Automated Modeling with FEniCS

L. Ridgway Scott

The Institute for Biophysical Dynamics,
The Computation Institute, and the
Departments of Computer Science and Mathematics,
The University of Chicago
Partial differential equations (PDEs) used pervasively to model phenomena of interest

Analytical techniques for solving PDEs limited in scope
- able to solve only the simplest model problems.

Development of reliable numerical methods facilitate PDE solution
- Modern computers and software techniques help

Most widely used technique is finite element method (FEM)

FEniCS Project automates generation of FEM software
PDE’s

- applied: separation of variables
- theory: requires measure theory (Lions Red Book, 1969)

Numerical approximation

- applied: finite differences, simple PDEs
- theory: Sobolev spaces with lots of indices (Babuska and Aziz, Maryland Conference, 1972)
New goal

A lot of theory has been developed in 50 years

So why can’t we

- Combine theory for both PDE’s and numerical methods
- Use software that automates generation of PDE/FEM software
- Focus on description of theory and critical PDE problems
- PDE models as variables (new materials)
The finite element method is based on the variational formulation of partial differential equations (PDEs).

The variational formulation has two advantages:

- It provides a language to define PDEs suitable for compilation into executable code
- It provides a basis for a theory of PDEs that allows one to know whether or not a given model is well posed.

We explain both these points via a simple example, Laplace’s equation.

Subsequently, a large variety of problems will be shown to fit into this framework.
Define a function \( u \) in a domain \( \Omega \subset \mathbb{R}^d \) by

\[-\Delta u = f \text{ in } \Omega \quad (1)\]

together with boundary conditions

\[u = 0 \text{ on } \Gamma \subset \partial \Omega \quad \text{(Dirichlet)}\]

\[\frac{\partial u}{\partial n} = 0 \text{ on } \partial \Omega \setminus \Gamma \quad \text{(Neumann)}\]

where \( \frac{\partial u}{\partial n} \) denotes the derivative of \( u \) in the direction normal to the boundary, \( \partial \Omega \) \( (\frac{\partial u}{\partial n} = n \cdot \nabla u. ) \)

This is known variously as Poisson’s equation or Laplace’s equation (especially when \( f \equiv 0 \)).
This equation forms the basis of a remarkable number of physical models.

It serves as a basic equation for diffusion, elasticity, electrostatics, gravitation, and many more domains.

In potential flow, the gradient of $u$ is the velocity of incompressible, inviscid, irrotational fluid flow.

- The boundary $\partial \Omega$ is the surface of an obstacle moving in the flow, and one solves the equation on the exterior of $\Omega$. 
Right place to look for solution of such an equation is a Sobolev space denoted $H^1(\Omega)$ defined by

$$H^1(\Omega) = \{ v \in L^2(\Omega) : \nabla v \in L^2(\Omega)^d \},$$  \hspace{1cm} (3)

where $L^2(\Omega)$ means functions square integrable on $\Omega$:

$$\| v \|_{L^2(\Omega)} = \left( \int_{\Omega} v(x)^2 \, dx \right)^{1/2} < \infty,$$

$L^2(\Omega)^d$ means $d$ copies of $L^2(\Omega)$ (Cartesian product). There is a natural inner-product on $L^2(\Omega)$ defined by

$$(v, w)_{L^2(\Omega)} = \int_{\Omega} v(x) w(x) \, dx, \hspace{1cm} (4)$$
Inner-product and associated norm on $H^1(\Omega)$ defined by

$$(v, w)_{H^1(\Omega)} = (v, w)_{L^2(\Omega)} + \int_{\Omega} \nabla v(x) \cdot \nabla w(x) \, dx$$

$$\|v\|_{H^1(\Omega)} = \sqrt{(v, v)_{H^1(\Omega)}}$$

For a vector-valued function $w$, e.g., $w = \nabla v$, we define

$$\|w\|_{L^2(\Omega)} = \|w\|_{L^2(\Omega)} = \left( \int_{\Omega} |w(x)|^2 \, dx \right)^{1/2},$$

where $|\xi|$ denotes Euclidean norm of vector $\xi \in \mathbb{R}^d$, and

$$(v, w)_{L^2(\Omega)} = \int_{\Omega} v(x) \cdot w(x) \, dx.$$
Now consider equation (1) with boundary conditions (2). Assume $\Gamma$ has nonzero measure (length or area, or even volume, depending on dimension).

Later, we will return to the case when $\Gamma$ is empty, the pure Neumann case.

Typical $\Omega$ shown in Figure 1, with $\Gamma$ shown in red.
To formulate the variational equivalent of (1) with boundary conditions (2), we define a variational space that incorporates the essential, i.e., Dirichlet, part of the boundary conditions in (2):

\[ V := \left\{ v \in H^1(\Omega) : v|_\Gamma = 0 \right\}. \tag{5} \]

See Table 1 for an explanation of the various names used to describe different boundary conditions.

