.dat.data_with_halos[:] = pc.evaluate(f1)

fig, ax = plt.subplots(1, 2, figsize=[8, 4], subplot_kw=dict(projection='3d'))
ts1 = fd.trisurf(f1, axes=ax[0])
ts2 = fd.trisurf(f2, axes=ax[1])
```



计算误差

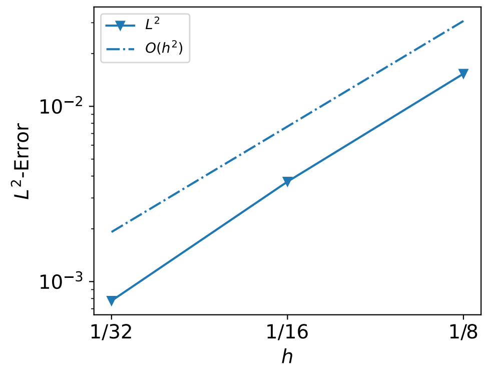
[24]:
```python
from fdutils.tools import errornorm as my_errornorm

my_errors_0 = []
for i, u in enumerate(us[:-1]):
    # 和相邻层结果比较
    my_errors_0.append(my_errornorm(u, us[i+1], tolerance=1e-12))

my_errors_0
```

[24]:
```
[0.012284003212205774, 0.003100763847789645, 0.0007770614201378605]
```

[25]:
```
from fdutils.tools import errornorm as my_errornorm

my_errors = []
for i, u in enumerate(us[:-1]):
    # 和最密层结果比较
    my_errors.append(my_errornorm(u, us[-1], tolerance=1e-12))

my_errors
```

[25]:
```
[0.015349062780286471, 0.003718192030819568, 0.0007770614201378605]
```

[26]:
```
from py.intro_utils import plot_errors
plot_errors(hs, my_errors, expect_order=2)
```



1.4 网格尺寸和质量

1.4.1 网格尺寸

网格尺寸 `CellDiameter` 和 `CellSize` 一样, 均为最长边.

也可以直接用 `mesh.cell_sizes` , 这个函数是 `CellSize` 在连续空间 P1 的投影.

内切圆半径 `Circumradius`

注: 只能作用于线性网格

[27]:
```
from firedrake import *

mesh = RectangleMesh(1, 1, 1, 1)
V = FunctionSpace(mesh, 'DG', 0)

d = CellDiameter(mesh)
d_int = Function(V).interpolate(d)

r = Circumradius(mesh)    # 内切圆半径
r_int = Function(V).interpolate(r)

size = mesh.cell_sizes
```

[28]:
```
d_int.dat.data, size.dat.data, r_int.dat.data,
```

[28]:
```
(array([1.41421356, 1.41421356]),
 array([1.41421356, 1.41421356, 1.41421356, 1.41421356]),
 array([0.70710678, 0.70710678]))
```

[29]:
```
CellDiameter?
```

```
Init signature: CellDiameter(domain)
Docstring:
UFL geometry representation: The diameter of the cell, i.e.,
maximal distance of two points in the cell.
File:           ~/firedrake/real-int32-mkl-debug/src/ufl/ufl/geometry.py
Type:           type
Subclasses:
```

[30]:
```
Circumradius?
```

```
Init signature: Circumradius(domain)
Docstring:      UFL geometry representation: The circumradius of the cell.
File:           ~/firedrake/real-int32-mkl-debug/src/ufl/ufl/geometry.py
Type:           type
Subclasses:
```

1.4.2 网格质量

仅作用于线性网格

[31]:
```
from firedrake import *

def get_quality_3d(mesh):
    kernel = r'''
    void get_quality(double coords[4][3], double v[1], double q[1]){
        double a, b, c, p;
        double ls[6];
        double s, r, R, _tmp;
        double v1[3], v2[3], v3[3];
        int idx[6][2] = {{0, 1}, {2, 3}, {0, 2}, {1, 3}, {0, 3}, {1, 2}};
        int idx2[4][3] = {{0, 1, 2}, {0, 2, 3}, {1, 2, 3}, {0, 1, 3}};
        for (int i=0; i < 6; i++){
            _tmp = 0;
            for (int j=0; j < 3; j++){
                _tmp += pow(coords[idx[i][0]][j] - coords[idx[i][1]][j], 2.0);
            }
            ls[i] = sqrt(_tmp);
        }
        a = ls[0]*ls[1];
        b = ls[2]*ls[3];
        c = ls[4]*ls[5];
        p = (a + b + c)/2;

        s = 0;
        for (int i=0; i < 4; i++){
            for (int j = 0; j < 3; j++){
                v1[j] = coords[idx2[i][2]][j] - coords[idx2[i][0]][j];
                v2[j] = coords[idx2[i][2]][j] - coords[idx2[i][1]][j];
            }
            v3[0] =   v2[1]*v1[2] - v2[2]*v1[1];
            v3[1] = - v2[0]*v1[2] + v2[2]*v1[0];
            v3[2] =   v2[0]*v1[1] - v2[1]*v1[0];
            s += sqrt(pow(v3[0], 2.0) + pow(v3[1], 2.0) + pow(v3[2], 2.0))/2;
        }

        R = sqrt(p*(p-a)*(p-b)*(p-c))/v[0]/6.0;
        r = 3*v[0]/s;
        q[0] = r/R;
    }
    '''

    coords =  mesh.coordinates
    V = FunctionSpace(mesh, 'DG', 0)
    volume = Function(V).interpolate(CellVolume(mesh))
    quality = Function(V)

    cell_node_map = quality.cell_node_map()
    op2.par_loop(op2.Kernel(kernel, 'get_quality'), cell_node_map.iterset,
                 coords.dat(op2.READ, coords.cell_node_map()),
                 volume.dat(op2.READ, cell_node_map),
                 quality.dat(op2.WRITE, cell_node_map))

    return quality

def get_quality_2d(mesh):
    V = FunctionSpace(mesh, 'DG', 0)
    quality = Function(V)
    kernel = '''
    // B[2] - B[0], B[3] - B[1]
    // B[4] - B[0], B[5] - B[1]
    double S, a, b, c, R, r;
    S = fabs((B[5] - B[1])*(B[2] - B[0])  - (B[3] - B[1])*(B[4] - B[0]));
    a = sqrt(pow(B[2] - B[0], 2.) + pow(B[3] - B[1], 2.));
    b = sqrt(pow(B[4] - B[2], 2.) + pow(B[5] - B[3], 2.));
    c = sqrt(pow(B[0] - B[4], 2.) + pow(B[1] - B[5], 2.));
    R = a*b*c/(2*S);
    r = S/(a+b+c);
    A[0] = r/R;
    '''

    par_loop(kernel, \
             dx, \
             {'A': (quality, WRITE), 'B' :(mesh.coordinates, READ)})

    return quality

def get_quality_2d_surface(mesh):
    kernel = r'''
    void get_quality(double coords[3][3], double v[1], double q[1]){
        double p, _tmp, R, r, ls[3];
        double S = v[0];
        int idx[3][2] = {{0, 1}, {1, 2}, {0, 2}};
        for (int i=0; i < 3; i++){
            _tmp = 0;
            for (int j=0; j < 3; j++){
                _tmp += pow(coords[idx[i][0]][j] - coords[idx[i][1]][j], 2.0);
            }
            ls[i] = sqrt(_tmp);
        }
        p = (ls[0] + ls[1] + ls[2])/2;

        // S = sqrt(p*(p-ls[0])*(p-ls[1])*(p-ls[2]));
        R = ls[0]*ls[1]*ls[2]/(4*S);
        r = S/p;
        q[0] = r/R;
    }
    '''

    coords =  mesh.coordinates
    V = FunctionSpace(mesh, 'DG', 0)
    volume = Function(V).interpolate(CellVolume(mesh))
    quality = Function(V)

    cell_node_map = quality.cell_node_map()
    op2.par_loop(op2.Kernel(kernel, 'get_quality'), cell_node_map.iterset,
                 coords.dat(op2.READ, coords.cell_node_map()),
                 volume.dat(op2.READ, cell_node_map),
                 quality.dat(op2.WRITE, cell_node_map))
    return quality
```

2d 和 3d

[32]:
```
mesh2d = RectangleMesh(1, 1, 1, 1)
mesh3d = UnitCubeMesh(1, 1, 1)

q2 = get_quality_2d(mesh2d)
q3 = get_quality_3d(mesh3d)
```

[33]:
```
q2.dat.data, q3.dat.data
```

[33]:
```
(array([0.41421356, 0.41421356]),
 array([0.23914631, 0.23914631, 0.23914631, 0.23914631, 0.23914631,
        0.23914631]))
```

2d 正三角形

[34]:
```
from firedrake.petsc import PETSc
from pyop2.datatypes import IntType

cells = np.array([[0, 1, 2]], dtype=IntType)
coords = np.array([[0.0, 0.0],
                   [1.0, 0.0],
                   [1/2, np.sqrt(3)/2]])

plex = PETSc.DMPlex()
plex.createFromCellList(2, cells, coords)
mesh = Mesh(plex)
q_mesh = get_quality_2d(mesh)
q_mesh.dat.data
```

[34]:
```
array([0.5])
```

曲面网格

[35]:
```
mesh_surf = IcosahedralSphereMesh(1)
q_surf = get_quality_2d_surface(mesh_surf)
q_surf.dat.data
```

[35]:
```
array([0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5,
       0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5])
```

[36]:
```
from firedrake.petsc import PETSc
from pyop2.datatypes import IntType

cells = np.array([[0, 1, 2]], dtype=IntType)
coords = np.array([[0.0, 0.0, 0.0],
                   [1.0, 0.0, 0.0],
                   [1/2, np.sqrt(3)/2, 0.0]])

plex = PETSc.DMPlex()
plex.createFromCellList(2, cells, coords)
mesh = Mesh(plex, dim=3)
q_mesh = get_quality_2d_surface(mesh)
q_mesh.dat.data
```

[36]:
```
array([0.5])
```

1.5 构造等参元

Firedrake 中坐标是通过函数 `Function` 给出的, 可以通过更改该函数的值来移动网格或者构造等参元对应的映射.

1.5.1 修改网格坐标 (移动网格)

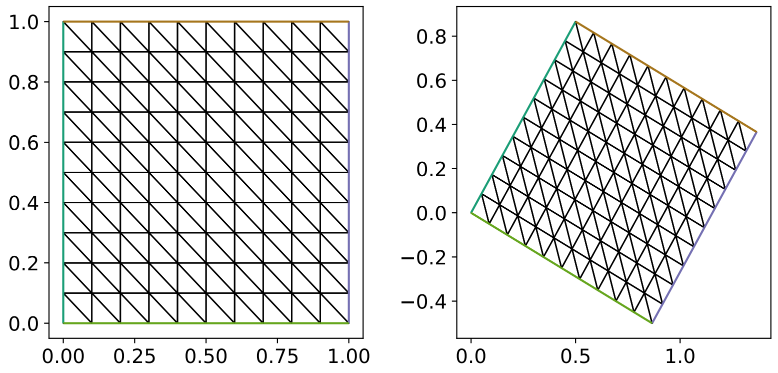
坐标的存储 (numpy 数组)

```
mesh = RectangleMesh(10, 10, 1, 1)
mesh.coordinates.dat.data
mesh.coordinates.dat.data_ro
mesh.coordinates.dat.data_with_halos
mesh.coordinates.dat.data_ro_with_halos
```

单进程运行时 `data` 和 `data_with_halos` 相同. 关于 `halos` 请参考 https://op2.github.io/PyOP2/mpi.html.

[37]:
```
import numpy as np

# test_mesh = UnitDiskMesh(refinement_level=3)
test_mesh = RectangleMesh(10, 10, 1, 1)

fig, ax = plt.subplots(1, 2, figsize=[8, 4])
handle = triplot(test_mesh, axes=ax[0])

theta = np.pi/6
R = np.array([[np.cos(theta), - np.sin(theta)],
              [np.sin(theta),   np.cos(theta)]])

# test_mesh.coordinates.dat.datas[:] = test_mesh.coordinates.dat.data_ro[:]@R
test_mesh.coordinates.dat.data_with_halos[:] = test_mesh.coordinates.dat.data_ro_with_halos[:]@R
```

```
handle = triplot(test_mesh, axes=ax[1])
fig.tight_layout()
```



1.5.2 简单映射边界点

等参元映射通过更改坐标向量场实现: 从线性网格开始构造, 把边界上的自由度移动到边界上. 以单位圆为例:

```
def points2bdy(points):
    r = np.linalg.norm(points, axis=1).reshape([-1, 1])
    return points/r

def make_high_order_mesh_map_bdy(m, p):
    coords = m.coordinates
    V_p = VectorFunctionSpace(m, 'CG', p)
    coords_p = Function(V_p, name=f'coords_p{i}').interpolate(coords)

    bc = DirichletBC(V_p, 0, 'on_boundary')
    points = coords_p.dat.data_ro_with_halos[bc.nodes]
    coords_p.dat.data_with_halos[bc.nodes] = points2bdy(points)

    return Mesh(coords_p)
```

1.5.3 同时移动边界单元的内点

Reference:

1. M. Lenior, Optimal Isoparametric Finite Elements and Error Estimates For Domains Involving Curved Boundaries. SIAM. J. Numer. Anal. 23(3). 1986. pp 562–580.

等参元映射通过更改坐标向量场实现: 从线性网格开始构造, 把边界上的自由度移动到边界上, 同时移动边界单元的内部自由度.

