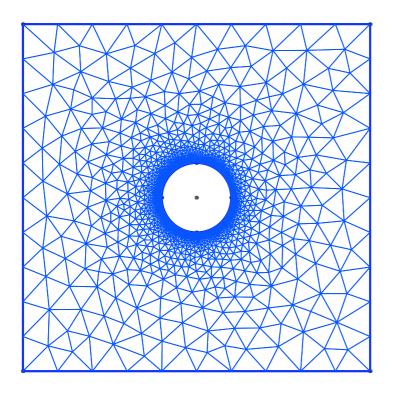
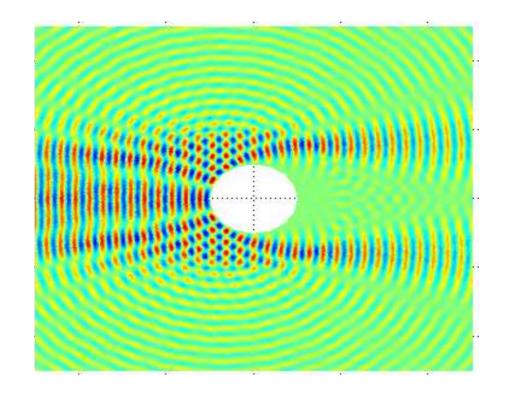
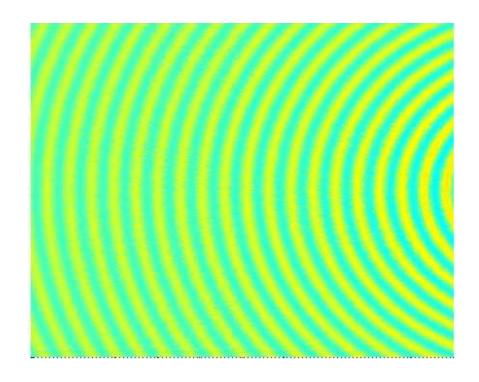
Rapidly Iterating from Prototype to Near-C Performance in Julia: A Finite Element Method Case Study

Reid Atcheson June 26, 2014







Traditional FEM Workflow

- Mathematical formulation.
- Translate into sparse linear system.
- Program sparse matrix assembly.
- Send to external solver package.

Traditional FEM Workflow

- Excellent tools already exist which specifically target this workflow:
 - Petsc, Deal.ii, DUNE, Trillinos, libMesh, FEniCS...
 (many, many more).
- I'm going to talk about a different workflow, and why Julia is uniquely qualified to targeting it.

Fix what isn't broken?

- Sparse matrix assembly can store excessive amounts of redundant information.
- Sparse linear solvers are "black box," they do not (typically) use domain information to speed up solution.

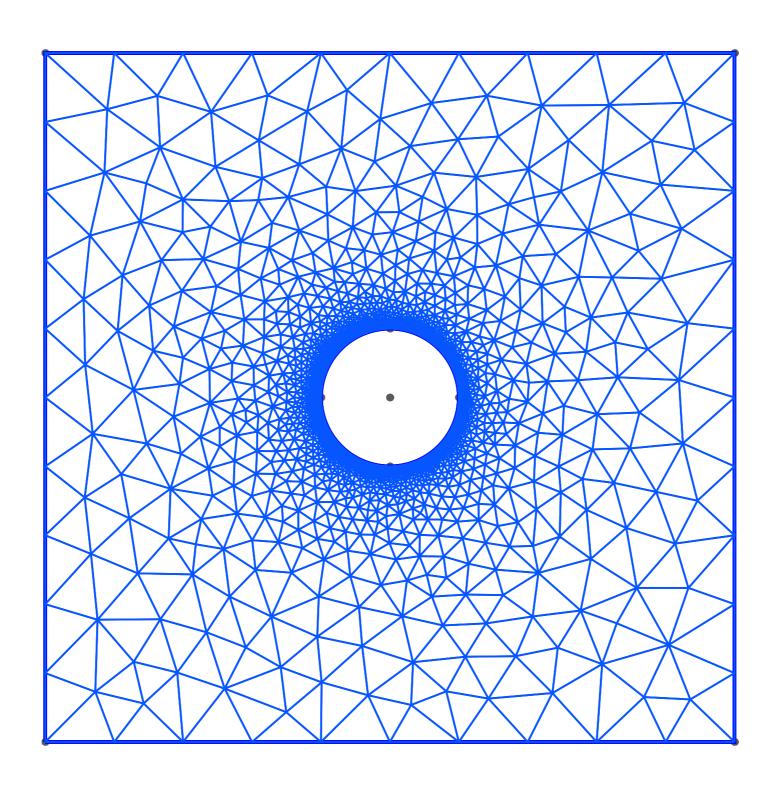
(Potentially) Improved FEM Workflow

- Mathematical formulation.
- Program operator evaluation
 - Sparse matrix-vector without assembling sparse matrix.
- Custom physics based solver.
 - e.g. Multigrid, Additive/Multiplicative Schwarz.

