A practical view of the classical FEM

(and some FEM software)

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Outline

nonlinear Poisson problems with general boundary conditions

assembly of FEM system

solving the equations

modern software: Gmsh, Firedrake, PETSc

fluid flow example

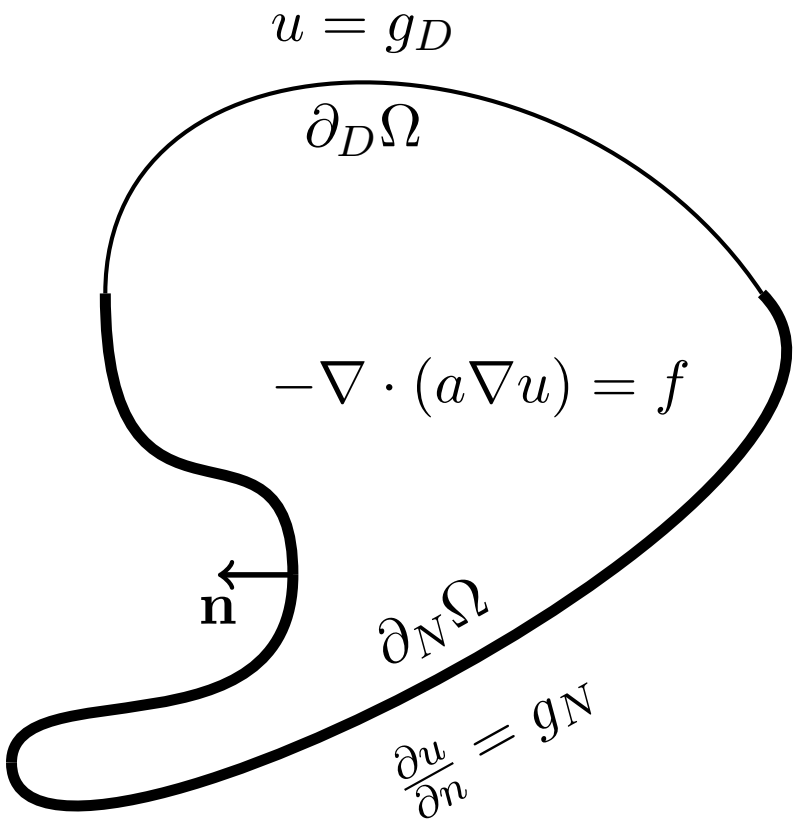
general, nonlinear Poisson problem

- $\Omega \subset \mathbb{R}^2$
- recall our usual problem: $\triangle u = f$, $u = 0$ on $\partial\Omega$
- these slides cover a nonlinear version with general boundary conditions:

$$\begin{aligned} -\nabla \cdot (a(u)\nabla u) &= f(u) && \text{on } \Omega, \\ u &= g_D && \text{on } \partial_D\Omega, \\ \frac{\partial u}{\partial n} &= g_N && \text{on } \partial_N\Omega. \end{aligned}$$

- $a(u,x,y)$, $f(u,x,y)$, $g_N(x,y)$, $g_D(x,y)$ are given (data)
- nonlinear because $a = a(u)$ and/or $f = f(u)$ is allowed

general, nonlinear Poisson problem



weak form

- $u \in H^1_g(\Omega) = \{u \in H^1(\Omega) \,:\, u = g_D \text{ on } \partial_D\Omega\}$
  - Dirichlet data g_D is used in defining $H^1_g(\Omega)$
- test functions: $H^1_0(\Omega) = \{v \in H^1(\Omega) \,:\, v = 0 \text{ on } \partial_D\Omega\}$
- for $v \in H^1_0(\Omega)$, multiply PDE by v and integrate by parts:

$$\int_\Omega a(u)\nabla u \cdot \nabla v - \int_{\partial\Omega} \frac{\partial u}{\partial n} v = \int_\Omega f(u)v$$

- apply boundary conditions:

$$\int_\Omega a(u)\nabla u \cdot \nabla v = \int_\Omega f(u)v + \int_{\partial_N\Omega} g_N v \qquad \text{(WF)}$$

  - Neumann data g_N appears here

examples

some examples of $-\nabla \cdot (a(u)\nabla u) = f(u)$:

- Poisson equation:

$$-\triangle u = f(x, y), \quad u = 0 \text{ on } \partial\Omega$$

- Liouville-Bratu equation:

$$-\triangle u = \lambda e^u$$

  - critical λ for well-posedness

- porous-medium equation:

$$-\nabla \cdot \Big((u^{m-1} + \epsilon)\nabla u \Big) = f$$

  - regularized with $\epsilon > 0$ for uniform ellipticity
  - $\epsilon = 0$: degeneracies within domain

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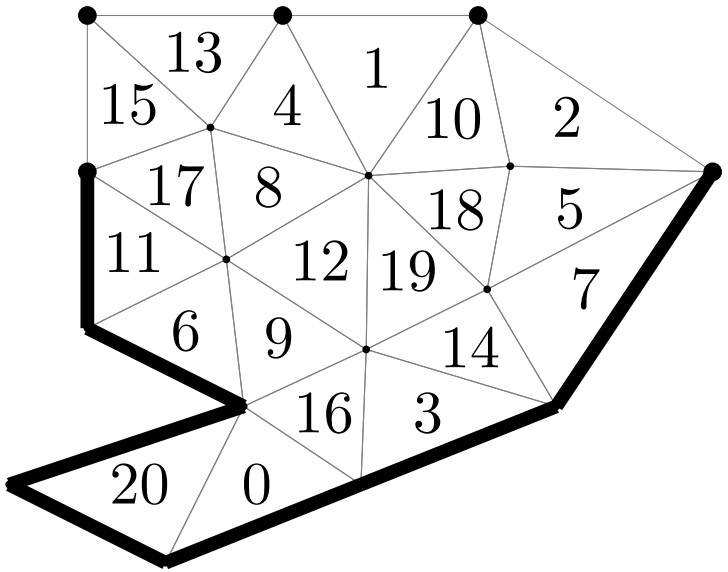
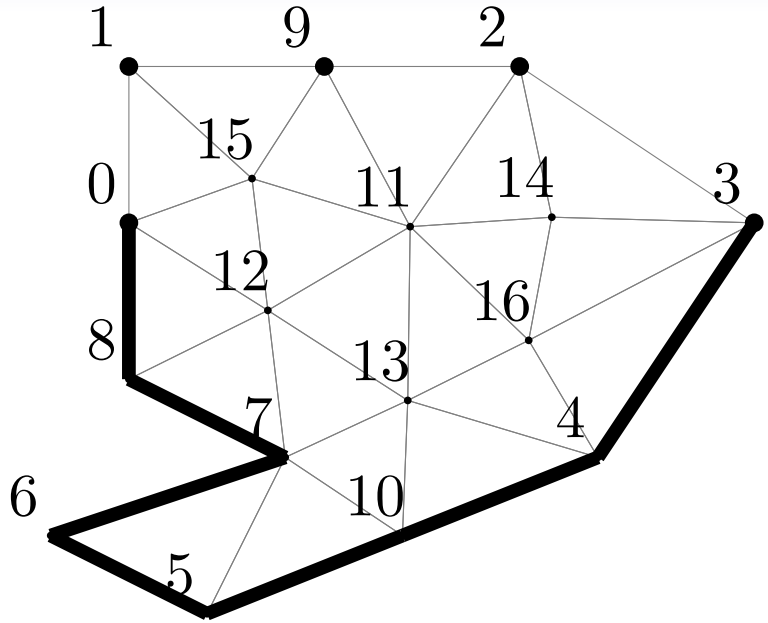
meshes and numbering

