PETSc for Python

http://petsc4py.googlecode.com

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What is **petsc4py**?

Python bindings for **PETSc**, the *Portable Extensible Toolkit for Scientific Computation*.

A *good friend* of **petsc4py** is:

- **mpi4py**: Python bindings for **MPI**, the *Message Passing Interface*.

Other two projects depend on petsc4py:

- **slepc4py**: Python bindings for **SLEPc**, the *Scalable Library for Eigenvalue Problem Computations*.
- **tao4py**: Python bindings for **TAO**, the *Toolkit for Advanced Optimization*.

Implementation

Implemented with Cython `http://www.cython.org`

- Code base far easier to write, maintain, and extend.
- Faster than other solutions (mixed Python and C codes).
- Easier to cross language boundaries (reuse C/C++/Fortran).

Implementation - Cython [1]

```
cdef import from "petsc.h":

    ctypedef int   PetscInt
    ctypedef float PetscScalar

    ctypedef void* PetscVec "Vec"
    ctypedef void* PetscMat "Mat"
    ctypedef void* PetscKSP "KSP"

    int VecDot(PetscVec x,PetscVec y, PetscScalar *val)
    int MatMult(PetscMat A, PetscVec x, PetscVec y)
    int KSPSolve(PetscKSP ksp, PetscVec b, PetscVec x)

cdef inline int CHKERR(int ierr) except -1:
    if ierr != 0:
        raise RuntimeError("error code %d" % ierr)
    return 0
```

Implementation - Cython [2]

```
cdef class Vec:
    cdef PetscVec vec
    ...
    def dot(self, Vec other):
        cdef PetscScalar val
        ierr = VecDot(self.vec, other.vec, &val); CHKERR(ierr)
        return val
...
cdef class Mat:
    cdef PetscMat mat
    ...
    def mult(self, Vec x, Vec y):
        ierr = MatMult(self.mat, x.vec, y.vec); CHKERR(ierr)
...
cdef class KSP:
    cdef PetscKSP ksp
    ...
    def solve(self, Vec b, Vec x):
        ierr = KSPSolve(self.ksp, b.vec, x.vec); CHKERR(ierr)
```

Features – PETSc components

- **Index Sets**: permutations, indexing into vectors, renumbering.
- **Vectors**: sequential and distributed.
- **Matrices**: sequential and distributed, sparse and dense.
- **Distributed Arrays**: regular grid-based problems.
- **Linear Solvers**: Krylov subspace methods.
- **Preconditioners**: sparse direct solvers, multigrid
- **Nonlinear Solvers**: line search, trust region, matrix-free.
- **Timesteppers**: time-dependent, linear and nonlinear PDE's.

Features – Interoperability

Support for wrapping other PETSc-based codes.

- You can use **Cython** (`from petsc4py` **cimport** `PETSc`).
- You can use **SWIG** (*typemaps* provided).
- You can use **F2Py** (`fortran` attribute).

(more on this later . . .)

Features – Easy installation

```
$ virtualenv --no-site-packages ENV
$ source ENV/bin/activate

(ENV) $ pip install slepc4py
Downloading/unpacking slepc4py
Downloading/unpacking petsc4py (from slepc4py)
Downloading/unpacking slepc (from slepc4py)
Downloading/unpacking petsc (from petsc4py->slepc4py)
Downloading/unpacking numpy (from petsc4py->slepc4py)
Installing collected packages: numpy, petsc, petsc4py,
                               slepc, slepc4py

(ENV) $
```

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Vectors (Vec) – Conjugate Gradients Method

$cg(A, x, b, i_{max}, \epsilon)$:

$i \Leftarrow 0$

$r \Leftarrow b - Ax$

$d \Leftarrow r$

$\delta_0 \Leftarrow r^T r$

$\delta \Leftarrow \delta_0$

while $i < i_{max}$ and

$\delta > \delta_0 \epsilon^2$ do :

