Introduction to Firedrake

2022 年 10 月 1 日

目录

1 Poisson equation

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

1.1 Dirichlet 问题

求解如下 Poisson 方程

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

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

试验和测试函数空间

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

变分问题

求解 $u \in H^1_E$, 使得

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

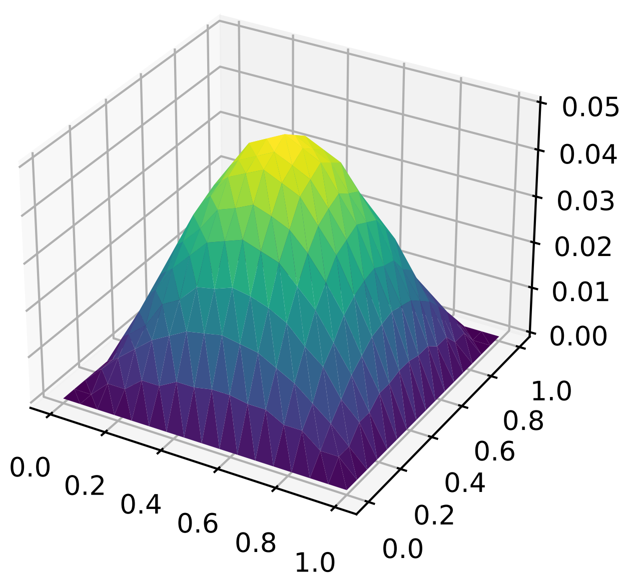
1.1.1 简单算例

- 区域 $\Omega = (0,1) \times (0,1)$,
- 右端项 $f = \sin(\pi x)\sin(\pi y)$

- 边界条件: $\partial\Omega_N = \emptyset, \quad g_D = 0$ (齐次 Dirichlet)

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

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')
solve(a == L, u_h, bcs=bc)          # 有不同求解方式， 可添加求解参数
# solve(a == L, u_h, bcs=(bc,))

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

[2]:
```
<mpl_toolkits.mplot3d.art3d.Poly3DCollection at 0x7fa87ed27400>
```



1.1.2 Firedrake 内建网格生成函数

UnitDiskMesh, IntervalMesh, RectangleMesh, CubeMesh …

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

pprint(utility_meshes.__all__)
```

```
['IntervalMesh',
 'UnitIntervalMesh',
 'PeriodicIntervalMesh',
 'PeriodicUnitIntervalMesh',
 'UnitTriangleMesh',
 'RectangleMesh',
 'TensorRectangleMesh',
 'SquareMesh',
 'UnitSquareMesh',
 'PeriodicRectangleMesh',
 'PeriodicSquareMesh',
 'PeriodicUnitSquareMesh',
 'CircleManifoldMesh',
 'UnitDiskMesh',
 'UnitTetrahedronMesh',
 'BoxMesh',
 'CubeMesh',
 'UnitCubeMesh',
 'PeriodicBoxMesh',
 'PeriodicUnitCubeMesh',
 'IcosahedralSphereMesh',
 'UnitIcosahedralSphereMesh',
 'OctahedralSphereMesh',
 'UnitOctahedralSphereMesh',
 'CubedSphereMesh',
 'UnitCubedSphereMesh',
 'TorusMesh',
 'CylinderMesh']
```

查看帮助 1. `?<fun-name>` 2. `help(<fun-name>)`

[4]:
```python
?CubeMesh
```

```
Signature:
CubeMesh(
    nx,
    ny,
    nz,
    L,
    reorder=None,
    distribution_parameters=None,
    comm=<mpi4py.MPI.Intracomm object at 0x7fa88bdc2f10>,
    name='firedrake_default',
)
Call signature: CubeMesh(*args, **kwargs)
Type:           cython_function_or_method
String form:    <cyfunction CubeMesh at 0x7fa884559c70>
File:           ~/software/firedrake-mini-petsc/src/firedrake/firedrake/utility_meshes.py
Docstring:
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 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.

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

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

      2. vector

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

      3. tensor

         设 $\mathbf{T}$ 为秩为 r 的张量, 那么

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

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

非线性函数 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
```

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, ... (https://firedrakeproject.org/variational-problems.html#supported-finite-elements)

1.1.5 线性方程组参数设置

求解的三种书写形式 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 possion_example1.py`

[5]:
```
# %load 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',
```

```python
                '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)
print('Done!')
```

```
Case: solve
Done!
```

- KSP scalable linear equations solvers, Krylov subspace solver with preconditioner

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

- PC

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

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

命令行参数　终端演示: 设置命令行参数控制线性方程组的求解

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

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

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

1.1.6 查看高斯积分公式

[6]:
```python
import FIAT
import finat

ref_cell = FIAT.reference_element.UFCTriangle()

from pprint import pprint
ret = {}
for i in range(0, 5):
    qrule = finat.quadrature.make_quadrature(ref_cell, i)
    ret[i] = {'points': qrule.point_set.points, 'weights': qrule.weights}

pprint(ret)
```

```
{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])},
 4: {'points': array([[0.81684757, 0.09157621],
       [0.09157621, 0.81684757],
       [0.09157621, 0.09157621],
       [0.10810302, 0.44594849],
       [0.44594849, 0.10810302],
       [0.44594849, 0.44594849]]),
     'weights': array([0.05497587, 0.05497587, 0.05497587, 0.11169079,
0.11169079,
       0.11169079])}}
```

显示选择积分公式

[7]:
```python
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(rule=qrule))
    print(f'degree={i}, v = {v}', )

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

```
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
```

