# ngsPETSc: NGS meets PETSc

UNIVERSITY OF OXFORD
Mathematical Institute

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Oxford Mathematics

## Overview

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- We will see how to use **PETSc KSP** to solve linear systems in **NGSolve**. We will also how to impose a near nullspace.
- We will see how to use **PETSc PC** as a preconditioners building block inside **NGSolve**. In particular, we will see how to use Hypre in a vertex patch preconditioner and as an auxiliary space preconditioner.
- We will see how to use **PETSc SNES** to solve non-linear problems in **NGSolve**. In particular, we will see how to solve the Naghdi shell problem.

All codes are available on Github:
`https://github.com/UZerbinati/PETSc24`

## Netgen/NGSolve

**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** representation, which conform to the geometry.
- A wide variety of mesh splits are available also for curved geometries, such as Alfeld splits and Powell-Sabin splits.
- High flexibility in the mesh generation and mesh refinement.

## Netgen/NGSolve

**NGSolve** is a high-performance multiphysics finite element software with an extremely flexible Python interface.

- Wide range of finite elements available, including and not limited to hierarchical $H^1$ elements, $H(div)$ Raviart-Thomas and Brezzi-Douglas-Marini elements, and $H(curl)$ Nédélec elements.
- The variational formulation can be easily defined using an analogous language to the unified form language (UFL).
- Many extensions are available, including **ngsxfem** for unfitted finite element discretizations, **ngsTreffetz** for Treffetz methods and **ngsTents** for spacetime tents schemes.

## ngsPETSc – NETGEN/NGSolve

**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 KSP

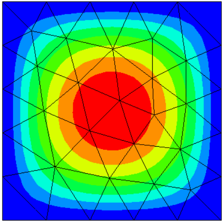
## An NGsolve Example – Poisson

```
from ngsolve import *
import netgen.gui
import netgen.meshing as ngm
from mpi4py.MPI import COMM_WORLD

if COMM_WORLD.rank == 0:
    mesh = Mesh(unit_square.GenerateMesh(maxh=0.2).Distribute(COMM_WORLD))
else:
    mesh = Mesh(ngm.Mesh.Receive(COMM_WORLD))
fes = H1(mesh, order=3, dirichlet="left|right|top|bottom")
u,v = fes.TnT()
a = BilinearForm(grad(u)*grad(v)*dx).Assemble()
f = LinearForm(fes)
f += 32 * (y*(1-y)+x*(1-x)) * v * dx
```

## PETSc KSP – Direct solve with MUMPS

- We can perform a direct solve using MUMPS.

```python

from ngsPETSc import KrylovSolver
opts = {'ksp_type': 'preonly',
        'pc_type': 'lu',
        'pc_factor_mat_solver_type': 'mumps'}
solver = KrylovSolver(a,fes, solverParameters=opts)
gfu = solver.solve(f)
Draw(gfu,mesh, "solution")
```



Solution of Poisson problem computed with MUMPS

# PETSc KSP – Iterative Jacobi method

- We can use a wide variety of iterative solvers, for example, the Jacobi method, i.e.

$$x^{(k+1)} = D^{-1}(b - (A - D)x^{(k)}).$$

```
opts = {'ksp_type': 'richardson',
        'ksp_richardson_scale': 1.0,
        'pc_type': 'jacobi'}
solver = KrylovSolver(a,fes, solverParameters=opts)
gfu = solver.solve(f)
Draw(gfu,mesh, "solution")
```

- Analogously we can implement the Gauss-Seidel method.

## PETSc KSP – Galerkin Algebraic MultiGrid (GAMG)

- Inside of a classical iterative method such as conjugate gradient, we can play with different preconditioners such as PETSc GAMG.

```
opts = {'ksp_type': 'cg',
        'pc_type': 'gamg'}
solver = KrylovSolver(a,fes, solverParameters=opts)
gfu = solver.solve(f)
```

- As we will see in a moment we have a wide variety of preconditioners available, such as: **Hypre (AMG)**, **BDDC**, **...**

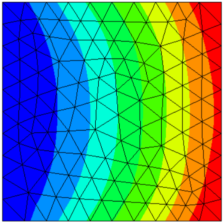
# An NGsolve Example – Linear Elasticity

```python
E, nu = 210, 0.2
mu  = E / 2 / (1+nu)
lam = E * nu / ((1+nu)*(1-2*nu))

def Stress(strain):
    return 2*mu*strain + lam*Trace(strain)*Id(2)

fes = VectorH1(mesh, order=1, dirichlet="left")
u,v = fes.TnT()

a = BilinearForm(InnerProduct(Stress(Sym(Grad(u))), Sym(Grad(v)))*dx)
a.Assemble()

force = CF( (0,1) )
f = LinearForm(force*v*ds("right")).Assemble()
```