```
def make_high_order_mesh_simple(m, p):
    if p == 1:
        return m

    coords_1 = m.coordinates
    coords_i = coords_1
    for i in range(2, p+1):
        coords_im1 = coords_i
        V_i = VectorFunctionSpace(m, 'CG', i)
        bc = DirichletBC(V_i, 0, 'on_boundary')
        coords_i = Function(V_i, name=f'coords_p{i}').interpolate(coords_im1)
        coords_i.dat.data_with_halos[bc.nodes] = \
            points2bdy(coords_i.dat.data_ro_with_halos[bc.nodes])

    return Mesh(coords_i)
```

注: 这是一个简单的实现, 并不完全符合文献 [1] 中等参元映射构造方式, 一个完整的实现方式见文件 py/make_mesh_circle_in_rect.py 中的函数 make_high_order_coords_for_circle_in_rect: 该函数实现了内部具有一个圆形界面的矩形区域上的等参映射.

1.5.4 数值实验

精确解为 $u = 1 - (x^2 + y^2)^{3.5}$

[38]:
```
%run py/possion_convergence_circle.py -max_degree 3 -exact "1 - (x[0]**2 + x[1]**2)**3.5"
```

output
```
Exact solution:  1 - (x[0]**2 + x[1]**2)**3.5

p = 1; Use iso: False; Only move bdy: False.
    Rel. H1 errors: [0.21472147 0.10953982 0.05505367]
            orders: [0.99748178 1.00490702]
    Rel. L2 errors: [0.02973733 0.00764636 0.00192565]
            orders: [2.01284532 2.01420929]

p = 2; Use iso: False; Only move bdy: False.
    Rel. H1 errors: [0.02567607 0.00823192 0.00274559]
            orders: [1.68586184 1.60384374]
    Rel. L2 errors: [0.00804638 0.00197793 0.00048968]
            orders: [2.07953304 2.0391775 ]

p = 2; Use iso: True; Only move bdy: False.
    Rel. H1 errors: [0.02049517 0.00516031 0.0012846 ]
            orders: [2.04399704 2.03112667]
    Rel. L2 errors: [1.32436157e-03 1.65779996e-04 2.05806815e-05]
            orders: [3.07968268 3.04739627]

p = 3; Use iso: False; Only move bdy: False.
    Rel. H1 errors: [0.01465085 0.00517696 0.00182789]
            orders: [1.54172011 1.52063516]
    Rel. L2 errors: [0.00786267 0.00195543 0.00048687]
            orders: [2.06225863 2.03084755]

p = 3; Use iso: True; Only move bdy: True.
    Rel. H1 errors: [2.88080070e-03 5.12223863e-04 9.06665015e-05]
            orders: [2.5595478  2.52924769]
    Rel. L2 errors: [1.06566715e-04 9.18124027e-06 7.97431433e-07]
            orders: [3.63334435 3.56916446]

p = 3; Use iso: True; Only move bdy: False.
    Rel. H1 errors: [1.02564343e-03 1.25126956e-04 1.52758197e-05]
            orders: [3.11780384 3.07186088]
    Rel. L2 errors: [4.46595130e-05 2.69981492e-06 1.63948920e-07]
            orders: [4.15838886 4.09188043]
```

1.6 间断有限元方法

1.6.1 UFL 符号

- +:

  `u('-')`

- -:

  `u('+')`

- avg:

  `(u('+') + u('-'))/2`

- jump:

  `jump(u, n) = u('+')*n('+') + u('-')*n('-')`

  `jump(u) = u('+') - u('-')`

- FacetNormal:

  边界法向

- CellDiameter:

  网格尺寸

1.6.2 UFL 测度

1. `ds` 外部边
2. `dS` 内部边

1.6.3 变分形式

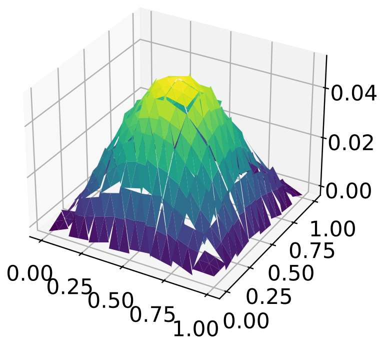
$$\begin{aligned}\int_\Omega \nabla u\cdot\nabla v - \int_{EI}(\{\nabla u\}[vn] + [un]\{\nabla v\}) - \frac{\alpha}{h}\int_{EI}[un][vn] \\ - \int_{EO}(vn\nabla u + un\nabla v) - \frac{\alpha}{h}\int_{EO} uv \\ - \int_\Omega fv - \int_{\partial\Omega_N} g_N v = 0\end{aligned} \tag{7}$$

其中 $[vn] = v^+n^+ + v^-n^-, \{u\} = (u^+ + u^-)/2$

[39]:
```python
mesh = RectangleMesh(8, 8, 1, 1)

DG1 = FunctionSpace(mesh, 'DG', 1)
u, v = TrialFunction(DG1), TestFunction(DG1)

x, y = SpatialCoordinate(mesh)
f = sin(pi*x)*sin(pi*y)

h = Constant(2.0)*Circumradius(mesh)
alpha = Constant(1)
```

```
gamma = Constant(1)

n = FacetNormal(mesh)

a = inner(grad(u), grad(v))*dx \
  - dot(avg(grad(u)), jump(v, n))*dS \
  - dot(jump(u, n), avg(grad(v)))*dS \
  + alpha/avg(h)*dot(jump(u, n), jump(v, n))*dS \
  - dot(grad(u), v*n)*ds \
  - dot(u*n, grad(v))*ds \
  + gamma/h*u*v*ds

L = f*v*dx

u_h = Function(DG1, name='u_h')
bc = DirichletBC(DG1, 0, 'on_boundary')
solve(a == L, u_h, bcs=bc)
```

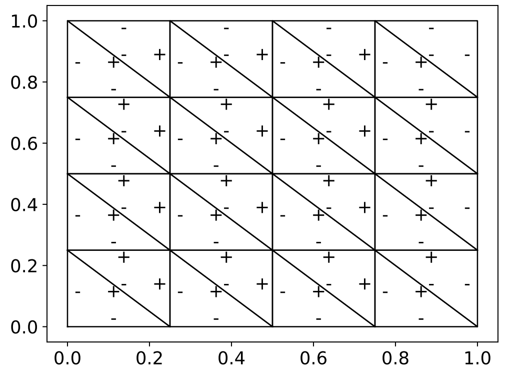
[40]:
```
fig, ax = plt.subplots(figsize=[8, 4], subplot_kw=dict(projection='3d'))
ts = trisurf(u_h, axes=ax)
```



1.6.4 Positive and negative part of inner boundary

[41]:
```
from firedrake import *
from firedrake.petsc import PETSc

import os, sys
import numpy as np
import matplotlib.pyplot as plt
# plt.rcParams.update({'font.size': 14})

N = PETSc.Options().getInt('N', default=4)

m = RectangleMesh(N, N, 1, 1)
V = FunctionSpace(m, 'DG', 0)
Vc = VectorFunctionSpace(m, 'DG', 0)
V_e = FunctionSpace(m, 'HDivT', 0)
V_ec = VectorFunctionSpace(m, 'HDivT', 0)

x, y = SpatialCoordinate(m)
u = Function(V, name='u')
uc = Function(Vc).interpolate(m.coordinates)
u_e = Function(V_e, name='u_e')
```

```
u_ec = Function(V_ec).interpolate(m.coordinates)

ncell = len(u.dat.data_ro)

factor = 0.7
for i in range(ncell):
    cell = V.cell_node_list[i][0]
    u.dat.data_with_halos[:] = 0
    u.dat.data_with_halos[cell] = 1
    es = V_e.cell_node_list[i]
    cc = uc.dat.data_ro_with_halos[cell, :]

    vertex = m.coordinates.dat.data_ro_with_halos[
        m.coordinates.function_space().cell_node_list[i]
    ]
    vertex = np.vstack([vertex, vertex[0]])
    plt.plot(vertex[:, 0], vertex[:, 1], 'k', lw=1)

    for e in es:
        u_e.dat.data_with_halos[:] = 0
        u_e.dat.data_with_halos[e] = 1
        ec = u_ec.dat.data_ro_with_halos[e, :]
        dis = ec - cc

        v_p, v_m = assemble(u('+')*u_e('+')*dS), assemble(u('-')*u_e('-')*dS)
        _x = cc[0] + factor*dis[0]
        _y = cc[1] + factor*dis[1]

        plt.text(_x, _y, '+' if v_p > 0 else '-', ha='center', va='center')

rank, size = m.comm.rank, m.comm.size
if not os.path.exists('figures'):
    os.makedirs('figures')
plt.savefig(f'figures/dgflag_{size}-{rank}.pdf')
```



1.7 Dirac Delta 函数

1.7.1 通过数值积分公式实现 dirac delta 函数

[42]:
```python
from firedrake import *

from firedrake.petsc import PETSc
from pyop2 import op2
from pyop2.datatypes import ScalarType
from mpi4py import MPI
import finat
import numpy as np

import matplotlib.pyplot as plt

set_level(CRITICAL) # Disbale warnings

class DiracOperator(object):
    def __init__(self, m, x0):
        """Make Dirac delta operator at point

        Args:
            m: mesh
            x0: source point

        Example:
            delta = DiracOperator(m, x0)
            f = Function(V)
            f_x0 = assemble(delta(f))
        """
        self.mesh = m
        self.x0 = x0
        self.operator = None

    def __call__(self, f):
        if self.operator is None:
            self._init()
        return self.operator(f)

    def _init(self):
        m = self.mesh
        x0 = self.x0
        V = FunctionSpace(m, 'DG', 0)
        cell_marker = Function(V, name='cell_marker', dtype=ScalarType)
        qrule = finat.quadrature.make_quadrature(V.finat_element.cell, 0)
        cell, X = m.locate_cell_and_reference_coordinate(x0, tolerance=1e-6)

        # c = 0 if X is None else 1
        n_cell_local = len(cell_marker.dat.data)
        if X is not None and cell < n_cell_local:
            c = 1
        else:
            c = 0

        comm = m.comm
        s = comm.size - comm.rank
        n = comm.allreduce(int(s*c), op=MPI.MAX)
        if n == 0:
            raise BaseException("Points not found!")

        k = int(comm.size - n) # get the lower rank which include the point x0

        if c == 1 and comm.rank == k:
            X[X<0] = 0
            X[X>1] = 1
            cell_marker.dat.data[cell] = 1
            comm.bcast(X, root=k)
        else:
            cell_marker.dat.data[:] = 0 # we must set this otherwise the process will hangup
            X = comm.bcast(None, root=k)


        cell_marker.dat.global_to_local_begin(op2.READ)
        cell_marker.dat.global_to_local_end(op2.READ)

        qrule.point_set.points[0] = X
        qrule.weights[0] = qrule.weights[0]/np.real(assemble(cell_marker*dx))

        self.operator = lambda f: f*cell_marker*dx(scheme=qrule)
```

1.7.2 测试 DiracOperator

[43]:
```
def test_dirca_delta_1D():
    test_mesh = IntervalMesh(8, 1)
    V = FunctionSpace(test_mesh, 'CG', 3)
    x1 = 0.683
    source = Constant([x1,])
    delta = DiracOperator(test_mesh, source)

    x, = SpatialCoordinate(test_mesh)
    g = Function(V).interpolate(x**2)

    expected_value =  g.at([x1])
    value = assemble(delta(g))
    PETSc.Sys.Print(f"value = {value}, expected value = {expected_value}")


test_dirca_delta_1D()
```

output
```
value = 0.46648900000000015, expected value = 0.4664890000000098
```

output
```
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
```

[44]:
```
def test_dirca_delta_2D():
    test_mesh = RectangleMesh(8, 8, 1, 1)
    V = FunctionSpace(test_mesh, 'CG', 3)
    x1 = 0.683
    x2 = 0.333
    source = Constant([x1,x2])
    x0 = source
    delta = DiracOperator(test_mesh, source)

    x, y = SpatialCoordinate(test_mesh)
    g = Function(V).interpolate(x**3 + y**3)

    expected_value =  g.at([x1, x2])
    value = assemble(delta(g))
    PETSc.Sys.Print(f"value = {value}, expected value = {expected_value}")


test_dirca_delta_2D()
```

output

```
value = 0.3555380240000009, expected value = 0.3555380240000011
```

output

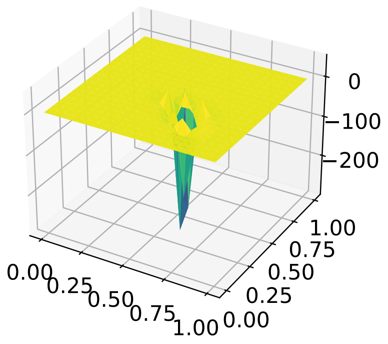
```
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
```

1.7.3 Dirac delta 函数的 L2 投影

[45]:
```
test_mesh = RectangleMesh(10, 10, 1, 1)
V = FunctionSpace(test_mesh, 'CG', 3)
delta = DiracOperator(test_mesh, [0.638, 0.33])
bc = DirichletBC(V, 0, 'on_boundary')
u, v = TrialFunction(V), TestFunction(V)
sol = Function(V)
solve(u*conj(v)*dx == delta(conj(v)), sol, bcs=bc)

fig, ax = plt.subplots(figsize=[8, 4], subplot_kw=dict(projection='3d'))
ts = trisurf(sol, axes=ax) # 为什么负值那么大？
```

output

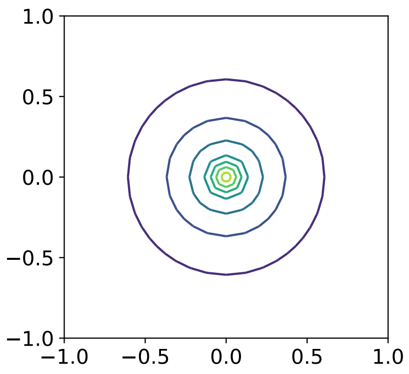
```
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
```



1.7.4 求解源项为 Dirca delta 函数的 Possion 方程

[46]:
```
x0 = [0, 0]
# N = 500
# m = SquareMesh(N, N, 1)

m = UnitDiskMesh(refinement_level=3)

V = FunctionSpace(m, 'CG', 1)

v = TestFunction(V)
u = TrialFunction(V)

a = inner(grad(u), grad(v))*dx
L = DiracOperator(m, x0)(v)
u = Function(V, name='u')

bc = DirichletBC(V, 0, 'on_boundary')

solve(a == L, u, bcs=bc)

# solve(a == L, u)
fig, ax = plt.subplots(figsize=[4, 4])
ts = tricontour(u, axes=ax)
```

output
```
/home/yzz/firedrake/real-int32-mkl-debug/src/ufl/ufl/utils/sorting.py:94:
UserWarning: Applying str() to a metadata value of type QuadratureRule, don't
know if this is safe.
  warnings.warn("Applying str() to a metadata value of type {0}, don't know if
this is safe.".format(type(value).__name__))
```



1.8 自由度映射关系

1.8.1 Cell node map

- `V.dim()`: Number of dofs
- `V.cell_node_list`: an array of cell node map (same with `V.cell_node_map().values`)

[47]:
```
mesh = RectangleMesh(8, 8, 1, 1)
V = FunctionSpace(mesh, 'CG', 1)

