Firedrake Notes

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Key Notes to NEVER FORGET

"Integration by Parts"

This comes up constantly in FEM stuff, when expressing problems in variational form. The usual spiel is to say "multiply by a test function v and then integrate by parts", to obtain the desired form. This hides a number of key subtle steps that otherwise look like magic.

First to note is that "integrate by parts" really means "apply (a corollary of) the Divergence Theorem":

Theorem 1.1 (Divergence Theorem)**.** If Ω is a compact subset of $\mathbb{R}^N$ with a piecewise smooth boundary $\partial\Omega = \Gamma$, and if $\boldsymbol{F}$ is a continuously differentiable vevctor field defined on a neighbourhood of Ω then we have:

$$\int_\Omega (\nabla \cdot \boldsymbol{F}) \; d\Omega = \oiint_\Gamma (\boldsymbol{F} \cdot \boldsymbol{n}) \; d\Gamma$$

where $\boldsymbol{n}$ is the outward pointing unit normal field of the boundary Γ.

Corollary 1.1. Replacing $\boldsymbol{F}$ with $\boldsymbol{F}g$ in the theorem, where g is a scalar function, we get:

$$\int_\Omega \boldsymbol{F} \cdot (\nabla g) \; d\Omega + \int_\Omega g(\nabla \cdot \boldsymbol{F}) \; d\Omega = \oiint_\Gamma g\boldsymbol{F} \cdot \boldsymbol{n} \; d\Gamma$$

We can apply this corollary to the LHS (i.e. to the terms involving u) to rewrite it as the sum of a different volume integral and a surface integral, which can often be made to vanish by applying boundary conditions.

Example: Linear Poisson Equation

Let us take an initial easy example of the basic linear Poisson problem:

$$\begin{aligned}(-\Delta u) &= f, \text{ on } \Omega \\ u &= 0, \text{ on } \partial\Omega = \Gamma\end{aligned}$$

We multiply both sides by the test function v and integrate to obtain:

$$\int_\Omega (-\Delta u)v \; d\Omega = \int_\Omega fv \; d\Omega$$

Now we apply the Corollary to the LHS (replacing $\boldsymbol{F}$ with ∇u and g with v) to get:

$$\int_\Omega \nabla u \cdot \nabla v \; d\Omega + \oiint_\Gamma v\nabla u \cdot \boldsymbol{n} \; d\Omega = \int_\Omega (-\Delta u)v \; d\Omega = \int_\Omega fv \; d\Omega$$

The second term in the new LHS is a <u>closed</u> line integral of a grad function and thus equal to the difference of its endpoints, which are the same, hence the term is zero, leaving us with the desired variational form $a(u,v) = L(v)$:

$$\int_\Omega \nabla u \cdot \nabla v \; d\Omega = \int_\Omega fv \; d\Omega$$

Example: Nonlinear Poisson Equation

Let's now look at the following nonlinear Poisson problem:

$$
\begin{aligned}
-\nabla \cdot \big((1+u)\nabla u\big) &= f, \text{ in } \Omega \\
u &= 0, \text{ on } \partial\Omega = \Gamma
\end{aligned}
$$

We multiply by the test function v and integrate both sides:

$$\int_\Omega \Big(-\nabla \cdot \big((1+u)\nabla u\big)\Big) v \; d\Omega = \int_\Omega fv \; d\Omega$$

Again we apply the Corollary to the LHS (replacing $\boldsymbol{F}$ with $\big((1+u)\nabla u\big)$ and g with v) to get:

$$\int_\Omega \big((1+u)\nabla u\big) \cdot \nabla v \; d\Omega + \oiint_\Gamma v\Big(\big((1+u)\nabla u\big)\Big) \cdot \boldsymbol{n} \; d\Gamma = \int_\Omega \Big(-\nabla \cdot \big((1+u)\nabla u\big)\Big) v \; d\Omega = \int_\Omega fv \; d\Omega$$

Looking again at the surface integral term on the new LHS, we recall the initial condition $u = 0$ on Γ and thus this term simplifies to:

$$\oiint_\Gamma v\big(\nabla u \cdot \boldsymbol{n}\big) \; d\Gamma = 0 \qquad \text{(closed line integral of a grad function)}$$

Leaving us with the desired variational form $F(u; v) = 0$:

$$\int_\Omega \big((1+u)\nabla u\big) \cdot \nabla v \; d\Omega = \int_\Omega fv \; d\Omega$$

Solving Navier Stokes in Firedrake

This section is based on material from the Navier Stokes tutorials from [1].