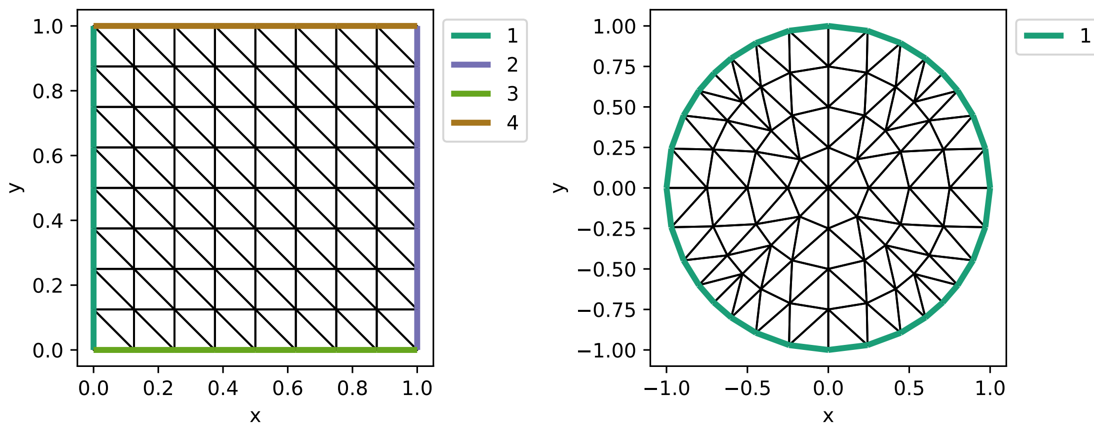
1.1.7 边界条件设置

内建网格边界编号

`RectangleMesh`:

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

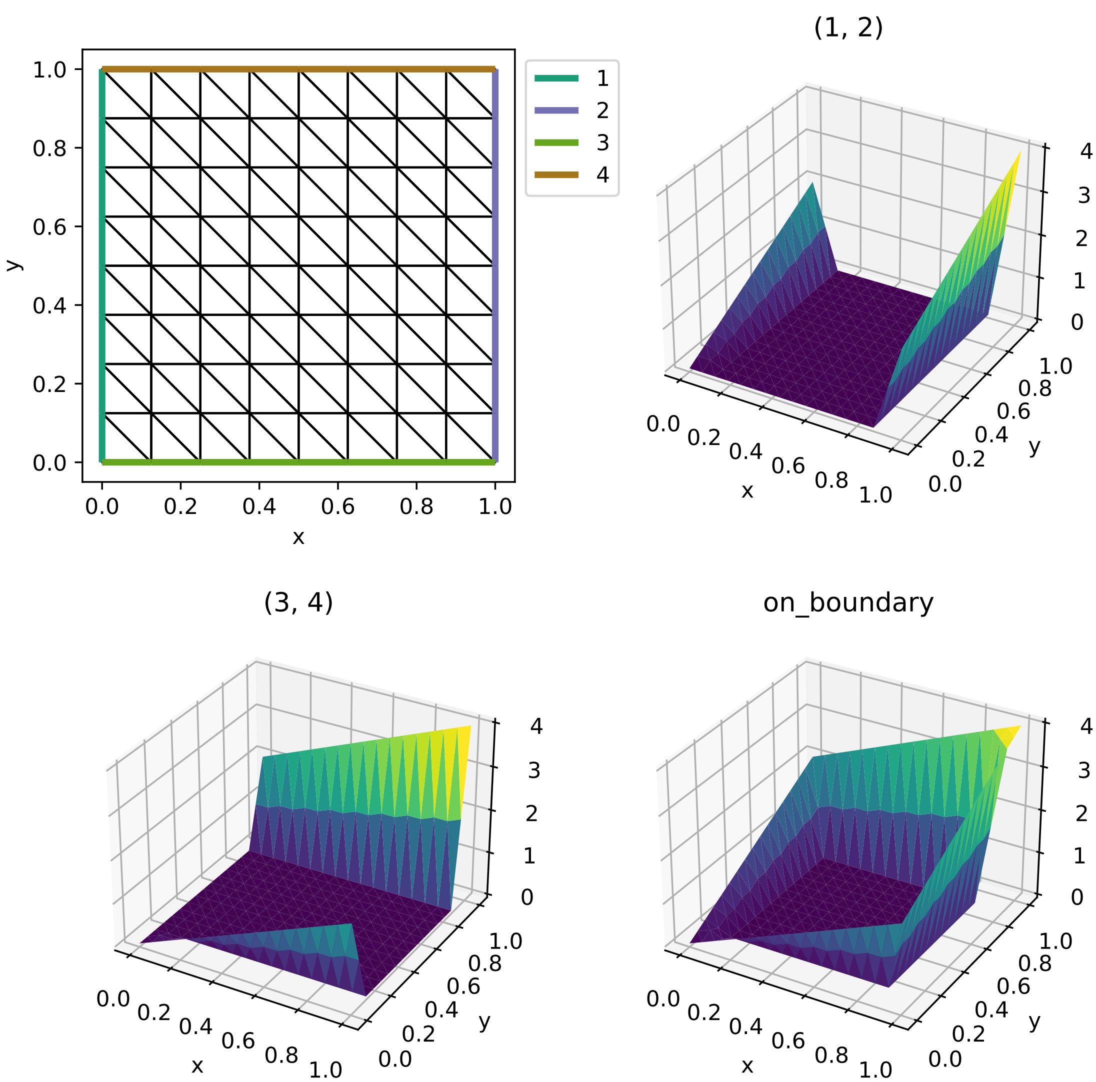
[8]:
```
from firedrake import *
import matplotlib.pyplot as plt


def plot_mesh_with_label(mesh, axes=None):
    if axes is None:
        fig, axes = plt.subplots(figsize=[4, 4])
    triplot(mesh, axes=axes, boundary_kw={'lw': 3})
    axes.set_aspect(aspect='equal')
    # ax.set_axis_off()
    axes.legend(loc='upper left', bbox_to_anchor=(1, 1))
    axes.set_xlabel('x')
    axes.set_ylabel('y')

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()
```