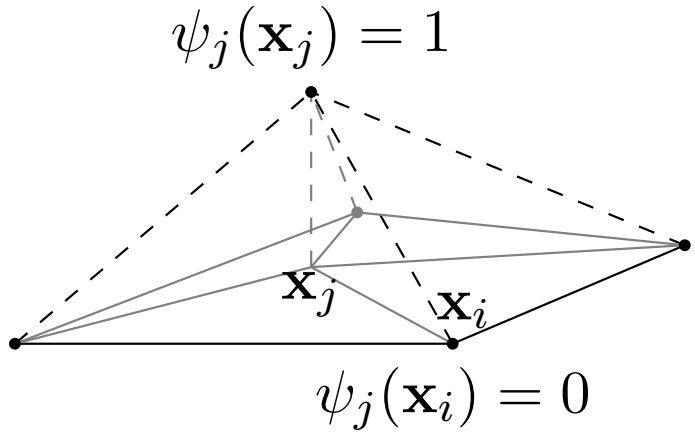




- triangulation $\mathcal{T}_h$ of a polygonal domain Ω
- numbering:
  - K elements ($= 21$ above; left)
  - N nodes ($= 17$ above; right)
  - P segments in Neumann boundary ($= 7$ above; bold)
  - n_D nodes in Dirichlet boundary ($= 5$ above)
- to fully describe mesh, also need node locations $\mathbf{x}_i = (x_i, y_i)$

FEM spaces

- hat functions satisfy:
  - $\psi_j(\mathbf{x})$ continuous
  - $\psi_j \in P_1$ on each element
  - $\psi_j(\mathbf{x}_i) = \delta_{ij}$



- use hat functions to approximate $g_D(\mathbf{x})$:

$$\hat{g}_D(\mathbf{x}) = \sum_{l=0}^{n_D-1} g_D(\mathbf{x}_{j_l})\psi_{j_l}(\mathbf{x}) \quad \in C(\overline{\Omega})$$

- use hat functions to define test function space:

$$S_0^h = \operatorname{span}\langle \psi_j \,:\, \mathbf{x}_j \notin \partial_D\Omega \rangle \subset H_0^1(\Omega)$$

- . . . and trial function space:

$$S_g^h = \left\{ \hat{g}_D + w \,:\, w \in S_0^h \right\} \overset{?}{\subset} H_g^1(\Omega)$$

FEM spaces

- expand the FEM solution u^h:

$$u^h(\mathbf{x}) = \hat{g}_D(\mathbf{x}) + \sum_{\mathbf{x}_j \notin \partial_D \Omega} u_j \, \psi_j(\mathbf{x})$$

- discrete weak form: for all i such that $\mathbf{x}_i \notin \partial_D \Omega$,

$$\int_\Omega a(u^h) \nabla u^h \cdot \nabla \psi_i = \int_\Omega f(u^h) \psi_i + \int_{\partial_N \Omega} g_N \psi_i \qquad \text{(DWF)}$$

- $\dim(S_0^h) = \dim(S_g^h) = N - n_D$
- however, it is easier to also make Dirichlet boundary nodes into degrees of freedom
  - we assemble a nonlinear system of N equations in N unknowns

element residuals

- for each element $\triangle_k$ and ψ_i, define an *element residual*:

$$F_i^k(\mathbf{u}) = \int_{\triangle_k} a(u^h)\nabla u^h \cdot \nabla\psi_i - f(u^h)\psi_i$$

- for each edge s_ν in the Neumann boundary we define

$$\varphi_i^\nu = \int_{s_\nu} g_N\psi_i$$

- (DWF) becomes:

$$F_i(\mathbf{u}) = \sum_{k=0}^{K-1} F_i^k(\mathbf{u}) - \sum_{\nu=0}^{P-1} \varphi_i^\nu = 0 \qquad \text{for } \mathbf{x}_i \notin \partial_D\Omega$$

- for Dirichlet boundary nodes have easy equation:

$$F_i(\mathbf{u}) = u_i - g_D(\mathbf{x}_i) \qquad \text{for } \mathbf{x}_i \in \partial_D\Omega$$

assembled FEM system of equations

- recall: N is number of nodes in mesh
- P^1 FEM generates an algebraic system of N equations in N unknowns:

$$\mathbf{F}(\mathbf{u}) = 0 \qquad (*)$$

  - one equation $F_i(\mathbf{u}) = 0$ per node
  - one unknown u_i per node
  - nonlinear system if $\partial a/\partial u \neq 0$ and/or $\partial f/\partial u \neq 0$
  - sparse because support of a hat function ψ_i only overlaps with a few triangles $\triangle_k$, and thus only a few nodal values $\mathbf{u} = \{u_j\}$ enter into a given $F_i^k(\mathbf{u})$
  - $J_{\mathbf{F}} = (\partial \mathbf{F}_i/\partial u_j)$ is the *Jacobian*, a sparse matrix

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nonlinear residual

- the result of FEM assembly is a nonlinear system:

$$\mathbf{F}(\mathbf{u}) = 0 \qquad (*)$$

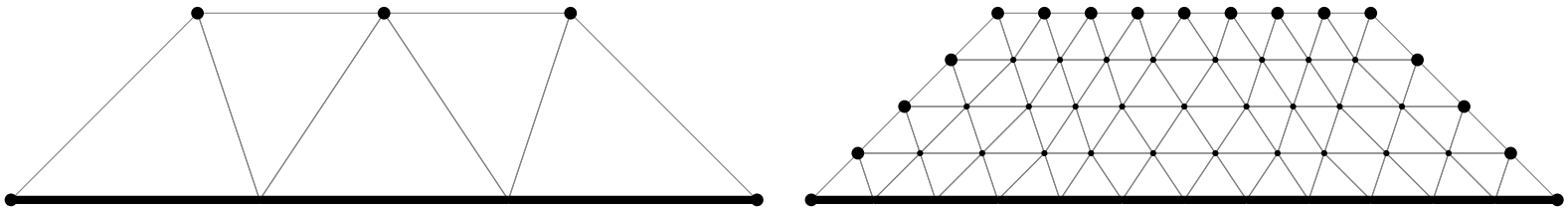
- the function $\mathbf{F} : \mathbb{R}^N \to \mathbb{R}^N$ is called the *residual*
  - continuous and differentiable if a, f are
- propose to solve $(*)$ by Newton method:

$$J_{\mathbf{F}}(\mathbf{u}_k)\mathbf{p} = -\mathbf{F}(\mathbf{u}_k)$$
$$\mathbf{u}_{k+1} = \mathbf{u}_k + \alpha\mathbf{p}$$

  - find α using line search based on *merit function* $\Phi(\mathbf{u}) = \frac{1}{2}\|\mathbf{F}(\mathbf{u})\|^2$
  - converges in one step if $a = a(x, y)$ and $f = f(x, y)$ [linear]
  - converges quadratically if a, f smooth