(Potentially) Improved FEM Workflow

- This style is mathematically and algorithmically challenging.
 - But by using more domain knowledge, potentially large payoff.
- Need to rapidly generate prototypes to ensure correctness.
 - But if a bug happens, need to be able to say: Is my math wrong, or is my code wrong?

"Mathematical Formulation"



Operator Evaluation

```
for k = 1: nElements
21
22
23
24
           #Map reference operators to general triangle.
25
           stiffness = mapstiffness(metric, jacobian, refstiff, k);
26
27
           #Calculate internal contributions.
28
           gradp = -gradient(p,stiffness,k);
           divu = -divergence(u,stiffness,k);
29
30
31
32
           for f = 1: nFaces
33
               (facemassP, facemassM) = mapface(facejacobian, refface, EToE, EToF, k, f);
34
35
               #Compute inter-element jumps.
               du = jump(u, facemassP, facemassM, EToE, EToF, k, f);
36
37
               dp = jump(p, facemassP, facemassM, EToE, EToF, k, f);
38
               ndotdu = ndot(du,normal,k,f);
               ndp = ntimes(dp,normal,k,f);
39
40
               nndotdu = ntimes(ndotdu,normal,k,f);
41
42
               #Update internal contributions with approximate boundary conditions.
               divu = divu + 0.5*(ndotdu-dp);
43
44
               qradp = qradp + 0.5*(ndp-nndotdu);
45
46
           end
47
           #Fill output.
48
           outp[:,k] = divu;
49
           outu[:,:,k] = gradp;
50
       end
```

Operator Evaluation

- Very slow.
 - Inner loop generates many temporaries.
- Plan of attack: @profile to identify bottlenecks.
 - Devectorize anything amenable to @devec.
 - Replace rest with C.

Eliminating Temporaries

```
#Preallocate operator memory.
23
       stiffness = zeros((Np,Np,dim));
24
25
       facemassM = zeros((Np,Np));
26
       facemassP = zeros((Np,Np));
27
28
       #Preallocate workspace.
       gradp = zeros((Np,dim));
29
       bdryu = zeros((Np,));
30
       bdryp = zeros((Np,dim));
31
       divu = zeros((Np,));
32
       du = zeros((Np,dim));
33
       dp = zeros((Np,));
34
       ndotdu = zeros((Np,));
35
36
       nndotdu = zeros((Np,dim));
       ndp = zeros((Np,dim));
37
```

```
#Map reference operators to general triangle.

stiffness = mapstiffness(metric,jacobian,refstiff,k);

#Calculate internal contributions.

gradp = -gradient(p,stiffness,k);

divu = -divergence(u,stiffness,k);
```

Becomes

```
#Map reference operators to general tetrahedron.
49
50
           ccall((:mapstiffness, "C/dgacoustic.so"), Void,
           (Ptr{Float64},Ptr{Float64},Int64,Int64,Ptr{Float64}),
51
52
           metric,refstiff,Np,nElements,k,stiffness);
53
54
           #Calculate internal contributions.
55
           #gradp = gradient(p,stiffness,k);
56
           ccall((:gradient, "C/dgacoustic.so"), Void,
57
           (Ptr{Float64},Ptr{Float64},Int64,Int64,Ptr{Float64}),
58
           p,stiffness,k,Np,gradp);
59
60
           #divu = divergence(u,stiffness,k);
61
           ccall((:divergence, "C/dgacoustic.so"), Void,
62
63
           (Ptr{Float64},Ptr{Float64},Int64,Int64,Ptr{Float64}),
64
           u,stiffness,k,Np,divu);
```

```
(facemassP, facemassM) = mapface(facejacobian, refface, EToE, EToF, k, f);

#Compute inter-element jumps.
du = jump(u, facemassP, facemassM, EToE, EToF, k, f);
dp = jump(p, facemassP, facemassM, EToE, EToF, k, f);
```

Becomes

```
ccall((:mapface, "C/dgacoustic.so"), Void,
(Ptr{Float64}, Ptr{Float64}, Ptr{Float64}, Ptr{Int64}, Ptr{Int64}, Int64, Int64, Int64, Int64, Ptr{Float64}, Ptr{Float64}),
facejacobian, jacobian, refface, ETOE, ETOF, nElements, Np, k, f, facemassP, facemassM);

#Compute inter-element jumps.
ccall((:vector_jump, "C/dgacoustic.so"), Void,
(Ptr{Float64}, Ptr{Float64}, Ptr{Float64}, Ptr{Int64}, Int64, Int64, Int64, Int64, Ptr{Float64}),
u, facemassP, facemassM, ETOE, nElements, Np, k, f, du);

ccall((:scalar_jump, "C/dgacoustic.so"), Void,
(Ptr{Float64}, Ptr{Float64}, Ptr{Float64}, Ptr{Int64}, Int64, Int64, Int64, Int64, Ptr{Float64}),
p, facemassP, facemassM, ETOE, nElements, Np, k, f, dp);
```