# the global numers of the dofs in the first 2 elements
for i in range(2):
    print(f"cell {i}: ", V.cell_node_list[i])
```

output

```
cell 0:  [0 1 2]
cell 1:  [1 2 3]
```

Example: 第一个三角形的坐标

[48]:
```
coords = mesh.coordinates
V_c = coords.function_space()
dof_numbers = V_c.cell_node_list[0]

for i in dof_numbers:
    print(f"vertex {i}:", coords.dat.data_ro_with_halos[i])
```

output

```
vertex 0: [0. 0.]
vertex 1: [0.    0.125]
vertex 2: [0.125 0.   ]
```

1.8.2 Finite element (dofs on reference cell)

[49]:
```
V = FunctionSpace(mesh, 'CG', 2)
element = V.finat_element

print("cell: ",  element.cell)
print("degree: ", element.degree)
```

output

```
cell:  <FIAT.reference_element.UFCTriangle object at 0x7f9f705c8490>
degree:  2
```

[50]:
```
element.entity_dofs() # dofs for every entity (vertex, edge, face, volume)
```

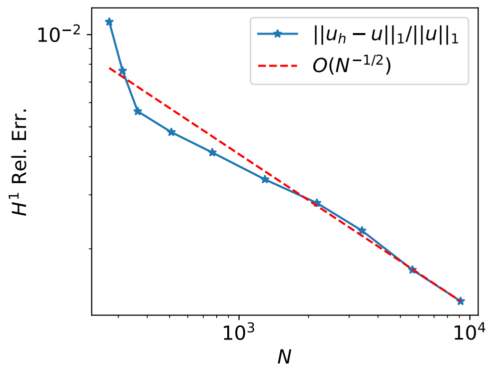
[50]:
```
{0: {0: [0], 1: [1], 2: [2]}, 1: {0: [3], 1: [4], 2: [5]}, 2: {0: []}}
```

1.9 Adaptive Finite Element Methods

1.9.1 Possion on Lshape

[51]:
```
# %load py/adapt_possion.py
from firedrake import *
from firedrake.petsc import PETSc, flatten_parameters
from pyop2.datatypes import IntType, RealType, ScalarType, \
                            as_cstr, as_ctypes, as_numpy_dtype

import numpy as np
import matplotlib.pyplot as plt

def solve_possion(mesh, u_handle, f_handle):
    x = SpatialCoordinate(mesh)
    u_e = u_handle(x)
    f = f_handle(x)

    V = FunctionSpace(mesh, 'CG', 1)
    u, v = TrialFunction(V), TestFunction(V)
    L = inner(f, v)*dx
    a = inner(grad(u), grad(v))*dx
    sol = Function(V, name='u_h')

    bc = DirichletBC(V, u_e, 'on_boundary')

    solve(a == L, sol, bcs=bc)

    err = errornorm(u_e, sol, norm_type='H1')/norm(u_e, norm_type='H1')

    return sol, err


def estimate(mesh, sol, u_handle, f_handle, alpha, beta):
    x = SpatialCoordinate(mesh)
    u_e = u_handle(x)
    f = f_handle(x)

    V_eta_K = FunctionSpace(mesh, 'DG', 0)
    V_eta_e = FunctionSpace(mesh, 'HDivT', 0)

    phi_K = TestFunction(V_eta_K)
    phi_e = TestFunction(V_eta_e)

    phi = div(grad(sol)) + f
    g = jump(grad(sol), FacetNormal(mesh))

    ksi_K = assemble(inner(phi**2, phi_K)*dx)
    ksi_e = assemble(inner(g**2, avg(phi_e))*dS)
    ksi_outer = assemble(inner((sol-u_e)**2, phi_e)*ds)

    h_e = assemble(conj(phi_e)*ds)
    h_K = Function(V_eta_K).interpolate(CellDiameter(mesh))

    eta_K = assemble_eta_K_op2(ksi_K, ksi_e, ksi_outer, h_K, h_e, alpha=alpha, beta=beta)
    # eta_K2 = assemble_eta_K_py(ksi_K, ksi_e, ksi_outer, h_K, h_e, alpha=alpha, beta=beta)
    # assert np.allclose(eta_K.dat.data_ro_with_halos, eta_K2.dat.data_ro_with_halos)

    return eta_K


def assemble_eta_K_py(ksi_K, ksi_e, ksi_outer, h_K, h_e, alpha, beta):
    V_eta_K = ksi_K.function_space()
    V_eta_e = ksi_e.function_space()

    cell_node_list_K = V_eta_K.cell_node_list
    cell_node_list_e = V_eta_e.cell_node_list

    ne_per_cell = V_eta_e.cell_node_list.shape[1]

    s1 = np.zeros_like(ksi_K.dat.data_ro_with_halos)
    for i in range(0, ne_per_cell):
        s1 += ksi_e.dat.data_ro_with_halos[cell_node_list_e[:, i]]

    s2 = np.zeros_like(ksi_K.dat.data_ro_with_halos)
    for i in range(0, ne_per_cell):
        s2 += h_e.dat.data_ro_with_halos[cell_node_list_e[:, i]] * ksi_outer.dat.
↪data_ro_with_halos[cell_node_list_e[:, i]]
```

```
    eta_K = Function(V_eta_K)
    eta_K.dat.data_with_halos[:] = np.sqrt(
        alpha * h_K.dat.data_ro_with_halos**2 * ksi_K.dat.data_ro_with_halos \
        + beta * h_K.dat.data_ro_with_halos * s1
        # + beta * (h_K.dat.data_ro_with_halos * s1 + s2)
    )

    return eta_K


def assemble_eta_K_op2(ksi_K, ksi_e, ksi_outer, h_K, h_e, alpha, beta):
    V_eta_K = ksi_K.function_space()
    V_eta_e = ksi_e.function_space()

    kernel_str = '''
void assemble_eta_K({type} eta_K[1], {type} ksi_K[1], {type} ksi_e[{dim}],
              {type} ksi_outer[{dim}], {type} h_K[1], {type} h_e[{dim}])
{{
    {type} s = 0;
    {type} s1 = 0;
    for (int i = 0; i < {dim}; i++) s += ksi_e[i];
    for (int i = 0; i < {dim}; i++) s1 += h_e[i]*ksi_outer[i];
    eta_K[0] = sqrt({alpha}*h_K[0]*h_K[0]*ksi_K[0] + {beta}*h_K[0]*s);
}}
'''.format(type=as_cstr(ScalarType), dim=V_eta_e.cell_node_list.shape[1],
           # double or complex       number of edges per element
           alpha=alpha, beta=beta)

    kernel = op2.Kernel(kernel_str, 'assemble_eta_K')

    eta_K = Function(ksi_K)
    iterset = eta_K.cell_node_map().iterset
    with PETSc.Log.Event("assemble_eta_K"):
        op2.par_loop(kernel, iterset, \
                     eta_K.dat(op2.WRITE, eta_K.cell_node_map()), \
                     ksi_K.dat(op2.READ, ksi_K.cell_node_map()), \
                     ksi_e.dat(op2.READ, ksi_e.cell_node_map()), \
                     ksi_outer.dat(op2.READ, ksi_outer.cell_node_map()), \
                     h_K.dat(op2.READ, h_K.cell_node_map()),
                     h_e.dat(op2.READ, h_e.cell_node_map())
                    )

    return eta_K


def mark_cells(mesh, eta_K, theta):
    plex = mesh.topology_dm
    cell_numbering = mesh._cell_numbering

    if plex.hasLabel('adapt'):
        plex.removeLabel('adapt')

    with eta_K.dat.vec_ro as vec:
        eta = vec.norm()
        eta_max = vec.max()[1]

    cell_node_list_K = eta_K.function_space().cell_node_list
    tol = theta*eta_max
    eta_K_data = eta_K.dat.data_ro_with_halos
    with PETSc.Log.Event("ADD_ADAPT_LABEL"):
        plex.createLabel('adapt')
        cs, ce = plex.getHeightStratum(0)
        for i in range(cs, ce):
            c = cell_numbering.getOffset(i)
            dof  = cell_node_list_K[c][0]
            if eta_K_data[dof] > tol:
                plex.setLabelValue('adapt', i, 1)

    return plex


def adapt_possion():
    opts = PETSc.Options()
    opts.insertString('-dm_plex_transform_type refine_sbr')

    def u_exact(x):
        mesh = x.ufl_domain()
        U = FunctionSpace(mesh, 'CG', 1)
        u = Function(U)
        coords = mesh.coordinates
        x1, x2 = np.real(coords.dat.data_ro[:, 0]), np.real(coords.dat.data_ro[:, 1])
        r = np.sqrt(x1**2 + x2**2)
        theta = np.arctan2(x2, x1)
        u.dat.data[:] = r**(2/3)*np.sin(2*theta/3)
        return u

    def f_handle(x):
        return Constant(0)

    mesh = Mesh('gmsh/Lshape.msh')
    ret = []
    parameters = {}
    parameters["partition"] = False
    for i in range(10):
        # PETSc.Sys.Print(f'It: {i}')
        if i != 0:
            with PETSc.Log.Event("ADAPT"):
                new_plex = plex.adaptLabel('adapt')
                new_plex.viewFromOptions('-dm_view')
                # Remove labels to avoid errors
                new_plex.removeLabel('adapt')
                new_plex.removeLabel("pyop2_core")
                new_plex.removeLabel("pyop2_owned")
                new_plex.removeLabel("pyop2_ghost")

            # mesh = Mesh(new_plex, distribution_parameters=parameters)
            mesh = Mesh(new_plex)
        sol, err = solve_possion(mesh, u_exact, f_handle)
        eta_K = estimate(mesh, sol, u_exact, f_handle, alpha=0.15, beta=0.15)
        plex = mark_cells(mesh, eta_K, theta=0.2)

        ndofs = sol.function_space().dim()

        ret.append((ndofs, np.real(err)))
    return ret

def plot_adapt_result(ret):
    data = np.array(ret)
    if COMM_WORLD.rank == 0:
        plt.figure(figsize=[5, 4])
        # plt.rcParams.update({'font.size': 12})
        plt.loglog(data[:, 0], data[:, 1], '*-', label=r'$||u_h - u||_1/||u||_1$')

        plt.loglog(data[:, 0], data[:, 0]**(-1/2)*data[-1, 1]/data[-1, 0]**(-1/2), 'r--',␣
 ↪label='$O(N^{-1/2})$')
        plt.savefig('figures/adapt_solver.pdf')
        plt.xlabel('$N$')
        plt.ylabel('$H^1$ Rel. Err.')
        plt.legend()


if __name__ == '__main__':
    ret = adapt_possion()
    plot_adapt_result(ret)
```



1.9.2 Update coordinates of DMPlex

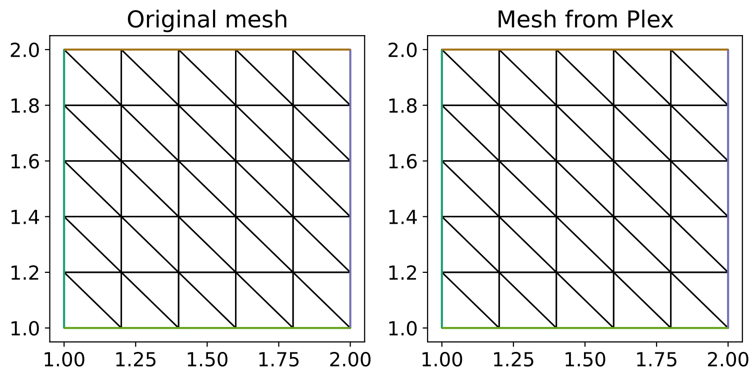
如果移动了网格, DMPlex 中存储的坐标和 Firedrake 的坐标将会不一致, 这时候做自适应加密需要把同步 Firedrake 中的坐标 DMPlex 中.

[52]:
```
from firedrake import *
import numpy as np

def remove_pyop2_label(plex):
    # Delete lables before create mesh with the plex,
    # otherwise error occurs when run in parallel
    plex.removeLabel("pyop2_core")
    plex.removeLabel("pyop2_owned")
    plex.removeLabel("pyop2_ghost")
    return plex

def get_plex_with_update_coordinates(mesh):
    """
    Update the coordinates of the plex in mesh, and then return a clone without pyop2 label
    """
    mesh.topology.init()
    dm = mesh.topology_dm
```

```python
    # cdm = dm.getCoordinateDM()
    # dim = dm.getCoordinateDim()
    csec = dm.getCoordinateSection()
    coords_vec = dm.getCoordinatesLocal()

    s, e = dm.getDepthStratum(0)
    sec = mesh._vertex_numbering

    data = mesh.coordinates.dat.data_ro_with_halos
    dest = np.zeros_like(data)
    n = mesh.geometric_dimension()
    m = csec.getFieldComponents(0)
    assert m == n
    for i in range(s, e):
        dof = sec.getDof(i)
        offset = sec.getOffset(i)
        cdof = csec.getDof(i)
        coffset = csec.getOffset(i)

        dest[coffset//m] = data[offset, :]

    coords_vec.array_w[:] = dest.flatten()
    # dm.setCoordinatesLocal(coords_vec)
    dm = dm.clone()
    remove_pyop2_label(dm)

    return dm

# # A simple method to update the coordinates is using section
# # Ref: https://github.com/firedrakeproject/firedrake/pull/2796/files
# # however, there are bugs in firedrake to read plex with user defined section
# # see: https://github.com/lrtfm/firedrake/tree/fixbug-coordinates
# # We can use the following code if the bug is fixed!
# def get_plex_with_update_coordinates(mesh):
#     tdim = mesh.topological_dimension()
#     gdim = mesh.geometric_dimension()
#     entity_dofs = np.zeros(tdim + 1, dtype=np.int32)
#     entity_dofs[0] = gdim
#     coord_section = mesh.create_section(entity_dofs)
#     plex = mesh.topology_dm
#     coord_dm = plex.getCoordinateDM()
#     coord_dm.setSection(coord_section)
#
#     coords_local = coord_dm.createLocalVec()
#     coords_local.array[:] = np.reshape(
#         mesh.coordinates.dat.data_ro_with_halos, coords_local.array.shape
#     )
#     plex.setCoordinatesLocal(coords_local)
#     plex = plex.clone()
#     remove_pyop2_label(plex)
#
#     return plex
```

下面使用移动网格进行测试

[53]:
```
def save_mesh(mesh, name):
    V = FunctionSpace(mesh, 'CG', 1)
    f = Function(V, name='f')
    File(name).write(f)

mesh_init = RectangleMesh(5, 5, 1, 1)