<table>
<thead>
<tr>
<th>generic name</th>
<th>example</th>
<th>honorific name</th>
</tr>
</thead>
<tbody>
<tr>
<td>essential</td>
<td>( u = 0 )</td>
<td>Dirichlet</td>
</tr>
<tr>
<td>natural</td>
<td>( \frac{\partial u}{\partial n} = 0 )</td>
<td>Neumann</td>
</tr>
</tbody>
</table>

Table 1: Nomenclature for different types of boundary conditions.
The appropriate bilinear form for the variational problem is determined by multiplying Poisson’s equation by a suitably smooth function, integrating over \( \Omega \) and then integrating by parts:

\[
(f, v)_{L^2(\Omega)} = \int_{\Omega} (-\Delta u)v \, dx \\
= \int_{\Omega} \nabla u \cdot \nabla v \, dx - \int_{\partial \Omega} v \frac{\partial u}{\partial n} \, ds \\
= \int_{\Omega} \nabla u \cdot \nabla v \, dx := a(u, v).
\]  \hspace{1cm} (6)

The boundary term in (6) vanishes for \( v \in V \) because either \( v \) or \( \frac{\partial u}{\partial n} \) is zero on any part of the boundary.
The integration-by-parts formula derives from the divergence theorem

\[ \int_{\Omega} \nabla \cdot w(x) \, dx = \oint_{\partial \Omega} w(s) \cdot n(s) \, ds \]  

(7)

applied to \( w = v \nabla u \), together with \( \frac{\partial u}{\partial n} = (\nabla u) \cdot n \) and \( \Delta u = \nabla \cdot (\nabla u) \) (\( n \) is the outward-directed normal to \( \partial \Omega \)). More precisely, we observe that

\[ \nabla \cdot (v \nabla u) = \sum_{i=1}^{d} ((v \nabla u)_i)_i = \sum_{i=1}^{d} (v u_{i,i})_i \]

\[ = \sum_{i=1}^{d} v_{i,i}u_{i,i} + v u_{ii} = \nabla v \cdot \nabla u + v \Delta u. \]
Thus the divergence theorem applied to $w = v \nabla u$ gives

$$\oint_{\partial \Omega} v \nabla u(s) \cdot n(s) \, ds = \int_{\Omega} (\nabla \cdot (v \nabla u))(x) \, dx$$

$$= \int_{\Omega} (\nabla v \cdot \nabla u + v \Delta u)(x) \, dx,$$

which means that

$$\int_{\Omega} -v(x) \Delta u(x) \, dx = \int_{\Omega} \nabla v(x) \cdot \nabla u(x) \, dx$$

$$- \oint_{\partial \Omega} v \frac{\partial u}{\partial n} \, ds$$

$$= a(u, v) - \oint_{\partial \Omega} v \frac{\partial u}{\partial n} \, ds.$$
Thus, \( u \) can be characterized via

\[
u \in V \quad \text{satisfying} \quad a(u, v) = (f, v)_{L^2(\Omega)} \quad \forall v \in V. \tag{9}
\]

The companion result, namely

\[
\text{a solution to the variational problem in (9) solves Poisson’s equation}
\]

can also be proved [2], under suitable regularity conditions on \( u \).

These regularity conditions guarantee the relevant expressions in (1) and (2) are well defined.

We will show how this is done in detail in the one-dimensional case.
The variational code

from dolfin import *
# Create mesh and define function space
mesh = UnitSquareMesh(32, 32)
V = FunctionSpace(mesh, "Lagrange", 1)
# Define boundary condition
u0 = Constant(0.0)
bc = DirichletBC(V, u0, "on_boundary")
# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
you = Expression("(sin(3.141592*x[0]))*(sin(3.141592*x[1]))")
a = inner(grad(u), grad(v))*dx
L = (2*3.141592*3.141592)*you*v*dx
# Compute solution
u = Function(V)
solve(a == L, u, bc)
plot(u, interactive=True)
The code $f \star dx$ means

$$\int_{\Omega} f(x) \, dx$$

where $\Omega$ is the domain associated with the function space of which $f$ is a member:

$$f \in V, \quad \Omega = \text{domain}(V)$$

In our example, $V$ is defined by

$$V = \text{FunctionSpace}(\text{mesh}, \text{"Lagrange"}, 1)$$

and $\text{mesh}$ contains the domain information.
We have seen that Laplace’s equation can be expressed as a variational formulation

Find $u \in V$ such that

$$a(u, v) = F(v) \text{ for all } v \in V$$

and furthermore that the variational formulation can be used as a language to describe the problem in code.

Now we want to show that this formulation is universal for a broad range of problems.
Pure Neumann (or natural) boundary conditions

\[
\frac{\partial u}{\partial n} = 0 \text{ on } \partial \Omega \tag{10}
\]

(i.e., when \( \Gamma = \emptyset \)) varies the definition of \( V \).