设置边界条件

[9]:
```
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)
```

[10]:
```
# plot the mesh and boundry conditons
fig, ax = plt.subplots(2, 2, figsize=[7, 7], subplot_kw=dict(projection='3d'))
ax = ax.flat

ax[0].remove()
ax[0] = fig.add_subplot(2, 2, 1)
plot_mesh_with_label(test_mesh, ax[0])

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()
```



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`

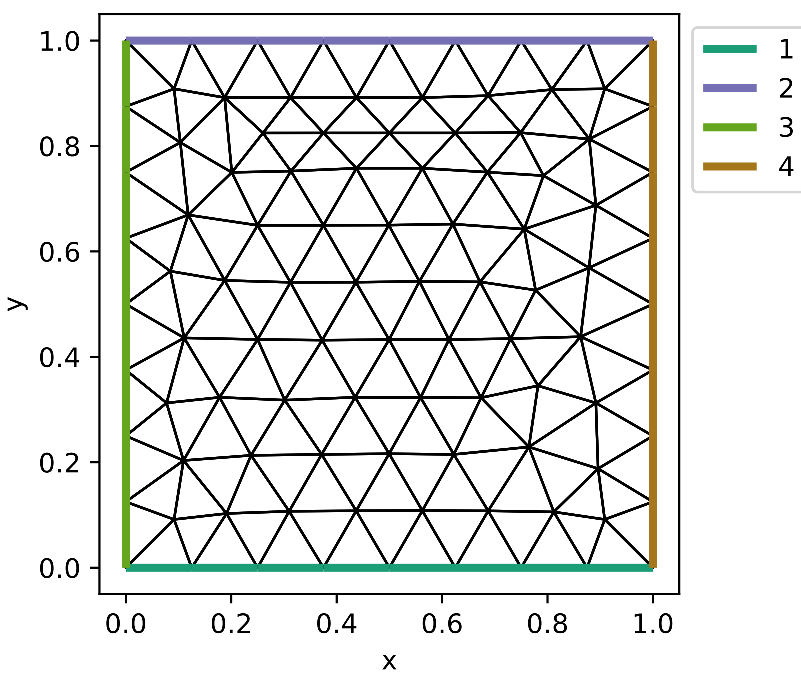
```
// Gmsh project created on Tue Sep 30 15:09:53 2022
SetFactory("OpenCASCADE");
//+
Rectangle(1) = {0, 0, 0, 1, 1, 0};
//+
Physical Curve("lower", 1) = {1};
```

```
//+
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`

[11]:

```python
# 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: `make_mesh_circle_in_rect.py`

[12]:

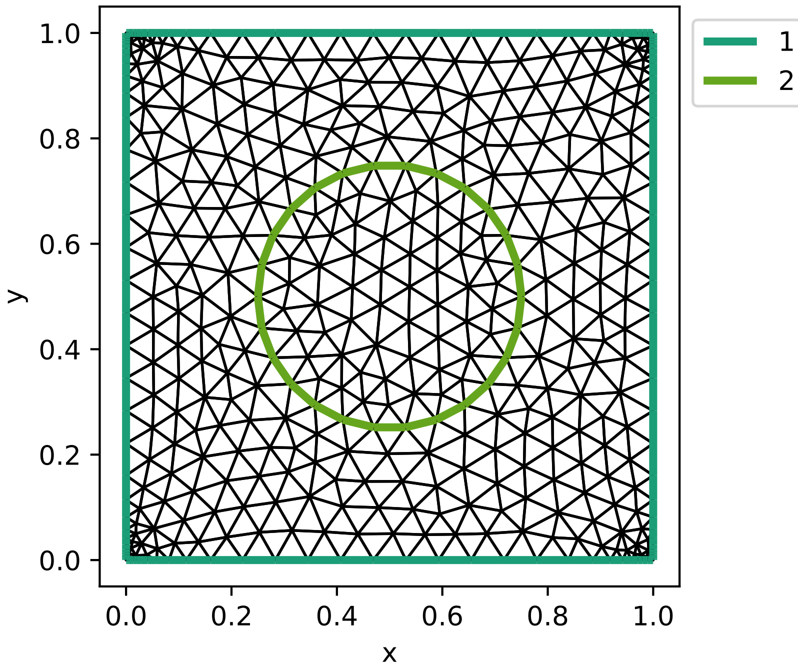
```python
from make_mesh_circle_in_rect import make_circle_in_rect
```

