Anatomy of PyClaw

Motivation

- Complete example of modernizing a serial Fortran code for large-scale computing
- Start with Clawpack, a serial grid-based Fortran code
- Wrap legacy Fortran code using f2py
- Prototype, visualize, and test from Python
- Scale serial grid code using petsc4py

Prototyping Example

(Live demo of PyClaw notebook)

Clawpack Overview

- **C**onservation **L**aws **Pack**age:
  - *General hyperbolic PDEs in 1/2/3 dimensions*
- Developed by Randy LeVeque, Marsh Berger, and various others over the past 15 years in Fortran 77
- Dozens of “Riemann solvers” by numerous additional contributors
- Includes adaptive mesh refinement (AMRClaw)
- Textbook and many examples available
- Models tidal waves, storm surges, acoustic waves, and pyroclastic flows/surges
- Available at: www.clawpack.org

Wrapping Clawpack with f2py

- We wrap at the hyperbolic solver level, Fortran code for advancing the solution on a grid by one time step
- The solver is generic over different physics, it accepts a pointer to a Fortran subroutine for computing the Riemann kernel at each interface
- We use f2py to wrap both the `step` subroutine and the `rp` Riemann kernel. We don't call the Riemann kernel from Python, it is simply passed as an argument to the f2py-wrapped `step` function.

Wrapping 1-D Wave Propagation Kernels with f2py

```
subroutine step1(num_eqn,num_waves,num_ghost,num_aux,mx,q,aux,dx, &
                 dt,method,mthlim,cfl,f,wave,s,amdq,apdq,dtdx,use_fwave,rp1)
```

We need to give f2py a little information about how we intend to use the data to avoid making unnecessary copies. We do this by adding f2py directives after the function declaration.

`!f2py intent(in,out) q !f2py intent(out) cfl !f2py intent(in) num_eqn !f2py intent(in) num_ghost !f2py intent(in) mx !f2py optional f, amdq, apdq, dtdx, s, wave`
The variables `num_eqn`, `num_waves`, and `num_aux` are automatically inferred from the dimensions of the input arrays.

Wrapping 2-D Wave Propagation Kernels with f2py

The 2-D picture is only slightly more complicated:

```
subroutine step2(maxm,num_eqn,num_waves,num_aux,num_ghost,mx,my, &
qold,qnew,aux,dx,dy,dt,method,mthlim,cfl, &
qadd,fadd,gadd,q1d,dtdx1d,dtdy1d, &
aux1,aux2,aux3,work,mwork,use_fwave,rpn2,rpt2)
```

Note that we're being slightly less verbose here, only explicitly specifying the output variable `cfl` as well as the modified array `qnew`.

```
!f2py intent(out) cfl
!f2py intent(in,out) qnew
!f2py optional q1d, qadd, fadd, gadd, dtdx1d, dtdy1d
```

Wrapping Riemann Fortran Kernels as Function Pointers with f2py

```
subroutine rp1(maxm,meqn,mwaves,mbc,mx,ql,qr,auxl,auxr, &
               wave,s,amdq,apdq,num_aux)
```

The function pointer is wrapped as-is!

Calling f2py-Wrapped Wave Propagation Kernels from Python

Here's the original Fortran interface:

```
subroutine step1(num_eqn,num_waves,num_ghost,num_aux,mx,q,aux,dx, &
                 dt,method,mthlim,cfl,f,wave,s,amdq,apdq,dtdx,use_fwave,rp1)
```

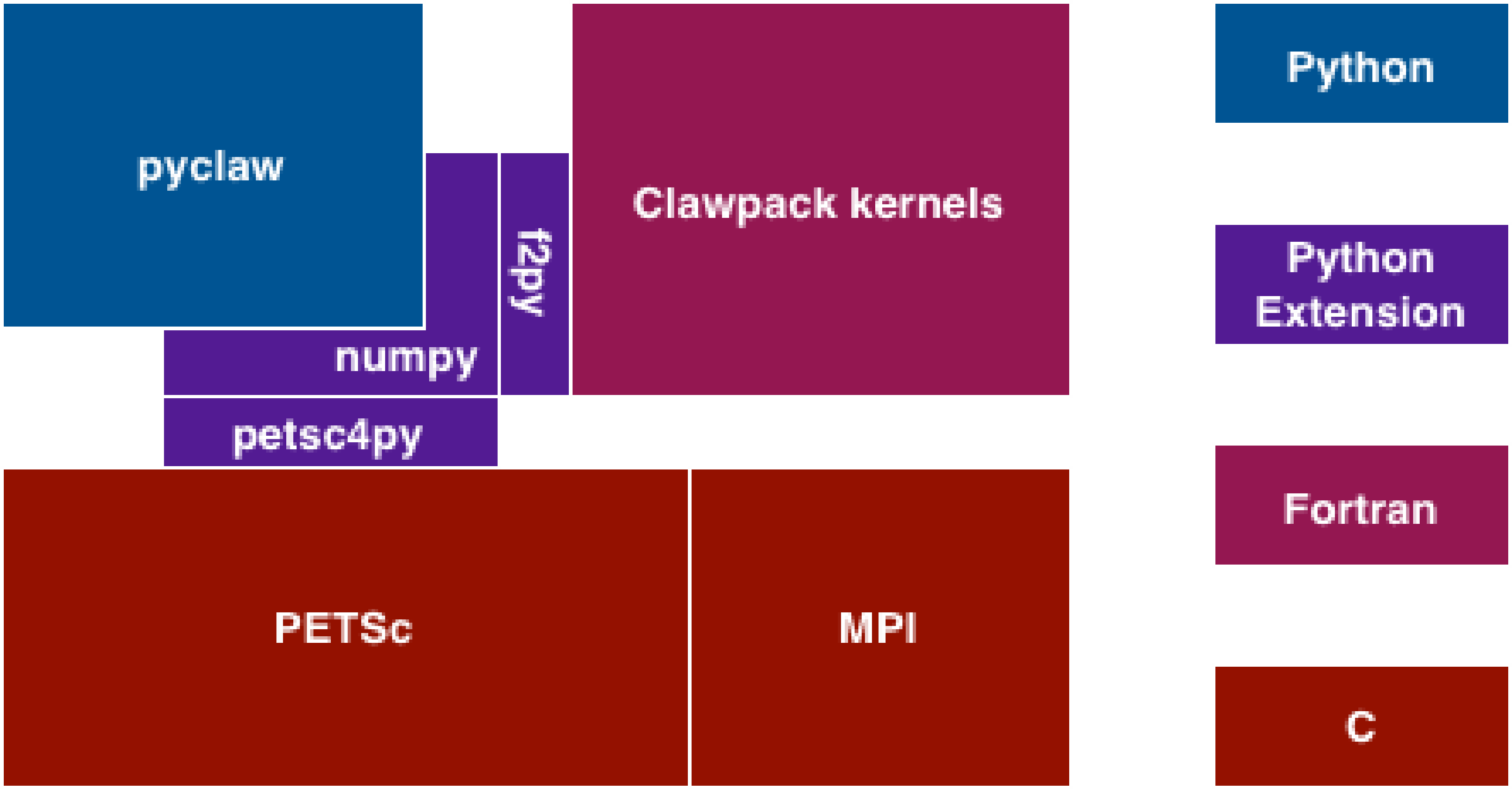
Here's the function call from Python.

```
rp1 = self.rp.rp1._cpointer
self.qbc,cfl = self.fmod.step1(num_ghost,mx,self.qbc,self.auxbc,dx,
               dt,self._method,self._mthlim,self.fwave,rp1)
```