# move mesh
mesh_init.coordinates.dat.data[:] += 1
save_mesh(mesh_init, 'pvd/mesh_init.pvd')

# recreate mesh from the plex
plex = get_plex_with_update_coordinates(mesh_init)
mesh = Mesh(plex, distribution_parameters={"partition": False})
save_mesh(mesh, 'pvd/mesh_with_update_plex.pvd')

fig, ax = plt.subplots(1, 2, figsize=[9, 4], subplot_kw={})
tp0 = triplot(mesh_init, axes=ax[0])
tp1 = triplot(mesh, axes=ax[1])
t0 = ax[0].set_title('Original mesh')
t1 = ax[1].set_title('Mesh from Plex')
```



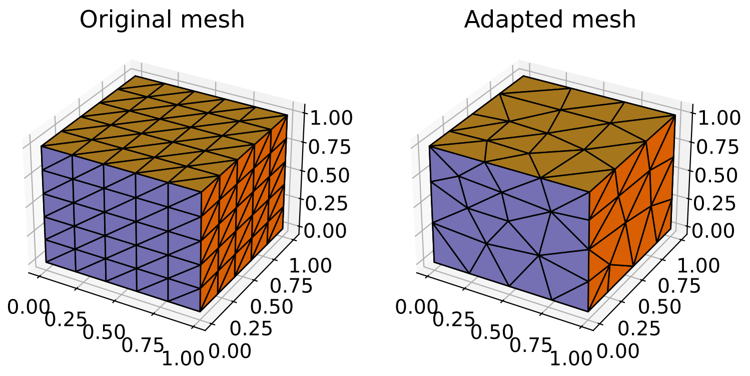
1.9.3 Using adaptMetric of dmplex

[54]:
```
# %load py/test_adapt_metric.py
from firedrake import *
from firedrake.petsc import PETSc, OptionsManager
import numpy as np
import matplotlib.pylab as plt


def to_petsc_local_numbering(vec, V):
    section = V.dm.getGlobalSection()
    out = vec.duplicate()
    varray = vec.array_r
    oarray = out.array
    dim = V.value_size
    idx = 0
    start, end = vec.getOwnershipRange()
    for p in range(*section.getChart()):
        dof = section.getDof(p)
        if dof > 0:
            off = section.getOffset(p)
            assert off >= 0
            off *= dim
            for d in range(dof):
                for k in range(dim):
                    oarray[idx] = varray[off + dim * d + k - start]
                    idx += 1
    assert idx == (end - start)

    return out


def create_metric_from_indicator(indicator):
    """
    Create an metric for adpative mesh from and indicator

    indicator: Function defined on cells, < 1 coarsen, > 1 refine
    """

    mesh = indicator.ufl_domain()
    V = FunctionSpace(mesh, 'DG', 0)
    U = FunctionSpace(mesh, 'CG', 1)
    W = TensorFunctionSpace(mesh, 'CG', 1)

    metric = Function(W, name='metric')

    tv = Function(U, name='total_volume')
    cv = Function(V, name='cell_volume').interpolate(CellVolume(mesh))

    par_loop(('{[i] : 0 <= i < A.dofs}',  'A[i] = B[0]'),
            dx, {'A' : (tv, INC), 'B' : (cv, READ)}, is_loopy_kernel=True)

    mesh = indicator.ufl_domain()

    degree = mesh.coordinates.function_space().ufl_element().degree()
    if degree != 1:
        raise Exception("We only support P1 mesh")

    coords = mesh.coordinates.dat.data_with_halos.real

    data = metric.dat.data_with_halos
    total_volume = tv.dat.data_with_halos.real
    cell_volume = cv.dat.data_with_halos.real
    Vc = mesh.coordinates.function_space()
    ind = indicator.dat.data_with_halos

    dim = mesh.geometric_dimension()

    if dim == 2:
        edge2vec = lambda e: [ e[0]**2, 2*e[0]*e[1], e[1]**2 ]
        vec2tensor = lambda g: [[g[0], g[1]], [g[1], g[2]]]
    elif dim == 3:
        edge2vec = lambda e:  [ e[0]**2, 2*e[0]*e[1], 2*e[0]*e[2], e[1]**2, 2*e[1]*e[2], e[2]**2␣
↪]
        vec2tensor = lambda g: [[g[0], g[1], g[2]], [g[1], g[3], g[4]], [g[2], g[4], g[5]]]
    else:
        raise Exception

    pair = []
```

```python
    for i in range(dim+1):
        for j in range(i):
            pair.append([i, j])

    for i, nodes in enumerate(Vc.cell_node_list):
        vertex = coords[nodes, :]
        edge = []
        for i, j in pair:
            edge.append(vertex[i, :] - vertex[j, :])

        mat = []
        for e in edge:
            mat.append(edge2vec(e))

        mat = np.array(mat)
        b = np.ones(len(edge))
        g = np.linalg.solve(mat, b)

        c = cell_volume[i] * ind[i]
        for n in nodes:
            data[n, :] += c/total_volume[n]*np.array(vec2tensor(g))

    return metric


def adapt(indicator):
    mesh = indicator.ufl_domain()
    metric = create_metric_from_indicator(indicator)
    size = metric.dat.dataset.layout_vec.getSizes()
    data = metric.dat._data[:size[0]]
    v = PETSc.Vec().createWithArray(data, size=size, bsize=metric.dat.cdim, comm=metric.comm)
    reordered = to_petsc_local_numbering(v, metric.function_space())
    v.destroy()
    plex_new = mesh.topology_dm.adaptMetric(reordered, "Face Sets", "Cell Sets")
    mesh_new = Mesh(plex_new)

    return mesh_new


def test_adapt(dim=2, factor=2):
    if dim == 2:
        mesh = UnitSquareMesh(5, 5)
    elif dim == 3:
        mesh = UnitCubeMesh(5, 5, 5)
    else:
        raise Exception("")

    V = FunctionSpace(mesh, 'DG', 0)
    indicator = Function(V, name='indicator')
    indicator.dat.data[:] = factor
    mesh_adapt = adapt(indicator)

    mesh.topology_dm.viewFromOptions('-dm_view')
    mesh_adapt.topology_dm.viewFromOptions('-dm_view_new')
    return mesh, mesh_adapt


def test_adapt_with_option(dim=2, factor=0.5):
    # adaptors: pragmatic, mmg, parmmg
    #   -dm_adaptor pragmatic
    #   -dm_adaptor mmg
    #   -dm_adaptor parmmg
    #   -dm_adaptor cellrefiner -dm_plex_transform_type refine_sbr
    parameters = {
        "dm_adaptor": "mmg",
        # "dm_plex_metric_target_complexity": 400,
        # "dm_view": None,
        # "dm_view_new": None,
    }

    om = OptionsManager(parameters, options_prefix="")
    with om.inserted_options():
        mesh, mesh_new = test_adapt(dim=dim, factor=factor)

    return mesh, mesh_new
```

[55]:

```
mesh, mesh_new = test_adapt_with_option(dim=3, factor=0.3)

if mesh.geometric_dimension() == 3:
    subplot_kw = dict(projection='3d')
else:
    subplot_kw = {}
fig, ax = plt.subplots(1, 2, figsize=[9, 4], subplot_kw=subplot_kw)
tp = triplot(mesh, axes=ax[0])
tp_new = triplot(mesh_new, axes=ax[1])
t0 = ax[0].set_title('Original mesh')
t1 = ax[1].set_title('Adapted mesh')
```



2 NS 方程

Navier-Stocks 方程:

$$\begin{cases} \partial_t u - \mu\Delta u + (u\cdot\nabla)u + \nabla p = f, & \text{in} \quad \Omega\times(0,T] \\ \nabla\cdot u = 0, & \text{in} \quad \Omega\times(0,T] \end{cases} \tag{8}$$

初边值条件

$$\begin{cases} u = 0, & \text{on} \quad \partial\Omega\times(0,T] \\ u_0 = (y,-x) & \text{in} \quad \Omega \quad \text{at} \quad t=0 \end{cases} \tag{9}$$

[56]:
```python
from firedrake import *

mu = 1
T = 0.25

N_S = 16
N_T = 128

tau = T/N_T
h = 1/N_S

mesh = RectangleMesh(N_S, N_S, 1, 1)

x = SpatialCoordinate(mesh)
# u_0 = as_vector((x[1] - 0.5, - x[0] + 0.5))
u_0 = as_vector((x[1], - x[0]))
f = as_vector([0, -1])
```

2.1 函数空间

采用 MINI 元, 即 P1 × P1b.

P1b 由 P1 加上 Bubble 组成.

`NodalEnrichedElement`, `EnrichedElement`

`VectorFunctionSpace` 构造向量空间

[57]:
```python
cell = mesh.ufl_cell()
tdim = cell.topological_dimension()

# Mini element: P1 X P1b
P1 = FiniteElement("CG", cell, 1)
B = FiniteElement("B", cell, tdim+1)
P1b = P1 + B # or P1b = NodalEnrichedElement(P1, B)

V_u = VectorFunctionSpace(mesh, P1b)
V_p = FunctionSpace(mesh, "CG", 1)
V = MixedFunctionSpace([V_u, V_p])
```

2.2 弱形式

$$\begin{cases}\dfrac{1}{\tau}(u^n - u^{n-1}, v) + \mu(\nabla u^n, \nabla v) + ((u^n\cdot\nabla)u^n, v) - (p^n, \nabla\cdot v) = (f^n, v)\\(q, \nabla\cdot u^n) = 0\end{cases} \tag{10}$$

- `TrialFunctions`, `TestFunctions`:

  以 `tuple` 返回函数空间中的试验/测试函数,

  主要用于 `MixedFunctionSpace`.

- `split`

– split: 以索引的方式获取 MixedFunctionSpace 中函数的分量 (保留 UFL 关联信息, 用于定义变分形式)

由于该问题是非线性问题, 我们打算用 NonlinearVariationalSolver 进行求解, 所以下面定义 w 使用了 Function 而不是 TrialFunction/TrialFunctions.

[58]:
```python
w = Function(V) # u and p
u, p = split(w)

v, q = TestFunctions(V)

w_nm1 = Function(V)
u_nm1, p_nm1 = w_nm1.subfunctions
u_nm1.rename('u_h') # for visualization in paraview
p_nm1.rename('p_h')

Re = Constant(mu)

F = \
      Constant(1/tau)*inner(u - u_nm1, v)*dx \
    + Re*inner(grad(u+u_nm1)/2, grad(v))*dx \
    + inner(dot(grad(u), (u+u_nm1)/2), v)*dx \
    - p*div(v)*dx \
    + div(u)*q*dx \
    - inner(f, v)*dx
```

2.3 定义 Solver

类似于纯 Neumann 问题, 我们将使用 nullspace 参数.

注意下面混合空间中, 边界条件和 nullspace 的定义.

[59]:
```python
bc = DirichletBC(V.sub(0), 0, 'on_boundary')
nullspace = MixedVectorSpaceBasis(V, [V.sub(0), VectorSpaceBasis(constant=True, comm=mesh.comm)])

problem = NonlinearVariationalProblem(F, w, bcs=bc)  # F = 0
solver = NonlinearVariationalSolver(problem,
                                    options_prefix='ns',
                                    solver_parameters=None, # {'snes_converged_reason': None,␣
 ↪'snes_max_it': 100},
                                    nullspace=nullspace
                                   )
```

2.4 时间循环和保存结果到 pvd 文件

[60]:
```python
u_, p_ = w.subfunctions

output = File('pvd/ns-equation.pvd')

u_nm1.project(u_0)
output.write(u_nm1, p_nm1, time=0)

for i in ProgressBar('T', bar_prefix=" |", bar_suffix="| ", empty_fill=" ", fill="#").
 ↪iter(range(N_T)):
    t = tau*(i+1)

    solver.solve()

    u_nm1.assign(u_)
    p_nm1.assign(p_)

    (i+1)%32 or output.write(u_nm1, p_nm1, time=t)
```

output
```
T |###################################################| 128/128 [0:00:01]
```

2.4.1 Constant 用于时间依赖的表达式

[61]:
```
from firedrake import *
mesh = RectangleMesh(10, 10, 1, 1)
C1 = Constant(0)

x, y = SpatialCoordinate(mesh)
expr = C1*(x+y)

v = []
for i in range(5):
    t = i*0.1
    C1.assign(t)
    v.append(
        assemble(expr*dx)
    )

print(v)
```

output
```
[0.0, 0.0999999999999999, 0.1999999999999998, 0.2999999999999997,
0.3999999999999996]
```

2.5 ParaView 可视化计算结果

Pipeline 和 Filter

2.5.1 二维结果 (surf 图)

Filter: Wrap by scalar

2.5.2 选择部分区域显示

View -> Find Data

2.5.3 并行数据显示各进程区域

Filter -> Connectivity

3 Cahn–Hilliard 方程

算子分裂方法

TODO Add more details

file: py/cahn_hilliard.py

[62]:
```
from firedrake import *
from firedrake.petsc import PETSc
import matplotlib.pyplot as plt

class Bar(ProgressBar):
    suffix = '%(index)s/%(max)s [%(elapsed_td)s/%(eta_td)s]'
    bar_prefix = ' |'
    bar_suffix = '| '
    empty_fill = ' '
    fill = '#'
    color = None
```

[63]:
```
def u0(x, y):
    return 0.05*cos(2*pi*x)*cos(2*pi*y)

def f_plus(u):
    return u**3

def f_minus(u):
    return u
```

[64]:
```
opts = PETSc.Options()
degree = opts.getInt('degree', default=1)
N = opts.getInt('N', default=100)
M = opts.getInt('M', default=200)  # M = 1600
tau = opts.getReal('tau', default=1e-4)
epsilon = opts.getReal('epsilon', default=0.05)
periodic = opts.getBool('periodic', default=True)

dt = Constant(tau)
```

[65]:
```
if periodic:
    filename = 'pvd/test_ch_periodic.pvd'
    mesh = PeriodicRectangleMesh(N, N, 2, 2)
else:
    filename = 'pvd/test_ch_neumann.pvd'
    mesh = RectangleMesh(N, N, 2, 2)