$q \Leftarrow Ad$

$\alpha \Leftarrow \dfrac{\delta}{d^T q}$

$x \Leftarrow x + \alpha d$

$r \Leftarrow r - \alpha q$

$\delta_{old} \Leftarrow \delta$

$\delta \Leftarrow r^T r$

$\beta \Leftarrow \dfrac{\delta}{\delta_{old}}$

$d \Leftarrow r + \beta d$

$i \Leftarrow i + 1$

```
1   def cg(A, b, x, imax=50, eps=1e-6):
2       """
3       A, b, x   : matrix, rhs, solution
4       imax      : maximum iterations
5       eps       : relative tolerance
6       """
7       # allocate work vectors
8       r = b.duplicate()
9       d = b.duplicate()
10      q = b.duplicate()
11      # initialization
12      i = 0
13      A.mult(x, r)
14      r.aypx(-1, b)
15      r.copy(d)
16      delta_0 = r.dot(r)
17      delta = delta_0
18      # enter iteration loop
19      while (i < imax and
20             delta > delta_0 * eps**2):
21          A.mult(d, q)
22          alpha = delta / d.dot(q)
23          x.axpy(+alpha, d)
24          r.axpy(-alpha, q)
25          delta_old = delta
26          delta = r.dot(r)
27          beta = delta / delta_old
28          d.aypx(beta, r)
29          i = i + 1
30      return i, delta**0.5
```

Matrices (Mat) [1]

```
1  from petsc4py import PETSc
2
3  # grid size and spacing
4  m, n  = 32, 32
5  hx = 1.0/(m-1)
6  hy = 1.0/(n-1)
7
8  # create sparse matrix
9  A = PETSc.Mat()
10 A.create(PETSc.COMM_WORLD)
11 A.setSizes([m*n, m*n])
12 A.setType('aij') # sparse
13 A.setFromOptions()
14
15 # precompute values for setting
16 # diagonal and non-diagonal entries
17 diagv = 2.0/hx**2 + 2.0/hy**2
18 offdx = -1.0/hx**2
19 offdy = -1.0/hy**2
```

Matrices (Mat) [2]

```
# loop over owned block of rows on this
# processor and insert entry values
Istart, Iend = A.getOwnershipRange()
for I in range(Istart, Iend) :
    A[I,I] = diagv
    i = I//n    # map row number to
    j = I - i*n # grid coordinates
    if i> 0  : J = I-n; A[I,J] = offdx
    if i< m-1: J = I+n; A[I,J] = offdx
    if j> 0  : J = I-1; A[I,J] = offdy
    if j< n-1: J = I+1; A[I,J] = offdy

# communicate off-processor values
# and setup internal data structures
# for performing parallel operations
A.assemblyBegin()
A.assemblyEnd()
```

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Linear Solvers (KSP+PC)

```
1  # create linear solver,
2  ksp = PETSc.KSP()
3  ksp.create(PETSc.COMM_WORLD)
4
5  # use conjugate gradients method
6  ksp.setType('cg')
7  # and incomplete Cholesky
8  ksp.getPC().setType('icc')
9
10 # obtain sol & rhs vectors
11 x, b = A.getVecs()
12 x.set(0)
13 b.set(1)
14
15 # and next solve
16 ksp.setOperators(A)
17 ksp.setFromOptions()
18 ksp.solve(b, x)
```

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Nonlinear Solvers (SNES) [1]

```
1  from petsc4py import PETSc
2  from numpy import exp
3
4  m, n = 32, 32 # grid sizes
5  alpha = 6.8   # parameter
6
7  def Bratu2D(snes, X, F, alpha, m, n):
8      # NumPy array <- Vec
9      x = X.array.reshape(m, n)
10     f = F.array.reshape(m, n)
11     # setup 5-points stencil
12     u  = x[1:-1, 1:-1] # center
13     uN = x[1:-1,  :-2] # north
14     uS = x[1:-1, 2:  ] # south
15     uW = x[ :-2, 1:-1] # west
16     uE = x[2:,   1:-1] # east
17     # compute nonlinear function
18     hx = 1.0/(m-1) # x grid spacing
19     hy = 1.0/(n-1) # y grid spacing
20     f[:,:] = x
21     f[1:-1, 1:-1] = \
22          (2*u - uE - uW) * (hy/hx) \
23        + (2*u - uN - uS) * (hx/hy) \
24        - alpha * exp(u)  * (hx*hy)
```

Nonlinear Solvers (SNES) [2]

```
1  # create  nonlinear solver
2  snes = PETSc.SNES().create()
3  # register the function in charge of
4  # computing the nonlinear residual
5  f = PETSc.Vec().createSeq(m*n)
6  snes.setFunction(Bratu2D, f, args=(alpha, m, n))
7
8  # configure the nonlinear solver
9  # to use a matrix-free Jacobian
10 snes.setUseMF(True)
11 snes.getKSP().setType('cg')
12 snes.setFromOptions()
13
14 # solve the nonlinear problem
15 b = None # rhs = 0
16 x = f.duplicate() # solution
17 snes.solve(b, x)
```