[13]:

```python
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)
```

```
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

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

变分问题

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

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

兼容性条件

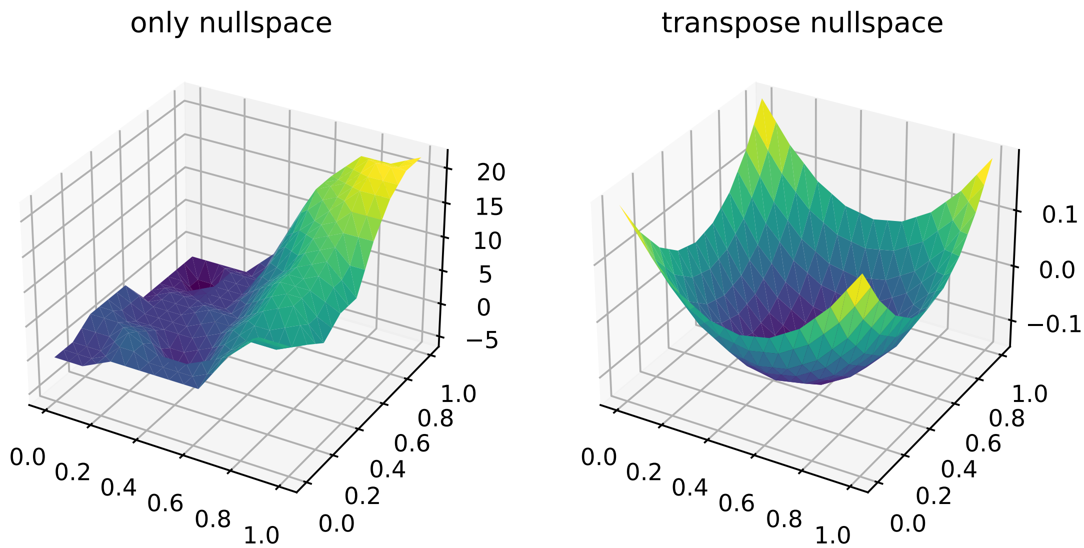
$$
\int_\Omega fv + \int_{\partial\Omega} g_N v = 0
$$

1.2.1 Use nullspace of solve

[14]:
```python
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 True:
    # 不满足兼容性条件
    g = Constant(1)
else:
    # 满足兼容性条件
    L = assemble(1*ds(domain=test_mesh, subdomain_id=subdomain_id))
    g = Constant(-assemble(f*dx)/L)

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)

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

nullspace = VectorSpaceBasis(constant=True)

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)


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

```
Residual norms for test1_ solve.
0 KSP Residual norm 7.133205795309e-01
1 KSP Residual norm 4.463009742158e+01
Residual norms for test2_ solve.
0 KSP Residual norm 5.188828525840e-01
1 KSP Residual norm 1.256141430046e-14
```

[14]: Text(0.5, 0.92, 'transpose nullspace')