mesh.coordinates.dat.data[:] = mesh.coordinates.dat.data_ro - 1
```

[66]:
```
V = FunctionSpace(mesh, 'CG', degree)
W = V*V
v, v_test = Function(W), TestFunction(W)
u, w = split(v)
u_test, w_test = split(v_test)

vn = Function(W)
un, wn = vn.subfunctions
un.rename('u')
```

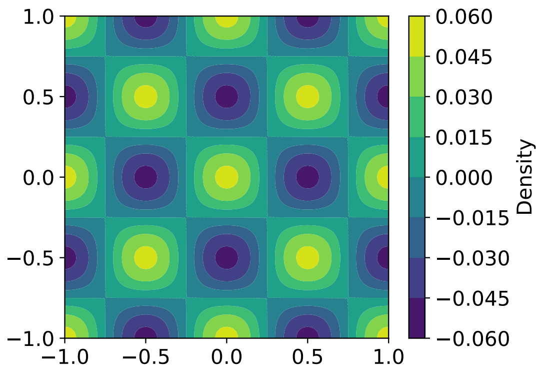
```
wn.rename('w')
```

[67]:
```
t = 0
x, y = SpatialCoordinate(mesh)
un.interpolate(u0(x,y))
```

[67]:
```
Coefficient(WithGeometry(IndexedProxyFunctionSpace(<firedrake.mesh.MeshTopology
object at 0x7f9f708475b0>, FiniteElement('Lagrange', triangle, 1), name=None,
index=0, component=None), Mesh(VectorElement(FiniteElement('Discontinuous
Lagrange', triangle, 1, variant='equispaced'), dim=2, variant='equispaced'),
605)), 1324)
```

[68]:
```
# plot init value
# colorbar:
#   https://matplotlib.org/stable/gallery/images_contours_and_fields/contourf_demo.html
fig, ax = plt.subplots(figsize=[5, 4])
cs = tricontourf(un, axes=ax)
cbar = fig.colorbar(cs)
cbar.ax.set_ylabel('Density')
```

[68]:
```
Text(0, 0.5, 'Density')
```



定义变分形式和非线性求解器

[69]:
```
a = 1/dt*inner(u - un, u_test)*dx + inner(grad(w), grad(u_test))*dx \
    + inner(w, w_test)*dx - epsilon**2*inner(grad(u), grad(w_test))*dx \
    - inner(f_plus(u) - f_minus(un), w_test)*dx

prob = NonlinearVariationalProblem(a, v)
solver = NonlinearVariationalSolver(prob, options_prefix="ch") # ␣
↪solver_parameters={'snes_monitor': None, 'snes_view': None})
```

[70]:
```
PETSc.Sys.Print(f'Will save result in {filename}')
output = File(filename)
output.write(un, wn, time=t)
```

output
```
Will save result in pvd/test_ch_periodic.pvd
```

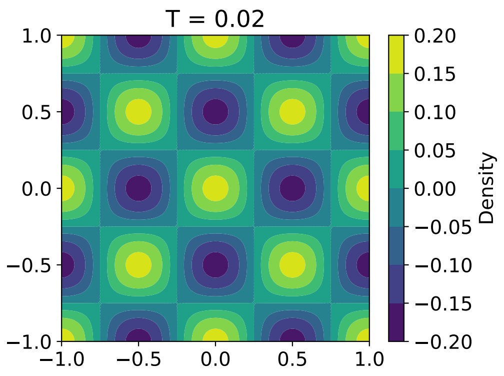
时间层循环

[71]:
```
for i in Bar('Timestep').iter(range(M)):
    t = (i+1)*tau
    solver.solve()

    vn.assign(v)
    if (i+1)%100 == 0:
        output.write(un, wn, time=t)
```

output
```
Timestep |##################################################| 200/200
[0:00:33/0:00:00]
```

[72]:
```
fig, ax = plt.subplots(figsize=[5, 4])
cs = tricontourf(un, axes=ax)
cbar = fig.colorbar(cs)
cbar.ax.set_ylabel('Density')
ax.set_title(f'T = {M*tau}')
```

[72]:
```
Text(0.5, 1.0, 'T = 0.02')
```



4 多进程并行 (MPI)

在终端使用 `mpiexec -n <np>` 运行 python 文件即可:

```
mpiexec -n 2 python myscript.py
```

4.1 Run code parallelly in jupyter

我们使用 `ipyparallel` 介绍并行程序的一些内容, 需要先安装 `ipyparallel`

4.1.1 Install ipyparallel

1. Install ipyparallel in firedrake env:

   ```
   pip install ipyparallel
   ```

2. create profile mpi

   ```
   ipython profile create --parallel --profile=mpi
   ```

Your will see the following output

```
[ProfileCreate] Generating default config file:
    PosixPath('/home/<your-user-name>/.ipython/profile_mpi/ipython_config.py')
[ProfileCreate] Generating default config file:
    PosixPath('/home/<your-user-name>/.ipython/profile_mpi/ipython_kernel_config.py')
[ProfileCreate] Generating default config file:
    PosixPath('/home/<your-user-name>/.ipython/profile_mpi/ipcontroller_config.py')
[ProfileCreate] Generating default config file:
    PosixPath('/home/<your-user-name>/.ipython/profile_mpi/ipengine_config.py')
[ProfileCreate] Generating default config file:
    PosixPath('/home/<your-user-name>/.ipython/profile_mpi/ipcluster_config.py')
```

3. Edit file `.ipython/profile_mpi/ipengine_config.py`. Add the following code at the begining of the file:

```
from firedrake import *
from firedrake.petsc import PETSc
```

4. Set the default engines to mpi in file `.ipython/profile_mpi/ipcluster_config.py`. You can search `engine_launcher_class` in the file, and the result file should looks like this:

```
#    - sshproxy: ipyparallel.cluster.launcher.SSHProxyEngineSetLauncher
#    - winhpc: ipyparallel.cluster.launcher.WindowsHPCEngineSetLauncher
#  Default: 'ipyparallel.cluster.launcher.LocalEngineSetLauncher'
c.Cluster.engine_launcher_class = 'mpi'
```

5. Test:

```
import ipyparallel as ipp
import os

cluster = ipp.Cluster(profile="mpi", n=2)
client = cluster.start_and_connect_sync()
```

The output should looks like

```
Starting 2 engines with <class 'ipyparallel.cluster.launcher.MPIEngineSetLauncher'>
```

```
%%px --block
from firedrake import *
from firedrake.petsc import PETSc
from mpi4py import MPI

mesh = RectangleMesh(8, 8, 1, 1)
PETSc.Sys.syncPrint(mesh.comm.rank, mesh.comm.size)
PETSc.Sys.syncFlush()
```

The output should looks like:

```
[stdout:0] 0 2
1 2
```

4.1.2 Example

[73]:
```python
import ipyparallel as ipp
import os

cluster = ipp.Cluster(profile="mpi", n=2)
client = cluster.start_and_connect_sync()
```

output
```
Starting 2 engines with <class
'ipyparallel.cluster.launcher.MPIEngineSetLauncher'>
```

```
  0%|          | 0/2 [00:00<?, ?engine/s]
```

[74]:
```python
%%px --block
from firedrake import *
from firedrake.petsc import PETSc
from mpi4py import MPI

mesh = RectangleMesh(8, 8, 1, 1)
PETSc.Sys.syncPrint(mesh.comm.rank, mesh.comm.size)
PETSc.Sys.syncFlush()
```

```
[stdout:0] 0 2
1 2
```

[75]:
```python
%%px --block

PETSc.Sys.syncPrint(COMM_WORLD.rank, COMM_WORLD.size)
PETSc.Sys.syncFlush()
```

```
[stdout:0] 0 2
1 2
```

有些时候需要在某个进程上, 做指定的操作或运算, 如只在第 0 个进程上画图

```python
if COMM_WORLD.rank == 0:
    plot(...)
```

4.2 并行输出

py/intro_utils.py

[76]:
```python
%%px --block
from firedrake import *
from firedrake.petsc import PETSc
from mpi4py import MPI

PETSc.Sys.Print('This is first line (from rank 0)')
```

```
[stdout:0] This is first line (from rank 0)
```

[77]:
```python
%%px --block
PETSc.Sys.syncPrint('This is second line (from all rank)')
PETSc.Sys.syncFlush()
```

```
[stdout:0] This is second line (from all rank)
This is second line (from all rank)
```

[78]:
```
%%px --block
print('This msg from all rank')
```

```
[stdout:0] This msg from all rank
```

```
[stdout:1] This msg from all rank
```

5 PETSc

Course:

1. Introduction to PETSc https://learn.tacc.utexas.edu/mod/page/view.php?id=96
2. DOC: https://web.corral.tacc.utexas.edu/CompEdu/pdf/pcse/petsc_p_course.pdf

PETSc git repo:

1. petsc4py demo https://gitlab.com/petsc/petsc/-/tree/main/src/binding/petsc4py/demo

PETSc 目录中有用的工具, 如 `h5dump`, `petsc_gen_xdmf.py`, `PetscBinaryIO.py` 等.

在 PETSc 环境中, 运行如下命令添加这些工具所在路径到 `PATH`:

```
export PATH="$PATH:$PETSC_DIR/lib/petsc/bin"
export PATH="$PATH:$PETSC_DIR/${PETSC_ARCH-default}/bin"
```

在激活的 firedrake 环境下, 可以运行如下命令的输出, 添加这些工具所在路径到环境变量 `PATH`.

```
python -c "from firedrake import *; \
           import os; \
           PETSC_DIR = os.environ['PETSC_DIR']; \
           PETSC_ARCH = os.environ['PETSC_ARCH']; \
           print('\nRun the follwoing code to add petsc/bin to path:\n'); \
           print(f'  export PATH=\"\$PATH:{PETSC_DIR}/lib/petsc/bin\"'); \
           print(f'  export PATH=\"\$PATH:{PETSC_DIR}/{PETSC_ARCH}/bin\"'); \
           print('');"
```

5.1 Vector and Matirx

保存矩阵到文件: matvecio.py

[79]:
```
from firedrake import *
from firedrake.petsc import PETSc

test_mesh = RectangleMesh(nx=4, ny=4, Lx=1, Ly=1)
x, y = SpatialCoordinate(test_mesh)
f = sin(pi*x)*sin(pi*y)

V = FunctionSpace(test_mesh, 'CG', degree=1)

u, v = TrialFunction(V), TestFunction(V)
```

```
a = inner(grad(u), grad(v))*dx
L = inner(f, v)*dx
```

[80]:
```
A = assemble(a)
b = assemble(L)
type(A), type(b)
```

[80]:
```
(firedrake.matrix.Matrix, firedrake.function.Function)
```

5.1.1 Matrix

[81]:
```
type(A.petscmat)
```

[81]:
```
petsc4py.PETSc.Mat
```

单进程运行且矩阵不大时, 可以把 PETSc 矩阵转换为 `numpy` 数组

[82]:
```
import numpy as np
from scipy.sparse import csr_matrix

m, n = A.petscmat.getSize()
indptr, indices, data = A.petscmat.getValuesCSR()

A_numpy = csr_matrix((data, indices, indptr), shape=(m, n)).toarray()
```

[83]:
```
A.petscmat.getRow(0), A_numpy[0, :]
```

[83]:
```
((array([0, 1, 2], dtype=int32), array([ 1. , -0.5, -0.5])),
 array([ 1. , -0.5, -0.5,  0. ,  0. ,  0. ,  0. ,  0. ,  0. ,  0. ,  0. ,
         0. ,  0. ,  0. ,  0. ,  0. ,  0. ,  0. ,  0. ,  0. ,  0. ,  0. ,
         0. ,  0. ,  0. ]))
```

保存矩阵到文件 MatViewFromOptions

https://petsc.org/main/manualpages/Mat/MatViewFromOptions/

在代码中加入如下行

```
A.petscmat.viewFromOptions('-A_view')
```

那么在命令行可以通过选项 `-A_view binary:A.bin` 保存 `A` 到文件 `A.bin`.

5.1.2 Vector

[84]:
```
with b.dat.vec_ro as vec:
    print(type(vec))
```

output
```
<class 'petsc4py.PETSc.Vec'>
```

5.1.3 ISLocalToGlobalMapping

Create a local to global map

[85]:
```
import firedrake as fd
from firedrake.petsc import PETSc
from pyop2.datatypes import IntType, ScalarType
import numpy as np


rank = COMM_WORLD.rank

owned_sz = np.array(rank+3, dtype=IntType)
offset = np.empty_like(owned_sz)
COMM_WORLD.Scan(owned_sz, offset)
offset -= owned_sz
indices = np.arange(offset, offset + owned_sz, dtype=IntType)


lgmap = PETSc.LGMap()
lgmap.create(indices, bsize=1, comm=COMM_WORLD)
lgmap.view()
```

output
```
ISLocalToGlobalMapping Object: 1 MPI process
  type not yet set
[0] 0 0
[0] 1 1
[0] 2 2
```

5.2 KSP

自定义 KSP 进行线性方程组求解请参考 PETSc 的文档

1. 求解完成需要检查是否收敛

[86]:
```
from firedrake.exceptions import ConvergenceError
from firedrake.petsc import OptionsManager, PETSc
from firedrake.solving_utils import KSPReasons
import numpy as np

def _make_reasons(reasons):
    return dict([(getattr(reasons, r), r)
                 for r in dir(reasons) if not r.startswith('_')])

PCFailedReason = _make_reasons(PETSc.PC.FailedReason())

def get_ksp_reason(ksp):
    r = ksp.getConvergedReason()
    pc = ksp.getPC()
    r_pc = pc.getFailedReason()
    return KSPReasons[r], PCFailedReason[r_pc]

A = PETSc.Mat()
A.create(PETSc.COMM_WORLD)
A.setSizes([2, 2])
A.setType('aij') # sparse
# A.setPreallocationNNZ(4)
A.setUp()
A.setValue(1, 0, 1)
A.setValue(0, 1, np.inf) # to make the solver failed
A.assemble()
```

