A goal-oriented error-controlled solver for biomedical flows

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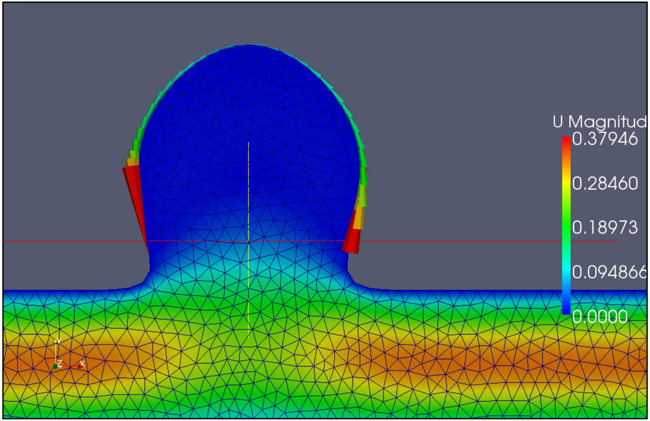
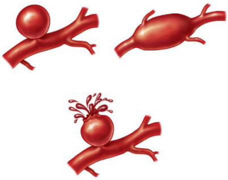


This talk will examine how quantities related to the growth of aneurysms can be accurately computed

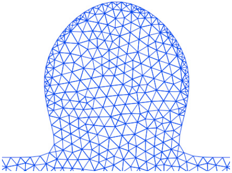


What are aneurysms? What are the quantities implicated in their growth?

Error indicator:

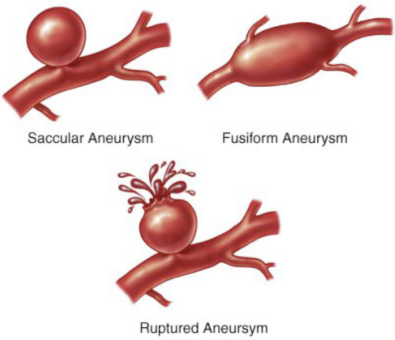
$$
\begin{aligned}
S_{\mathrm{n,t}}\left(\boldsymbol{\sigma}(\boldsymbol{u},p)\right) - S_{\mathrm{n,t}}\left(\boldsymbol{\sigma}(\boldsymbol{u}^h,p^h)\right) \leq\ & \textstyle\sum_K C_1\, h_K\, ||Dw||_K\, ||\underbrace{\mathrm{div}\left(\sigma(u^h,p^h)\right)}_{R_1} \\
& + \textstyle\sum_K C_2\, h_K\, ||Dr||_K\, ||\underbrace{\mathrm{div}(u^h)}_{R_2}||_K \\
& + \textstyle\sum_K C_3\, \sqrt{h_K}\, ||Dw||_{\omega_K}\, ||[\partial_n u_h]||_{\partial K} \\
& + \textstyle\sum_K C_4\, \sqrt{h_K}\, ||Dw||_{\omega_K}\, ||[p_h n]||_{\partial K}
\end{aligned}
$$

How do we control the error in the computation of these quantities?



What does this mean for computational domains?

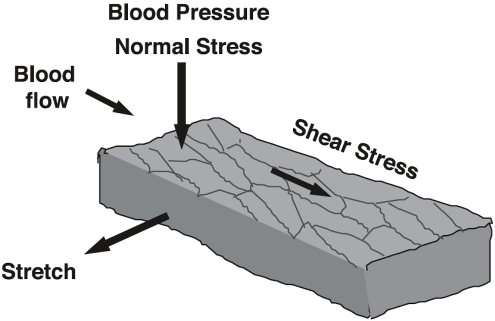
Accurate computation of the fluid shear stress and circumferential stress is of principal importance



- Shear stress drives apoptotic behaviour of muscle cells
- Cells remodel arterial walls under constant tension

[Chien, 2007]

Accurate computation of the fluid shear stress and circumferential stress is of principal importance



- Shear stress drives apoptotic behaviour of muscle cells
- Cells remodel arterial walls under constant tension

[Chien, 2007]

We introduce our quantity of interest as a *goal functional* through an auxiliary problem

- Abstract (linear) *primal* problem in weak form:
  Find $u \in \mathrm{V} : a(u, v) = L(v) \; \forall \; v \in \hat{\mathrm{V}}$