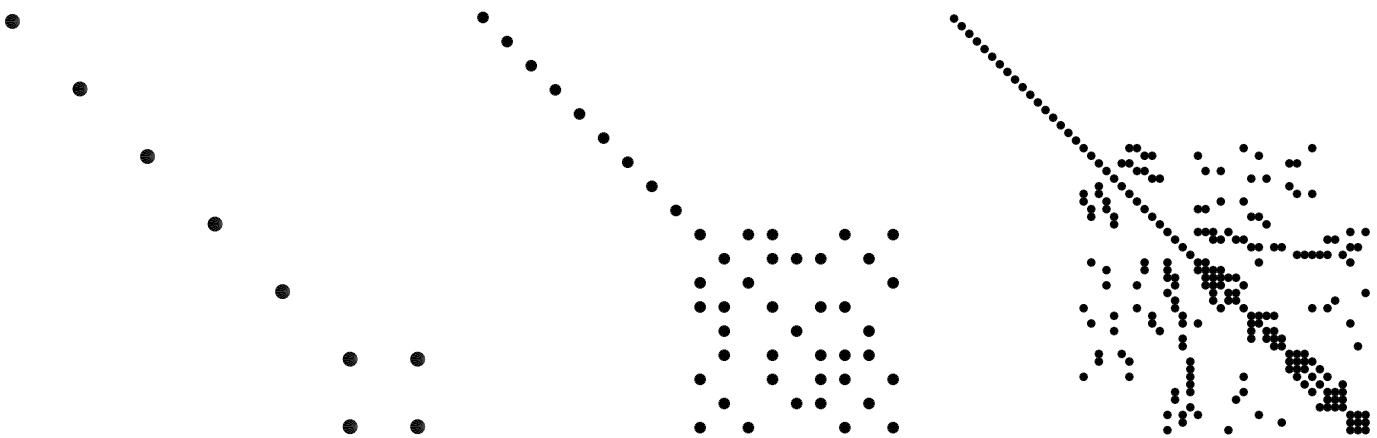
the Jacobian is the FEM stiffness matrix

- $J_{\mathbf{F}}(\mathbf{u})$ is the FEM "stiffness matrix"
- example: meshes with $N = 7, 18, 55$ nodes



  - generated by uniform refinement of $N = 7$ mesh
  - $N = 18$ mesh not shown

- sparsity patterns for corresponding $J_{\mathbf{F}}(\mathbf{u})$:



the Newton step is a sparse linear system

- $J_{\mathbf{F}}(\mathbf{u}_k)\mathbf{p} = -\mathbf{F}(\mathbf{u}_k)$ is a sparse linear system
  - solve it for the Newton step $\mathbf{p}$
  - actually take the step after line search: $\mathbf{u}_{k+1} = \mathbf{u}_k + \alpha\mathbf{p}$
- so, how to solve?:

$$A\mathbf{p} = \mathbf{b}$$

  - always: $A = J_{\mathbf{F}}(\mathbf{u}_k)$ is sparse $N \times N$ matrix
  - if PDE is well-posed: $A = J_{\mathbf{F}}(\mathbf{u}_k)$ is invertible
  - if uniformly elliptic and assembled as described: $A = J_{\mathbf{F}}(\mathbf{u}_k)$ is symmetric positive-definite

solving sparse linear systems

- the Newton step is $A\mathbf{p} = \mathbf{b}$ where $A = J_{\mathbf{F}}(\mathbf{u}_k)$
- $O(N^3)$ dense algorithms are possible:
  - Gaussian elimination (LU decomposition)
  - Cholesky decomposition
- . . . but they struggle for big N
  - variable reordering (minimum degree, nested dissection) helps a lot . . . but is still slow
- modern expectation: use Krylov methods
  - $\mathcal{K}_m(A, \mathbf{b}) = \left\langle \mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \ldots, A^{m-1}\mathbf{b} \right\rangle$ is *Krylov space*
  - CG and GMRES are best-known Krylov methods

solving sparse linear systems

- actually one uses *preconditioned* Krylov methods
- a *preconditioner* is an M which is spectrally-equivalent to A and such that $M\mathbf{p} = \mathbf{c}$ can be rapidly solved
- for $A\mathbf{p} = \mathbf{b}$ the preconditioned system is $M^{-1}A\mathbf{p} = M^{-1}\mathbf{b}$
  - $\mathcal{K}_m(M^{-1}A, M^{-1}\mathbf{b})$ contains good approximation of $\mathbf{p}$
- preconditioners include:
  - diagonal of A — *Jacobi*
  - incomplete factorization — *ILU,IC*
  - approximate block inverse — *ASM*
  - application of multigrid cycles — *GMG,AMG*

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modern FEM software

- slogan: modern FEM software should make FEM easy
- application packages:
  - COMSOL Multiphysics ← grew out of a Matlab toolbox
  - ABACUS
  - Autodesk Simulation
  - *I don't actually know much about these packages* . . .
- open source libraries:
  - deal.II [C++]
  - libmesh [C++]
  - Elmer [Fortran90]
  - FEniCS [Python]
  - Firedrake [Python]

tool stacks

- one needs 4 levels of tools:

mesh generation
↓
FEM assembly[a]
↓
solver library[b]
↓
visualization

- commercial packages may partially hide this structure, but libraries always allow separate control of these levels
- notes:
  - a includes weak form declaration/implementation, element definitions, and actual assembly
  - b includes both nonlinear solvers (e.g. Newton method) and linear solvers (e.g. CG and preconditioners too)

tool stacks I have actually used

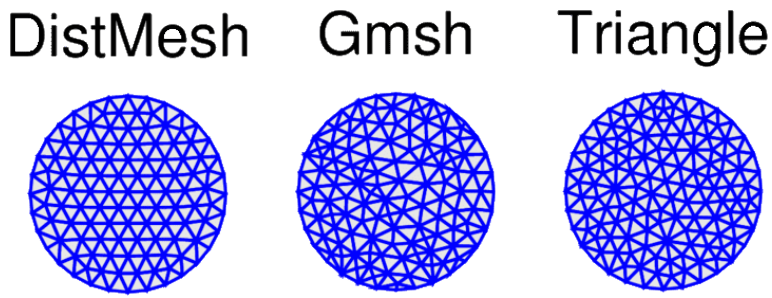
- stacks I have actually used:

	1.	2.	3.
mesh generation	Distmesh	Gmsh	Gmsh
↓	↓	↓	↓
FEM assembly	Matlab code*	C code*	Firedrake
↓	↓	↓	↓
solver library	Matlab	PETSc	PETSc
↓	↓	↓	↓
visualization	Matlab	my own tools	Paraview

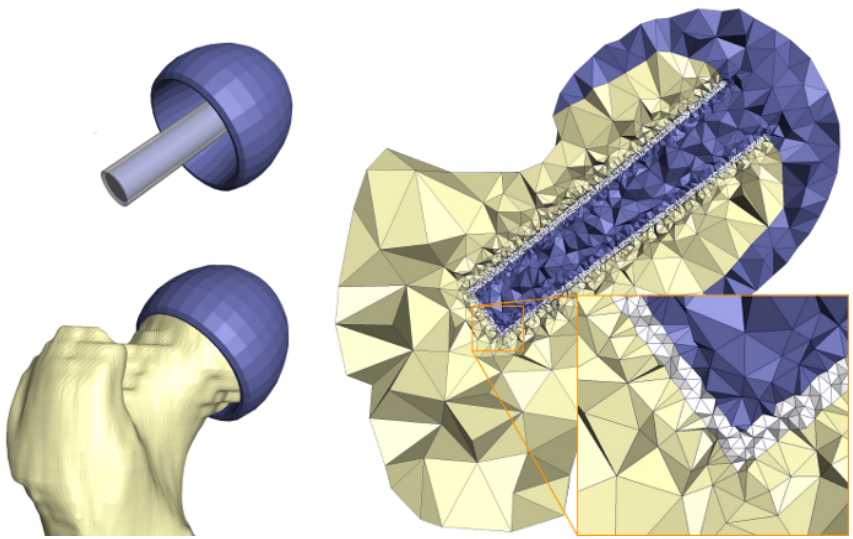
- $*$ = (hand-coded FEM assembly)
- I will show examples using 2. and 3.

mesh generation

- mesh generation varies:



  - 2004 FEM seminar used DistMesh in Matlab
- I'll demonstrate Gmsh (`gmsh.info`), a standard choice for "real" applications . . .