```
ksp = PETSc.KSP().create()
ksp.setOperators(A) # solve A*x=b by ksp.solve(b,x)

om = OptionsManager(
    {
        'ksp_type': 'preonly',
        'pc_type': 'lu',
        # 'ksp_view': None,
        'pc_factor_mat_solver_type': 'mumps',
        # 'ksp_error_if_not_converged': None,
    },
    options_prefix='test')
om.set_from_options(ksp)

x, b = A.createVecs()
b.setValue(0, 1)
# ksp.view()
with om.inserted_options():
    try:
        ksp.solve(b, x)
        r = ksp.getConvergedReason()
        if r < 0:
            raise ConvergenceError(KSPReasons[r])
    except ConvergenceError as e:
        r, r_pc = get_ksp_reason(ksp)
        PETSc.Sys.Print(f"Error: solver did not converged: {r}, PC: {r_pc}")
    except PETSc.Error as e:
        if e.ierr == 91: # https://petsc.org/release/include/petscerror.h.html
            PETSc.Sys.Print(f"Error from PETSc: solver did not converged: {KSPReasons[ksp.
↪getConvergedReason()]}")
        elif e.ierr == 76:
            PETSc.Sys.Print(f"Error from PETSc:")
            PETSc.Sys.Print(f"  ksp reason: {KSPReasons[ksp.getConvergedReason()]}")
            PETSc.Sys.Print(f"  error in library called by PETSc:")
            PETSc.Sys.Print("  "*4 + str(e).replace("\n", "\n" + " "*4))
        # We should terminate the process when an error occured in petsc
        # as suggested by Matt https://lists.mcs.anl.gov/pipermail/petsc-users/2023-March/048146.
↪html
        raise
```

output

```
Error: solver did not converged: DIVERGED_PCSETUP_FAILED, PC:
FACTOR_NUMERIC_ZEROPIVOT
```

2. 查看特征值和残差变化, 并保存图片

```
python test.py -ksp_type gmres -pc_type jacobi -ksp_view_eigenvalues draw -ksp_monitor
 ↪  draw::draw_lg -draw_save .png
```

5.2.1 Check ksp status in Firedrake

[87]:
```
from firedrake import *
from firedrake.petsc import PETSc
from firedrake.solving_utils import KSPReasons
import numpy as np
```

```python
def printf(*args, **kwargs):
    PETSc.Sys.Print(*args, **kwargs)

def get_ksp_reason(solver):
    r = solver.snes.getKSP().getConvergedReason()
    return KSPReasons[r]

rank, size = COMM_WORLD.rank, COMM_WORLD.size

opts = PETSc.Options()
N = opts.getInt('N', 32*size)

test_mesh = RectangleMesh(nx=N, ny=N, Lx=1, Ly=1)
x, y = SpatialCoordinate(test_mesh)
f = sin(pi*x)*sin(pi*y)

V = FunctionSpace(test_mesh, 'CG', degree=1)
u, v = TrialFunction(V), TestFunction(V)
a = inner(grad(u), grad(v))*dx - inner(f, v)*dx
bc = DirichletBC(V, 0, sub_domain='on_boundary')

u_h = Function(V, name='u_h')
problem = LinearVariationalProblem(lhs(a), rhs(a), u_h, bcs=bc)

solver_parameters = {'ksp_type': 'cg',
                     'ksp_max_it': 4,
                     'ksp_converged_reason': None,
                     # 'ksp_error_if_not_converged': None,
                     'pc_type': 'none'}
solver = LinearVariationalSolver(problem, solver_parameters=solver_parameters, options_prefix='')

for i in range(3):
    printf(f"Loop i = {i}")
    try:
        solver.solve()
    except ConvergenceError:
        printf(f"  Error from Firedrake: solver did not converged: {get_ksp_reason(solver)}")
    except PETSc.Error as e:
        if e.ierr == 91: # https://petsc.org/release/include/petscerror.h.html
            printf(f"  Error from PETSc: solver did not converged: {get_ksp_reason(solver)}")
        elif e.ierr == 76:
            PETSc.Sys.Print(f"Error from PETSc:")
            PETSc.Sys.Print(f"  ksp reason: {KSPReasons[ksp.getConvergedReason()]}")
            PETSc.Sys.Print(f"  error in library called by PETSc:")
            PETSc.Sys.Print(" "*4 + str(e).replace("\n", "\n" + " "*4))
        # We should terminate the process when an error occured in petsc
        # as suggested by Matt https://lists.mcs.anl.gov/pipermail/petsc-users/2023-March/048146.
 ↪html
        raise
```

output

```
Loop i = 0
  Linear  solve did not converge due to DIVERGED_ITS iterations 4
  Error from Firedrake: solver did not converged: DIVERGED_MAX_IT
Loop i = 1
  Linear  solve did not converge due to DIVERGED_ITS iterations 4
  Error from Firedrake: solver did not converged: DIVERGED_MAX_IT
Loop i = 2
  Linear  solve did not converge due to DIVERGED_ITS iterations 4
```

```
Error from Firedrake: solver did not converged: DIVERGED_MAX_IT
```

5.3 DMPlex

并行时, 网格会被划分成不同的块, 分配到各个进程.

网格由 PETSc 中的 DMPlex 管理.

DMPlex Reference:

1. Lange, M., Mitchell, L., Knepley, M. G., & Gorman, G. J. Efficient mesh management in firedrake using PETSC DMPLEX. SISC, 2016, 38(5), S143-S155.
2. Hapla, V., Knepley, M. G., Afanasiev, M., Boehm, C., van Driel, M., Krischer, L., & Fichtner, A. Fully parallel mesh I/O using PETSc DMPlex with an application to waveform modeling. SISC, 2021, 43(2), C127-C153.

5.3.1 网格粗化

```python
import sys
import petsc4py
petsc4py.init(sys.argv)
from petsc4py import PETSc

def output_vtk(dmplex, filename):
    viewer = PETSc.Viewer().createVTK(filename, 'w')
    viewer.view(dmplex)

opts = PETSc.Options()
N = opts.getInt('N', 4)
dim = opts.getInt('dim', 3)
overlap = opts.getInt('overlap', 1)

faces = [N for _ in range(dim)]
plex = PETSc.DMPlex().createBoxMesh(faces, simplex=True)
plex.setName('Init DM')
plex.viewFromOptions('-init_dm_view')

sf = plex.distribute(overlap=overlap)
plex.setName('Distribue DM')
plex.viewFromOptions('-dist_dm_view')

new_plex = plex.coarsen()
new_plex.setName('Coarsen DM')
new_plex.viewFromOptions('-coarsen_dm_view')

# mpiexec -n 2 python test_coarsen.py -dim 3 -overlap 0 -dm_adaptor parmmg -coarsen_dm_view
↪  vtk:data/test.vtu
```

5.4 Viewer

1. https://petsc.org/main/manualpages/Sys/PetscObjectViewFromOptions/

Option values for Viewer:

```
If no value is provided ascii:stdout is used

ascii[:[filename][:[format][:append]]]    defaults to stdout - format can be one of ascii_info,
 ↪ ascii_info_detail, or ascii_matlab,
                                          for example ascii::ascii_info prints just the
                                           ↪ information about the object not all details
                                          unless :append is given filename opens in write mode,
                                           ↪ overwriting what was already there
binary[:[filename][:[format][:append]]]   defaults to the file binaryoutput
draw[:drawtype[:filename]]                for example, draw:tikz, draw:tikz:figure.tex or draw:x
socket[:port]                             defaults to the standard output port
saws[:communicatorname]                   publishes object to the Scientific Application
                                          Webserver (SAWs)
```

2. https://petsc.org/main/manualpages/Draw/PetscDrawSetFromOptions/

```
-nox                                          - do not use X graphics (ignore graphics calls, but
 ↪ run program correctly)
-nox_warning                                  - when X Windows support is not installed this
 ↪ prevents the warning message from being printed
-draw_pause <pause amount>                   -- -1 indicates wait for mouse input,
                                                -2 indicates pause when window is to be destroyed
-draw_marker_type - <x,point>
-draw_save [optional filename]                - (X Windows only) saves each image before it is
 ↪ cleared to a file
-draw_save_final_image [optional filename]   - (X Windows only) saves the final image displayed in
 ↪ a window
-draw_save_movie                              - converts image files to a movie  at the end of the
 ↪ run. See PetscDrawSetSave()
-draw_save_single_file                        - saves each new image in the same file, normally
 ↪ each new image is saved in a new file with 'filename/filename_%d.ext'
-draw_save_on_clear                           - saves an image on each clear, mainly for debugging
-draw_save_on_flush                           - saves an image on each flush, mainly for debugging
```

5.4.1 Load mesh file and view (petsc4py)

[88]:
```python
import sys
import petsc4py
petsc4py.init(sys.argv)

from petsc4py import PETSc
import numpy as np

dm = PETSc.DMPlex().createFromFile('gmsh/Lshape.msh', plexname='test')
dm.view()

# hdf5 for load
viewer = PETSc.Viewer().createHDF5('data/Lshape.h5', mode='w')
viewer(dm)

# hdf5 for visualization:
# You can generate xdmf file from this file by
#     `petsc/lib/petsc/bin/petsc_gen_xdmf.py`
# Then load the xdmf file to paraview to visualize the mesh.
viewer = PETSc.Viewer().createHDF5('data/Lshape_xdmf.h5', mode='w')
viewer.pushFormat(viewer.Format.HDF5_XDMF)
```

```
viewer(dm)
viewer.popFormat()

# vtk file
viewer = PETSc.Viewer().createVTK('data/Lshape.vtk', mode='w')
viewer(dm)

# draw on X window
# viewer = PETSc.Viewer().createDraw()
# viewer(dm)
```

output

```
DM Object: test 1 MPI process
  type: plex
test in 2 dimensions:
  Number of 0-cells per rank: 274
  Number of 1-cells per rank: 755
  Number of 2-cells per rank: 482
Labels:
  celltype: 3 strata with value/size (0 (274), 3 (482), 1 (755))
  depth: 3 strata with value/size (0 (274), 1 (755), 2 (482))
```

[89]:
```
# since the petsc_draw is not in petsc4py, we use options to save the images

opts = PETSc.Options()
opts_old = opts.getAll()
opts.insertString('-dm_view draw:tikz:data/Lshape.tex')
dm.viewFromOptions('-dm_view')
```

5.4.2 View mesh of firedrake by DMPlex

[90]:
```
%%px --block
from firedrake import *

mesh = RectangleMesh(8, 8, 1, 1)
mesh.topology_dm.view()
```

```
[stdout:0] DM Object: firedrake_default_topology 2 MPI processes
  type: plex
firedrake_default_topology in 2 dimensions:
  Number of 0-cells per rank: 45 45
  Number of 1-cells per rank: 108 108
  Number of 2-cells per rank: 64 64
Labels:
  depth: 3 strata with value/size (0 (45), 1 (108), 2 (64))
  celltype: 3 strata with value/size (0 (45), 1 (108), 3 (64))
  Face Sets: 2 strata with value/size (1 (8), 3 (8))
  exterior_facets: 1 strata with value/size (1 (16))
  interior_facets: 1 strata with value/size (1 (92))
```

5.5 Star Forest

Reference:

[1] J. Zhang et al., The PetscSF Scalable Communication Layer, IEEE Transactions on Parallel and Distributed Systems, 33(4), 2022.

[91]:

```
%%px --block
from firedrake import *
from firedrake.petsc import PETSc

from petsc4py import PETSc
import numpy as np

# 6--------7--------8
# |        |        |
# 3--------4--------5
# |        |        |
# 0--------1--------2

def test_SFDistributeSection():
    comm = COMM_WORLD
    if comm.rank == 0:
        cells = np.asarray(
            [[0, 1, 3],
             [1, 2, 4],
             [1, 4, 3],
             [2, 5, 4],
             [3, 4, 6],
             [4, 5, 7],
             [4, 7, 6],
             [5, 8, 7]], dtype=np.int32)
        coords = np.asarray(
            [[0. , 0. ],
             [0.5, 0. ],
             [1. , 0. ],
             [0. , 0.5],
             [0.5, 0.5],
             [1.0, 0.5],
             [0. , 1. ],
             [0.5, 1. ],
             [1. , 1. ]], dtype=np.double)
    else:
        cells = np.zeros([0, 3], dtype=np.int32)
        coords = np.zeros([0, 2], dtype=np.double)
    dim = 2
    plex = PETSc.DMPlex().createFromCellList(dim, cells, coords, comm=comm)
    rootSection = PETSc.Section().create(comm=comm)
    pStart, pEnd = plex.getHeightStratum(2)
    rootSection.setChart(*plex.getChart())
    for p in range(pStart, pEnd):
        rootSection.setDof(p, 1)
    rootSection.setUp()
    rootSection.viewFromOptions('-section_view')

    dplex = plex.clone()
    msf = dplex.distribute()

    if msf is None:
        PETSc.Sys.Print("Warning: plex has not been distributed!")
        return
    dplex.viewFromOptions('-dm_view')

    def isEqualSF(ssf0, ssf1):
        nroots0, local0, remote0 = ssf0.getGraph()
        nroots1, local1, remote1 = ssf1.getGraph()
        return (nroots0 == nroots1) \
                and np.array_equal(local0, local1) \
                and np.array_equal(remote0, remote1)

    remoteOffsets0, leafSection0 = msf.distributeSection(rootSection)
    ssf0 = msf.createSectionSF(rootSection, remoteOffsets0, leafSection0)

    remoteOffsets1, leafSection1 = msf.distributeSection(rootSection, None)
    ssf1 = msf.createSectionSF(rootSection, remoteOffsets1, leafSection1)

    leafSection2 = PETSc.Section()
    remoteOffsets2, leafSection2 = msf.distributeSection(rootSection, leafSection2)
    ssf2 = msf.createSectionSF(rootSection, remoteOffsets2, leafSection2)

    leafSection3 = PETSc.Section()
    remoteOffsets3, _ = msf.distributeSection(rootSection, leafSection3)
    ssf3 = msf.createSectionSF(rootSection, remoteOffsets3, leafSection3)

    leafSection4 = PETSc.Section().create(dplex.getComm())
    remoteOffsets4, leafSection4 = msf.distributeSection(rootSection, leafSection4)
    ssf4 = msf.createSectionSF(rootSection, remoteOffsets4, leafSection4)

    leafSection5 = PETSc.Section().create(dplex.getComm())
    remoteOffsets5, _ = msf.distributeSection(rootSection, leafSection5)
    ssf5 = msf.createSectionSF(rootSection, remoteOffsets5, leafSection5)

    assert isEqualSF(ssf0, ssf1)
    assert isEqualSF(ssf0, ssf2)
    assert isEqualSF(ssf0, ssf3)
    assert isEqualSF(ssf0, ssf4)
    ssf0.view()
```

[92]:
```
%%px --block
# Add back after upgrad the firedrake
test_SFDistributeSection()
```