In particular, solutions are unique only up to an additive constant, and they can exist only if the right-hand side \( f \) in (1) satisfies

\[
\int_{\Omega} f(x) \, dx = \int_{\Omega} -\Delta u(x) \, dx = \int_{\Omega} \nabla u(x) \cdot \nabla 1 \, dx - \oint_{\partial \Omega} \frac{\partial u}{\partial n} \, ds = 0. \tag{11}
\]
A variational space appropriate for the present case is

\[ V = \left\{ v \in H^1(\Omega) : \int_{\Omega} v(x) \, dx = 0 \right\}. \]  \hspace{1cm} (12)

For any integrable function \( g \), we define its mean, \( \bar{g} \), as follows:

\[ \bar{g} := \frac{1}{\text{meas}(\Omega)} \int_{\Omega} g(x) \, dx. \]  \hspace{1cm} (13)

For any \( v \in H^1(\Omega) \), note that \( v - \bar{v} \in V \).

Then \( u - \bar{u} \) satisfies the variational formulation (9) with \( V \) defined as in (12).
Conversely, if \( u \in H^2(\Omega) \) solves (9) then \( u \) solves Poisson’s equation (1) with a right-hand-side given by

\[
\tilde{f}(x) := f(x) - \bar{f} \quad \forall x \in \Omega
\]  

(14)

with boundary conditions (10).

Variational form \( a(\cdot, \cdot) \) coercive on the space \( V \) [2]: there is a constant \( C \) depending only on \( \Omega \) and \( \Gamma \) such that

\[
\|v\|_{H^1(\Omega)}^2 \leq C a(v, v) \quad \forall v \in V.
\]  

(15)

Coercivity implies solution is unique: \( f \equiv 0 \implies \)

\[
0 = (f, u)_{L^2} = a(u, u) \geq \frac{1}{C} \|u\|_{H^1(\Omega)}^2.
\]
In the finite-dimensional case, this uniqueness also implies existence, and a similar result (Lax-Milgram Theorem) holds in the setting of infinite dimensional Hilbert spaces such as $V$.

Moreover, the coercivity condition immediately implies a stability result, namely

$$
\|u\|_{H^1(\Omega)} \leq \frac{Ca(u, u)}{\|u\|_{H^1(\Omega)}} = C \frac{(f, u)_{L^2}}{\|u\|_{H^1(\Omega)}} \leq C \|f\|_{V'}, \quad (16)
$$

where the dual norm is defined by

$$
\|F\|_{V'} := \sup_{0 \neq v \in V} \frac{|F(v)|}{\|v\|_V}.
$$
When coercivity holds, the Lax-Milgram theorem guarantees variational problem (9) has unique solution.

Additional **continuity condition** required:

\[
|a(u, v)| \leq C \|u\|_{H^1(\Omega)} \|v\|_{H^1(\Omega)} \quad \text{for all } u, v \in V. \quad (17)
\]

Usually this condition is evident, but consider

\[
-\frac{1}{2} \Delta u(r_1, r_2) + (\kappa(r_1) + \kappa(r_2)) u(r_1, r_2) = f(r_1, r_2)
\]

in \( \Omega = [0, \infty] \times [0, \infty] \), where \( \kappa(r) = r^{-2} - r^{-1} + \frac{1}{2} \).

Here coercivity is easy but continuity requires Hardy’s inequality (assuming \( u = 0 \) on \( \partial \Omega \)).
Lax-Milgram Theorem Suppose that the variational form $a(\cdot, \cdot)$ is coercive (15) and continuous (17) (bounded) on $H^1(\Omega)$. Then the variational problem (9) has a unique solution $u$ for every continuous (bounded) $F$ defined on $H^1(\Omega)$. Moreover,

$$
\|u\|_{H^1(\Omega)} \leq c_1 c_0 \sup_{v \in H^1(\Omega)} \frac{|F(v)|}{\|v\|_{H^1(\Omega)}},
$$

(18)

where $c_0$ is the constant in (15) and $c_1$ is the constant in (17).

The combination of continuity and coercivity correspond to the stability of the numerical scheme.
Many models balance advection and diffusion:

$$-\epsilon \Delta u + \beta \cdot \nabla u = f \text{ in } \Omega$$

(19)

where $\beta$ is a vector-valued function.

Assume that we have boundary conditions

$$u = g \text{ on } \Gamma \subset \partial \Omega \quad \text{(Dirichlet)}$$

(20)

$$\frac{\partial u}{\partial n} = 0 \text{ on } \partial \Omega \setminus \Gamma \quad \text{(Neumann)}$$

The quantity $u$ is being advected in the direction of $\beta$.

There are in-flow and out-flow parts of the boundary.