The following is the time-dependent Navier Stokes equation:

$$\rho\Big(\frac{\partial u}{\partial t} + u \cdot \nabla u\Big) = \nabla \cdot \sigma(u,p) + f \tag{1.1}$$

$$\nabla \cdot u = 0 \tag{1.2}$$

where

$$\sigma(u,p) = 2\mu\epsilon(u) - pI,$$

$$\epsilon(u) = \frac{\nabla u + (\nabla u)^T}{2},$$

f is a given force per unit volume.

We could choose to discretize this in time by replacing the time derivative with a difference quotient. There are complications to such a method though, since it has a "saddle-point" structure, and requires particular pre-conditioners and iterative methods to solve properly. Instead, we shall use one example of what is known as a *splitting method*, which essentially 'splits' the above nonlinear problem into numerous easier problems to be solved in sequence.

Time-Dependent Navier Stokes via "Chorin's Method (IPCS)"

We shall use a variant of what is known as *Chorin's Method*. This variant, called IPCS, solves three linear problems per timestep:

P1: We compute a 'tentative velocity' u^* by advancing the momentum equation by a midpoint finite difference scheme in time, but using the previous pressure p^n and linearising the nonlinear convective term using u^n.

P2: We use the tentative velocity u^* to compute the new pressure p^{n+1}.

P3: We use the new pressure p^{n+1} to compute the new velocity u^{n+1}.

Each of these steps has some individual complexity, so we will discuss them in detail:

P1 - Computing the Tentative Velocity

We can express this as a linear variational problem, using the following variational form:

$$\underbrace{\Big\langle \frac{\rho(u^* - u^n)}{\delta t}, v \Big\rangle + \Big\langle \rho u^n \cdot \nabla u^n, v \Big\rangle}_{1\ \&\ 2} + \underbrace{\Big\langle \sigma(u^{n+\frac{1}{2}}, p^n), \epsilon(v) \Big\rangle + \Big\langle p^n n, v \Big\rangle_{\partial\Omega} - \Big\langle \mu \nabla u^{n+\frac{1}{2}} \cdot n, v \Big\rangle_{\partial\Omega}}_{3,\ 4\ \&\ 5} = \Big\langle f^{n+1}, v \Big\rangle \tag{1.3}$$

where

$$u^{n+\frac{1}{2}} = \frac{u^n + u^{n+1}}{2} \text{ (arithmetic mean)}$$

Let's break down this variational form a little to see where each term comes from:

<u>Terms 1 & 2</u> come from the LHS of the first equation in the initial problem. We write $\frac{u^*-u^n}{\delta t}$ for $\frac{\partial u}{\partial t}$ and then just integrate after multiplying by a test function v:

$$\rho\Big(\frac{\partial u}{\partial t} + u\cdot\nabla u\Big) \rightsquigarrow \int_\Omega \frac{\rho(u^* - u^n)}{\delta t} v\ dx + \int_\Omega \rho(u\cdot\nabla u)v\ dx$$

$$= \underbrace{\Big\langle \frac{\rho(u^*-u^n)}{\delta t}, v\Big\rangle}_{1} + \underbrace{\Big\langle \rho u^n\cdot\nabla u^n, v\Big\rangle}_{2}$$

<u>Terms 3, 4 & 5</u> come from the term $\nabla\cdot\sigma(v,p)$ from the RHS of the initial expression. We multiply by v and integrate by parts to obtain:

$$-\int_\Omega (\nabla\cdot\sigma)v\ dx = \int_\Omega \sigma\cdot\nabla v\ dx - \int_{\partial\Omega} v(\sigma\cdot n)\ ds$$