```
[stdout:0] PetscSF Object: 2 MPI processes
  type: basic
  [0] Number of roots=9, leaves=6, remote ranks=1
  [0] 0 <- (0,0)
  [0] 1 <- (0,1)
  [0] 2 <- (0,3)
  [0] 3 <- (0,4)
  [0] 4 <- (0,6)
  [0] 5 <- (0,7)
  [1] Number of roots=0, leaves=6, remote ranks=1
  [1] 0 <- (0,1)
  [1] 1 <- (0,2)
  [1] 2 <- (0,4)
  [1] 3 <- (0,5)
  [1] 4 <- (0,7)
  [1] 5 <- (0,8)
  MultiSF sort=rank-order
```

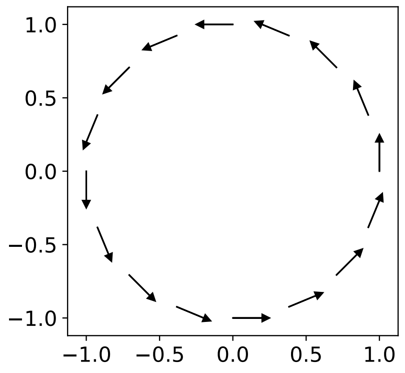
6 Surface problems

6.1 Line in plane

6.1.1 Cell orientation for line in plane

[93]:
```
def set_cell_orientations(mesh):
    from ufl.classes import ReferenceGrad
    import firedrake as fd

    V0 = fd.FunctionSpace(mesh, 'DG', 0)
    X = fd.SpatialCoordinate(mesh)
    flag = fd.Function(V0)
    flag.interpolate(fd.dot(X, fd.as_vector((-ReferenceGrad(X)[1, 0], ReferenceGrad(X)[0, 0]))))
    cell_orientations = fd.Function(V0, dtype=np.int32)
    cell_orientations.dat.data[:] = (flag.dat.data_ro < 0)
    mesh.topology._cell_orientations = cell_orientations


def plot_orientations_1d(mesh):
    import matplotlib.pyplot as plt

    plt.figure(figsize=[4, 4])
    Vc = mesh.coordinates.function_space()
    cell_orientations = mesh.cell_orientations()
    for i, index in enumerate(Vc.cell_node_list):
        coord = mesh.coordinates.dat.data_ro_with_halos[index].real
        o = cell_orientations.dat.data_ro_with_halos[i]

        _x = coord[:, 0]
        _y = coord[:, 1]
        if o > 1/2:
            plt.arrow(_x[0], _y[0], (_x[1]-_x[0])/2, (_y[1]-_y[0])/2, head_width=0.05,␣
 ↪head_length=0.05, fc='k', ec='k')
        else:
            plt.arrow(_x[1], _y[1], (_x[0]-_x[1])/2, (_y[0]-_y[1])/2, head_width=0.05,␣
 ↪head_length=0.05, fc='k', ec='k')
    bbox = plt.axis('equal')
```

[94]:
```
from firedrake import *
import matplotlib.pyplot as plt

# mesh = Mesh("gmsh/circle_1d.msh", dim=2)
# set_cell_orientations(mesh)

mesh = CircleManifoldMesh(16)
x = SpatialCoordinate(mesh)
# mesh.init_cell_orientations(x)

set_cell_orientations(mesh)

V = VectorFunctionSpace(mesh, 'CG', degree=1)
n_h = Function(V, name='n_h')
n_h.project(as_vector([-x[1], x[0]]))

plt.figure(figsize=[4, 4])
for coord, vector in zip(mesh.coordinates.dat.data_ro.real, n_h.dat.data_ro.real):
    plt.arrow(coord[0], coord[1], 0.2*vector[0], 0.2*vector[1], head_width=0.05, head_length=0.
  ↪05, fc='k', ec='k')
bbox = plt.axis('equal')
```



[95]:
```
def test_cell_orientation_curve():
    m = CircleManifoldMesh(3)
    x = SpatialCoordinate(m)
    # m.init_cell_orientations(x)
    set_cell_orientations(m)

    U = VectorFunctionSpace(m, 'CG', degree=1)
    V = VectorFunctionSpace(m, 'CG', degree=2)
    f = project(CellNormal(m), U)

    g = interpolate(f, V)
    h = project(f, V)

    assert abs(g.dat.data - h.dat.data).max() < 1e-2

    print(g.dat.data - h.dat.data)
```

[96]:
```
test_cell_orientation_curve()
```

output
```
[[ 0.00000000e+00 -2.22044605e-16]
 [ 1.22124533e-15  1.72988663e-17]
 [-2.77555756e-16  7.77156117e-16]
 [ 1.11022302e-16  4.36425264e-17]
 [-3.88578059e-16 -7.77156117e-16]
 [-5.55111512e-17  5.55111512e-17]]
```

6.2 Surface in 3D space

7 Debug

7.1 常见问题

7.1.1 DIVERGED_LINEAR_SOLVE

The errors are like this.

```
File "/home/yzz/firedrake/src/firedrake/firedrake/adjoint/solving.py", line 50, in wrapper
    output = solve(*args, **kwargs)
```

```
  File "/home/yzz/firedrake/src/firedrake/firedrake/solving.py", line 129, in solve
    _solve_varproblem(*args, **kwargs)
  File "/home/yzz/firedrake/src/firedrake/firedrake/solving.py", line 161, in _solve_varproblem
    solver.solve()
  File "/home/yzz/firedrake/src/firedrake/firedrake/adjoint/variational_solver.py", line 75, in
   ↪  wrapper
    out = solve(self, **kwargs)
  File "/home/yzz/firedrake/src/firedrake/firedrake/variational_solver.py", line 278, in solve
    solving_utils.check_snes_convergence(self.snes)
  File "/home/yzz/firedrake/src/firedrake/firedrake/solving_utils.py", line 139, in
   ↪  check_snes_convergence
    raise ConvergenceError(r"""Nonlinear solve failed to converge after %d nonlinear iterations.
firedrake.exceptions.ConvergenceError: Nonlinear solve failed to converge after 0 nonlinear
 ↪  iterations.
Reason:
   DIVERGED_LINEAR_SOLVE
```

Reasons for this:

1. You equation is not closed. May be you write wrong boundary conditions. Check the boundary condition carefully.
2. External package?
3. The resulting system is singular? (Maybe)
4. ...

We can add flag `-ksp_error_if_not_converged` to make PETSc print more infomation on the error. Below is an example of error `DIVERGED_LINEAR_SOLVE`

Exmaple 1 (Error of MUMPS)

Reference:

1. Doc of MUMPS: https://graal.ens-lyon.fr/MUMPS/index.php?page=doc
2. MATSOLVERMUMPS: https://petsc.org/main/manualpages/Mat/MATSOLVERMUMPS/

Below is an example on error occured in package mumps, we can look up the meaning of the error message in doc of mumps

```
[63]PETSC ERROR: --------------------- Error Message
 ↪  --------------------------------------------------------------
[63]PETSC ERROR: Error in external library
[63]PETSC ERROR: Error reported by MUMPS in numerical factorization phase: INFOG(1)=-9,
 ↪  INFO(2)=26
[63]PETSC ERROR: See https://petsc.org/release/faq/ for trouble shooting.
[63]PETSC ERROR: Petsc Development GIT revision: v3.4.2-38777-g979cc68729  GIT Date: 2022-06-22
 ↪  21:18:23 +0100
[63]PETSC ERROR: ../hsolver/hsolver.py on a default named AMAs4 by z2yang Tue Nov  8 16:03:18
 ↪  2022
```

```
[63]PETSC ERROR: Configure options
↪ PETSC_DIR=/home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/petsc PETSC_ARCH=default
↪ --download-ptscotch --with-zlib --download-hwloc --with-c2html=0
↪ --download-eigen="/home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/eigen-3.3.3.tgz
↪ " --download-mpich --download-hdf5 --with-fortran-bindings=0 --with-64-bit-indices
↪ --download-bison --with-cxx-dialect=C++11 --download-metis --download-openblas
↪ --download-openblas-make-options="'USE_THREAD=0 USE_LOCKING=1 USE_OPENMP=0'"
↪ --download-pastix --download-mumps --with-shared-libraries=1 --with-scalar-type=complex
↪ --download-cmake --download-scalapack --with-debugging=0 --download-netcdf
↪ --download-superlu_dist --download-suitesparse --download-pnetcdf
[63]PETSC ERROR: #1 MatFactorNumeric_MUMPS() at
↪ /home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/petsc/src/mat/impls/aij/mpi/mumps/mumps.c:1664
[63]PETSC ERROR: #2 MatLUFactorNumeric() at
↪ /home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/petsc/src/mat/interface/matrix.c:3177
[63]PETSC ERROR: #3 PCSetUp_LU() at
↪ /home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/petsc/src/ksp/pc/impls/factor/lu/lu.c:135
[63]PETSC ERROR: #4 PCSetUp() at
↪ /home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/petsc/src/ksp/pc/interface/precon.c:993
[63]PETSC ERROR: #5 KSPSetUp() at
↪ /home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/petsc/src/ksp/ksp/interface/itfunc.c:407
[63]PETSC ERROR: #6 KSPSolve_Private() at
↪ /home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/petsc/src/ksp/ksp/interface/itfunc.c:843
[63]PETSC ERROR: #7 KSPSolve() at
↪ /home/z2yang/opt/firedrake-env/firedrake-complex-int64/src/petsc/src/ksp/ksp/interface/itfunc.c:1078
```

The doc of mumps on `INFOG(1) = -9` and `INCTL(14)`:

```
The main internal real/complex workarray S is too small. If INFO(2) is positive, then the number
of entries that are missing in S at the moment when the error is raised is available in INFO(2).
If INFO(2) is negative, then its absolute value should be multiplied by 1 million. If an error -9
occurs, the user should increase the value of ICNTL(14) before calling the factorization (JOB=2)
again, except if LWK_USER is provided LWK_USER should be increased.
```

```
ICNTL(14) corresponds to the percentage increase in the estimated working space.
Phase: accessed by the host both during the analysis and the factorization phases.
Default value: between 20 and 35 (which corresponds to at most 35 % increase) and depends on
               the number of MPI processes. It is set to 5 % with SYM=1 and one MPI process.
Related parameters: ICNTL(23)
Remarks: When significant extra fill-in is caused by numerical pivoting, increasing ICNTL(14)
         may help
```

We can set mumps' parameter through `-mat_mumps_icntl_<num>`, such as `-mat_mumps_icntl_14 40`, see manual page on `MATSOLVERMUMPS` and doc of MUMPS for details.

Tips

添加标志 `ksp_view`, `ksp_monitor`, `ksp_converged_reason`, `ksp_error_if_not_converged`.

Example 2 (Mumps)

```
petsc4py.PETSc.Error: error code 76
[0] SNESSolve() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/snes/interface/snes.c:4693
[0] SNESSolve_KSPONLY() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/snes/impls/ksponly/ksponly.c:48
[0] KSPSolve() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/ksp/ksp/interface/itfunc.c:1070
```

```
[0] KSPSolve_Private() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/ksp/ksp/interface/itfunc.c:824
[0] KSPSetUp() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/ksp/ksp/interface/itfunc.c:405
[0] PCSetUp() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/ksp/pc/interface/precon.c:994
[0] PCSetUp_LU() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/ksp/pc/impls/factor/lu/lu.c:120
[0] MatLUFactorNumeric() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/mat/interface/matrix.c:3215
[0] MatFactorNumeric_MUMPS() at
↪ /home/yzz/firedrake/real-int32-mkl-debug/src/petsc/src/mat/impls/aij/mpi/mumps/mumps.c:1683
[0] Error in external library
[0] Error reported by MUMPS in numerical factorization phase: INFOG(1)=-10, INFO(2)=4464
```

```
INFOG(1)=-10: Numerically singular matrix. INFO(2) holds the number of eliminated pivots.
```

Add option `-mat_mumps_icntl_24 1` may fix this error.

```
ICNTL(24) controls the detection of ``null pivot rows''.
    Phase: accessed by the host during the factorization phase
    Possible variables/arrays involved: PIVNUL LIST
    Possible values :
        0: Nothing done. A null pivot row will result in error INFO(1)=-10.
        1: Null pivot row detection.
    Other values are treated as 0.
    Default value: 0 (no null pivot row detection)
```

7.1.2 Currently no support for ReferenceGrad in CoefficientDerivative

在使用高阶网格时, 不能对单元边界法向进行求导. 对高阶网格的单元边界法向求导会有如下错误:

```
ufl.log.UFLException: Currently no support for ReferenceGrad in CoefficientDerivative.
```

[97]:
```python
from firedrake import *

def get_s12(mesh, u, v):
    n = FacetNormal(mesh)
    s1 = dot(n, dot(n, grad(grad(grad(u)))))
    s2 = dot(n, dot(n, grad(grad(grad(v)))))
    return s1, s2

def get_s12_v2(mesh, u, v):
    n = FacetNormal(mesh)
    s1 = dot(n, grad(dot(n, grad(grad(u)))))
    s2 = dot(n, grad(dot(n, grad(grad(v)))))
    return s1, s2

def test_grad_n(high_order_mesh=True, fun=get_s12):
    p = 3
    N = 10

    mesh = RectangleMesh(N, N, 1, 1)

    if high_order_mesh:
        V = VectorFunctionSpace(mesh, 'CG', 2)
        coords = Function(V).interpolate(mesh.coordinates)
        mesh = Mesh(coords)

    V = FunctionSpace(mesh, 'CG', p)

    u, v = TrialFunction(V), TestFunction(V)

    s1, s2 = fun(mesh, u, v)
    a = inner(grad(u), grad(v))*dx + inner(s1('+'), s2('+'))*dS + inner(s1('-'), s2('-'))*dS
    L = inner(Constant(0), v)*dx

    sol = Function(V)
    prob = LinearVariationalProblem(a, L, sol)
    solver = LinearVariationalSolver(prob)

    solver.solve()

for f in [get_s12, get_s12_v2]:
    for hom in [False, True]:
        try:
            test_grad_n(high_order_mesh=hom, fun=f)
            print(f.__name__, f': High order mesh: {hom}, ', "TEST OK!")
        except Exception as e:
            print(f.__name__, f': High order mesh: {hom}, ', "TEST ERROR: ", e)
```

output