1.2.2 Using Lagrange multiplier

变分问题

求 $u \in H^1, \mu \in R$ 使得

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

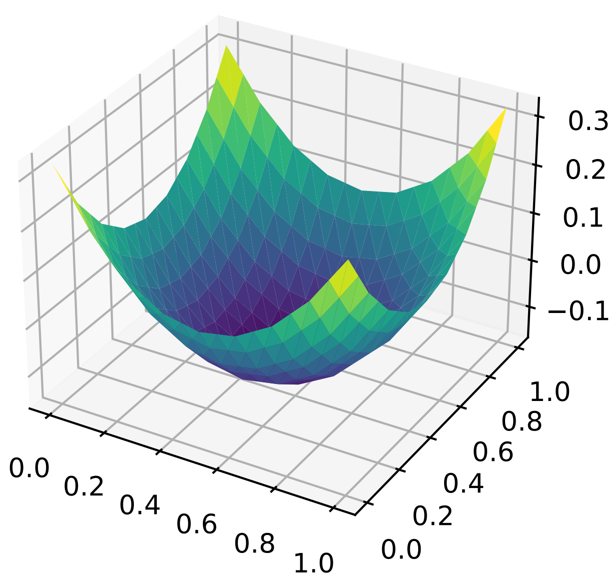
[15]:
```
# %load possion_neumann_lagrange.py
from firedrake import *
from firedrake.petsc import PETSc

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)
g_N = Constant(1)

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)
```

```python
a = inner(grad(u), grad(v))*dx + inner(mu, v)*dx + inner(u, eta)*dx
L = inner(f, v)*dx + inner(g_N, v)*ds

w_h = Function(W)
solve(a == L, w_h, options_prefix='test')

u_h, mu_h  = w_h.split()

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

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

[16]:
```python
fig, ax = plt.subplots(figsize=[4, 4], subplot_kw=dict(projection='3d'))
trisurf(u_h, axes=ax)
```

[16]:
```
&lt;mpl_toolkits.mplot3d.art3d.Poly3DCollection at 0x7fa879624700&gt;
```



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

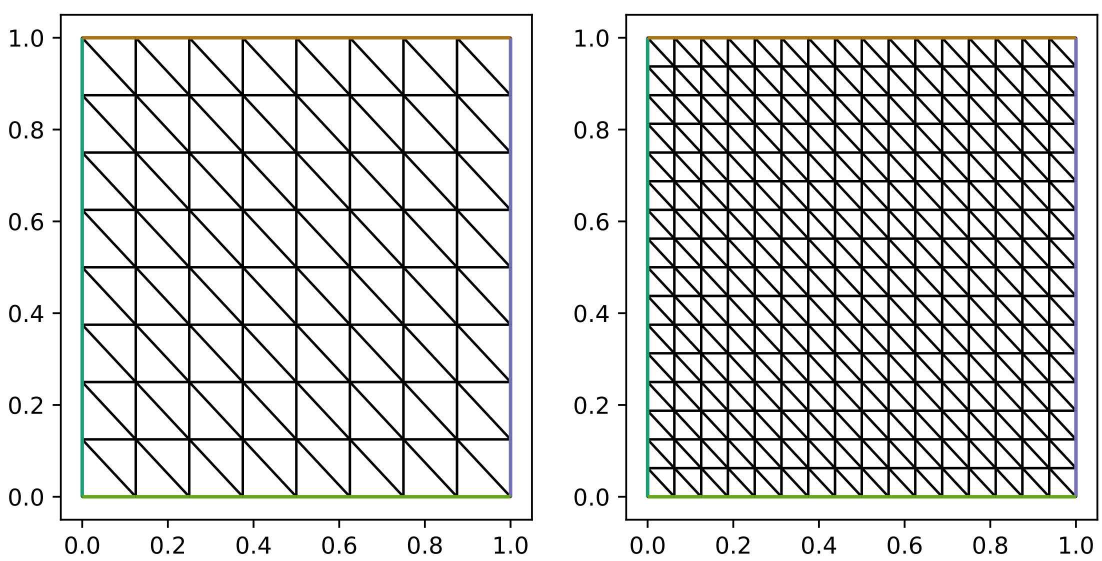
- 和真解对比
- 和参考解对比
- 相邻三层之间对比 (Cauchy 序列): possion_convergence.py

1.3.1 生成网格序列

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

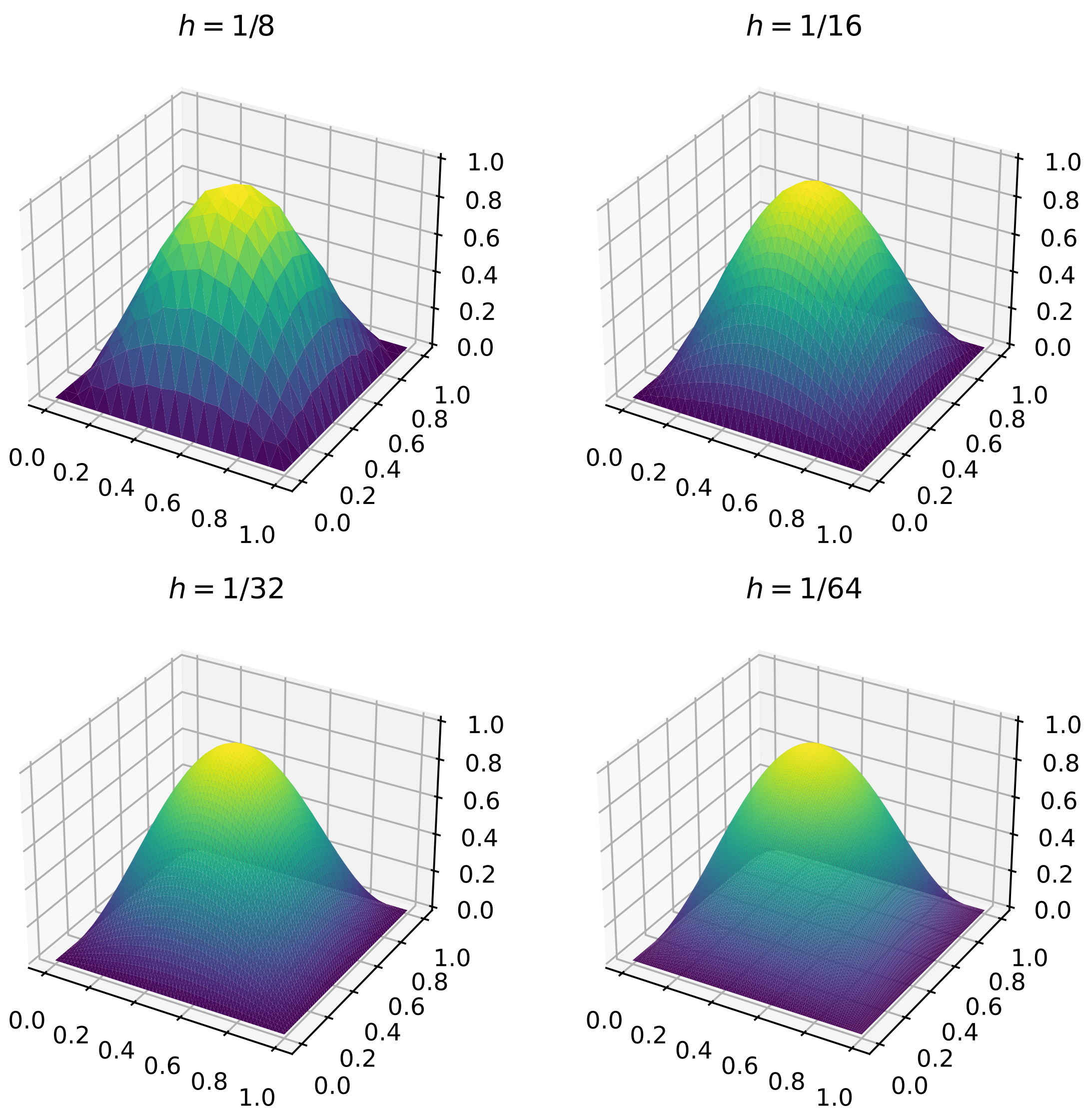
[17]:

```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])
```



[18]:

```
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(2, 2, figsize=[4*2, 4*2], 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