- Finite element discretisation:
  Find $u_h \in \mathrm{V_h} : a(u_h, v) = L(v) \; \forall \; v \in \hat{\mathrm{V}}_\mathrm{h}$

- Let $\mathcal{M}(u)$ be the *goal functional* we are interested in, e.g.,
  - Shear stress on the aneurysm surface
  - Point value of the fluid pressure
  - Outward normal flow across a given area

  We want $\mathcal{M}(u) - \mathcal{M}(u_h) \leq \mathtt{TOL}$

- We introduce the goal functional through the *dual problem*:
  Find $z \in \hat{\mathrm{V}} : a^*(z, v) = \mathcal{M}(v) \; \forall \; v \in \mathrm{V} - \mathrm{V}_h$

[Eriksson and Johnson, 1988 & 1991]

Solution of the dual problem provides information about the error in the goal functional

The error in the goal functional,

$$\begin{aligned}\mathcal{M}(u_h) - \mathcal{M}(u) &= \mathcal{M}(u_h - u) \\ &= a^*(z, u_h - u) \\ &= a(u_h - u, z) \\ &= a(u_h, z) - a(u, z) \\ &= a(u_h, z) - L(z) \\ &= r(z)\end{aligned}$$

is the residual of the dual solution! Furthermore,

$$\begin{aligned}r(z) &= r(z - \Pi_h z) \\ &= (z - \Pi_h z, \hat{r}) \\ &\leq ||Dz||\,||h\,\hat{r}||\end{aligned}$$

[Becker and Rannacher, 2001]

Applying the theory to the steady-state Stokes equations provides estimates of the error

The Stokes equations for fluid flow:

$\operatorname{div}(\boldsymbol{\sigma}(\boldsymbol{u},p)) + \boldsymbol{f} = \boldsymbol{0}$; $\operatorname{div}(\boldsymbol{u}) = 0$,

where $\boldsymbol{\sigma}(\boldsymbol{u},p) = 2\ \mu\ \operatorname{grad}_{\mathrm{s}}(\boldsymbol{u}) - p\ \mathbf{1}$

Rewritten in weak form, find $(\boldsymbol{u},p) \in \mathrm{V}_{\boldsymbol{u}} \times \mathrm{V}_{\mathrm{p}}$:

$a((\boldsymbol{u},p),(\boldsymbol{v},q)) = L((\boldsymbol{v},q))\ \forall\ (\boldsymbol{v},q) \in \hat{\mathrm{V}}_{\boldsymbol{u}} \times \hat{\mathrm{V}}_{p}$,

where $L = (\boldsymbol{v},\boldsymbol{f})$ and

$a = (2\ \mu\ \operatorname{grad}(\boldsymbol{v}), \operatorname{grad}(\boldsymbol{u})) - (\operatorname{div}(\boldsymbol{v}), p) + (q, \operatorname{div}(\boldsymbol{u}))$

Introduce the goal functional, e.g., *shear component* of the traction:

$$\mathcal{M}((\boldsymbol{u},p)) = \int_{\Gamma} (\boldsymbol{\sigma}(\boldsymbol{u},p)\ \boldsymbol{n}) \cdot \boldsymbol{t}\, ds$$

The dual problem: Find $(\boldsymbol{w},r) \in \hat{\mathrm{V}}_{\boldsymbol{u}} \times \hat{\mathrm{V}}_{p}$:

$$a^*((\boldsymbol{w},r),(\boldsymbol{v},q)) = \mathcal{M}((\boldsymbol{v},q))\ \forall\ (\boldsymbol{v},q) \in \tilde{\mathrm{V}}_{\boldsymbol{u}} \times \tilde{\mathrm{V}}_{p}$$

