ngsPETSc: NETGEN meets PETSc

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Oxford Mathematics

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Overview

- Reynolds and pressure robust Hood-Taylor discretisation with high-order mesh.
- Reynolds robust geometric multigrid on curved meshes.
- Easy implementation:

All codes are available on Github: `https://github.com/UZerbinati/DD28`

NETGEN

NETGEN is an advancing front 2D/3D-mesh generator, with many interesting features.

- The geometry we intend to mesh can be described by **Constructive Solid Geometry** (CSG), in particular we can use **Opencascade** to describe our geometry.
- It is able to construct isoparametric meshes, which conform to the geometry.

Joachim Scöberl

PETSc

PETSc stands for Portable, Extensible Toolkit for Scientific Computation, is a library for the scalable (parallel) solution of scientific applications modeled by partial differential equations (PDEs).

- **PETSc KSP** provides access to extremly efficent Krylov solvers.
- **PETSc SNES** provides access to extremly efficent non-linear solvers, with line-searching and trust region capabilities.

Stefano Zampini

ngsPETSc – NETGEN/NGSolve

Mathematical Institute

ngsPETSc is an interface between NETGEN/NGSolve and **PETSc**. In particular, **ngsPETSc** provides new capabilities to **NETGEN/NGSolve** such as:

- Access to all linear solver capabilities of **KSP**.
- Access to all preconditioning capabilities of **PC**.
- Access to all non-linear solver capabilities of **SNES**.
- Access to all mesh refinement capabilities of **DMPLEX**.

PETSc DMPlex

PETSc DMPlex handles unstructured grids using the generic **PETSc** interface for hierarchy and multi-physics.

- **PETSc DMPlex** provides a wide variety of primitive mesh operations such as: *meet*, *closure*, *cone*, etc $+$
- **PETSc DMPlex** provides a wide variety of mesh refinement operations such as: *uniform refinement*, *Alfeld refinement*, *box refinement*, etc

Matthew G. Knepley

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

- Variational formulation can be easily defined using the **UFL** language.
- Wide class of finite elements are available, including $H(div)$, $H(curl)$, H^1 and H^2.
- Provides access to **PETSc** linear solvers and non-linear solvers.

ngsPETSc provides new capabilities to **Firedrake** such as:

- Access to all Netgen generated linear meshes and high order meshes.
- Splits for macro elements, such as Alfeld splits and Powell-Sabin splits (even on curved geometries).
- Adaptive mesh refinement capabilities, that conform to the geometry.
- High order mesh hierarchies for multigrid solvers.

Examples – Opencascade via NETGEN

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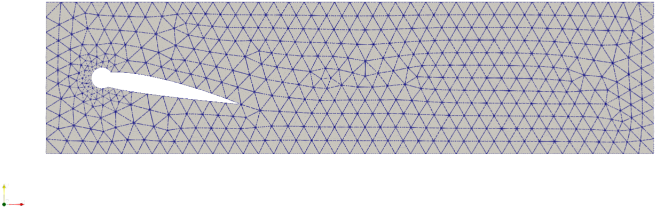
```
n = 140
profile = "2412"
xNACA = naca(profile, n, False, False)[0]
yNACA = naca(profile, n, False, False)[1]
pnts = [Pnt(xNACA[i], yNACA[i], 0) for i in range(len(
    xNACA))]
spline = SplineApproximation(pnts)
airfoil = Face(Wire(spline)).Move((0.3,0.5,0)).Rotate(
    Axis((0.3,0.5,0), Z), -10)
circle = Circle(Pnt(0.37,0.5),0.07).Face()
shape = (Rectangle(4, 1).Face()-airfoil-circle)
shape.edges.name="wall"
shape.edges.Min(X).name="inlet"
```

Examples – Opencascade via NETGEN


```
shape.edges.Max(X).name="outlet"
geo = OCCGeometry(shape, dim=2)
ngmesh = geo.GenerateMesh(maxh=0.1)
```



Stokes flow – Weak formulation

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Find $(\boldsymbol{u}, p) \in V \times Q$ such that

$$\begin{aligned} \nu \int_\Omega \varepsilon(\boldsymbol{u}) : \varepsilon(\boldsymbol{v}) - \int_\Omega p \nabla \cdot \boldsymbol{v} &= \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v} && \forall \boldsymbol{v} \in V \\ - \int_\Omega q \nabla \cdot \boldsymbol{u} &= 0 && \forall q \in Q \end{aligned}$$

where V and Q are the velocity and pressure spaces respectively, i.e. $V = H_0^1(\Omega)^2$ and $Q = L_0^2(\Omega)$.