# PETSc KSP – Near Nullspace

- We can pass a near nullspace to a **KrylovSolver**, informing the solver that there is a near nullspace.

```
from ngsPETSc import KrylovSolver, NullSpace
rbms = []
for val in [(1,0), (0,1), (-y,x)]:
    rbm = GridFunction(fes)
    rbm.Set(CF(val))
    rbms.append(rbm.vec)
nullspace = NullSpace(fes, rbms, near=True)
opts = {'ksp_type': 'cg',
        'pc_type': 'gamg'}
```



Solution of lienar elasticity fixing SO(3) to be in the near nullspace.

```
solver = KrylovSolver(a,fes, solverParameters=opts, nullspace=nullspace)
gfu = solver.solve(f)
```

# PETSc PC

# PETSc PC – Hypre

- We can use PETSc preconditioners as normal preconditioners in NGSolve, for example we can wrap a PETSc PC of type Hypre in NGSolve and use it inside NGSolve Krylov solvers.

```python
from ngsPETSc import pc
from ngsolve.krylovspace import CG
pre = Preconditioner(a, "PETScPC", pc_type="hypre")
gfu = GridFunction(fes)
gfu.vec.data = CG(a.mat, rhs=f.vec, pre=pre.mat,
 printrates=True)
Draw(gfu)
```

| Degrees of Freedom (p=1) | 7329 | 1837569 |
|---|---|---|
| PETSc PC (HYPRE) | 22 (5.19e-13) | 31 (6.82e-13) |
| NGSolve Geometric MultiGrid | 14 (4.08e-13) | 16 (1.30e-12) |

# PETSc PC – Hypre

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from ngsPETSc import pc
from ngsolve.krylovspace import CG
pre = Preconditioner(a, "PETScPC", pc_type="hypre")
gfu = GridFunction(fes)
gfu.vec.data = CG(a.mat, rhs=f.vec, pre=pre.mat,
 printrates=True)
Draw(gfu)
```

| | | |
|---|---|---|
| Degrees of Freedom (p=3) | 64993 | 259009 |
| PETSc PC (HYPRE) | 40 (6.48e-13) | 69 (2.53e-13) |
| NGSolve Geometric MultiGrid | 19 (8.89e-13) | 19 (7.78e-13) |

# PETSc PC – Vertex Patch

- We can use PETSc preconditioner as one of the building blocks of a more complex preconditioner. For example, we can use it as a two-level additive Schwarz preconditioner. In this case, we will use as fine space correction, the inverse of the local matrices associated with the patch of a vertex, i.e.

$$\mathcal{P} = \sum_{i=1}^{n} I_i A_i^{-1} I_i^T.$$

```
blocks = VertexPatchBlocks(mesh, fes)
blockjac = a.mat.CreateBlockSmoother(blocks)
gfu.vec.data = CG(a.mat, rhs=f.vec, pre=blockjac,
 printrates=True)
Draw(gfu)
```

# PETSc PC – Two level additive Schwarz

- We can also use the PETSc PC inside a two-level additive Schwarz preconditioner. In particular, we will use a PETSc PC of type HYPRE to do a coarse grid correction on the vertex degree of freedom.

$$\mathcal{P} = I_H A_H^{-1} I_H^T + \sum_{i=1}^{n} I_i A_i^{-1} I_i^T.$$

```
vertexdofs = VertexDofs(mesh, fes)
preCoarse = Preconditioner(a, "PETScPC", pc_type="hypre", restrictedTo=vertexdofs)
pretwo = preCoarse.mat + blockjac
gfu.vec.data = CG(a.mat, rhs=f.vec, pre=pretwo, printrates=True)
```

# An NGsolve Example – Discontinuous Galerkin

