ngsPETSc

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Oxford Mathematics

NGSolve-PETSc

January 2023 — First NetGen to DMPlex interface for Firedrake.

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Why PETSc?

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PETSc is a suite of data structures and routines developed by Argonne National Laboratory for the scalable (parallel) solution of scientific applications modeled by partial differential equations.

- PETSc implementation have **scalability** in mind, for this reason most linear algebra operations have **efficient parallel** implementation.
- Wide variety of **Krylov linear solvers (KSP)**.
- Wide variety of **preconditioners (PC)**.
- PETSc easily **wraps** many external libraries, such as: **HYPRE**, **MUMPS**, **H2OPUS**, **Intel MKL**, **...**

Setting up ngsPETSc

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MPI Support

To interface NGSolve with PETSc, you need to have NGSolve compiled with a MPI support, you achieve this using the **USE_MPI** flag, when building from source.

pip install will <u>not</u> work !

PETSc/SLEPc

You need to have PETSc and SLEPc configured on your system with slepc4py and petsc4py installed as well.

https://ngspetsc.readthedocs.io/en/latest/ngsPETSc.html

ngsPETSc - Basic Components

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ngsPETSc wraps the following PETSc objects in such a way that can be used easily in NGSolve:

- **PETSc Vec** and **PETSc Mat**, those are the basic linear algebra object corresponding to vectors and matrices.
- **PETSc KSP**, this is the object representing a **large sparse linear solver**.
- **PETSc DMPlex**, this is the object representing meshes in PETSc.
- **SLEPc EPS**, this is the object representing an eigenvalue problem solver in SLEPc.

ngsPETSc - PETSc Vec

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ngsPETSc is capable of creating a PETSc **Vec** from a NGSolve **BaseVector** and **ParallelVector** using the **VectorMapping** object.

```
from ngsPETSc import VectorMapping
Map = VectorMapping(fes)
petscVec = Map.petscVec(ngsVec)
```

ngsPETSc - PETSc Mat

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ngsPETSc is capable of creating a PETSc **Mat** from a NGSolve **BaseMatrix** object, thanks to the **Matrix** class.

```
a = BilinearForm(grad(u)*grad(v)*dx).Assemble()
M = a.mat
from ngsPETSc import Matrix
M = Matrix(m.mat, fes.FreeDofs(), matType="aij")
M.view()
```

- We can easily host PETSc **Mat** on devices, in particular PETSc support using **Kokkos** GPU manufactured by **NVIDIA**, **INTEL** and **AMD**.

ngsPETSc - PETSc KSP

ngsPETSc is capable of creating a PETSc **KSP** from a NGSolve **BilinearForm** object, thanks to the **KrylovSolver** class.

```
f = LinearForm(fes)
f += 32 * (y*(1-y)+x*(1-x)) * v * dx
from ngsPETSc import KrylovSolver
sol = KrylovSolver(a, fes, solverParameters={
           'ksp_type': 'cg',
           'pc_type': 'lu',
           'pc_factor_mat_solver_type': 'mumps'
          })
gfu = sol.solve(f)
```

ngsPETSc - PETSc KSP

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Algorithm	Associated Type	External Packages	Parallel	Complex
Richardson	KSPRICHARDSON	—	X	X
Chebyshev	KSPCHEBYSHEV	—	X	X
GMRES	KSPGMRES	—	X	X
Flexible GMRES	KSPFGMRES	—	X	X
LGMRES	KSPLGMRES	—	X	X
Deflated GMRES	KSPDGMRES	—	X	
Two-stage with least squares residual minimization	KSPTSIRM	—	X	X
Conjugate Gradient	KSPCG	—	X	X
Conjugate Gradient Squared	KSPCGS	—	X	X
Conjugate Gradient for Least Squares	KSPCGLS	—	X	X
Conjugate Gradient on Normal Equations	KSPCGNE	—	X	X