Stokes flow – Inf-sup condition

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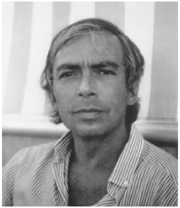
We can also look for a discrete solution, i.e. find $(\boldsymbol{u}_h, p_h) \in V_h \times Q_h$ such that

$$\nu \int_\Omega \varepsilon(\boldsymbol{u}) : \varepsilon(\boldsymbol{v}) - \int_\Omega p \nabla \cdot \boldsymbol{v} = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v}$$
$$- \int_\Omega q \nabla \cdot \boldsymbol{u} = 0$$

for all $(\boldsymbol{v}, q) \in V_h \times Q_h$.

$$\inf_{q \in Q_h} \sup_{\boldsymbol{v} \in V_h} \frac{\int_\Omega q \nabla \cdot \boldsymbol{v}}{\|q\|_{L^2} \|\boldsymbol{v}\|_{H^1}} \geq \beta > 0$$



Franco Brezzi

Stokes flow – UFL


```python
u, p = TrialFunctions(Z)
v, q = TestFunctions(Z)
nu = Constant(1e-3)
a = (nu*inner(eps(u), eps(v)) - p * div(v) - div(u) * q)*dx
L = inner(Constant((0, 0)), v) * dx
```

Stokes flow – Scott–Vogelius element

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We can use the Scott–Vogelius pair, which is a mixed finite element of order k for the velocity and order $k-1$ for the pressure. Such an element is inf-sup stable for $k \geq 2$, under certain assumptions on the mesh. Such pair is **divergence-free**.

When $k=2$ we need **Alfeld splits**.

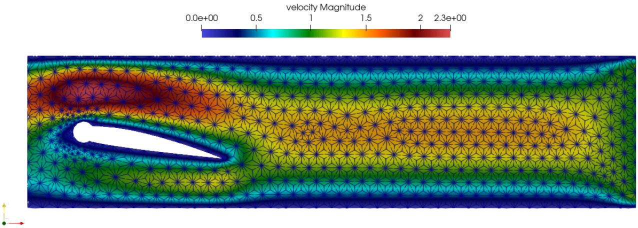
```
geo = OCCGeometry(shape, dim=2)
ngmesh = geo.GenerateMesh(maxh=0.1)
ngmesh.SplitAlfeld()
```

```
V = VectorFunctionSpace(mesh, "CG", 2)
W = FunctionSpace(mesh, "DG", 1)
Z = V * W
```

Ridgway Scott

Stokes flow – Scott–Vogelius

```
bcs = [DirichletBC(Z.sub(0), inflowoutflow,
    labelsInlet),
       DirichletBC(Z.sub(0), zero(2), labelsWall)]
nullspace = MixedVectorSpaceBasis(Z, [Z.sub(0),
    VectorSpaceBasis(constant=True)])
solve(a == L, sol0, bcs=bcs, solver_parameters=
    paramsLU)
```

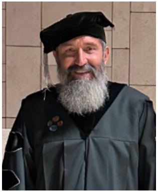


Stokes flow – Hood–Taylor element

Another element pair we will use is the Hood–Taylor pair, which has **no restrictions** on the mesh in two dimensions.

```
V = VectorFunctionSpace(mesh, "CG", 2)
W = FunctionSpace(mesh, "CG", 1)
Z = V * W
```

We lose the point-wise divergence-free property! This is not an issue because the same would happen for Scott-Vogelius on curved meshes.