We need to know how we are allowed to pick $\Gamma$. 
As before, using the three-step recipe, we define

\[ a(u, v) = \int_\Omega \nabla u(x) \cdot \nabla v(x) \, dx \]

\[ b(u, v) = \int_\Omega (\beta(x) \cdot \nabla u(x)) v(x) \, dx. \]

(21)

Alternative formulation: integrate by parts in the advection term.

Consider coercivity of the bilinear form

\[ a_\beta(u, v) = \epsilon a(u, v) + b(u, v). \]

Coercivity will guide us regarding choices for \( \Gamma \).
Since we already know that $a(\cdot, \cdot)$ is coercive on

$$V = \{ v \in H^1(\Omega) : v = 0 \text{ on } \Gamma \},$$

one approach is to determine conditions under which

$$b(v, v) \geq 0 \text{ for all } v \in V.$$

Then

$$a_\beta(v, v) = \epsilon a(v, v) + b(v, v) \geq \epsilon a(v, v) \geq c\epsilon \|v\|_{H^1}^2.$$

The positivity of $b(v, v)$ will depend on the choice of $\Gamma$. 
Positivity of the advection form

We again invoke the divergence theorem:

\[ \oint_{\partial \Omega} u v \beta \cdot n \, ds = \int_{\Omega} \nabla \cdot (u v \beta) \, dx \]

\[ = \int_{\Omega} u \beta \cdot \nabla v + v \beta \cdot \nabla u + u v \nabla \cdot \beta \, dx. \quad (22) \]

In particular,

\[ b(u, v) + b(v, u) = \oint_{\partial \Omega} u v \beta \cdot n \, ds - \int_{\Omega} u v \nabla \cdot \beta \, dx. \quad (23) \]

From (23), we have

\[ 2b(v, v) = \oint_{\partial \Omega} v^2 \beta \cdot n \, ds - \int_{\Omega} v^2 \nabla \cdot \beta \, dx. \quad (24) \]
Define

$$\Gamma_0 = \{x \in \partial \Omega : \beta(x) \cdot n = 0\},$$

$$\Gamma_\pm = \{x \in \partial \Omega : \pm \beta(x) \cdot n > 0\}.$$  (25)

An important special case is when \(\beta\) is incompressible, meaning \(\nabla \cdot \beta = 0\).

We will assume \(\nabla \cdot \beta = 0\) from now on.
In the case $\nabla \cdot \beta = 0$, (24) simplifies to

$$2b(v, v) = \int_{\Gamma_- \cup \Gamma_+} v^2 \beta \cdot n \ ds \geq \int_{\Gamma_-} v^2 \beta \cdot n \ ds,$$

(26)
since, by definition,

$$\int_{\Gamma_+} v^2 \beta \cdot n \ ds \geq 0.$$

Thus $\Gamma_- \subset \Gamma$ implies

- $b(v, v) \geq 0$ for all $v \in V$, and thus
- $a_\beta(\cdot, \cdot)$ is coercive on $V$.

We need to control the inflow region of the boundary.
An example

Let $\Omega = [0, 1]^2$ and $\beta = (1, 0)$. Note that $\nabla \cdot \beta = 0$.

Figure 2: Diffusion-advection problem (19)–(20) with $\Gamma = \Gamma_- \cup \Gamma_+$ and $g(x, y) = y^2 \left(1 - \frac{2}{3}y\right)$ and $f(x, y) = 1 - x$. Left: $\epsilon = 0.1$, $u_\epsilon$ computed using piecewise linears on a $100 \times 100$ mesh. Right: $\epsilon = 0.001$, $u_\epsilon$ computed using piecewise linears on a $1000 \times 1000$ mesh.
Numerical pollution

Spurious oscillations with too few grid points (on the scale of the mesh, at the outflow boundary)

Figure 3: Diffusion-advection problem (19)–(20) with $\Gamma = \Gamma_- \cup \Gamma_+$ and $g(x, y) = y^2 \left(1 - \frac{2}{3}y\right)$ and $f(x, y) = 1 - x$. Left: $\epsilon = 0.01$, $u_\epsilon$ computed using piecewise linears on a $100 \times 100$ mesh. Right: $\epsilon = 0.01$, $u_\epsilon$ computed using piecewise linears on a $15 \times 15$ mesh.
Wrong boundary conditions

What if no boundary condition on in-flow part: $\Gamma = \Gamma_+$. 

![Figure 4: Diffusion-advection problem (19)–(20) with $\Gamma = \Gamma_+$ and $g(x, y) = y^2(1 - \frac{2}{3}y)$ and $f(x, y) = 1 - x$. The solution $u_\epsilon$ was computed using piecewise linears on a 100 × 100 mesh. Left: $\epsilon = 1.0$, Right: $\epsilon = 0.1.$]
Looks reasonable at first. However, look at the scale.

The solution is now extremely large.

And if we continue to reduce $\epsilon$ (exercise) the solution size becomes disturbingly large.