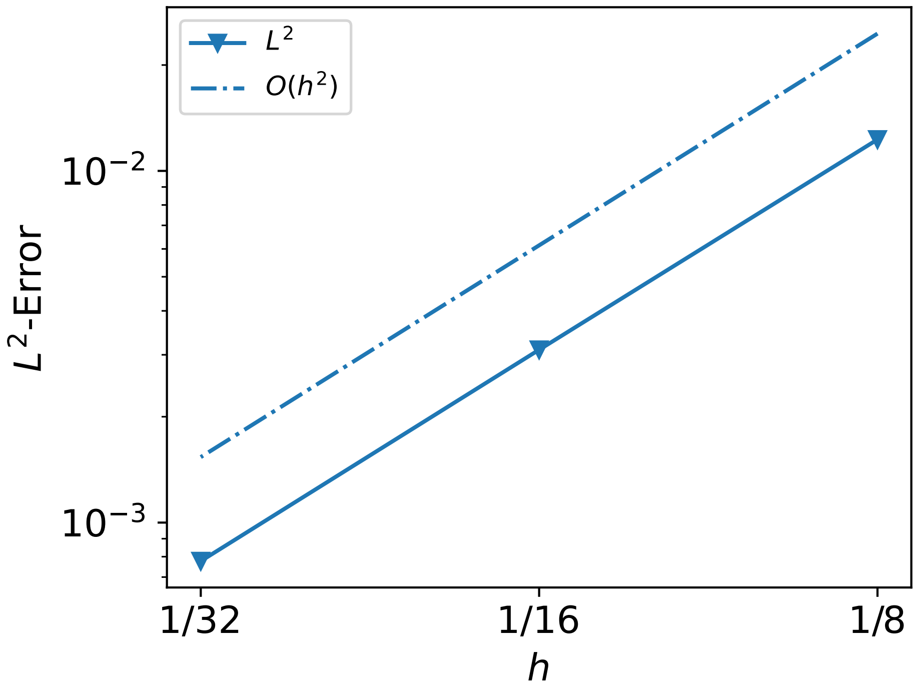
目前 Firedrake 只能投影函数到相邻层的网格上 (由 MeshHierarchy 生成的网格), 和最密网格比较时可以多次投影, 直至最密网格, 然后比较结果.

下面我们仅比较相邻层的误差

[19]:
```
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
```

[19]:
```
([0.125, 0.0625, 0.03125],
 [0.012284003199971324, 0.003100763810085325, 0.0007770614161052795])
```

[20]:
```
from intro_utils import plot_errors
plot_errors(hs, errors, expect_order=2)
```



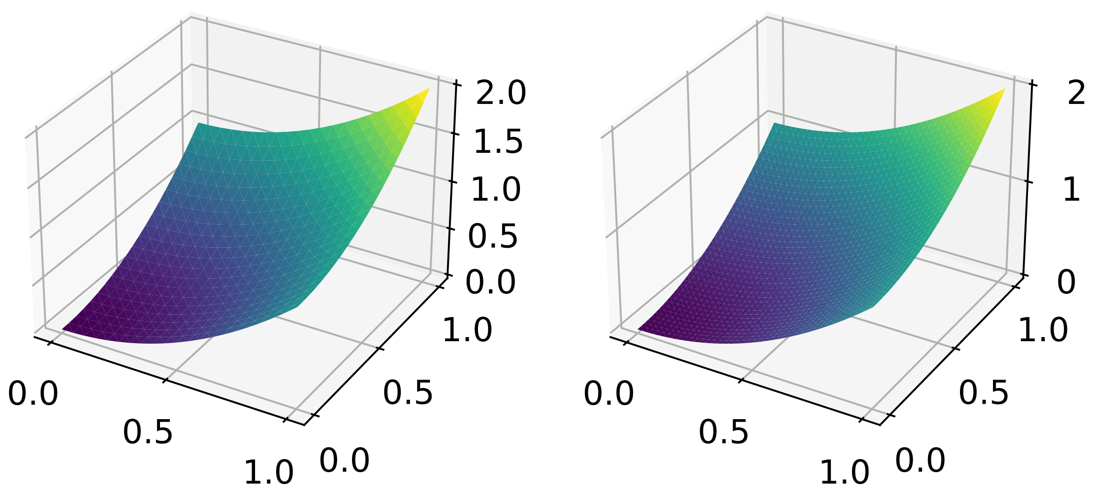
1.3.3 插值到细网格上的空间中

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

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

[21]:
```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'))
fd.trisurf(f1, axes=ax[0])
fd.trisurf(f2, axes=ax[1])
```

[21]:
```
<mpl_toolkits.mplot3d.art3d.Poly3DCollection at 0x7fa86b874fa0>
```



计算误差

[22]:
```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
```

[22]:

```
[0.012284003212205772, 0.003100763847789638, 0.0007770614201377909]
```

[23]:

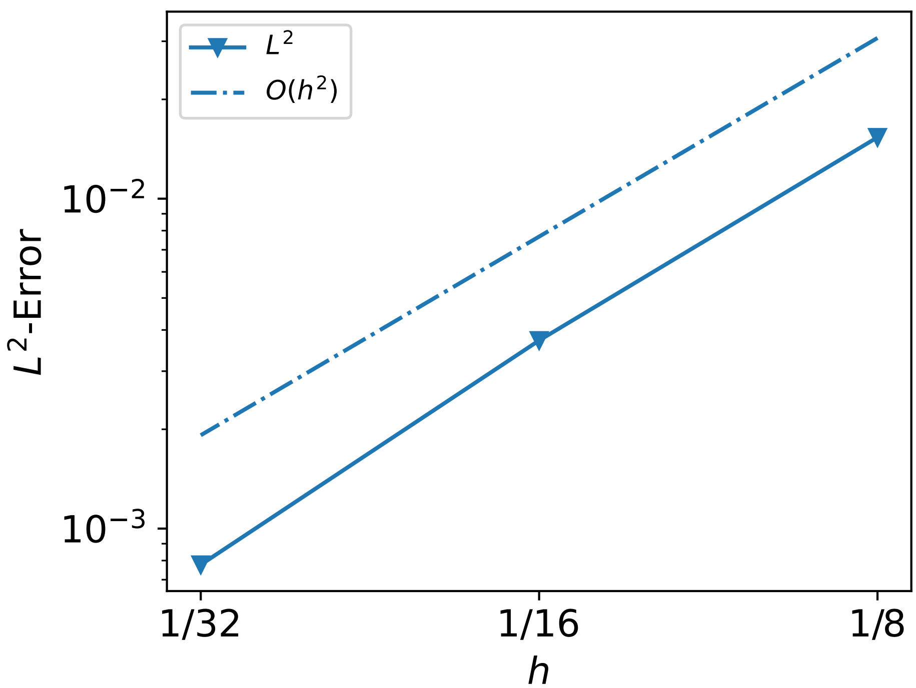
```
from fdutils.tools import errornorm as my_errornorm

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
```