The resulting error indicators:

$$\begin{aligned}
\mathcal{M}(\boldsymbol{\sigma}(\boldsymbol{u},p)) - \mathcal{M}\left(\boldsymbol{\sigma}(\boldsymbol{u}^h,p^h)\right) \quad &\le \textstyle\sum_K C_1\ h_K\ \|D\boldsymbol{w}\|_K\ \|\underbrace{\operatorname{div}\left(\boldsymbol{\sigma}(\boldsymbol{u}^h,p^h)+\boldsymbol{f}\right)}_{R_1}\|_K \\
&+ \textstyle\sum_K C_2\ h_K\ \|Dr\|_K\ \|\underbrace{\operatorname{div}(\boldsymbol{u}^h)}_{R_2}\|_K \\
&+ \textstyle\sum_K C_3\ \sqrt{h_K}\ \|D\boldsymbol{w}\|_{\omega_K}\ \|[\partial_n \boldsymbol{u}_h]\|_{\partial K} \\
&+ \textstyle\sum_K C_4\ \sqrt{h_K}\ \|D\boldsymbol{w}\|_{\omega_K}\ \|[p_h \boldsymbol{n}]\|_{\partial K}
\end{aligned}$$

The finite element scheme is implemented in FEniCS and the error indicators are used to suitably refine the mesh

```
# Define function spaces
V = VectorFunctionSpace(mesh, "CG", 2)
Q = FunctionSpace(mesh, "CG", 1)
W = V + Q

# Define boundary conditions
# bcs = ...

# Define variational problem
(v, q) = TestFunctions(W)
(u, p) = TrialFunctions(W)
f = Constant(mesh, (0, 0, 0))
a = 2*mu*inner(grad(v), grad(u))*dx
    - div(v)*p*dx + q*div(u)*dx
L = inner(v, f)*dx

# Compute solution
problem = VariationalProblem(a, L, bcs)
(u, p) = problem.solve().split()

# Plot solution
plot(u)
plot(p)
```

`while` $||E|| \geq$ `TOL` :

`compute primal solution`

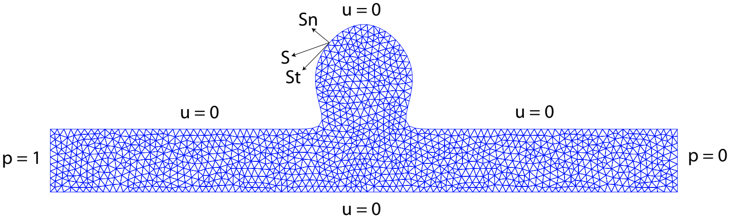
`compute dual solution`

`compute cell-wise error estimators`

`refine mesh where the local error is high`

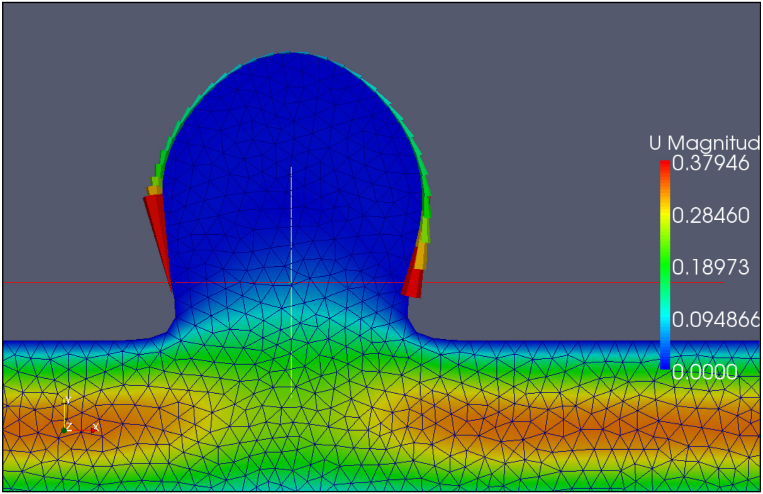
[www.fenics.org]

We return to our aneurysm problem to see what computational meshes our implementation suggests



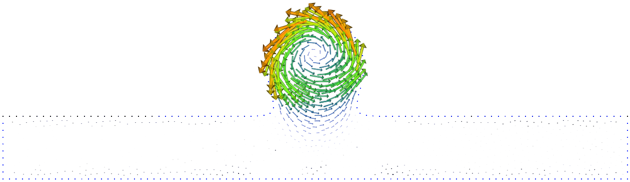
Initial mesh and boundary conditions

We return to our aneurysm problem to see what computational meshes our implementation suggests



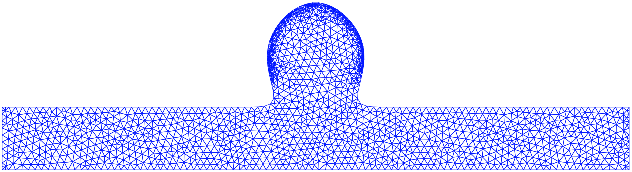
Flow velocity magnitude and shear stresses