Picking different orders of polynomials and values for $\epsilon$ tend to give random, clearly spurious results.

Thus we conclude that the coercivity condition provides good guidance regarding how to proceed.
The Stokes equations for the flow of a viscous, incompressible, Newtonian fluid can be written

\[-\Delta \mathbf{u} + \nabla p = 0\]
\[\nabla \cdot \mathbf{u} = 0.\]

(27)

in \(\Omega \subset \mathbb{R}^d\), where \(\mathbf{u}\) denotes fluid velocity and \(p\) denotes pressure [3].

Equations supplemented by boundary conditions, e.g., Dirichlet boundary conditions, \(\mathbf{u} = \gamma\) on \(\partial \Omega\).

Compatibility condition on data (divergence theorem):

\[\int_{\partial \Omega} \gamma \cdot \mathbf{n} \, ds = 0.\]

(28)
The variational formulation of (27) takes the form: Find \( u \) such that \( u - \gamma \in V \) and \( p \in \Pi \) such that

\[
a(u, v) + b(v, p) = 0 \quad \forall v \in V, \\
b(u, q) = 0 \quad \forall q \in \Pi,
\]

where e.g. \( a(\cdot, \cdot) = a_\nabla(\cdot, \cdot) \) and \( b(\cdot, \cdot) \) are given by

\[
a_\nabla(u, v) := \int_\Omega \sum_{i,j=1}^d u_{i,j}v_{i,j} \, dx, \quad b(v, q) := -\int_\Omega \sum_{i=1}^d v_{i,i}q \, dx.
\]

Derived by multiplying (27) by \( v \) with a “dot” product, and integrating by parts as usual. Note that the second equation in (27) and (29) are related by multiplying the former by \( q \) and integrating, with no integration by parts.
Stokes variational spaces

The spaces $V$ and $\Pi$ are as follows.

$V = H^1_0(\Omega)^d$

$\Pi = \text{subset of } L^2(\Omega) \text{ having mean zero.}$

Latter constraint fixes ambient pressure.

Inhomogeneous boundary data dealt with by writing $\mathbf{u} = \hat{\mathbf{u}} + \gamma$, $\hat{\mathbf{u}} \in V$, and (29) becomes

Find $\hat{\mathbf{u}}$ such that $\hat{\mathbf{u}} \in V$ and $p \in \Pi$ such that

$$a(\hat{\mathbf{u}}, \mathbf{v}) + b(\mathbf{v}, p) = -a(\gamma, \mathbf{v}) := F(\mathbf{v}) \quad \forall \mathbf{v} \in V,$$

$$b(\hat{\mathbf{u}}, q) = -b(\gamma, q) := G(q) \quad \forall q \in \Pi. \quad (30)$$

From now on, we will drop the drop the “hats” on $\mathbf{u}$. 

General formulation of discretization of \((29)\) is

\[
\begin{align*}
a(u_h, v) + b(v, p_h) &= F(v) &\forall v \in V_h \\
b(u_h, q) &= G(q) &\forall q \in \Pi_h,
\end{align*}
\tag{31}
\]

where \(F \in V'\) and \(G \in \Pi'\) (the “primes” indicate dual spaces [2]).

It is called a “mixed method” since the variables \(v\) and \(q\) are mixed together.

For the Stokes problem \((29)\), the natural variational formulation is already a mixed method, whereas it is an optional formulation in other settings.
We assume that the bilinear forms satisfy the standard continuity conditions

\[
\begin{align*}
a(u, v) & \leq C_a \|u\|_V \|v\|_V \quad \forall u, v \in V \\
b(v, p) & \leq C_b \|v\|_V \|p\|_\Pi \quad \forall v \in V, \ p \in \Pi.
\end{align*}
\]

(32)

We also assume appropriate coercivity conditions

\[
\begin{align*}
\alpha \|v\|_V^2 & \leq a(v, v) \quad \forall v \in Z \cup Z_h \\
\beta \|p\|_\Pi & \leq \sup_{v \in V_h} \frac{b(v, p)}{\|v\|_V} \quad \forall p \in \Pi_h.
\end{align*}
\]

(33)

Note the special spaces \( Z \) and \( Z_h \).
The spaces $Z$ and $Z_h$

$Z$ and $Z_h$ are defined by

$$Z = \{ v \in V : b(v, q) = 0 \quad \forall q \in \Pi \}$$  \hspace{1cm} (34)

and

$$Z_h = \{ v \in V_h : b(v, q) = 0 \quad \forall q \in \Pi_h \}$$  \hspace{1cm} (35)

respectively.

$Z$ is the set of divergence free functions in $H^1_0(\Omega)$, and

$$u \in Z \text{ such that } a(u, v) = F(v) \quad \forall v \in Z.$$  

Functions in $Z_h$ are not in general divergence free, but

$$u_h \in Z_h \text{ such that } a(u_h, v) = F(v) \quad \forall v \in Z_h.$$
Thus the variational problem for Stokes appears to be standard in the spaces $Z$ and $Z_h$:

$u_h \in Z_h$ such that $a(u_h, v) = F(v)$ \quad $\forall v \in Z_h$.