```
get_s12 : High order mesh: False,  TEST OK!
get_s12 : High order mesh: True,  TEST OK!
get_s12_v2 : High order mesh: False,  TEST OK!
get_s12_v2 : High order mesh: True,  TEST ERROR:  Currently no support for
ReferenceGrad in CoefficientDerivative.
```

7.1.3 PyErr_Occurred

```
python: src/petsc4py.PETSc.c:348918: __Pyx_PyCFunction_FastCall: Assertion `!PyErr_Occurred()'
↪  failed.
```

This may caused by your python code (with pragrammer error, such as undefined variables) called by PETSc

Tips

在程序开始添加如下代码, 可能会有更详细信息

```
from firedrake.petsc import PETSc
PETSc.Sys.popErrorHandler()
```

7.1.4 PETSc Error Code

https://petsc.org/release/manualpages/Sys/PetscErrorCode/

```
 {
  PETSC_SUCCESS                   = 0,
  PETSC_ERR_BOOLEAN_MACRO_FAILURE = 1, /* do not use */

  PETSC_ERR_MIN_VALUE = 54, /* should always be one less then the smallest value */

  PETSC_ERR_MEM             = 55, /* unable to allocate requested memory */
  PETSC_ERR_SUP              = 56, /* no support for requested operation */
  PETSC_ERR_SUP_SYS          = 57, /* no support for requested operation on this computer system */
  PETSC_ERR_ORDER            = 58, /* operation done in wrong order */
  PETSC_ERR_SIG              = 59, /* signal received */
  PETSC_ERR_FP               = 72, /* floating point exception */
  PETSC_ERR_COR              = 74, /* corrupted PETSc object */
  PETSC_ERR_LIB              = 76, /* error in library called by PETSc */
  PETSC_ERR_PLIB             = 77, /* PETSc library generated inconsistent data */
  PETSC_ERR_MEMC             = 78, /* memory corruption */
  PETSC_ERR_CONV_FAILED      = 82, /* iterative method (KSP or SNES) failed */
  PETSC_ERR_USER             = 83, /* user has not provided needed function */
  PETSC_ERR_SYS              = 88, /* error in system call */
  PETSC_ERR_POINTER          = 70, /* pointer does not point to valid address */
  PETSC_ERR_MPI_LIB_INCOMP = 87, /* MPI library at runtime is not compatible with MPI user
↪  compiled with */

  PETSC_ERR_ARG_SIZ          = 60, /* nonconforming object sizes used in operation */
  PETSC_ERR_ARG_IDN          = 61, /* two arguments not allowed to be the same */
  PETSC_ERR_ARG_WRONG        = 62, /* wrong argument (but object probably ok) */
  PETSC_ERR_ARG_CORRUPT      = 64, /* null or corrupted PETSc object as argument */
  PETSC_ERR_ARG_OUTOFRANGE   = 63, /* input argument, out of range */
  PETSC_ERR_ARG_BADPTR       = 68, /* invalid pointer argument */
  PETSC_ERR_ARG_NOTSAMETYPE  = 69, /* two args must be same object type */
  PETSC_ERR_ARG_NOTSAMECOMM  = 80, /* two args must be same communicators */
  PETSC_ERR_ARG_WRONGSTATE   = 73, /* object in argument is in wrong state, e.g. unassembled mat
↪  */
  PETSC_ERR_ARG_TYPENOTSET   = 89, /* the type of the object has not yet been set */
  PETSC_ERR_ARG_INCOMP       = 75, /* two arguments are incompatible */
  PETSC_ERR_ARG_NULL         = 85, /* argument is null that should not be */
  PETSC_ERR_ARG_UNKNOWN_TYPE = 86, /* type name doesn't match any registered type */

  PETSC_ERR_FILE_OPEN       = 65, /* unable to open file */
  PETSC_ERR_FILE_READ       = 66, /* unable to read from file */
  PETSC_ERR_FILE_WRITE      = 67, /* unable to write to file */
  PETSC_ERR_FILE_UNEXPECTED = 79, /* unexpected data in file */

  PETSC_ERR_MAT_LU_ZRPVT = 71, /* detected a zero pivot during LU factorization */
  PETSC_ERR_MAT_CH_ZRPVT = 81, /* detected a zero pivot during Cholesky factorization */

  PETSC_ERR_INT_OVERFLOW   = 84,
  PETSC_ERR_FLOP_COUNT     = 90,
  PETSC_ERR_NOT_CONVERGED  = 91,  /* solver did not converge */
  PETSC_ERR_MISSING_FACTOR = 92,  /* MatGetFactor() failed */
  PETSC_ERR_OPT_OVERWRITE  = 93,  /* attempted to over write options which should not be changed
↪  */
  PETSC_ERR_WRONG_MPI_SIZE = 94,  /* example/application run with number of MPI ranks it does not
↪  support */
  PETSC_ERR_USER_INPUT     = 95,  /* missing or incorrect user input */
  PETSC_ERR_GPU_RESOURCE   = 96,  /* unable to load a GPU resource, for example cuBLAS */
  PETSC_ERR_GPU            = 97,  /* An error from a GPU call, this may be due to lack of
↪  resources on the GPU or a true error in the call */
  PETSC_ERR_MPI            = 98,  /* general MPI error */
  PETSC_ERR_RETURN         = 99,  /* PetscError() incorrectly returned an error code of 0 */
  PETSC_ERR_MAX_VALUE      = 100, /* this is always the one more than the largest error code */

  /*
    do not use, exist purely to make the enum bounds equal that of a regular int (so conversion
    to int in main() is not undefined behavior)
  */
  PETSC_ERR_MIN_SIGNED_BOUND_DO_NOT_USE = INT_MIN,
  PETSC_ERR_MAX_SIGNED_BOUND_DO_NOT_USE = INT_MAX
} PETSC_ERROR_CODE_ENUM_NAME;
```

7.2 调试 Python 代码

运行中抛出异常, 定位出错代码, 检查相关的变量是否有异常值存在. 例如在 Jupyter notebook 中, `%debug` 可打开调试器, 检查相关变量.

7.3 调试 C 代码 (gdb)

由于 firedrake 基于 PETSc 进行网格管理和线性方程组求解, 有时出错会在 PETSc 中, 例如运行如下代码:

TODO: 找个示例, 这个示例不行

```
# filename: test.py
import sys
import petsc4py
petsc4py.init(sys.argv)
from petsc4py import PETSc
if PETSc.COMM_WORLD.rank == 0:
    PETSc.Vec().create(comm=PETSc.COMM_SELF).view()
```

出错信息如下:

```
$ python test.py
Vec Object: 1 MPI process
  type not yet set
Traceback (most recent call last):
  File "test.py", line 7, in <module>
    PETSc.Vec().create(comm=PETSc.COMM_SELF).view()
  File "PETSc/Vec.pyx", line 140, in petsc4py.PETSc.Vec.view
petsc4py.PETSc.Error: error code 56
[0] VecView() at
↪  /home/yzz/software/firedrake-mini-petsc/src/petsc/src/vec/vec/interface/vector.c:715
[0] No support for this operation for this object type
[0] No method view for Vec of type (null)
```

这时可以使用 gdb 等调试工具.

7.3.1 gdb 命令行说明

```
gdb [options] --args executable-file [inferior-arguments ...]
```

7.3.2 参数 (options)

1. `-x file`: 从文件中读取 gdb 命令
2. `-ex COMMAND`: 执行 gdb 命令
3. `--args exe [exe-args]` 传递参数给 exe
4. `--pid <pid>` 调试正在运行的程序

7.3.3 gdb 命令:

1. bt: 查看函数调用栈
2. run: 运行可执行文件
3. l: 查看代码
4. p: 打印变量

7.3.4 示例 (调试 test.py)

```
$ gdb  -ex run --args $(which python3) test.py
```

7.3.5 gdb 控制命令

一下命令可以保存 gdb 调试过程到文件, 可用于提交 issue.

1. 输出执行的 gdb 命令 `set trace-commands on`
   ref https://sourceware.org/gdb/onlinedocs/gdb/Messages_002fWarnings.html
2. 关闭分页 `set pagination off`
   ref https://sourceware.org/gdb/onlinedocs/gdb/Screen-Size.html
3. 设置日志文件，并开启日志 `set logging file my.logs`, `set logging enable on`
   ref https://sourceware.org/gdb/download/onlinedocs/gdb/Logging-Output.html

7.3.6 gdb 的 python 插件

在 ubuntu 上安装 `python3-dbg` 后, 文件夹 `/usr/share/gdb/auto-load/usr/bin/` 下会有如下插件

```
$ ls /usr/share/gdb/auto-load/usr/bin/
python3.10-dbg-gdb.py  python3.10dm-gdb.py  python3.10-gdb.py  python3.10m-gdb.py
```

其中定义了用于显示 python 调用栈的命令: `py-bt`.

在启动 gdb 调试时如果, gdb 没有自动加载该插件时 (为什么没有自动加载), 可以手动加载:

```
source /usr/share/gdb/auto-load/usr/bin/python3.10m-gdb.py
```

或者把该文件添加进 gdb 的初值化文件 `$HOME/.config/gdb/gdbinit` 或当前目录下的 `.gdbinit`:

```
source /usr/share/gdb/auto-load/usr/bin/python3.10m-gdb.py
```

7.3.7 Using commands from file

新建文件 `cmd.txt` 内容如下

```
source /usr/share/gdb/auto-load/usr/bin/python3.10m-gdb.py
set trace-commands on
set pagination off
set logging file my.logs
set logging enable on
py-bt
exit
```

使用 -x 参数运行 gdb 自动运行上面命令并退出.

```
gdb -x cmd.txt -p <pid>
```

7.4 并行程序调试

7.4.1 PETSc 的参数 -start_in_debugger

Reference:

1. https://petsc.org/main/manualpages/Sys/PetscInitialize/
2. https://petsc.org/main/manualpages/Sys/PetscSetDebugTerminal/

可以选择使用 PETSc 的参数 -start_in_debugger 给每个进程启动调试器如下:

```
mpiexec -n 3 $(which python) test.py  -start_in_debugger
```

默认会启动多个 xterm 窗口.

Notes: 修改 xterm 窗口显示效果 (Ref: http://www.futurile.net/2016/06/14/xterm-setup-and-truetype-font-configuration/)

```
$ cat ~/.Xdefaults
xterm*faceName: Monospace
xterm*faceSize: 12
xterm*foreground: rgb:a8/a8/a8
xterm*background: rgb:00/00/00
```

7.4.2 工具 tmux-mpi

Reference:

1. https://github.com/firedrakeproject/firedrake/wiki/Parallel-MPI-Debugging-with-tmux-mpi-(python-and-c!)
2. Tips of Firedrake Wiki: https://github.com/firedrakeproject/firedrake/wiki

另外我们也可以选择使用工具 tmux-mpi.

安装 tmux-mpi

1. 安装 tmux

   ```
   sudo apt-get install tmux
   ```

2. 安装 dtach (tmux-mpi 依赖)

   先编译 dtach, 然后拷贝二进制文件到某个在 PATH 中的路径, 如 $HOME/bin.

   ```
   git clone https://github.com/crigler/dtach
   cd dtach
   ./configure
   make
   mkdir -p $HOME/bin
   ```

```
cp dtach $HOME/bin
export PATH=$PATH:$HOME/bin
```

运行 `which dtach` 确认安装是否成功

3. 安装 tmux-mpi

   使用 pip 安装

   ```
   pip install --upgrade --no-cache-dir git+https://github.com/wrs20/tmux-mpi@master
   ```

调试命令

1. 启动调试器

   ```
   tmux-mpi 3 gdb -ex run --args $(which python) test.py
   ```

2. Attach 到相应的的伪终端, 每个进程一个窗口. (这里是 tmux 的一个 session, 有多个 window)

   ```
   tmux attach -t tmux-mpi
   ```

3. 使用 gdb 调试命令调试

7.5 编译 pyx 文件

7.5.1 firedrake 中的 pyx 文件

Recompile`dmcommon.pyx` after making modifications to it

```
python setup.py build_ext --inplace
```

8 Profiling

Reference:

1. https://www.firedrakeproject.org/optimising.html
2. https://petsc.org/main/manual/profiling/
3. https://petsc.org/main/manualpages/Sys/PetscInitialize/
4. https://petsc.org/main/manualpages/Profiling/PetscLogView/

8.1 `log_view`

1. `-log_view [:filename]` Prints summary of log information
2. `-log_view :filename.py:ascii_info_detail` Saves logging information from each process as a Python file
3. `-log_view :filename.xml:ascii_xml` Saves a summary of the logging information in a nested format (see below for how to view it)

4. `-log_view :filename.txt:ascii_flamegraph` Saves logging information in a format suitable for visualising as a Flame Graph (see below for how to view it)
5. `-log_view_memory` Also display memory usage in each event
6. `-log_view_gpu_time` Also display time in each event for GPU kernels (Note this may slow the computation)
7. `-log_all` Saves a file Log.rank for each MPI rank with details of each step of the computation
8. `-log_trace [filename]` Displays a trace of what each process is doing

8.1.1 Flame graph

运行代码时加上选项 `-log_view :profile.txt:ascii_flamegraph`, 将会生成文件 `profile.txt`, 该文件会记录某些代码块的运行时间, 可用于性能分析. 可以通过在线工具 https://www.speedscope.app/ 可视化该文件. 示例代码如下:

```
python test.py -log_view :profile.txt:ascii_flamegraph
```

可以通过 `PETSc.Log.Event` 和 `PETSc.Log.EventDecorator` 添加自定义事件, 用于测量代码块的运行事件. 如果如上运行代码, 事件名称和运行时间将会记录在上述 `profile.txt` 中.

1. `PETSc.Log.Event`

   ```
   from firedrake.petsc import PETSc

   with PETSc.Log.Event("foo"):
       do_something_expensive()
   ```

2. `PETSc.Log.EventDecorator`

   ```
   from firedrake.petsc import PETSc

   @PETSc.Log.EventDecorator("foo")
   def do_something_expensive():
       ...
   ```

8.1.2 `-log_view :profile.txt`

Ref: https://petsc.org/release/manual/profiling/#interpreting-log-view-output-parallel-performance

```
[ ]:
```