ngsPETSc - PETSc KSP

Nash Conjugate Gradient with trust region constraint	`KSPNASH`	—	X	X
Conjugate Gradient with trust region constraint	`KSPSTCG`	—	X	X
Gould et al Conjugate Gradient with trust region constraint	`KSPGLTR`	—	X	X
Steinhaug Conjugate Gradient with trust region constraint	`KSPQCG`	—	X	X
Left Conjugate Direction	`KSPLCD`	—	X	X
Bi-Conjugate Gradient	`KSPBICG`	—	X	X
Stabilized Bi-Conjugate Gradient	`KSPBCGS`	—	X	X
Improved Stabilized Bi-Conjugate Gradient	`KSPIBCGS`	—	X	X
Transpose-free QMR	`KSPTFQMR`	—	X	X

ngsPETSc - PETSc KSP

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Tony Chan QMR	KSPTCQMR	—	X	X
QMR BiCGStab	KSPQMRCGS	—	X	X
Flexible Conjugate Gradients	KSPFCG	—	X	X
Flexible stabilized Bi-Conjugate Gradients	KSPFBCGS	—	X	X
Flexible stabilized Bi-Conjugate Gradients with fewer reductions	KSPFBCGSR	—	X	X
Stabilized Bi-Conjugate Gradients with length ℓ recurrence	KSPBCGSL	—	X	X
Conjugate Residual	KSPCR	—	X	X
Generalized Conjugate Residual	KSPGCR	—	X	X
Generalized Conjugate Residual (with inner normalization and deflated restarts)	KSPHPDDM	HPDDM	X	X
Minimum Residual	KSPMINRES	—	X	X

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Minimum Residual	`KSPMINRES`	—	X	X
LSQR	`KSPLSQR`	—	X	X
SYMMLQ	`KSPSYMMLQ`	—	X	X
FETI-DP (reduction to dual-primal sub-problem)	`KSPFETIDP`	—	X	X
Gropp's overlapped reduction Conjugate Gradient	`KSPGROPPCG`	—	X	X

ngsPETSc - PETSc PC

It is now possible to use any PETSc **PC** in NGSolve using the **“PETScPC”** preconditioner in NGSolve.

```
pre = Preconditioner(a, "PETScPC", pc_type="hypre")
gfu = GridFunction(fes)
gfu.vec.data = CG(a.mat, rhs=f.vec, pre=pre, printrates=mesh.comm.rank==0)
```

ngsPETSc - PETSc PC

	Algorithm	Associated Type	Matrix Types	External Packages
Generic	Jacobi	PCJACOBI	MATAIJ, MATBAIJ, MATSBAIJ, MATDENSE	—
	Point Block Jacobi	PCPBJACOBI	MATAIJ, MATBAIJ, MATSBAIJ, MATKAIJ, MATMPISELL, MATIS	—
	Variable Point Block Jacobi	PCPBJACOBI	MATAIJ, MATBAIJ, MATSBAIJ	—
	Block Jacobi	PCBJACOBI	MATAIJ, MATBAIJ, MATSBAIJ	—
	SOR	PCSOR	MATAIJ, MATSEQDENSE, MATSEQSBAIJ	—

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	Point Block SOR		MATSEQBAIJ (only for bs = 2,3,4,5)	—
	Kaczmarz	PCKACZMARZ	MATAIJ	—
	Additive Schwarz	PCASM	MATAIJ, MATBAIJ, MATSBAIJ	—
	Vanka/overlapping patches	PCPATCH	MATAIJ	—
	Deflation	PCDEFLATION	All	—
Incomplete	ILU	PCILU	MATSEQAIJ, MATSEQBAIJ	—
	ILU with drop tolerance	PCILU	MATSEQAIJ	SuperLU Sequential ILU solver
		PCILU	MATAIJ	Euclid/hypre (PCHYPRE)

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	ICholesky	PCICC	MATSEQAIJ, MATSEQBAIJ, MATSEQSBAIJ	—
	Algebraic recursive multilevel	PCPARMS	MATSEQAIJ	pARMS
Matrix Free	Infrastructure	PCSHELL	All	—
Multigrid	Infrastructure	PCMG	All	—
	Geometric		All	—
	Smoothed Aggregation	PCGAMG	MATAIJ	—
	Smoothed Aggregation (ML)	PCML	MATAIJ	ML/Trilinos
	Structured Geometric	PCPFMG, PCSYSPFMG, PCSMG	MATHYPRESTRUCT	hypre