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Interoperability – **Cython**

```
1   from petsc4py.PETSc cimport *
2
3   cdef extern from "MyPDE.h":
4       ctypedef struct Params:
5           double alpha, beta, gamma
6       int FormFunction(PetscDA da, PetscVec x, PetscVec F, Params *p)
7       int FormJacobian(PetscDA da, PetscVec x, PetscMat J, Params *p)
8
9   cdef inline Params getParams(dict params):
10      cdef Params p
11      p.alpha = params.get('alpha', 0.0)
12      p.beta  = params.get('beta',  1.0)
13      p.gamma = params.get('gamma', 2.0)
14      return p
15
16  def computeFunction(DA da, Vec X, Vec F, **params):
17      cdef Params p = getParams(params)
18      ierr = FormFunction(da.da, X.vec, F.vec, &p)
19      assert ierr != 0
20
21  def computeJacobian(DA da, Vec X, Mat J, **params):
22      cdef Params p = getParams(params)
23      ierr = FormJacobian(da.da, X.vec, J.mat, &p)
24      assert ierr != 0
```

Interoperability – **SWIG**

```
1  %module MyPDE
2
3  %include petsc4py/petsc4py.i
4
5  %{
6  #include "MyPDE.h"
7  %}
8
9  typedef struct Params {
10   double alpha;
11   double beta;
12   double gamma;
13 } Params;
14
15 PetscErrorCode FormInitGuess(DA da, Vec x, Params *p);
16 PetscErrorCode FormFunction(DA da, Vec x, Vec F, Params *p);
17 PetscErrorCode FormJacobian(DA da, Vec x, Mat J, Params *p);
```

Interoperability – **F2Py**

```
1   python module MyPDE
2   interface
3
4       subroutine FormInitGuess(da, x, params, ierr)
5         integer, intent(in)       :: da, x
6         real(kind=8), intent(in) :: params(3)
7         integer, intent(out)      :: ierr
8       end subroutine FormInitGuess
9
10      subroutine FormFunction(da, x, F, params, ierr)
11        integer, intent(in)       :: da, x, F
12        real(kind=8), intent(in) :: params(3)
13        integer, intent(out)      :: ierr
14      end subroutine FormFunction
15
16      subroutine FormJacobian(da, x, J, params, ierr)
17        integer, intent(in)       :: da, x, J
18        real(kind=8), intent(in) :: params(3)
19        integer, intent(out)      :: ierr
20      end subroutine FormJacobian
21
22  end interface
23  end python module MyPDE
```

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Consider the following diffusive, unsteady, non-linear, scalar problem in the unit cube $\Omega = (x, y, z) = (0, 1)^3$

- PDE, boundary and initial conditions:

$$\begin{aligned} \frac{\partial \phi}{\partial t} - \nabla \cdot (\kappa(\phi) \nabla \phi) &= G \quad \text{on } \Omega \times (0, T] \\ \frac{\partial \phi}{\partial \mathbf{n}} &= 0 \quad \text{at } \partial\Omega \times [0, T] \\ \phi &= \phi^0 \quad \text{at } t = 0, \end{aligned} \tag{1}$$

- Nonlinear diffusion and line source term:

$$\kappa(\phi) = \begin{cases} 1 & \text{if } \phi \geq 0 \\ \frac{1}{1+\phi^2} & \text{if } \phi < 0 \end{cases} \tag{2}$$

$$G(x = \frac{1}{4}, y = \frac{1}{4}, \frac{1}{2} < z < 1) = -300$$

Performance –Discretization

- finite differences in space
- backward Euler in time

$$\frac{1}{\Delta t}(\phi^{n+1}_{i,j,k} - \phi^{n}_{i,j,k}) - L_{i,j,k}(\kappa, \phi^{n+1}) - G_{i,j,k} = 0 \tag{3}$$