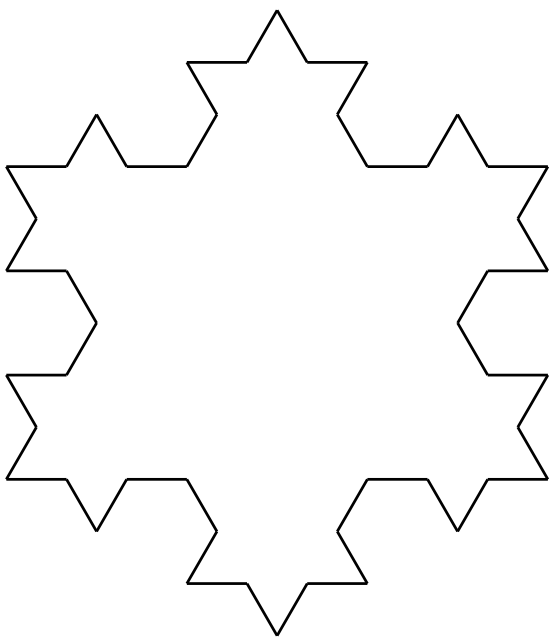
fractal Poisson: mesh generation

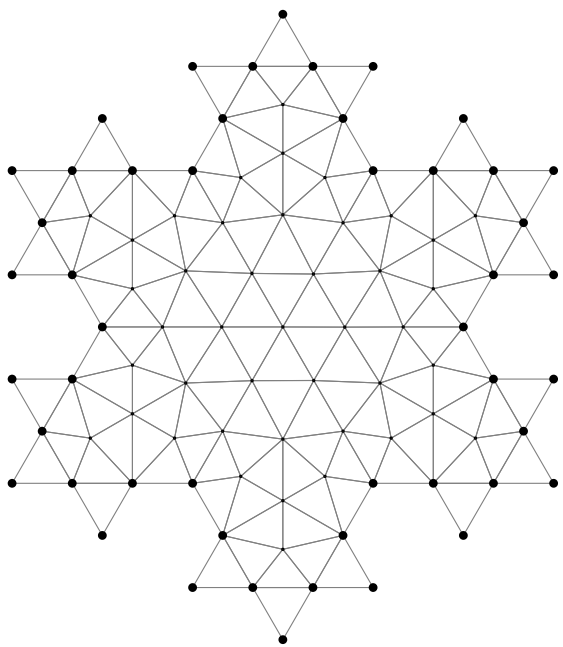
- problem:

$$-\triangle u = 1, \qquad u = 0 \text{ on } \partial\Omega$$

- generate polygon Ω (left figure) and ask Gmsh to triangulate it (right figure):

```
$ ./domain.py -l 2 -o koch2.geo
$ gmsh -2 koch2.geo
```





fractal Poisson: solving the PDE

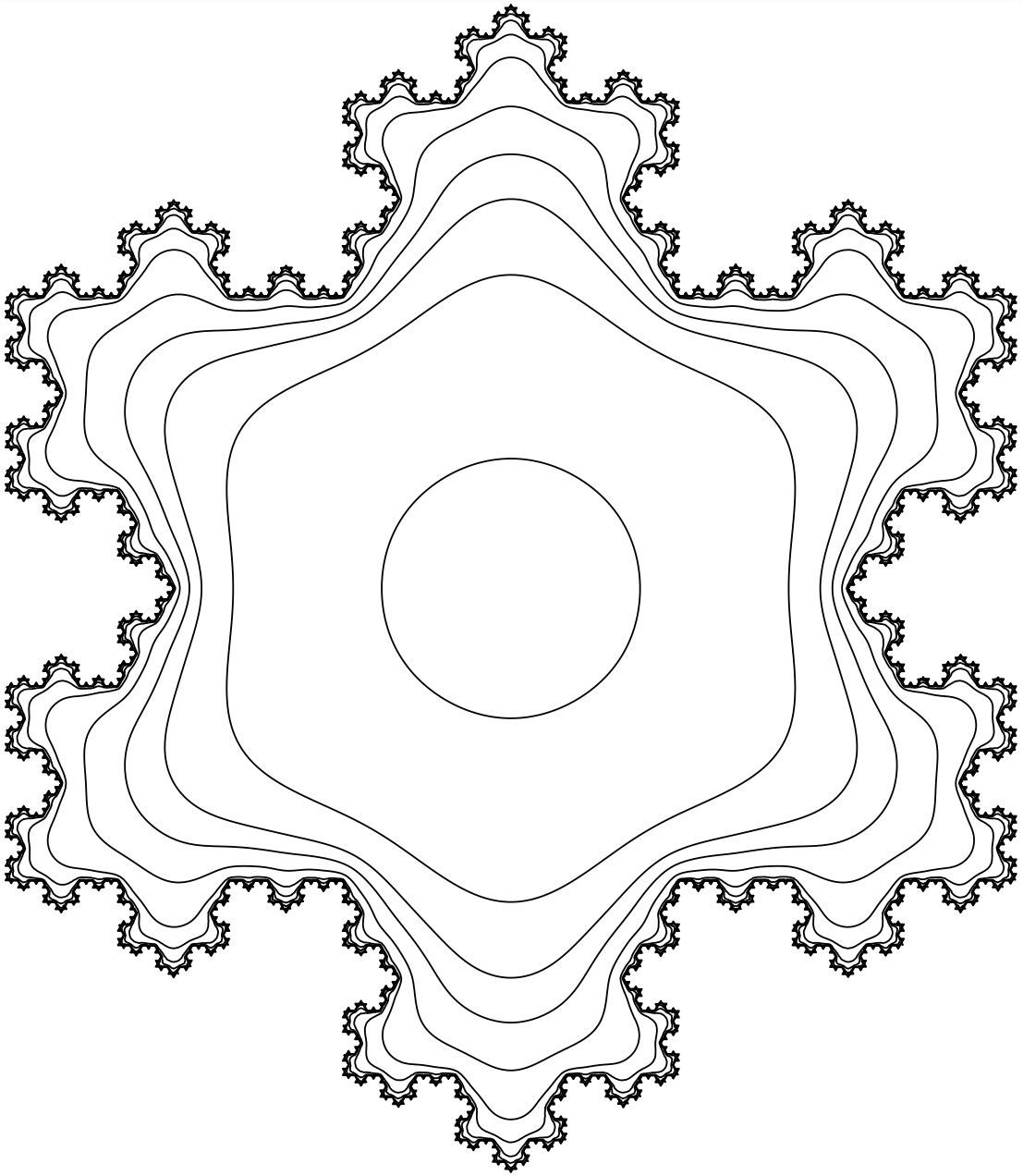
- in fact I wrote three codes:

`domain.py`	generates the boundary polygon
`msh2petsc.py`	converts Gmsh output to binary format
`unfem.c`	assemble the FEM residual using PETSc (`www.mcs.anl.gov/petsc`) data structures, including parallelization; then it calls a PETSc solver

- PDE solution by algebraic multigrid-preconditioned CG on the level-6 fractal domain with $N \approx 480{,}000$ nodes:

```
$ domain.py -l 6 -o koch6.geo
$ gmsh -2 koch6.geo
$ msh2petsc.py koch6
$ unfem -un_mesh koch6 \
    -snes_type ksponly -ksp_type cg -pc_type gamg
```

contours of solution



ugly code

- the result was pretty but the code was ugly
- even using PETSc, `unfem.c` was 900 lines of C code

```
for (k = 0; k < user->mesh->K; k++) {
    ...
    for (l = 0; l < 3; l++) {
        if (abf[en[l]] == 2) {
            ...
            aF[en[l]] = au[en[l]] - user->gD_fcn(xx,yy);
        } else {
            sum = 0.0;
            for (r = 0; r < q.n; r++) {
                psi = chi(l,q.xi[r],q.eta[r]);
                ip  = InnerProd(gradu,gradpsi[l]);
                sum += q.w[r] * ( ... );
            }
            aF[en[l]] += fabs(detJ) * sum;
        }
    }
}
```

better tools

- previous tool stack requires too much hand-coding
- want better tools for FEM assembly stage
- recall the second stack:

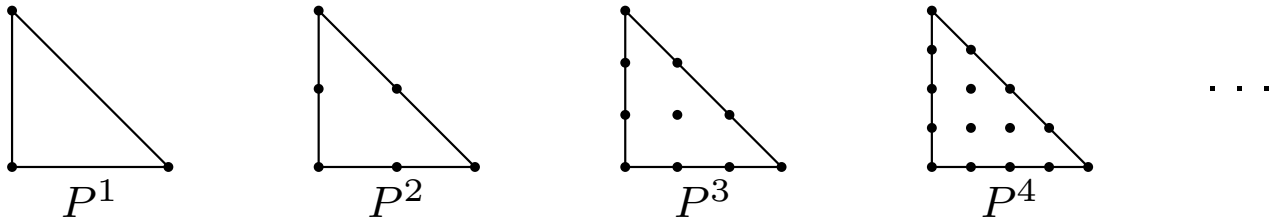
  Gmsh $\rightarrow$ Firedrake $\rightarrow$ PETSc $\rightarrow$ Paraview

- Firedrake: `www.firedrakeproject.org`

  . . . is an automated system for the solution of partial differential equations using the finite element method (FEM) . . . uses sophisticated code generation . . . Expressive specification of any PDE using the Unified Form Language from the FEniCS Project. Sophisticated, programmable solvers through seamless coupling with PETSc.

Unified Form Language (UFL) example

- UFL is an *expressive* language for weak forms
- choose function space $S^h = P^k$ for arbitrary degree k:



- Poisson problem ($-\triangle u = f$ on Ω) has b.c.s $u = g$ on $\partial\Omega$
- weak form:

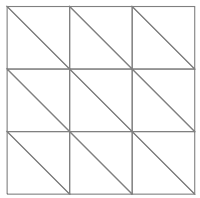
$$\int_\Omega \nabla u \cdot \nabla v - fv = 0$$

- Python UFL Firedrake code for above:

```
Sh = FunctionSpace(mesh,'CG',degree=k)       # Sh = P^k
bc = DirichletBC(Sh, g, bdry_ids)
u, v = Function(Sh), TestFunction(Sh)
F = (dot(grad(u), grad(v)) - f * v) * dx     # weak form
solve(F == 0, u, bcs=bc, ...)
```

solving the whole PDE problem

- for convergence analysis, use unit square $\Omega = (0,1)^2$ and consider regular triangulations only



- this time I wrote one code of only 70 lines:

`fish.py` uses UFL to define function space, boundary conditions, and weak form, and calls the Firedrake (PETSc) nonlinear solver . . . only a few important lines as before:

```
Sh = FunctionSpace(mesh,'CG',degree=k)
bc = DirichletBC(Sh, g, bdry_ids)
u, v = Function(Sh), TestFunction(Sh)
F = (dot(grad(u), grad(v)) - f * v) * dx
solve(F == 0, u, bcs=bc, ...)
```

- test problem: $u(x,y) = -xe^y$ is exact solution
  - very smooth solution
  - f is computed from u $\longleftarrow$ *manufactured exact solution*

refine and measure convergence

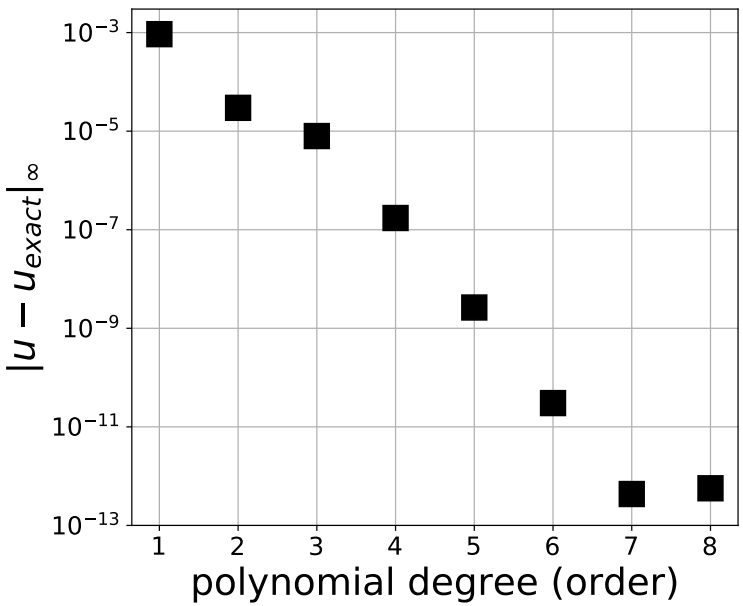
- one can approximate the continuum solution by either
  - h-refinement: make the triangles in `mesh` smaller
  - p-refinement: increase the polynomial degree `k`
- h-refinement chooses $m \times m$ grid where $m = 2^{\mathtt{X}+1} + 1$:

```
$ ./fish.py -refine X
```

- p-refinement (*spectral method*) chooses $P^{\mathtt{K}}$ on each element:

```
$ ./fish.py -k K
```

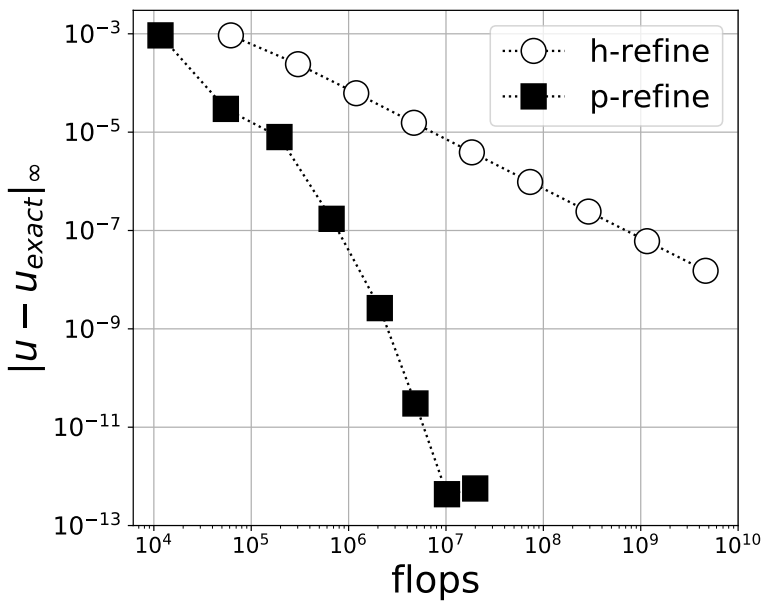
  - for example ...
  - fix $\mathtt{X} = 1$ for $m = 5$
  - vary k