We return to our aneurysm problem to see what computational meshes our implementation suggests



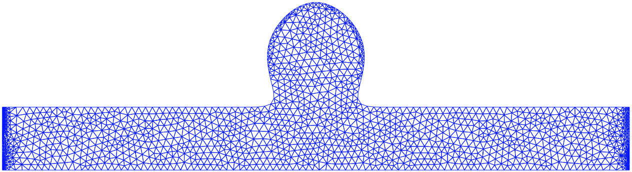
The dual “velocity” field driven by the shear stress

When optimising for the *shear component* of the stress, the mesh is dense near the aneurysm surface



After refining 5% of the cells with the highest local error-indicators 10 times

When optimising for the *normal component* of the stress, the mesh is dense near the pressure boundaries



After refining 5% of the cells with the highest local error-indicators 10 times

The *a posteriori* error analysis can be extended to general non-linear and time-dependent PDEs

- Approximate primal problem in weak form:
  Find $u_h \in \mathrm{V_h} : a(u_h; v) = L(v) \; \forall \; v \in \hat{\mathrm{V}}_h$

- $\mathcal{M}(u)$ is the goal functional we are interested in.
  Recall, we want $\mathcal{M}(u) - \mathcal{M}(u_h) \leq \mathtt{TOL}$

- The linearised dual problem in weak form:
  Find $z \in \hat{\mathrm{V}} : \bar{a'}^*[u, u_h](z, v) = \bar{\mathcal{M}}'[u, u_h](v) \; \forall \; v \in \mathrm{V} - \mathrm{V}_h$

- As before, the error in the goal functional:
  $\mathcal{M}(u_h) - \mathcal{M}(u) = r(z - \Pi_h z) \leq ||Dz|| \, ||h \, \hat{r}||$

[Verfürth, 1993, 1994 & 1991]

Applying the theory to the incompressible Navier-Stokes equations provides insight on controlling the error

The strong form of the Navier-Stokes equations:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\boldsymbol{\nabla} p}{\rho} - \nu \nabla^2 \boldsymbol{u} + (\boldsymbol{\nabla u})\, \boldsymbol{u} = \boldsymbol{f}\,;\; \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

A consistent splitting scheme *(CSS)* in weak form:

Find $(\boldsymbol{u}^{k+1}, p^{k+1}) \in V_u \times V_p$ such that

$$\left(\frac{D\boldsymbol{u}^{k+1}}{\Delta t}, \boldsymbol{v}\right) + \nu(\boldsymbol{\nabla u}^{k+1}, \boldsymbol{\nabla v}) - \left(\frac{p^{\bigstar,k+1}}{\rho}, \nabla \cdot \boldsymbol{v}\right) = (\boldsymbol{g}^{k+1}, \boldsymbol{v}) \quad \forall \boldsymbol{v} \in \hat{V}_u$$

$$\text{where} \quad \boldsymbol{g}^{k+1} = \boldsymbol{f}^{k+1} - ((\boldsymbol{\nabla u})\, \boldsymbol{u})^{\bigstar,k+1}$$

$$(\nabla \phi, \frac{\nabla \psi^{k+1}}{\rho}) = (\nabla \phi, \frac{D\boldsymbol{u}^{k+1}}{\Delta t}) \quad \forall \phi \in \hat{V}_\phi$$

$$(\frac{p^{k+1}}{\rho}, q) = (\frac{p^{\bigstar,k+1}}{\rho} + \frac{\psi^{k+1}}{\rho} - \nu \nabla \cdot \boldsymbol{u}^{k+1}, q) \quad \forall q \in \hat{V}_p$$

[Guermond and Shen, 2003]

Applying the theory to the incompressible Navier-Stokes equations provides insight on controlling the error