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	Classical Algebraic	PCHYPRE, PCAMGX	MATAIJ	BoomerAMG/hypre, AmgX
	Multi-group MG	PCHMG	MATAIJ	—
	Domain Decomposition	PCHPDDM	MATAIJ, MATBAIJ, MATSBAIJ, MATIS	HPDDM
Hierarchical matrices	$\mathcal{H}^2$	PCH2OPUS	MATHTOOL, MATH2OPUS	H2OPUS
Physics-based Splitting	Relaxation & Schur Complement	PCFIELDSPLIT	MATAIJ, MATBAIJ, MATNEST	—
	Galerkin composition	PCGALERKIN	Any	—
	Additive/multiplicative	PCCOMPOSITE	Any	—
	Least Squares Commutator	PCLSC	MATSCHURCOMPLEMENT	—

ngsPETSc - PETSc PC

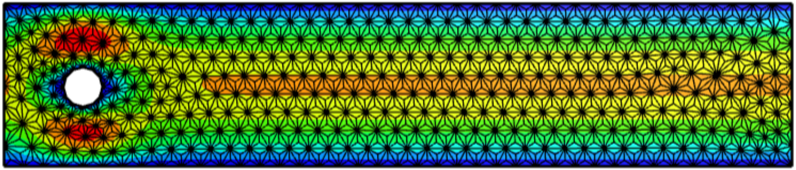
Parallel transformation	Redistribution	PCREDISTRIBUTE	MATAIJ	—
	Telescoping communicator	PCTELESCOPE	MATAIJ	—
	Distribute for MPI	PCMPI	MATAIJ	—
Approximate Inverse	AIV	PCHYPRE, PCSPAI	MATAIJ	Parasails/hypre, SPAI
Substructuring	Balancing Neumann-Neumann	PCNN	MATIS	—
	Balancing Domain Decomposition	PCBDDC	MATIS	—
	2-level Schwarz wire basket	PCEXOTIC	MATAIJ	—

ngsPETSc - PETSc DMPlex

ngsPETSc is capable of creating a mapping PETSc **DMPlex** and NGSolve **Mesh** object, thanks to the **MeshMapping** class. This will allow to apply **DMPlexTransform** to NGSolve Meshes.

```
Map = MeshMapping(mesh)
tr = PETSc.DMPlexTransform().create(comm=PETSc.COMM_WORLD)
tr.setType(PETSc.DMPlexTransformType.REFINEALFELD)
tr.setDM(Map.petscPlex)
tr.setUp()
newplex = tr.apply(Map.petscPlex)
mesh = Mesh(MeshMapping(newplex).ngMesh)
```

ngsPETSc - PETSc DMPlex



ngsPETSc - PETSc EPS

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ngsPETSc is capable of creating easily a SLEPc **EPS** one can use in NGSolve to solve eigenvalue problems. In particular, we are interested in solving an eigenvalue pencil

$$-\lambda(\vec{u}_h, \vec{v}_h) + (\nabla \vec{u}_h, \nabla \vec{v}_h) = 0$$

```
    solver = EigenSolver((m, a), fes, 4, solverParameters={"eps_type":SLEPc.EPS.Type.ARNOLDI,
                   "eps_smallest_magnitude":None,
                   "eps_tol": 1e-6,
                   "eps_target": 2,
                   "st_type": "sinvert",
                   "st_pc_type": "lu"})
```

ngsPETSc - Future Features

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- NGSolve **BaseMatrix** with block structures should be mapped to a PETSc **NestMat**. This will allow for **field split** preconditioning.
- Use PETSc **SNES** to solve non-linear system in NGSolve, this will allow for **line search** and **trust region**.
- Use PETSc **TS** to solve time dependent partial differential equations.
- Use SLEPc **PEP** to solve polynomial eigenvalue problems.

ngsPETSc - Other Solvers (It's a secret ...)

Having access to a PETSc **DMPlex** allows using NetGen meshes also in other finite element libraries,

- **Firedrake**, thanks to the ngsPETSc interface is now possible to use NetGen mesh and do **adaptive mesh refinement**.

```
ngmsh = unit_square.GenerateMesh(maxh=0.1)
msh = firedrake.Mesh(ngmsh)
File("output/MeshExample1.pvd").write(msh)
```

- **FEniCSx**, thanks to the ngsPETSc interface is now possible to use NetGen mesh.