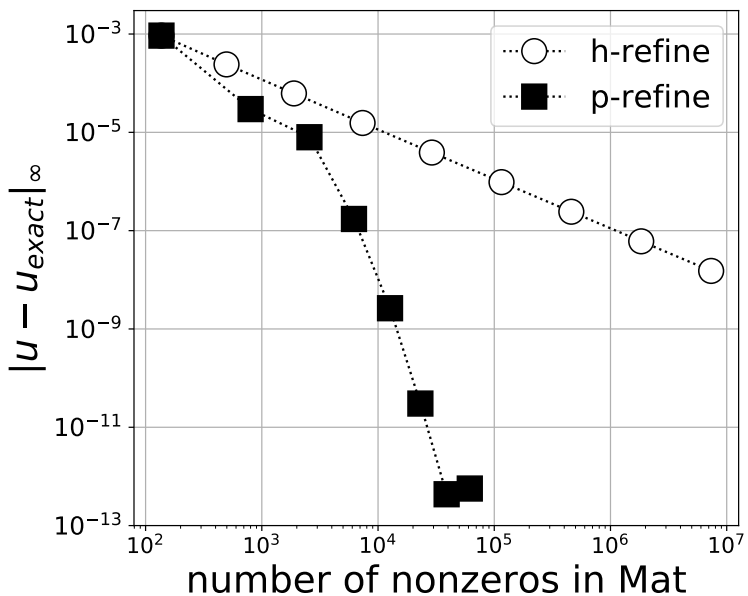


- combine options for h/p-refinement: `-refine X -k K`

measure performance

- performance runs use different solvers (educated choices!)
  - h-refinement runs use CG + (geometric multigrid)
  - p-refinement runs use Cholesky
- how to do a fair comparison of refinement modes?
- by error-vs-flops (left figure)
- by number of nonzeros in Jacobian matrix (right figure)





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Stokes equations for viscous, incompressible fluids

- the model for very-viscous fluids with viscosity $\mu > 0$
  - "very viscous" = (Reynold's number $\to 0$)
  - e.g. honey, motor oil, glacier ice
- solve for velocity $\mathbf{u}$ and pressure p on domain Ω:

$$-\mu \triangle \mathbf{u} + \nabla p = 0$$
$$\nabla \cdot \mathbf{u} = 0$$

- here only consider Dirichlet boundary conditions:

$$\mathbf{u} = \mathbf{g} \quad \text{on } \partial\Omega$$

Stokes weak form

- weak form from multiplying by test functions $\mathbf{v}$, q:

$$\int_\Omega \mu \nabla \mathbf{u} : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v} = 0, \qquad \int_\Omega q \nabla \cdot \mathbf{u} = 0$$

- can write this as one bilinear form,

$$k(\mathbf{u}, p; \mathbf{v}, q) = \mu\, a(\mathbf{u}, \mathbf{v}) + b(\mathbf{v}, p) + b(\mathbf{u}, q)$$

  where

$$a(\mathbf{w}, \mathbf{v}) = \int_\Omega \nabla \mathbf{w} : \nabla \mathbf{v}, \qquad b(\mathbf{v}, q) = -\int_\Omega q \nabla \cdot \mathbf{v}$$

- so $\mathbf{u}$, p satisfy: $\quad k(\mathbf{u}, p; \mathbf{v}, q) = \ell(\mathbf{v})$ for all $\mathbf{v}, q$

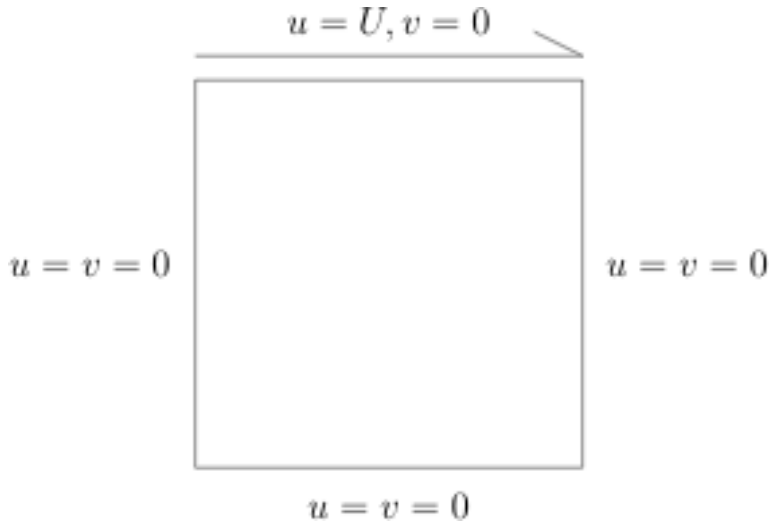
second UFL example

- suppose we choose $\mathbf{u} \in P^{k+2}$ and $p \in P^k$
  - "mixed" FEM for an incompressible fluid
  - nontrivial fact: these are a stable element choice
  - "Taylor-Hood"
- but Firedrake/UFL makes it easy to put into code ...

```
V = VectorFunctionSpace(mesh, 'CG', degree=k+2)  # velocity space
W = FunctionSpace(mesh, 'CG', degree=k)          # pressure space
Z = V * W
up = Function(Z)
u,p = split(up)
v,q = TestFunctions(Z)
F = (mu * dot(grad(u), grad(v)) - p * div(v) - div(u) * q) * dx
bc = ...
solve(F == 0, up, bcs=bc, ...)
```

lid-driven cavity problem

- choose a particular problem: lid-driven cavity
  - standard test problem
  - Dirichlet boundary conditions
  - $\Omega = (0,1)^2$

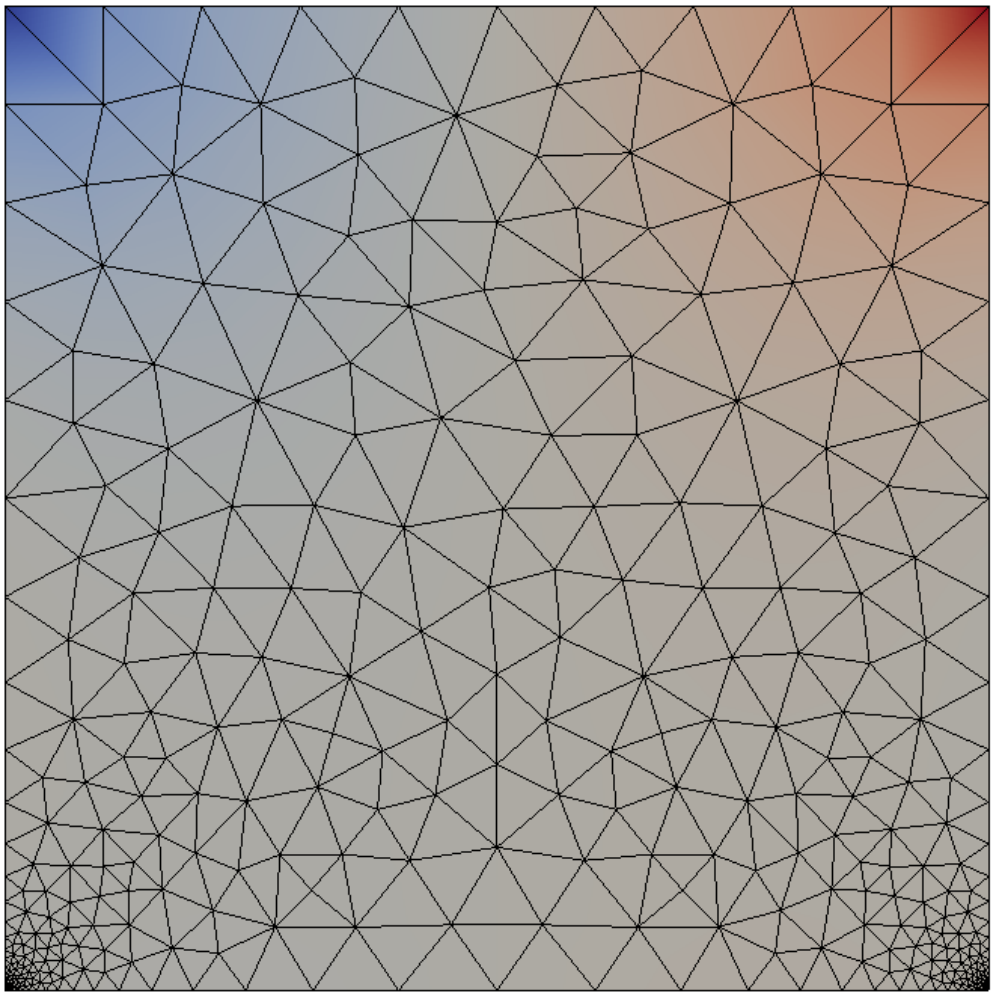


- boundary conditions code:

```
bc = [ DirichletBC(Z.sub(0), u_noslip, other),
       DirichletBC(Z.sub(0), u_lid,    lid)   ]
```