But there is a variational crime in general: $Z_h \not\subset Z$.

So there are two things of concern:

- The approximate flow $u_h$ will not necessarily be incompressible, and
- we do not know if $Z_h$ will provide good approximation.
Canonical variational form

The mixed formulation can be posed in the canonical variational form by writing

\[ A((u, p), (v, q)) := a(u, v) + b(v, p) + b(u, q) \]

(36)

\[ F((v, q)) := G(q) + F(v) \]

for all \((v, q) \in V := V \times \Pi\).

This can be solved by direct methods (Gaussian elimination), \textbf{but the system is not positive definite}.

However, other algorithms can be used in special cases, as we discuss subsequently.
The first general spaces used for the Stokes equations (29) were the so-called Taylor-Hood spaces, as follows.

Let $V_h^k$ denote $C^0$ piecewise polynomials of degree $k$ on a triangulation $T_h$ of a polygonal domain $\Omega \subset \mathbb{R}^d$.

Let

$$\tilde{V}_h = \left\{ \mathbf{v} \in (V_h^k)^d : \mathbf{v} = 0 \text{ on } \partial \Omega \right\}$$

and let

$$\Pi_h = \left\{ q \in V_h^{k-1} : \int_\Omega q(x) \, d\mathbf{x} = 0 \right\}.$$
It can be proved that (33) holds in both two and three dimensions under very mild restrictions on the mesh [1].

Note that $Z_h \not\subset Z$ in this case.

The main drawback of Taylor-Hood is that the divergence-free condition can be substantially violated, leading to a loss of mass conservation.

The loss of mass conservation can be avoided if we force the divergence constraint to be satisfied by a penalty method.
Another drawback of Taylor-Hood is that the linear system (36) is bigger and not positive definite. It represents a saddle-point problem.

We will see that an iterated penalty method has a symmetric, positive definite linear system that is well conditioned.

Thus we consider the question of how to force $Z_h \subset Z$ for a general space $V_h$. This can be done by choosing

$$\Pi_h = \nabla \cdot V_h.$$
Comparison of the matrix sizes

Taylor–Hood matrix

\[
\begin{bmatrix}
A & B \\
B^t & 0
\end{bmatrix}
\]

Iterated Penalty matrix

\[
A_\rho
\]
Under mesh restrictions, convergence of velocity can be proved \([8, 7, 6, 4]\)

<table>
<thead>
<tr>
<th>(d)</th>
<th>(k)</th>
<th>inf-sup</th>
<th>mesh restrictions</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
<td>NO</td>
<td>all crossed triangles</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>YES</td>
<td>some crossed triangles required</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>YES</td>
<td>\textbf{new conditions [Guzman, Scott]}</td>
</tr>
<tr>
<td>2</td>
<td>(\geq 4)</td>
<td>YES</td>
<td>no nearly singular vertices</td>
</tr>
<tr>
<td>3</td>
<td>(\geq 6)</td>
<td>YES</td>
<td>only one (T_h) known</td>
</tr>
</tbody>
</table>

Table 2: Mesh restrictions for exact divergence-free piecewise polynomials; \(d=\) dimension of \(\Omega\), \(k=\) degree of polynomials.
Taylor-Hood has no analog for the piecewise linear case.

Malkus crossed triangles show that the inf-sup condition is not necessary for well-posed mixed method.

Approximation by $Z_h$ based on Powell $C^1$ piecewise quadratic element.

We now turn to an algorithm for solving for the velocity and pressure without dealing explicitly with the pressure space $\Pi_h$.

The algorithm is a general optimization technique called the iterated penalty method.
Consider a mixed method for Stokes of the form (31):

\[ a(u_h, v) + b(v, p_h) = F(v) \quad \forall v \in V_h \]

\[ b(u_h, q) = G(q) \quad \forall q \in \Pi_h. \]

Let \( \rho' \in \mathbb{R} \) and \( \rho > 0 \). The iterated penalty method is

\[ a(u^n, v) + \rho (\nabla \cdot u^n, \nabla \cdot v)_{\Pi} = F(v) - (\nabla \cdot v, \nabla \cdot (w^n + \rho \gamma))_{\Pi} \quad \forall v \in V_h \quad (39) \]

\[ w^{n+1} = w^n + \rho' (u^n + \gamma), \]

The pressure is defined by

\[ p_h = P_{\Pi} \nabla \cdot w_h, \quad (40) \]

where \( w_h := w^n \) for terminal value of \( n \).
The convergence properties of (39) follow from [2].