The linearised dual problem for Navier-Stokes: Find $(\boldsymbol{w}, r) \in \hat{\mathrm{V}}_{\boldsymbol{u}} \times \hat{\mathrm{V}}_p$:

$$
\begin{aligned}
(\boldsymbol{v}(T), \boldsymbol{\Psi}) + \int_0^T ((\boldsymbol{v}, q), \boldsymbol{\Phi}) \; dt = \; & \int_0^T \left(\frac{\partial \boldsymbol{v}}{\partial t}, \boldsymbol{w} \right) dt + \int_0^T \left(\operatorname{grad}(\boldsymbol{u}_h)\boldsymbol{v} + \operatorname{grad}(\boldsymbol{v})\boldsymbol{u}_h, \boldsymbol{w} \right) dt \\
& - \int_0^T (\nu \; \operatorname{grad}_{\mathrm{s}}(\boldsymbol{v})\boldsymbol{n}, \boldsymbol{w})_N \; dt + \int_0^T (\boldsymbol{\sigma}(\boldsymbol{v}, q), \operatorname{grad}_{\mathrm{s}}(\boldsymbol{w})) \, dt \\
& + \int_0^T (\operatorname{div}(\boldsymbol{v}), r) \, dt, \quad \forall \; (\boldsymbol{v}, q) \in \tilde{\mathrm{V}}_{\boldsymbol{u}} \times \tilde{\mathrm{V}}_p
\end{aligned}
$$

Note here that:

$$
\int_0^T \left(\frac{\partial \boldsymbol{v}}{\partial t}, \boldsymbol{w} \right) dt = - \int_0^T \left(\boldsymbol{v}, \frac{\partial \boldsymbol{w}}{\partial t} \right) dt + (\boldsymbol{v}(T), \cancelto{\boldsymbol{\Psi}}{\boldsymbol{w}(T)}),
$$

which results in a dual problem in $t = [T, 0]$.

The global error estimate now becomes:

$$
\begin{aligned}
\int_0^T (\boldsymbol{e}, \boldsymbol{\Phi}) \, dt &= \int_0^T (\boldsymbol{R}_1, \boldsymbol{w}) \, dt + \int_0^T (R_2, r) \, dt \\
&\leq T \max_{[0,T]} ||h \, \boldsymbol{R}_1|| \; ||D\boldsymbol{w}|| + \int_0^T k \, ||\boldsymbol{R}_1|| \; ||\dot{\boldsymbol{w}}|| \; dt + \int_0^T ||R_2|| \; ||r|| \; dt
\end{aligned}
$$

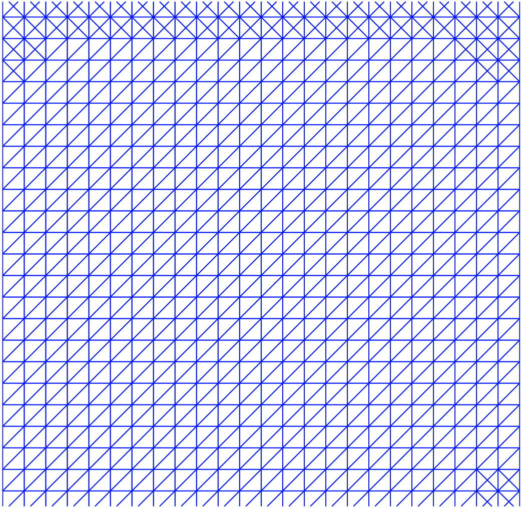
The primal equations describe the flow field

Flow velocity magnitude and direction

The dual equations describe the propagation of information

The dual “velocity” field driven by the shear stress on the top surface

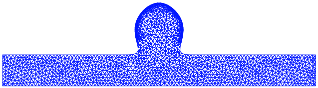
Information from the primal and dual problems are used to determine optimal computational meshes and time steps

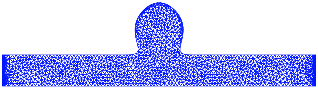


Optimal mesh refinement at the initial time

In conclusion, error control schemes can be used to accurately and efficiently compute quantities of interest

- We have the tools for a posteriori error control for general Navier-Stokes solution schemes (and CSS in particular)
- Optimising for different goals results in significantly different meshes





- For some kinds of flow, inexpensive Stokes calculations can serve as predictors for useful meshes

In conclusion, error control schemes can be used to accurately and efficiently compute quantities of interest

- We are continuing the error analysis to better adapt the mesh and time step sizes
- The implementation is being extended to incorporate all contributions to the error indicators, including jump terms
- We are also working on extensions to flow in realistic 3D domains