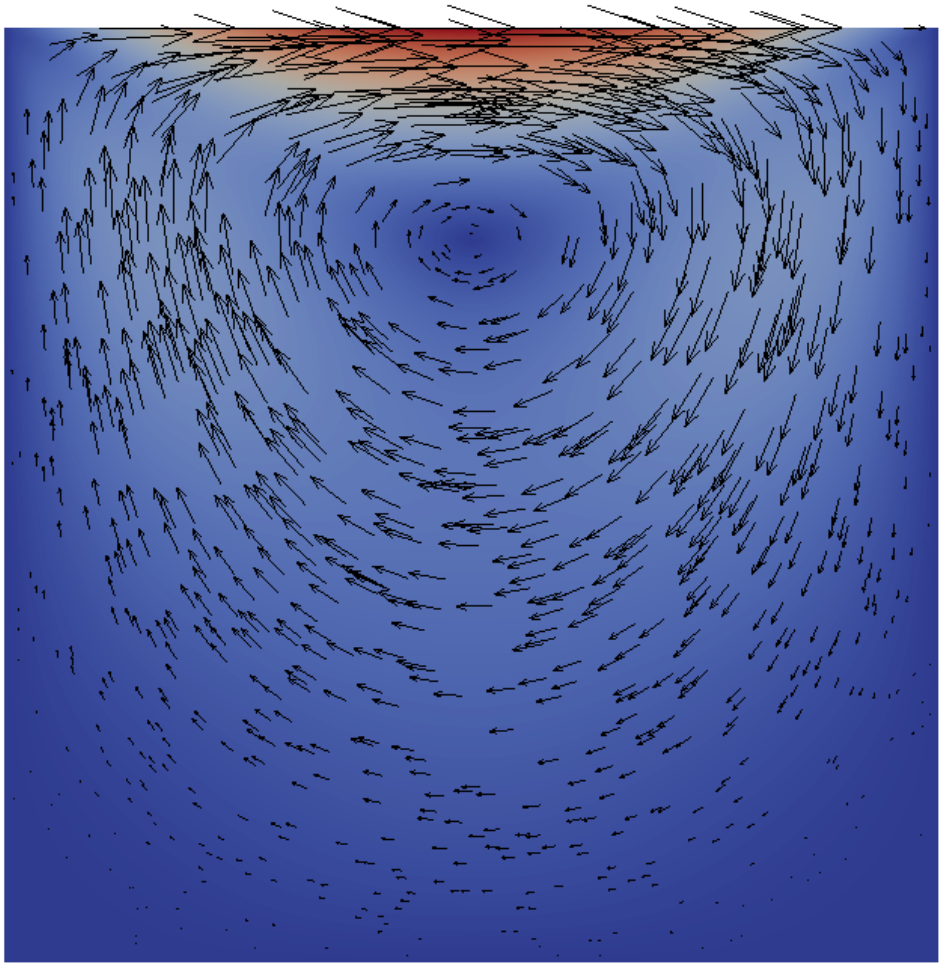
mesh and pressure

- non-uniform mesh: $N = 394$ nodes, $K = 686$ elements
- coloring by pressure



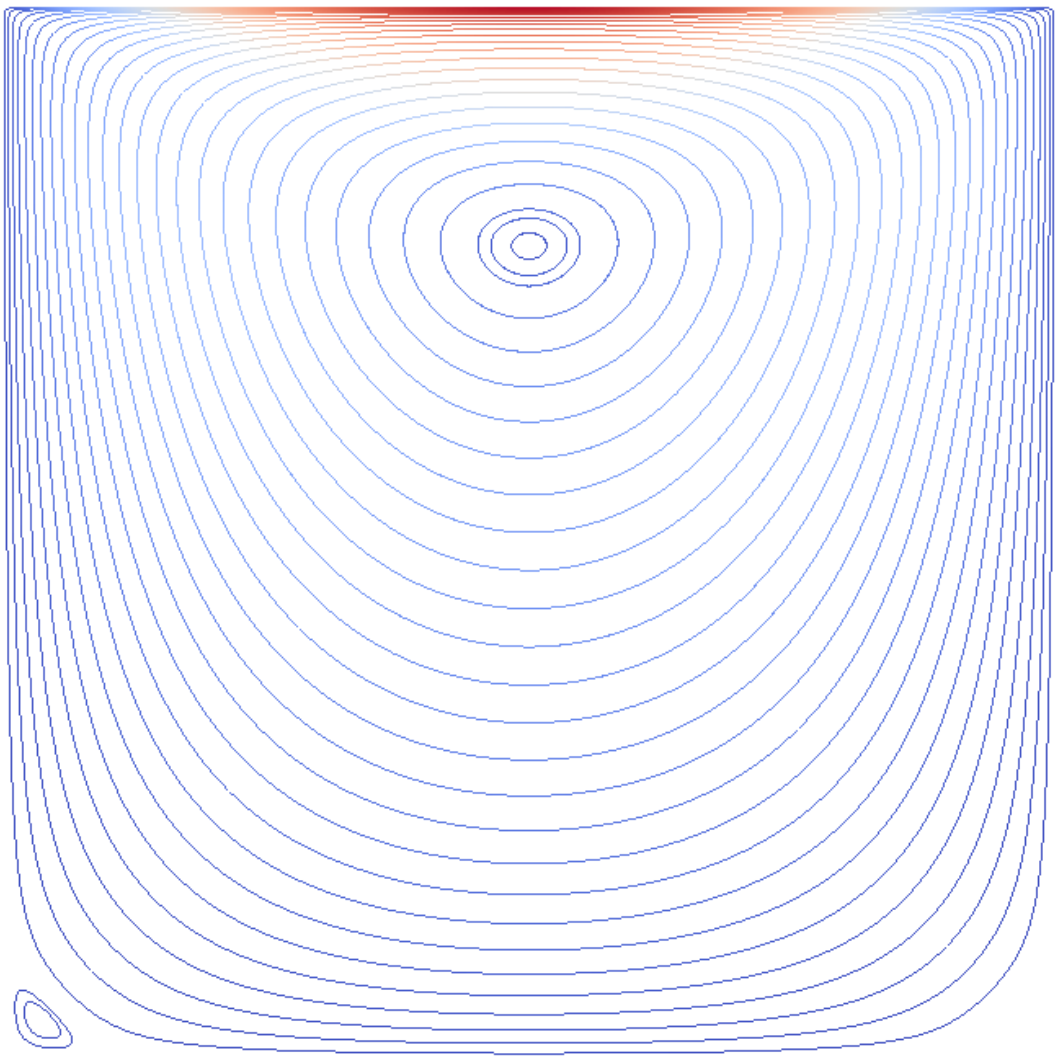
velocity vector field

- refined mesh: $N = 350{,}000$ nodes, $K = 700{,}000$ elements
- coloring by velocity magnitude