**Theorem 0.1** Suppose that the forms (31) satisfy (32) and (33). for $V_h$ and $\Pi_h = \nabla \cdot V_h$. Then the algorithm (39) converges for any $0 < \rho < 2\rho'$ for $\rho'$ sufficiently large. For the choice $\rho = \rho'$, (39) converges geometrically with a rate given by

$$C_a \left( \frac{1}{\beta} + \frac{C_a}{\alpha \beta} \right)^2 \rho.$$

The following stopping criterion follows from [2].
Theorem 0.2  Suppose that the forms (31) satisfy (32) and (33). for $V_h$ and $\Pi_h = \nabla \cdot V_h$. Then the errors in algorithm (39) can be estimated by

$$\|u^n - u_h\|_V \leq \left( \frac{1}{\beta} + \frac{C_a}{\alpha \beta} \right) \|\nabla \cdot u^n - P_{\Pi} G\|_{\Pi}$$

and

$$\|p^n - p_h\|_{\Pi} \leq \left( \frac{C_a}{\beta} + \frac{C_a^2}{\alpha \beta} + \rho'C_b \right) \|\nabla \cdot u^n - P_{\Pi} G\|_{\Pi}.$$  

When $G(q) = -b(\gamma, q)$, then $P_{\Pi} G = -P_{\Pi} \nabla \cdot \gamma$ and since $\nabla \cdot u^n \in \Pi_h$,

$$\|\nabla \cdot u^n - P_{\Pi} G\|_{\Pi} = \|P_{\Pi} \nabla \cdot (u^n + \gamma)\|_{\Pi} \leq \|\nabla \cdot (u^n + \gamma)\|_{\Pi}.$$  

(41)
The latter norm in (41) is easier to compute, avoiding the need to compute $P_{\Pi} G$.

We formalize this observation in the following result.

**Corollary 0.1**  *Under the conditions of Theorem (0.2) the errors in algorithm (39) can be estimated by*

$$
\| u^n - u_h \|_V \leq \left( \frac{1}{\beta} + \frac{C_a}{\alpha \beta} \right) \| \nabla \cdot (u^n + \gamma) \|_{\Pi}
$$

*and*

$$
\| p^n - p_h \|_{\Pi} \leq \left( \frac{C_a}{\beta} + \frac{C^2_a}{\alpha \beta} + \rho' C_b \right) \| \nabla \cdot (u^n + \gamma) \|_{\Pi}.
$$
Iterated penalty performance

Convergence of $\text{div}(u)$ is independent of mesh size or polynomial degree.

- $(C/r)^n$ with $C = 5$
- $h = 1/2, k = 4$
- $h = 1/16, k = 4$
- $h = 1/16, k = 6$
The iterated penalty code

```python
mesh = UnitSquareMesh(meshsize, meshsize, "crossed")
V = VectorFunctionSpace(mesh, "Lagrange", k)
u = TrialFunction(V)
v = TestFunction(V)
w = Function(V)
a = inner(grad(u), grad(v))*dx + r*div(u)*div(v)*dx
b = -div(w)*div(v)*dx
F = inner(f, v)*dx
u = Function(V)
pde = LinearVariationalProblem(a, F - b, u, bc)
solver = LinearVariationalSolver(pde)
# Scott-Vogelius iterated penalty method
iters = 0; max_iters = 10; div_u_norm = 1
while iters < max_iters and div_u_norm > 1e-10:
    # solve and update w
    solver.solve()
    w.vector().axpy(-r, u.vector())
    # find the L^2 norm of div(u) to check stopping condition
    div_u_norm = sqrt(assemble(div(u)*div(u) * dx(mesh)))
    print "norm(div u)=%.2e"%div_u_norm
    iters += 1
```
We can use FEniCS to test our algorithm. In our experiments, we try to recover an analytical solution of the Stokes equations

\[
\mathbf{u} = \begin{bmatrix}
\sin(4\pi x) \cos(4\pi y) \\
-\cos(4\pi x) \sin(4\pi y)
\end{bmatrix}
\]

\[
p = \pi \cos(4\pi x) \cos(4\pi y)
\]

by applying \( \mathbf{u} \) above as a boundary condition and letting

\[
\mathbf{f} = \begin{bmatrix}
28\pi^2 \sin(4\pi x) \cos(4\pi y) \\
-36\pi^2 \cos(4\pi x) \sin(4\pi y)
\end{bmatrix}.
\]

Next is a complete implementation on the unit square with mesh size \( h = \frac{1}{16} \) and polynomial order \( k = 6 \).
Unified Stokes solution for the pressure (left) and velocity (right);
Divergence comparison: smooth problem