[23]:

```
[0.015349062780286471, 0.0037181920308195534, 0.0007770614201377909]
```

[24]:

```
from intro_utils import plot_errors
plot_errors(hs, my_errors, expect_order=2)
```



1.4 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.

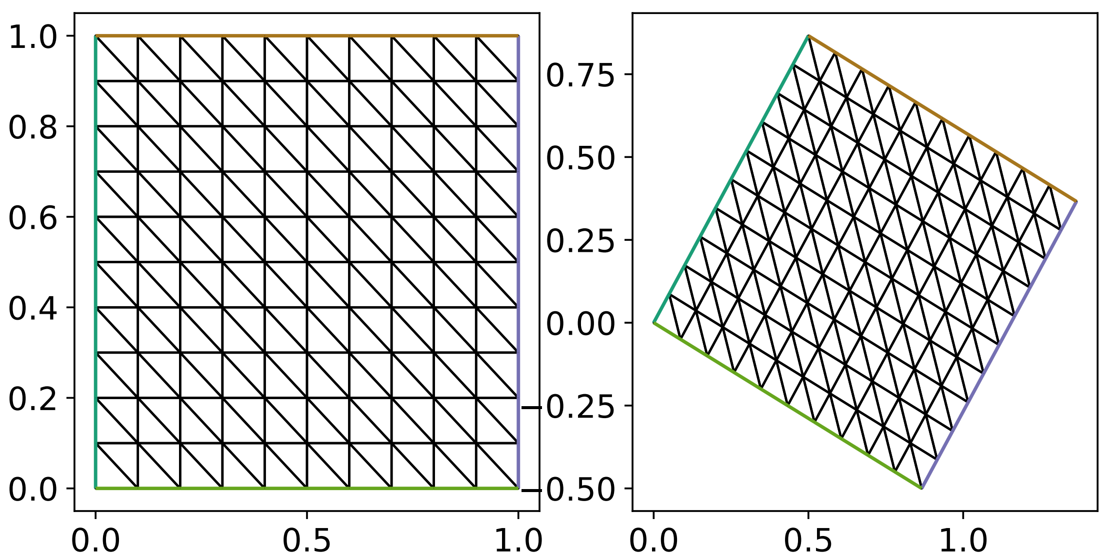
1.4.1 移动网格

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
```

[25]:

```python
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])
```



1.4.2 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.

```python
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)

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

1.4.3 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 `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.

1.4.4 数值实验

精确解为 \$ u = 1 - (x^2 + y$^{2)}${3.5}\$

[26]:
```
%run possion_convergence_circle.py
```

```
p = 1; Use iso: False; Only move bdy: False.
    orders: [2.01284527 2.01420928]

p = 2; Use iso: False; Only move bdy: False.
    orders: [2.07953299 2.0391775 ]

p = 2; Use iso: True; Only move bdy: False.
    orders: [3.07968268 3.04739627]

p = 3; Use iso: False; Only move bdy: False.
    orders: [2.06225857 2.03084755]

p = 3; Use iso: True; Only move bdy: True.
    orders: [3.63334435 3.56916446]
```

```
p = 3; Use iso: True; Only move bdy: False.
    orders: [4.15838886 4.09188043]

p = 4; Use iso: False; Only move bdy: False.
    orders: [2.05924173 2.02916455]

p = 4; Use iso: True; Only move bdy: True.
    orders: [3.50007466 3.49278383]

p = 4; Use iso: True; Only move bdy: False.
    orders: [5.19566749 5.10742164]
```

1.5 间断有限元方法

1.5.1 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

1.5.2 UFL 测度

1. `ds` 外部边
2. `dS` 内部边

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

[27]:

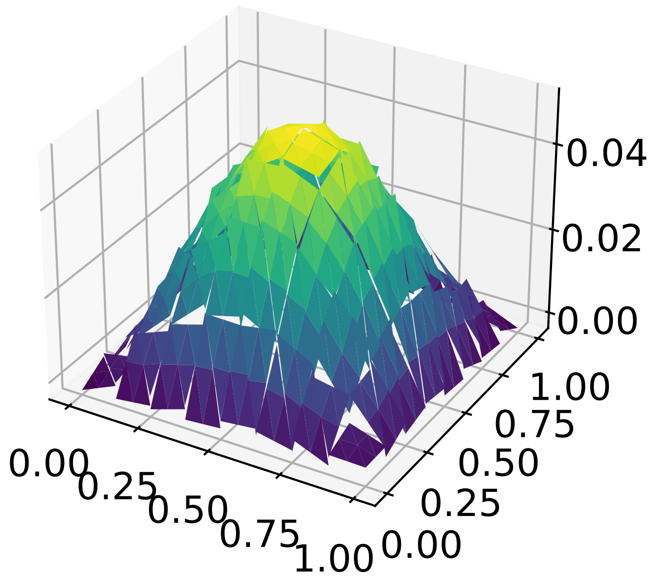
```
mesh = RectangleMesh(8, 8, 1, 1)

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)
```