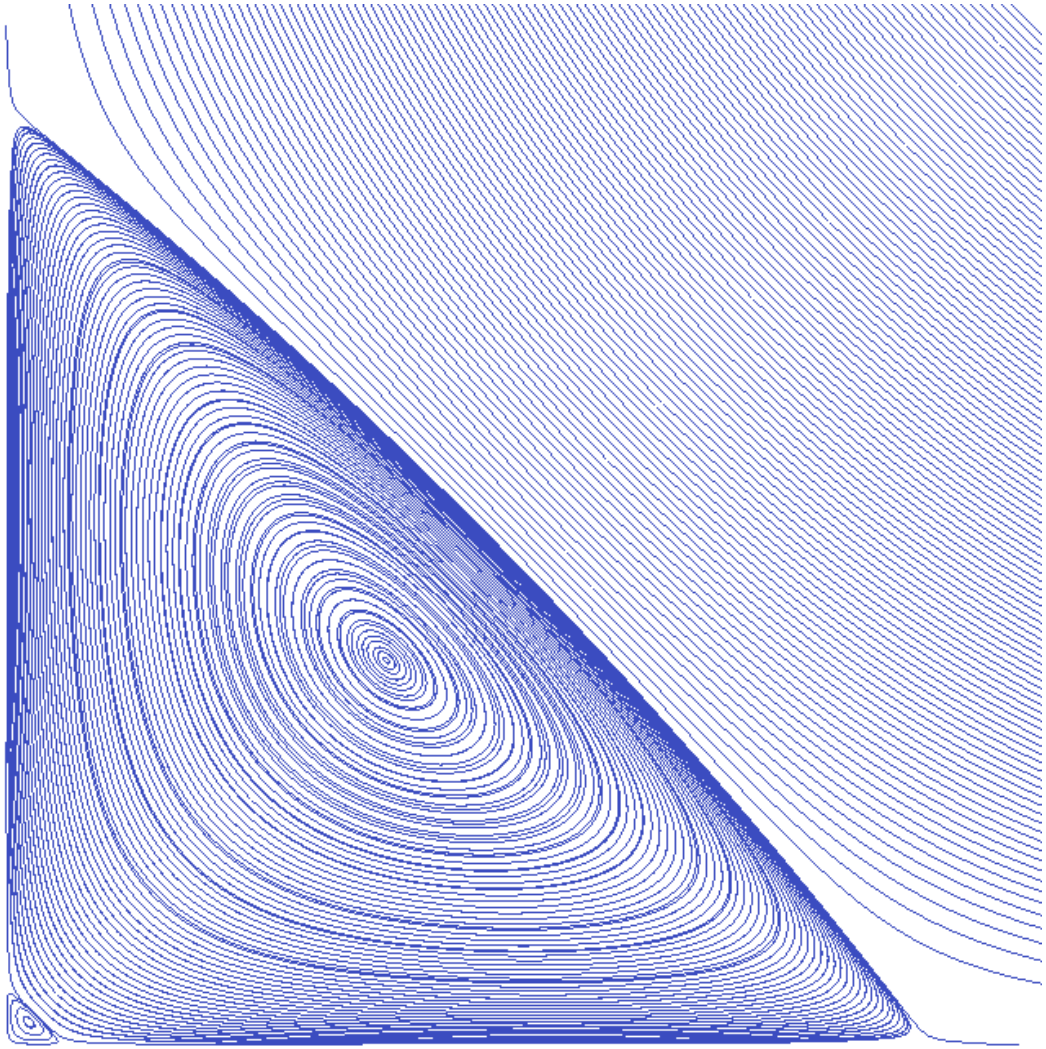
streamlines

- another view: streamlines



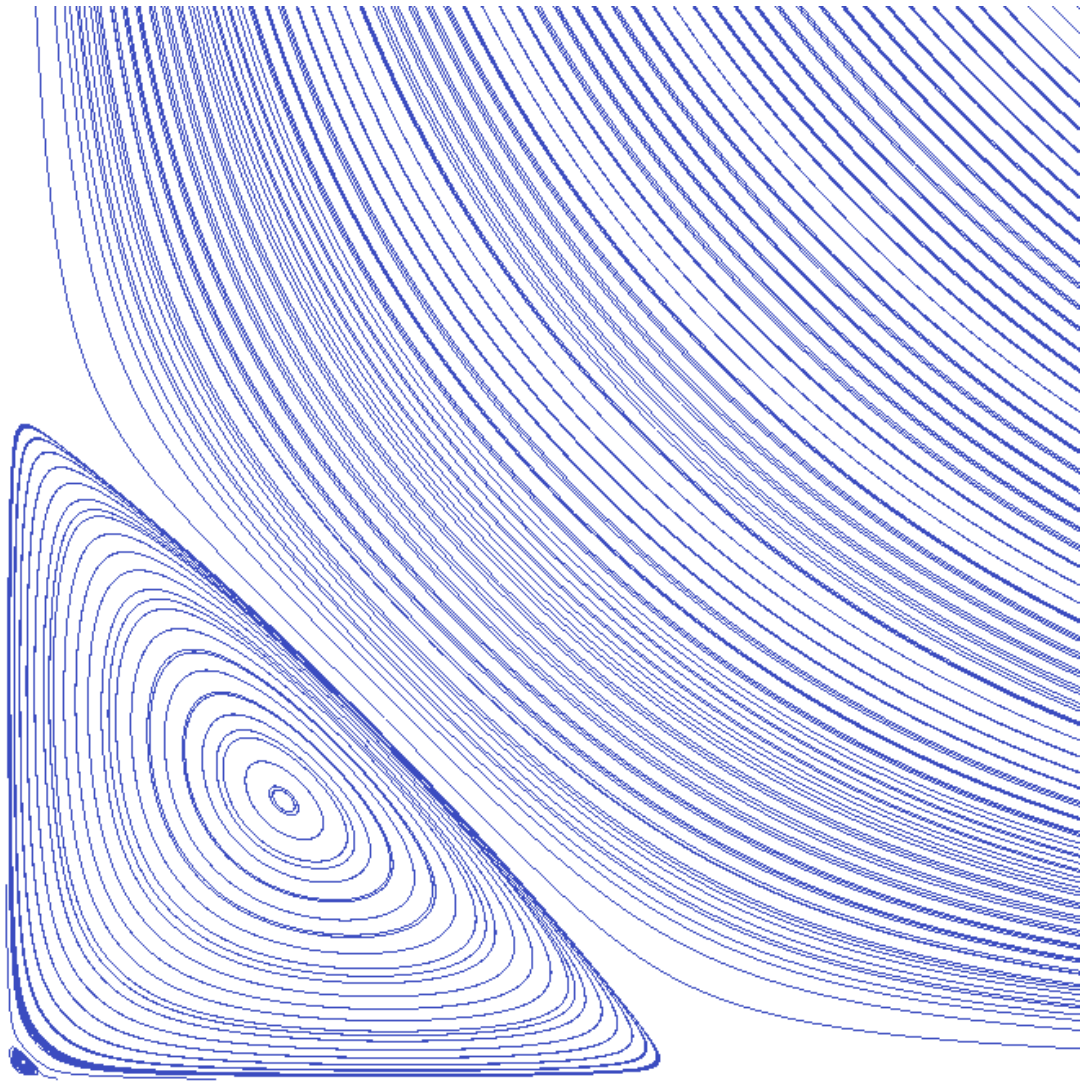
zoom to Moffat eddy

- zoom to show eddy in corner; add streamlines . . .



3 levels of Moffat eddies

- zoom again; third appears!



regarding Moffatt eddies

- Moffatt (1964): beautiful similarity solution analysis
- Acheson (1990), *Elementary Fluid Mechanics*:

  > *[if the corner angle is] below 146.3° . . . then a simple flow . . . is not possible and corner eddies occur instead. Indeed, as we probe deeper and deeper into each corner we find, in [Moffatt's] theory, not just one eddy but an infinite sequence of nested, alternately rotating eddies . . . each eddy is 1000 times weaker than the next; even with a 90 minute exposure time [a laboratory experiment] failed to detect the third eddy.*