```
fesDG = L2(mesh, order=3, dgjumps=True)
u,v = fesDG.TnT()
aDG = BilinearForm(fesDG)
jump_u = u-u.Other(); jump_v = v-v.Other()
n = specialcf.normal(2)
mean_dudn = 0.5*n * (grad(u)+grad(u.Other()))
mean_dvdn = 0.5*n * (grad(v)+grad(v.Other()))
alpha = 4
h = specialcf.mesh_size
aDG = BilinearForm(fesDG)
aDG += grad(u)*grad(v) * dx
aDG += alpha*3**2/h*jump_u*jump_v * dx(skeleton=True)
aDG += alpha*3**2/h*u*v * ds(skeleton=True)
aDG += (-mean_dudn*jump_v -mean_dvdn*jump_u)*dx(skeleton=True)
aDG += (-n*grad(u)*v-n*grad(v)*u)*ds(skeleton=True)
fDG = LinearForm(fesDG)
fDG += 1*v * dx
```

## PETSc PC – Auxiliary Space Preconditioner

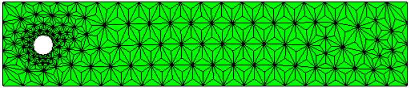
- We can now use the PETSc PC assembled for the conforming Poisson problem as an auxiliary space preconditioner for the DG discretisation. In particular, we will use as smoother a PETSc PC of type SOR.

```python
from ngsPETSc import pc
smoother = Preconditioner(aDG, "PETScPC", pc_type="sor")
transform = fes.ConvertL2Operator(fesDG)
preDG = transform @ pre.mat @ transform.T + smoother.mat
gfuDG = GridFunction(fesDG)
gfuDG.vec.data = CG(aDG.mat, rhs=fDG.vec, pre=preDG, printrates=True)
```

# Saddle Point Problems

# An NGsolve Example – Stokes flow

```
V = VectorH1(mesh, order=4, dirichlet="wall|inlet|cyl")
Q = H1(mesh, order=3)
u,v = V.TnT(); p,q = Q.TnT()
a = BilinearForm(InnerProduct(Grad(u),Grad(v))*dx+1e1*div(u)*div(v)*dx)
a.Assemble()
b = BilinearForm(div(u)*q*dx).Assemble()
gfu = GridFunction(V, name="u")
gfp = GridFunction(Q, name="p")
uin = CoefficientFunction( (1.5*4*y*(0.41-y)/(0.41*0.41), 0) )
gfu.Set(uin, definedon=mesh.Boundaries("inlet"))
```



## Fieldsplit Schur preconditioner – Mass matrix



It is well known that a field split preconditioner can be used to solve saddle point problems, i.e.

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

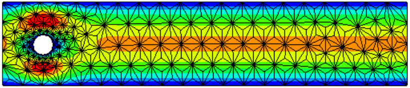
Thanks to the inf-sup condition we can prove that the Schur complement is spectrally equivalent to the mass matrix, hence we can use as preconditioner:

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

where $M$ is the mass matrix.

# PETSc PC – NGSolve Fieldsplit

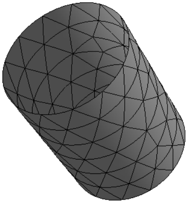
```
m = BilinearForm(p*q*dx)
K = BlockMatrix( [ [a.mat, b.mat.T], [b.mat, None] ] )
from ngsPETSc import pc
pre = Preconditioner(a, "PETScPC", pc_type="hypre")
mp = Preconditioner(m, "bddc")
m.Assemble()
C = BlockMatrix( [ [pre.mat, None], [None, mp.mat] ] )
rhs = BlockVector ( [f.vec, g.vec] )
sol = BlockVector( [gfu.vec, gfp.vec] )
solvers.MinRes (mat=K, pre=C, rhs=rhs, sol=sol,
                printrates=True, initialize=False,
```



# PETSc SNES

## An NGsolve Example – Naghdi Shell

```
geo = CSGeometry()
cyl   = Cylinder(Pnt(0,0,0),Pnt(1,0,0),0.4).bc("cyl")
left  = Plane(Pnt(0,0,0), Vec(-1,0,0))
right = Plane(Pnt(1,0,0), Vec(1,0,0))
finitecyl = cyl * left * right
geo.AddSurface(cyl, finitecyl)
geo.NameEdge(cyl,left, "left")
geo.NameEdge(cyl,right, "right")
if MPI.COMM_WORLD.rank == 0:
    mesh = Mesh(geo.GenerateMesh(maxh=0.3).Distribute(MPI.COMM_WORLD))
else:
    mesh = Mesh(ngm.Mesh.Receive(MPI.COMM_WORLD))
mesh.Curve(order)
```



Naghdi shell undeformed geometry.

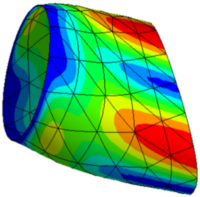
# An NGsolve Example – Naghdi Shell