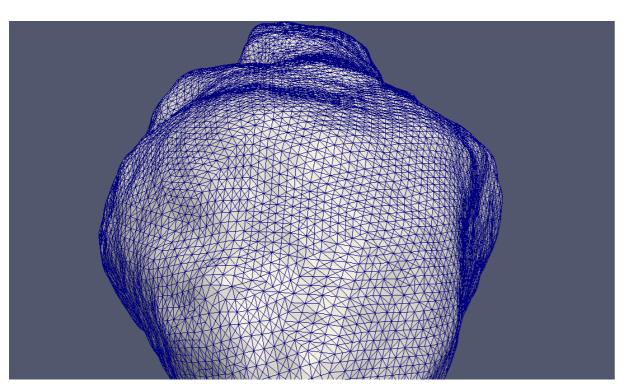
```
ndotdu = ndot(du,normal,k,f);
ndp = ntimes(dp,normal,k,f);
nndotdu = ntimes(ndotdu,normal,k,f);

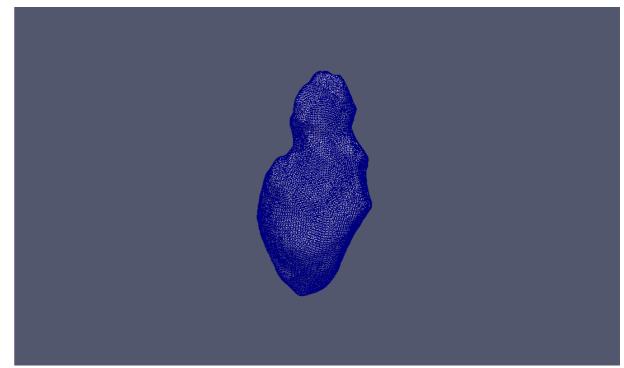
#Update internal contributions with approximate boundary conditions.
divu = divu + 0.5*(ndotdu-dp);
gradp = gradp + 0.5*(ndp-nndotdu);
```

Becomes

```
for i = 1: dim
95
                    nifk = normal[i,f,k];
96
                    @devec ndotdu = ndotdu + nifk.*du[:,i];
97
98
                    @devec ndp[:,i] = nifk.*dp;
99
                end
                for i = 1: dim
100
                    nifk = normal[i,f,k];
101
                    @devec nndotdu[:,i] = nifk.*ndotdu;
102
103
               end
104
105
                #Update internal contributions with approximate boundary conditions.
106
                @devec bdryu = bdryu + 0.5.*(ndotdu-dp);
107
                @devec bdryp = bdryp + 0.5.*(ndp-nndotdu);
108
```