[28]:

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

[28]:

```
<mpl_toolkits.mplot3d.art3d.Poly3DCollection at 0x7fa86b3f34f0>
```



1.6 自由度映射关系

1.6.1 编号

- V.dim(): 自由度个数
- V.cell_node_list: 局部编号与全局编号

[29]:
```
mesh = RectangleMesh(8, 8, 1, 1)
V = FunctionSpace(mesh, 'CG', 1)
V.dim(), V.cell_node_list[:5]
```

[29]:
```
(81,
 array([[0, 1, 2],
        [1, 2, 3],
        [2, 3, 4],
        [1, 3, 5],
        [3, 4, 6]], dtype=int32))
```

Example: 第一个三角形的坐标

[30]:
```
coords = mesh.coordinates
```

[31]:
```
# get the cell node map
V_c = coords.function_space()
V_c.cell_node_list[:2]
```

[31]:
```
array([[0, 1, 2],
       [1, 2, 3]], dtype=int32)
```

[32]:
```python
# another way to get the cell node map
coords.cell_node_map().values[:2]
```

[32]:
```
array([[0, 1, 2],
       [1, 2, 3]], dtype=int32)
```

[33]:
```python
coords.dat.data_ro_with_halos[[0, 1, 2]]
```

[33]:
```
array([[0.   , 0.   ],
       [0.   , 0.125],
       [0.125, 0.   ]])
```

1.6.2 有限元自由度

[34]:
```python
V = FunctionSpace(mesh, 'CG', 2)
# V.dim(), V.cell_node_list[:5]

element = V.finat_element

element.degree, element.cell,
```

[34]:
```
(2, <FIAT.reference_element.UFCTriangle at 0x7fa86be29a60>)
```

[35]:
```python
V.finat_element.entity_dofs()
```

[35]:
```
{0: {0: [0], 1: [1], 2: [2]}, 1: {0: [3], 1: [4], 2: [5]}, 2: {0: []}}
```

[36]:
```python
V.finat_element.entity_support_dofs()
```

[36]:
```
{0: {0: [0], 1: [1], 2: [2]},
 1: {0: [1, 2, 3], 1: [0, 2, 4], 2: [0, 1, 5]},
 2: {0: [0, 1, 2, 3, 4, 5]}}
```

1.6.3 查看矩阵和向量 (PETSc)

Introduction to PETSc

DOC: https://web.corral.tacc.utexas.edu/CompEdu/pdf/pcse/petsc_p_course.pdf

PETSc git repo: petsc4py demo

保存矩阵到文件: matvecio.py

[37]:
```python
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
```

[38]:
```
A = assemble(a)
b = assemble(L)
type(A), type(b)
```

[38]:
```
(firedrake.matrix.Matrix, firedrake.function.Function)
```

[39]:
```
type(A.petscmat)
```

[39]:
```
petsc4py.PETSc.Mat
```

[40]:
```
with b.dat.vec_ro as vec:
    print(type(vec))
```

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

2 NS 方程

Navier-Stokes 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

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

[41]:
```
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 $\times$ P1b.

P1b 由 P1 加上 Bubble 组成.

`NodalEnrichedElement`, `EnrichedElement`

VectorFunctionSpace 构造向量空间

[42]:
```
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

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

- TrialFunctions, TestFunctions:

  以 tuple 返回函数空间中的试验/测试函数,

  主要用于 MixedFunctionSpace.

- split, Function.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)
  - Function.split: 以存储共享的方式获取分量 (生成新的变量, 只是共享原存储空间)

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.

[43]:
```
w = Function(V) # u and p
u, p = split(w)

v, q = TestFunctions(V)

w_nm1 = Function(V)
u_nm1, p_nm1 = w_nm1.split()
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.

[44]:
```
bc = DirichletBC(V.sub(0), 0, 'on_boundary')
nullspace = MixedVectorSpaceBasis(V, [V.sub(0), VectorSpaceBasis(constant=True)])

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

[45]:
```
from tqdm.notebook import tqdm # progress bar

u_, p_ = w.split()

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

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

for i in  tqdm(range(N_T)):
    t = tau*(i+1)

    solver.solve()

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

    output.write(u_nm1, p_nm1, time=t)
```

```
0%|          | 0/128 [00:00<?, ?it/s]
```

2.4.1 Constant 用于时间依赖的表达式

[46]:
```
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)
```

```
[0.0, 0.09999999999999991, 0.19999999999999982, 0.29999999999999966,
0.39999999999999963]
```

2.5 ParaView 可视化计算结果

ParaView 演示

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

3 多进程并行

使用 `mpiexec` 运行 python 文件即可

此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.

[47]:
```
import ipyparallel as ipp
import os

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

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

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

3.1 DMPlex

[48]:
```
%%px --block
from firedrake import *

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

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

```
[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))
```

3.2 输出

intro_utils.py

[49]:
```
%%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)
```

[50]:
```
%%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)
```

[51]:
```
%%px --block
print('This msg from all rank')
```

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


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

3.3 communicator

[52]:
```
%%px --block

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

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

[53]:
```
%%px --block

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

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

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

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

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

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

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