PySE – Python Stencil Environment

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Outline

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Basic features of PySE

High–level tool for rapid development of FDM solvers.

- High–level syntax, Matlab-like.
- Code close to the math or pseudo code.
- Easy deployment on parallel computers.
- Written in python, uses extension modules for better performance.
- Available at http://pyfdm.sourceforge.net.
- Former know as paraStencils and pyFDM.

Priorities: 1. Abstractions, 2. Parallelization, 3. Efficiency

Some related works

PySE use ideas and concepts from many other tools:

- Diffpack
- *hypre*
- A++/P++
- cogito

- PETSc
- Trilinos
- Chombo

The abstractions

PySE defines the following abstractions.

- Grid; for the domain and FDM mesh.
- Field; for scalar fields over a Grid.
- Stencil; the action of the PDE in a point.
- StencilSet; set of stencils for a problem.

The first three abstractions are quite common.
Stencil and StencilSet are the most important abstractions in PySE.

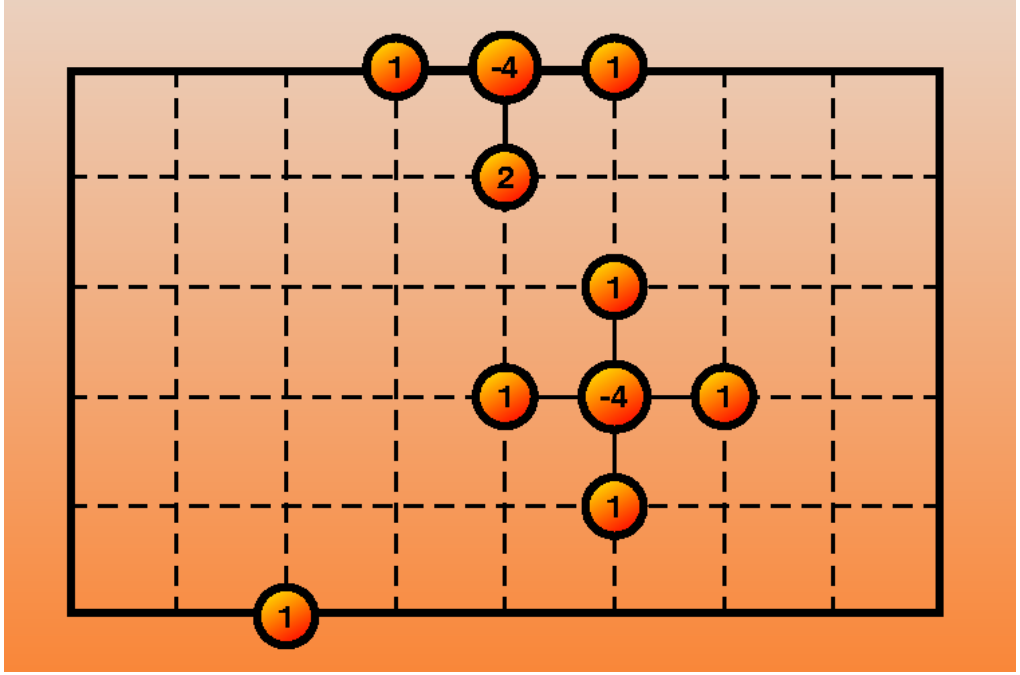
Outline

Consider a simple Heat equation:

$$
\begin{aligned}
u_t &= \nabla^2 u && x \in \Omega \\
u(x,0) &= f(x), && x \in \Omega \\
\frac{\partial u(x,t)}{\partial n} &= g_n(x,t), && x \in \partial\Omega_n \\
u(x,t) &= g_d(x,t), && x \in \partial\Omega_d
\end{aligned}
$$

Assume further that we want to solve this on the unit square with f and g given as initialfunc and neumannfunc, respectively.

A simple example, graphically



- Assume A is the StencilSet.
- One explicit step: $u_{n+1} = A(u_n)$.

Example code

This short code solves the problem on the previous slide:

```
from pyFDM import *

def neumannfunc(x,y): return sin(x)*cos(y)

def initialfunc(x,y): return sin(x)*cos(y)

g = Grid(domain=([0,1,[0,1]),division=(100,100))
u = Field(g)
t = 0; dt = T/n;
A = StencilSet(g)
innerstencil = Identity(g.nsd) + dt*Laplace(g)
innerind = A.addStencil(innerstencil, g.innerPoints())
A += createNeumannBoundary(innerstencil, g, neumannfunc)
u.fill(initialfunc)
for t < T:
    u = A(u)
    t += dt
plot(u)
```

Example code

Some remarks on the code

- Laplace and Identity are stencils defined in PySE
- The Neumann condition function is not time dependent
- It can be made time dependent by wrapping into a lambda:

```
def neumannfunc(x,y,t): return x*y*t

rt = 0
neumanncall = lambda x,y: neumannfunc(x,y,rt)
A += createNeumannBoundary(innerstencil, g, neumanncall)
while rt < T:
    u = A(u)
    t += dt
    A.updateDataStructures()
```

Outline

Stencil

You can easily build your own stencils

```
h = (dt**2/g.dx**2)
lap_5pt = Stencil(nsd=2, varcoeff=False,\
          nodes={             (0,1):  1.,\
                 (-1,0): 1., (0,0):  -4., (1,0): 1.,\
                             (0,-1): 1.})
id = Stencil(nsd=2, varcoeff=False, nodes={(0,0): 1.0})
inner = id + h*lap_5pt
```