Test Problem: Toutatis Asteroid



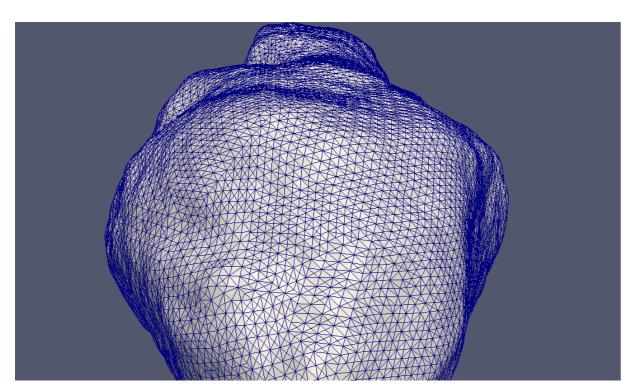


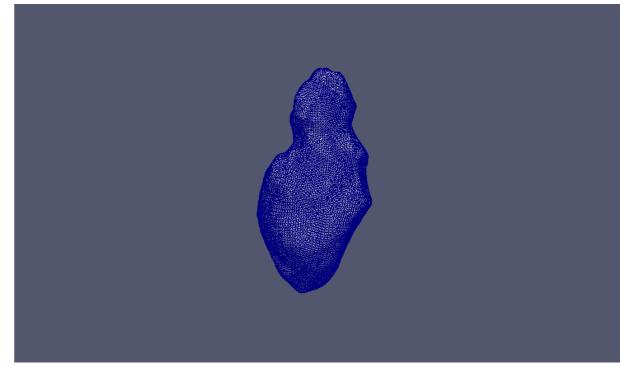
~500,000 Tetrahedra

One Prototype Operator Eval: 223s

One Optimized Operator Eval: 43s

Test Problem: Toutatis Asteroid





~500,000 Tetrahedra

One Prototype Operator Eval: 223s

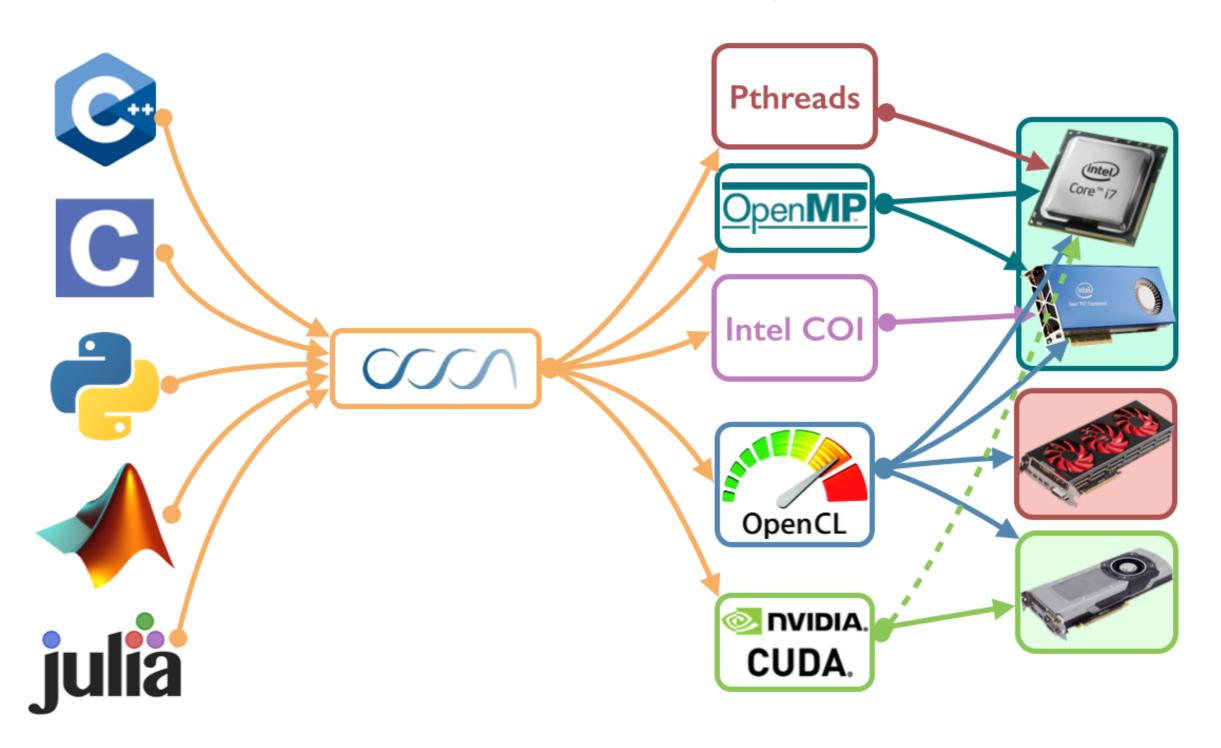
One Optimized Operator Eval: 43s

Speedup ~ 5x

Conclusions

- Prototype reads very straightforwardly from math.
 - Easy to separate math bugs from programming bugs.
 - Rapidly produce correct prototype.
- Devectorization and C interface provides straightforward optimization opportunities.
 - Start with slow correct code and use it as unit test for optimization iterations.

Future: Shared Memory Parallelism



https://github.com/tcew/OCCA2

Future: Distributed Parallelism

- Need native RDMA over infiniband, with seamless transition to TCP if unavailable.
 - MPI only real portable option.
 - https://github.com/lcw/MPI.jl

Future: Julia Package

- Would love to work with others to make this more accessible.
 - Orthogonal polynomials on: triangles, tetrahedra, quadrilaterals, hexahedra
 - Quadratures on all these shapes.
 - Mesh handling.
 - computational topology, computational geometry.
 - Visualization

Acknowledgements

- Jeff Bezanson, Stefan Karpinski, Viral Shah, Alan Edelman et al. Julia
- Dahua Lin et al. Devectorize.jl
- Toutatis mesh: gmsh
 - http://geuz.org/gmsh/
- Visualization: Paraview
 - http://www.paraview.org/
- Toutatis STL definition:
 - http://www.thingiverse.com/thing:4092
- VTK format I/O: My code + LightXML.jl
 - https://github.com/lindahua/LightXML.jl