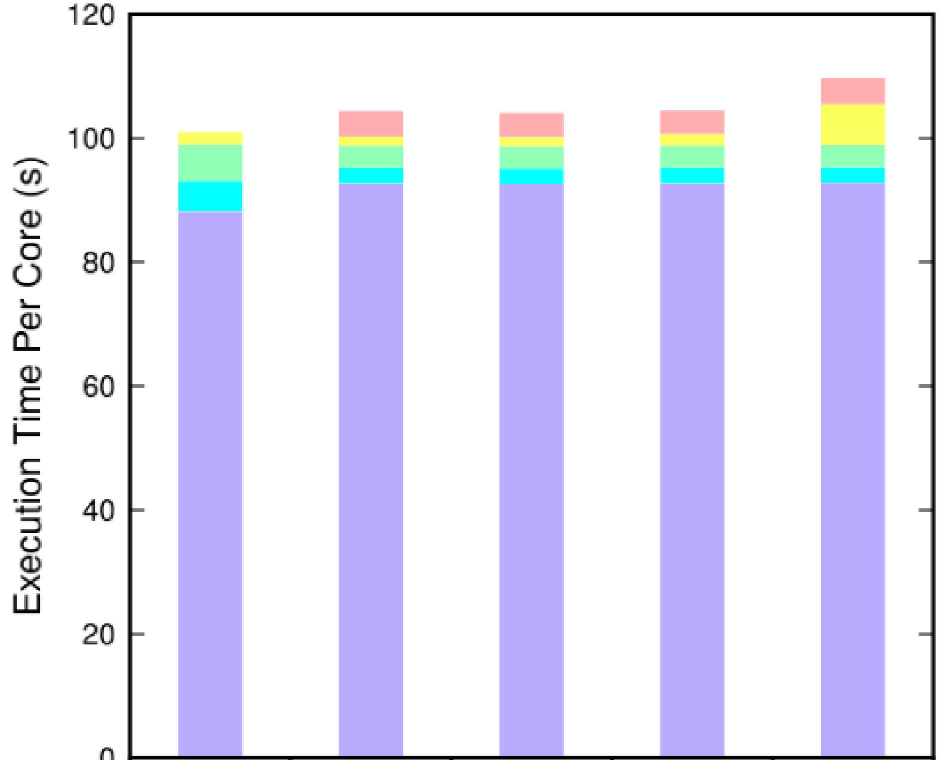
Enabling Grid-Based Parallelism with PETSc DMDA

- Grid-based serial solver operates on a grid augmented by "ghost cells"
- Exact same concept used by PETSc DMDA
  - *each process is responsible for one grid, exchanges boundary information with neighbors*
- Changes to PyClaw (Less than 100 LOC):
  - *Store grid data in DMDA instead of NumPy array*
  - *Calculate global CFL condition by reduction*
  - *Update neighbor information after successful time steps*

PyClaw Architecture



Scaling



	1	16	256	4096	65536
CFL Reduce	0.001	4.1	3.9	3.8	4.2
Parallel Initialization	2	1.5	1.5	1.9	6.6
Global to Local	5.9	3.6	3.6	3.6	3.6
Local to Global	4.9	2.5	2.5	2.5	2.5
Serial Computations	88.2	92.7	92.6	92.7	92.8
Total Efficiency	1.0	0.97	0.97	0.97	0.92

Number of Cores

Verification and Validation

- Code is prototyped and verified from Python scripts
- Validated against Clawpack
    - *which in turn has been validated against other codes and models*
- Verified by developers before commits
- Also verified continuously by Travis CI on GitHub