```
nsurf = specialcf.normal(3)
thickness = 0.1
Ptau = Id(3) - OuterProduct(nsurf,nsurf)
Ftau = grad(u).Trace() + Ptau
Ctautau = Ftau.trans * Ftau
Etautau = 0.5*(Ctautau - Ptau)
eps_beta = Sym(Ptau*grad(beta).Trace())
gradu = grad(u).Trace()
ngradu = gradu.trans*nsurf
gfn = nsurf
a = BilinearForm(fes, symmetric=True)
a += Variation( thickness*InnerProduct(Etautau, Etautau)*ds )
a += Variation( 0.5*thickness**3*InnerProduct(eps_beta-Sym(gradu.trans*grad(gfn)),eps_beta-Sym(gradu.trans*grad(gfn)))*ds )
a += Variation( thickness*(ngradu-beta)*(ngradu-beta)*ds )
factor = Parameter(0.0)
a += Variation( -thickness*factor*y*u[1]*ds )
```

# PETSc SNES

- We can use PETSc SNES to solve the non-linear Naghdi shell problem.

```
    factor.Set (1.5*(loadstep+1))
    opts = {"snes_type": "newtonls",
    "snes_max_it": 10,
    "snes_monitor": "",
    "ksp_monitor": "",
    "pc_type": "lu"}
    solver = NonLinearSolver(fes, a=a,solverParameters=opts)
    gfu = solver.solve(gfu)
```



Solution of Naghdi shell problem.

# PETSc DMPLEX

**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 – Firedrake

**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.

# SLEPc EPS

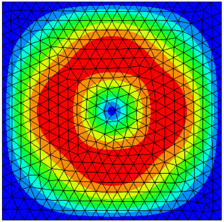
# An NGsolve Example – Mass conserving scheme

```
V1 = HDiv(mesh,order=order,dirichlet="rect",RT=True)
V2 = HCurlDiv(mesh, order=order, GGbubbles=True)
Q = L2(mesh, order=order, lowest_order_wb=el_int)
W = L2(mesh, order=order)
N = ng.FESpace("number", mesh)
V = V1 * V2 * Q * N * W
u, sigma, p, lam, w = V.TrialFunction()
v, tau, q, mu, r = V.TestFunction()
n = ng.specialcf.normal(mesh.dim)
h = ng.specialcf.mesh_size
a = ng.BilinearForm(V,eliminate_internal=el_int)
a += 1/(2*nu)*InnerProduct(dev(sigma),dev(tau))*dx
a += ((div(sigma) * v + div(tau) * u)) * dx
a += -(((sigma * n) * n) * (v * n) + ((tau * n) * n) *
       (u * n)) * dx(element_boundary=True)
a += (div(u) * q + div(v) * p) * dx
a += (lam * q + mu * p) * dx
a += (w * skw(tau) + skw(sigma) * r) * dx
m = ng.BilinearForm(V)
m += -1.*InnerProduct(u,v)*dx
```

# SLEPc ESP

- We easily solve the eigenvalue problem associated to the Stokes formulation using ngsPETSc EigenSolver.

```python
from ngsPETSc import EigenSolver
opts={"eps_type":"arnoldi",
      "st_type":"sinvert",
      "pc_type": "lu",
      "pc_factor_mat_solver_type": "mumps"}
solver = EigenSolver((m, a), V, 10, solverParameters=opts)
solver.solve()
print ("Eigenvalues")
for i in range(10):
    print(solver.eigenValue(i))
eigenMode, _ = solver.eigenFunction(0)
```



First eigenfunctions of the Stokes eigenvalue problem

# Conclusions

# What is new ?



- We exposed PETSc solver in NGSolve.
- PETSc preconditioners can be used as building blocks in NGSolve.
- Thanks to **PETSc SNES** we have a robust non-linear solver in NGSolve.
- Thanks to **SLEPc EPS** we have a robust eigenvalue solver in NGSolve.

# Future developments



- We plan to extend the interface to include time-stepping capabilities from **PETSc TS**.
- We plan to expriment with **HPDDM**.
- We plan to use **PETSc** as linear algebra backend in **NGSolve** to ensure cross-architecture compatibility and GPU acceleration.
- We plan to wrap also **SLEPc PEP** to solve polynomial eigenvalue problems.

# NGSolve User Meeting

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- Come to the 5th NGSolve User Meeting that will be held between the **17th of June** and the **19th of June** at **TU Wien**.

**Usually there are beers !**