Now expressing in $\langle\ ,\ \rangle$ notation we get:

$$-\Big\langle \nabla\cdot\sigma, v\Big\rangle = \overbrace{\Big\langle \sigma, \nabla v\Big\rangle}^{\substack{=\langle\sigma,\epsilon(v)\rangle\ \because\ \sigma \text{ is sym } \& \\ \epsilon(v) \text{ is sym part of } \nabla v}} - \Big\langle \sigma\cdot n, v\Big\rangle_{\partial\Omega}$$

$$\big(\text{expanding } \sigma\big) = \Big\langle \sigma, \epsilon(v)\Big\rangle + \Big\langle pn - \mu\nabla u\cdot n - \underbrace{\mu(\nabla u)^T\cdot n}_{\star}, v\Big\rangle_{\partial\Omega}$$

$$\left(\substack{\text{assuming } \star = 0 \text{ (see below),} \\ \text{and using } \nabla u = \left(\frac{\partial u_j}{\partial x_i}\right)_{ij} \text{ convention}}\right) = \underbrace{\Big\langle \sigma, \epsilon(v)\Big\rangle}_{3} + \underbrace{\Big\langle pn, v\Big\rangle_{\partial\Omega}}_{4} - \underbrace{\Big\langle \mu\nabla u\cdot n, v\Big\rangle_{\partial\Omega}}_{5}$$

We should avoid passing over $\star$ without remarking on what assumption we are making in allowing it to be zero. If we had been solving a problem with a free boundary we could simply set $\sigma\cdot n = 0$ on the boundary. However we are computing flow through a channel and hence our flow continues at the end into some 'imaginary' further channel or region, so we need to be a little more careful. We therefore make the assertion that "the derivative of the velocity in the direction of the channel is zero at the outflow"[1], which is what (assuming the $\nabla u = \big(\frac{\partial u_j}{\partial x_i}\big)_{ij}$ convention) yields $\star = 0$.

[1] `https://fenicsproject.org/pub/tutorial/html/._ftut1009.html`[1]

P2 - Computing p^{n+1} with the tentative velocity u^*

To compute the new pressure p^{n+1}, we solve the following linear variational problem, wherein q is a scalar-valued test function from the pressure function space:

$$\Big\langle \nabla p^{n+1}, \nabla q \Big\rangle = \Big\langle \nabla p^{n}, \nabla q \Big\rangle - \Delta t^{-1} \Big\langle \nabla \cdot u^*, q \Big\rangle \tag{1.4}$$

Again let's provide some intuition for where this comes from. Let us take the Navier Stokes momentum equation in terms of u^* and p^{n+1} and subtract it from the same equation expressed in terms of u^{n+1} and p^{n+1}:

$$\rho\Big(\frac{u^{n+1} - u^*}{\Delta t} + u^n \cdot \nabla u^n\Big) - \rho\Big(\frac{u^* - u^n}{\Delta t} + u^n \cdot \nabla u^n\Big) = \nabla \cdot \sigma(u^n, p^{n+1}) - \nabla \cdot \sigma(u^n, p^n)$$

which simplifies to:

$$\begin{aligned} \rho\ \frac{u^{n+1} - u^*}{\Delta t} &= \nabla \cdot \sigma(u^n, p^{n+1}) - \nabla \cdot \sigma(u^n, p^n) \\ \text{(by defn of } \sigma) &= \big(\nabla \cdot p^n I\big) - \big(\nabla \cdot p^{n+1} I\big) \\ &= \nabla p^n - \nabla p^{n+1} \end{aligned}$$

and hence yields:

$$\frac{u^{n+1} - u^*}{\Delta t} + \nabla p^{n+1} - \nabla p^n = 0 \tag{1.5}$$

(the ρ vanishes inexplicably because hey, physics!)

If we then take the divergence and require the $\nabla \cdot u^{n+1} = 0$ condition from the second Navier Stokes equation 1.2, we get:

$$\frac{-\nabla \cdot u^*}{\Delta t} + \nabla^2 p^{n+1} - \nabla^2 p^n = 0$$

which is a Poisson problem for p^{n+1}, yielding the variational problem 1.4 we were hoping to arrive at!

P3 - Computing the new velocity u^{n+1} with the new pressure p^{n+1}

Once again we seek a linear variational problem, this time to solve for u^{n+1} using the updated pressure p^{n+1} that we just solved in P2. If we look back at equation 1.5 we see that this provides exactly what we need! Multiplying by a test function v and integrating yields precisely:

$$\left\langle u^{n+1}, v \right\rangle = \left\langle u^{*}, v \right\rangle - \Delta t \left\langle \nabla (p^{n+1} - p^{n}), v \right\rangle \tag{1.6}$$

References

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- https://en.wikipedia.org/wiki/Divergence_theorem
- https://en.wikipedia.org/wiki/Surface_integral
- http://mathinsight.org/gradient_theorem_line_integrals

References

[1] H. P. Langtangen. Solving PDEs in Python: the FEniCS tutorial I. SpringerOpen, 2016.