Daniele Boffi

Fieldsplit Schur preconditioner

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The previous set of equations can be written in matrix form as

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ p \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ 0 \end{bmatrix}$$

We choose as preconditioner the **fieldsplit Schur preconditioner**, i.e.

$$\begin{bmatrix} I & -\hat{A}^{-1}B^T \\ 0 & I \end{bmatrix} \begin{bmatrix} \hat{A}^{-1} & 0 \\ 0 & \hat{S}^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -B\hat{A}^{-1} & I \end{bmatrix}$$

where S is the **Schur complement**, i.e. $S = -BA^{-1}B^T$.

```
    "fieldsplit_0_ksp_type": "preonly",
    "fieldsplit_0_pc_type": "mg",
    "fieldsplit_1_ksp_type": "preonly",
    "fieldsplit_1_pc_type": "python",
```

Fieldsplit Schur preconditioner – Mass matrix

Thanks to the inf-sup condition we can prove that the Schur complement is spectrally equivalent to the mass matrix, hence we can use as preconditioner:

$$\begin{bmatrix} I & -\hat{A}^{-1}B^T \\ 0 & I \end{bmatrix} \begin{bmatrix} \hat{A}^{-1} & 0 \\ 0 & -\nu\hat{M}^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -B\hat{A}^{-1} & I \end{bmatrix}$$

where M is the mass matrix.

```
class Mass(AuxiliaryOperatorPC):
    def form(self, pc, test, trial):
        a=1/nu*inner(test, trial)*dx
        bcs = None
        return (a, bcs)
```

Andrew Wathen

Multigrid on curved meshes

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ngsPETSc allows us to create a hierarchy of curved meshes for multigrid solvers.

```
mesh = Mesh(ngmesh)
from ngsPETSc import NetgenHierarchy
mh = NetgenHierarchy(ngmesh,2, 2)
```

We can then use a multigrid solver to compute $\hat{A}^{-1}$:

```
    "fieldsplit_0_pc_type": "mg",
    "fieldsplit_1_ksp_type": "preonly",
    "fieldsplit_1_pc_type": "python",
    "fieldsplit_1_pc_python_type": "__main__.Mass",
    "fieldsplit_1_aux_pc_type": "bjacobi",
    "fieldsplit_1_aux_sub_pc_type": "icc",
```

Navier-Stokes flow

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A more interesting example is the Navier-Stokes flow, which is a non-linear problem. In particular, we will consider the problem of finding $(\boldsymbol{u}, p) \in H^1(\Omega)^2 \times L^2(\Omega)$ such that

$$\int_\Omega \partial_t \boldsymbol{u} \cdot \boldsymbol{v} + \int_\Omega (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} \cdot \boldsymbol{v} + \nu \int_\Omega \nabla \boldsymbol{u} : \nabla \boldsymbol{v} - \int_\Omega p \nabla \cdot \boldsymbol{v} = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v}$$

$$-\int_\Omega q \nabla \cdot \boldsymbol{u} = 0$$

for all $(\boldsymbol{v}, q) \in H^1(\Omega)^2 \times L^2(\Omega)$.

Navier-Stokes flow – Augmented Lagrangian

We consider an augmented Lagrangian formulation for the discrete problem, i.e. find $(\boldsymbol{u}_h, p_h) \in V_h \times Q_h$ such that

$$\begin{aligned}(\partial_t \boldsymbol{u}, \boldsymbol{v})_0 + (\boldsymbol{u} \cdot \nabla \boldsymbol{u}, \boldsymbol{v})_0 + \nu(\nabla \boldsymbol{u}, \nabla \boldsymbol{v})_0 \\ - (p, \nabla \cdot \boldsymbol{v})_0 + \gamma(\nabla \cdot \boldsymbol{u}, \nabla \cdot \boldsymbol{v})_0 \quad &= (\boldsymbol{f}, \boldsymbol{v})_0\end{aligned}$$

and verifying the weak divergence free constraint $(\nabla \cdot \boldsymbol{u}, q)_0 = 0$, for all $(\boldsymbol{v}, q) \in V_h \times Q_h$.

Navier-Stokes flow – Fieldsplit Schour preconditioner

The linearized version of the Navier-Stokes equations can be written in matrix form as

$$\begin{bmatrix} A + \gamma B^T W B & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ p \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ 0 \end{bmatrix}$$

We choose as preconditioner the **fieldsplit Schur preconditioner**, i.e.

$$\begin{bmatrix} I & -\hat{A}_\gamma^{-1} B^T \\ 0 & I \end{bmatrix} \begin{bmatrix} \hat{A}_\gamma^{-1} & 0 \\ 0 & \hat{S}_\gamma^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -BA_\gamma^{-1} & I \end{bmatrix}$$

$$A_\gamma = A + \gamma B^T W B \qquad S_\gamma = -BA_\gamma^{-1} B^T.$$

In this case, we notice that $S_\gamma \sim -(\nu + \gamma)^{-1} M$, but $\mathcal{S} \not\sim \nu^{-1} M$.