<table>
<thead>
<tr>
<th>$\frac{1}{h}$</th>
<th>$k$</th>
<th>Taylor-Hood</th>
<th>Scott-Vogelius</th>
<th>Unified Stokes</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
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<td>1.86e-01</td>
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<tr>
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<td>6</td>
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<td>3.33e-11</td>
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<tr>
<td>4</td>
<td>4</td>
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<td>3.46e-11</td>
<td>3.30e-11</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
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<td>3.33e-11</td>
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</tr>
<tr>
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<tr>
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<td>6</td>
<td>5.73e-08</td>
<td>3.09e-11</td>
<td>3.07e-11</td>
</tr>
</tbody>
</table>

Table 3: $\| \nabla \cdot u \|_{L^2(\Omega)}$ for varying $h$ and $k$ with 4 iterations of the penalty method for Scott-Vogelius (and therefore also USA)
Divergence comparison: lid problem

<table>
<thead>
<tr>
<th>$\frac{1}{h}$</th>
<th>$k$</th>
<th>Taylor-Hood</th>
<th>$n = 1$</th>
<th>$n = 4$</th>
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<th>$n$</th>
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<tbody>
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<td>4.20e-03</td>
<td>8.10e-09</td>
<td>1.02e-11</td>
<td>6</td>
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<td>4</td>
<td>1.17e-01</td>
<td>4.58e-03</td>
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<tr>
<td>4</td>
<td>5</td>
<td>8.46e-02</td>
<td>4.89e-03</td>
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<td>5.78e-11</td>
<td>7</td>
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<td>5.18e-03</td>
<td>9.70e-08</td>
<td>3.00e-11</td>
<td>7</td>
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<td>5.48e-03</td>
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<td>7.43e-11</td>
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</tr>
<tr>
<td>16</td>
<td>6</td>
<td>1.27e-01</td>
<td>7.05e-03</td>
<td>6.64e-09</td>
<td>2.43e-12</td>
<td>6</td>
</tr>
</tbody>
</table>

Table 4: $\| \nabla \cdot u \|_{L^2(\Omega)}$ for Taylor-Hood and $\| \nabla \cdot u^n \|_{L^2(\Omega)}$ with $n$ iterations of the penalty method for Scott-Vogelius (and USA) for varying $h$ and $k$. 
Numerical results

Max $u$ and $p$ error vs. mesh size after 4 iterations, $k = 6$
The unified Stokes algorithm

Scott-Vogelius: very accurate velocity approximation with exact divergence zero, but pressure approximation is discontinuous.

Taylor-Hood: pressure approximation is continuous but the velocity does not preserve mass.

The unified Stokes algorithm combines the best of these two methods and eliminates the bad features.

Velocity approximation is same as for Scott-Vogelius, but pressure is projected onto the continuous pressure space (38) used in the Taylor-Hood method.
Pressure and velocity errors

$L^2 u$ and $p$ error vs. mesh size after 4 iterations, $k = 6$

- $L^2 p$ error Taylor-Hood
- $L^2 p$ error Scott-Vogelius
- $L^2 p$ error USA

$L^2 u$ error
- $L^2 u$ error Taylor-Hood
- $L^2 u$ error Scott-Vogelius
- $L^2 u$ error USA

mesh size

$1/2, 1/4, 1/8, 1/16$
Scott-Vogelius pressure $p_h = \nabla \cdot w$ for $w \in V_h$, computed via iterated penalty.

Then the unified Stokes pressure $\hat{p}_h$ is defined by

$$ (\hat{p}_h, q)_{L^2(\Omega)} = (\nabla \cdot w, q)_{L^2(\Omega)} \quad \forall q \in \Pi_h. $$

When the inf-sup condition holds independently of the mesh, the unified Stokes pressure $\hat{p}_h$ also satisfies [5]

$$ \|p - \hat{p}_h\|_{L^2(\Omega)} \leq \frac{C}{\beta} \left( \inf_{v \in V_h} \|u - v\|_{H^1(\Omega)} + \inf_{q \in \Pi_h} \|p - q\|_{L^2(\Omega)} \right). $$

**USA code is one line:**

```python
pUS = project(div(w), FunctionSpace(mesh, "Lagrange", uorder-1)
```
Iterated penalty solves well-conditioned, symmetric, positive-definite systems.

This makes Scott-Vogelius faster than Taylor-Hood.

<table>
<thead>
<tr>
<th>$1/h$</th>
<th>$k$</th>
<th>Taylor-Hood</th>
<th>Scott-Vogelius</th>
<th>Unified Stokes</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
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<td>4.33e+00</td>
<td>3.14e+00</td>
<td>3.12e+00</td>
</tr>
</tbody>
</table>

Table 5: Runtimes in seconds for varying mesh size $h$ and polynomial degree $k$ (one solve for Taylor-Hood, four iterations for Scott-Vogelius and unified Stokes).

Unified Stokes faster due to smaller pressure space.
Automated Modeling with FEniCS

- variational formulation provides language for PDEs
- also a basis for PDE theory
- automation allows complicated algorithms to be used
  - sophisticated optimization algorithms give better linear algebra performance
  - merger of NA, CS, OR
References