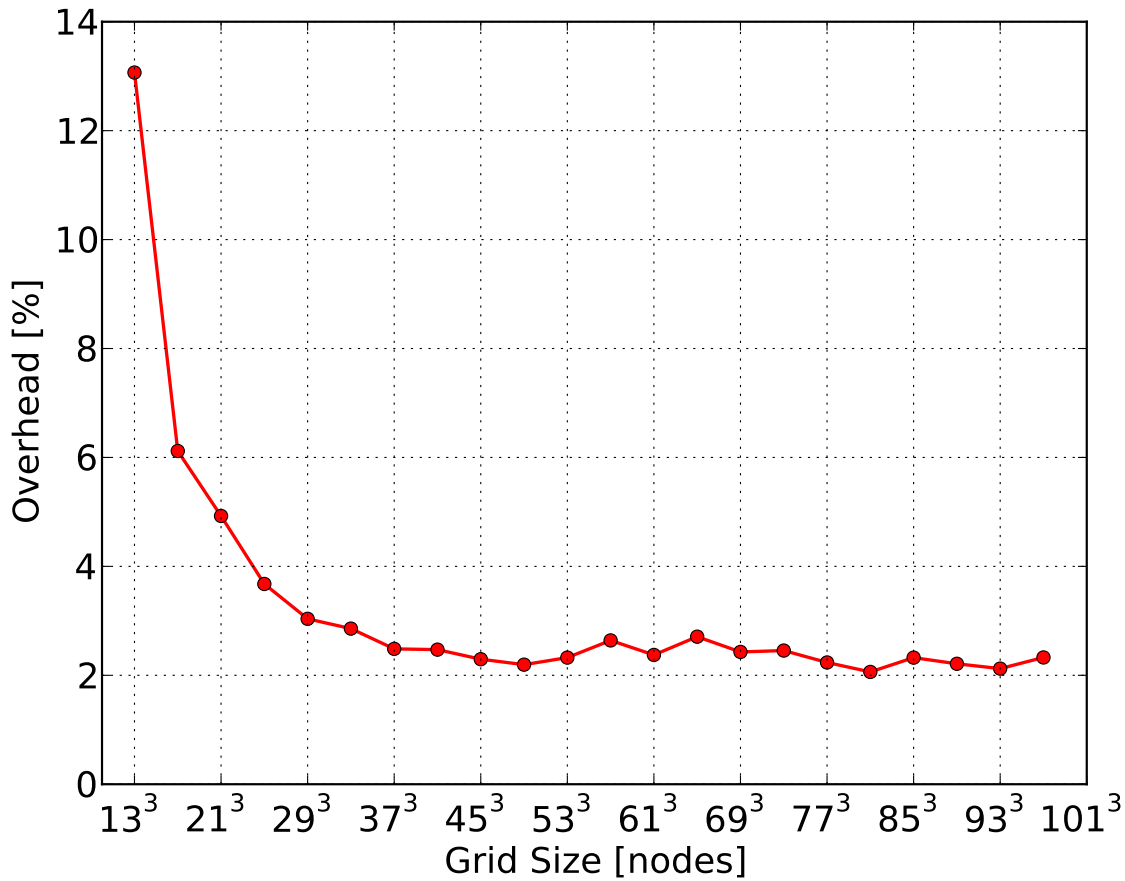
$$\begin{aligned} L_{i,j,k}(\kappa,\phi) =& \frac{\kappa[i-\frac{1}{2}]}{(\Delta x_1)^2}\phi[i-1] - \frac{\kappa[i-\frac{1}{2}]+\kappa[i+\frac{1}{2}]}{(\Delta x_1)^2}\phi[0] + \frac{\kappa[i+\frac{1}{2}]}{(\Delta x_1)^2}\phi[i+1] + \\ &+ \frac{\kappa[j-\frac{1}{2}]}{(\Delta x_2)^2}\phi[j-1] - \frac{\kappa[j-\frac{1}{2}]+\kappa[j+\frac{1}{2}]}{(\Delta x_2)^2}\phi[0] + \frac{\kappa[j+\frac{1}{2}]}{(\Delta x_2)^2}\phi[j+1] + \\ &+ \frac{\kappa[k-\frac{1}{2}]}{(\Delta x_3)^2}\phi[k-1] - \frac{\kappa[k-\frac{1}{2}]+\kappa[k+\frac{1}{2}]}{(\Delta x_3)^2}\phi[0] + \frac{\kappa[k+\frac{1}{2}]}{(\Delta x_3)^2}\phi[k+1] \end{aligned} \tag{4}$$

(notation: $[0] = (i,j,k)$, $[i \pm \frac{1}{2}] = (i \pm \frac{1}{2}, j, k)$, and so on)

Performance – Python+F90 versus C+F90

Basically a measure of Python calling overhead . . .

- equivalent Python and C codes for the drivers
- common Fortran 90 code for the nonlinear residual
- use matrix–free for the nonlinear problems



Do not hesitate to ask for help ...

- Mailing List: `petsc-users@mcs.anl.gov`
- Mail&Chat: `dalcinl@gmail.com`
- Project Page:
  `http://petsc4py.googlecode.com`

Thanks!