Navier-Stokes flow – Augmented Lagrangian

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- The augmented Lagrangian term helps enforce the divergence-free constraint, and makes the scheme pressure robust.
- We can use as preconditioner

$$\begin{bmatrix} I & -\hat{A}_\gamma^{-1}B^T \\ 0 & I \end{bmatrix} \begin{bmatrix} \hat{A}_\gamma^{-1} & 0 \\ 0 & -(\nu+\gamma)M^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -BA_\gamma^{-1} & I \end{bmatrix}$$

- How do we compute $\hat{A}_\gamma^{-1}$ efficiently ? Can we adopt a multigrid approach ?

Subspace correction methods for nearly singular problems

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To compute $\hat{A}_\gamma^{-1}$ we can use a subspace correction method. We decompose the space V_h as follows:

$$V_h = \sum_{i=1} V_i.$$

We consider a coarse space V_H and the projection and injection operators:

$$P_H : V_H \to V_h, \qquad I : V_h \to V_i.$$

We then consider as smoother the two–level additive Schwarz preconditioner defined as:

$$\hat{A}_\gamma^{-1} = P_H A_{\gamma,H}^{-1} P_H^T + \sum_{i=1} I_i A_{\gamma,i}^{-1} I_i^T.$$

Subspace correction methods for nearly singular problems

Robust relaxetion

We need the discrete kernel,

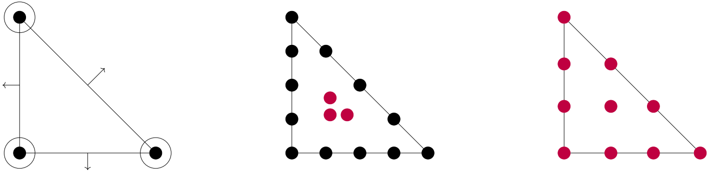
$$\mathbb{K}_h = \{\boldsymbol{v} \in V_h : B\boldsymbol{v} = 0\},$$

to decompose in a **stable** way as follows:

$$\mathbb{K}_h = \sum_{i=1} \mathbb{K}_h \cap V_i.$$

Robust relaxation via FEEC – Hood–Taylor

$$\begin{tikzcd}
0 \arrow[r] & \left[H^2(\Omega)\right]^2 \arrow[r, "\nabla\times"] \arrow[d] & \left[H^1_0(\Omega)\right]^2 \arrow[r, "\nabla\cdot"] \arrow[d] & L^2(\Omega) \arrow[r] \arrow[d] & 0 \\
0 \arrow[r] & \left[\mathbb{P}^5(\mathcal{T}_h)\right]^2 \arrow[r, "\nabla\times"] & \left[\mathbb{P}^4(\mathcal{T}_h)\right]^2 \arrow[r, "\nabla\cdot"] & \mathbb{P}^3_{disc}(\mathcal{T}_h) \arrow[r] & 0
\end{tikzcd}$$



Robust prolongation – Hood–Taylor

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Robust prolongation

If the space pair (V_h, Q_h) is inf-sup stable and the meshes are nested, we have a robust prolongation operator defined by:

$$\tilde{P}_H \boldsymbol{u}_H - \tilde{\boldsymbol{u}}_h = \boldsymbol{u}_H - \tilde{\boldsymbol{u}}_h,$$

where

$$a_\gamma(\tilde{\boldsymbol{u}}_h, \tilde{\boldsymbol{v}}_h) = \gamma(\nabla \cdot \tilde{\boldsymbol{u}}_h, \nabla \cdot \tilde{\boldsymbol{v}}_h)_{\pi_{Q_h} \pi_{Q_h}{}^T} \quad \forall \tilde{\boldsymbol{v}}_h \in \tilde{V}_h,$$

where π_{Q_h} is the L^2 projection onto Q_h and $\tilde{V}_h$ is the space of discrete velocity vanishing at the boundary of the coarse cells.

Firedrake' 24

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Join us at the Firedrake user and developer workshop that will be held between 16-18 September 2024 at the University of Oxford.