Stencils can be added together, scaled, and evaluated

StencilSet

- Stencils are added to a StencilSet together with an iterator for nodes.
- Grid have methods for various sets of nodes:
  - allPoints
  - innerPoints
  - boundary
  - corners
- innerPoints and boundary take an optional *region* argument:

```
A.addStencil(diricond, \
    grid.boundary(region=((-1,1),(-1,1)), \
                  type='circle', center=(0,0), \
                  radius=1, direction='in'))
```

StencilSet

During the first call to the call–operator A(u) in StencilSet, more efficient datastructures are build:

- Why:
  - Walking the iterators is time–consuming (in pure Python).
- Stencil–coefficients are assembled in a sparse matrix.
- Source information is assembled in a vector.
- We need to provide hooks to update for changes in coefficients and source:
  - updateDataStructures
  - updateSourceDatastructures
- These methods trigger reassembling of all or parts of the data.

StencilSet

- If present in StencilSet instances, the sparse matrix and vector will be used on subsequent calls to A(u) and A*u.
- A.direct_matvec(x): operate on a NumPy vector, returns a NumPy vector.
  - Less overhead (no Field creation), hence more efficient.
  - The interface for updating datastructures is (at least for now) less convenient in this case.
  - A Field u stores its data as u.data, a NumPy vector.
  - Remark, a dummy A(u) must be inserted to build datastructures.

Neumann boundary conditions

Creating Neumann boundary conditions can be tricky in the multidimensional case.

- The function createNeumanBoundary function can be used:

```
nSet = createNeumanBoundary(stencil, grid, condition)
```

- The Neumann creator also accept a region specification:

```
nSet = createNeumanBoundary(stencil, grid, condition,\
     region=((-1,1),(-1,1)), \
     type='circle', center=(0,0), \
     raduis=1, direction='out')
```

Parallel computations with PySE

All parts of PySE are inherently parallel.

- Parallelism is initated with

  ```
  grid.partition(StencilSet)
  ```

- The StencilSet supplied shoud be “ready”
- All Fields created on the grid, will be converted.
- Other StencilSets in the grid get the same partitioning with

  ```
  StencilSet.doInitParallel()
  ```

Outline

A more involved example

Consider the following problem:

$$
\begin{aligned}
u_t &= \nabla \cdot (k(x,y)\nabla u) + f(x,y,t), && (x,y) \in \Omega, && t \in \mathbb{R}^+, \\
u(x,y,t) &= h(x,y,t), && (x,y) \in \partial\Omega, && t \in \mathbb{R}^+, \\
u(x,y,0) &= g(x,y), && (x,y) \in \Omega. &&
\end{aligned}
$$

- We chose $f(x,y,t)$, $k(x,y)$, $h(x,y,t)$, and $g(x,y)$ such that

$$u(x,y,t) = e^{-t} sin(\pi x) cos(\pi y)$$

- Implementation follow the simple example.

Timing of the solver

# cpus:	1	4	16	24	32
1000×1000, 160 step:	7984	1998	498.5	332.0	249.3
speed–up:	1	3.99	16.0	24.0	32.0
1500×1500, 240 step:	26820	6728	1681	1125	838.8
speed–up:	1	3.98	15.9	23.8	31.9

CPU time in seconds and corresponding speed-up numbers.

- The solver uses the direct_matvec trick

Comparison with a C solver

We have created a (less flexible) solver in C:

Problem size	runtime	1-cpu P/C	32-cpu P/C
1000×1000, 160 steps:	107.3	74.4	2.32
1500×1500, 240 steps:	362.4	74.0	2.31

CPU time in seconds for the solver implemented in C, as well as speed– relative to the Python solver running on one and 32 processors.

- For certain applications, this is just fine
- If we do not assemble in sparse matrix and vector, multiply P/C numbers by O(10) (update source vs. all)
- Where do we loose that much?

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The bottelneck...

In this problem, the Dirichlet boundary condition and the source function are time dependent.

- For each timestep, we walk the iterators to update data.
- If we remove the time dependency (and hence the need for update of data), we get:

Problem size	C	Python
1000×1000, 160 time steps:	34.5	30.5

The modules we're using from Python for mat*vec, vec*vec are obviously smarter than my C program

The bottelneck can be removed!

- NumPy can fill an array with values from a function very fast!
- We can put source and boundary information in Fields, and use additional (static) StencilSet operators.
- Rewrite the explicit update as

```
u = A(u) + S(F) + B(H)
```

- The Fields F and H can be filled quickly with F.fill_vec(function).
- The direct_matvec trick improve performance further.

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When the bottelneck is gone, we get good performance

# cpus:	1	4	16	24	32
1000×1000, 160 steps:	365.0	93.90	23.51	16.05	12.52
speed–up:	1	3.89	15.5	22.7	29.2
1500×1500, 240 steps:	1226	315.7	78.42	52.33	40.73
speed–up:	1	3.88	15.6	23.4	30.1

CPU time in seconds and corresponding speed-up numbers for the improved Python solver.

Comparison with C of the faster solver

Problem size	runtime	1-cpu P/C	32-cpu P/C
1000×1000, 160 steps:	107.3	3.40	0.12
1500×1500, 240 steps:	362.4	3.38	0.11

- Is this fast enough?
- What did we loose? Only nice syntax.
- What's not there: limited support for higher order methods, no support for non–linear problems, only simple grids
- How can it be usefull in FEniCS?

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