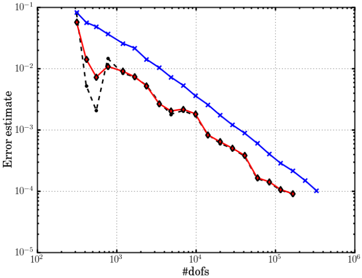
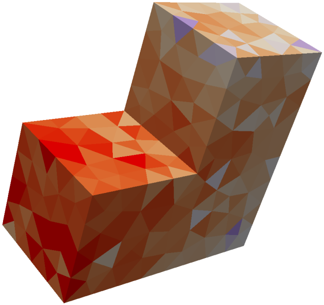
Automated goal-oriented error control for stationary variational problems

Marie E. Rognes and Anders Logg

Simula Research Laboratory





'Automated goal-oriented error control I: stationary variational problems'.

Marie E. Rognes and Anders Logg. In preparation. 2010.

The FEniCS project (www.fenics.org)

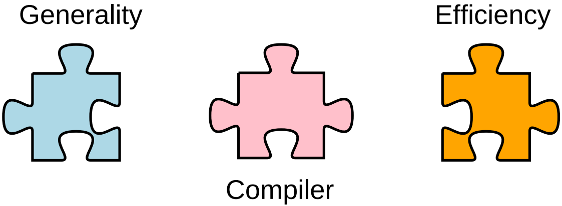
Free Software for Automated Scientific Computing

Agenda

1. Automation of discretization ✓
2. Automation of error control
3. ...

Key components

- High-level form language (UFL)
- Form compiler (FFC)
- Main interface (DOLFIN)



What is automated goal-oriented error control?

Input

- PDE: find $u \in V$ such that $a(v, u) = L(v) \quad \forall\, v \in V$
- Quantity of interest/Goal: $\mathcal{M} : V \to \mathbb{R}$
- Tolerance: $\epsilon > 0$

Challenge

Find $V_h \subset V$ such that $|\mathcal{M}(u) - \mathcal{M}(u_h)| < \epsilon$ where $u_h \in V_h$ is determined by

$$a(v, u_h) = L(v) \quad \forall\, v \in V_h$$

FEniCS/DOLFIN

```
pde = AdaptiveVariationalProblem(a - L, M)
u_h = pde.solve(1.0e-3)
```

The error measured in the goal is the residual of the dual solution

1. Define residual

$$r(v) := L(v) - a(v, u_h)$$

2. Introduce dual problem

$$\text{Find } z \in V\colon \quad a^*(v, z) = \mathcal{M}(v) \quad \forall\, v \in V$$

3. Dual solution + residual $\implies$ error

$$\mathcal{M}(u) - \mathcal{M}(u_h) = L(z) - a(z, u_h) = r(z) = r(z - z_h)$$

4. A good dual approximation $\tilde{z}_h$ gives computable error estimate

$$\eta_h = r(\tilde{z}_h)$$

5. Error indicators ... ?

Let us take Poisson's equation as an example for manual derivation of error indicators

$$a(v,u) = \int_\Omega \nabla v \cdot \nabla u \,\mathrm{d}x \quad L(v) = \int_\Omega v f \,\mathrm{d}x$$

Recall error representation:

$$\mathcal{M}(u) - \mathcal{M}(u_h) = r(z) = \int_\Omega z f - \nabla z \cdot \nabla u_h \,\mathrm{d}x$$

Residual decomposition

$$r(v) = \sum_{T \in \mathcal{T}_h} \int_T v \underbrace{(f + \mathrm{div}\,\nabla u_h)}_{R_T} + \int_{\partial T} v \underbrace{(-\nabla u_h \cdot n)}_{R_{\partial T}} \,\mathrm{d}s$$

Error indicators:

$$\eta_T = |\langle \tilde{z}_h - z_h, R_T \rangle_T + \langle \tilde{z}_h - z_h, [\![R_{\partial T}]\!] \rangle_{\partial T}|$$

The residual decomposition can be automatically computed for a class of residuals

Have: $a - L$ and $u_h \implies r$

Want: $\eta_T = |\langle \tilde{z}_h - z_h, R_T \rangle_T + \langle \tilde{z}_h - z_h, [\![R_{\partial T}]\!] \rangle_{\partial T}|$

Need: Residual decomposition R_T, $R_{\partial T}$ for each cell T

Assumptions

1. $r(v) = \sum_T r_T(v)$
2. $r_T(v) = \int_T v \cdot R_T + \int_{\partial T} v \cdot R_{\partial T}$
3. $R_T \in P_k(T)$, $R_{\partial T}|_e \in P_q(e)$ for some integer k, q

We can compute R_T and $R_{\partial T}$ by solving small local variational problems

Recall assumption:

$$r_T(v) = \int_T v \cdot R_T \, \mathrm{d}x + \int_{\partial T} v \cdot R_{\partial T} \quad \text{with} \quad R_T \in P_k(T)$$

Let

- $b_T : T \to \mathbb{R}$ such that $b_T|_{\partial T} = 0$ (Bubble)
- $\{\phi_i\}_{i=1}^n$ be a basis for $P_k(T)$

Lemma

R_T is uniquely determined by the equations

$$\int_T b_T \phi_i \cdot R_T \, \mathrm{d}x = r_T(b_T \phi_i)$$

$i = 1, \ldots, n$

An improved dual approximation can be computed by higher-order extrapolation

Dual problem

$$a^*(v, z_h) = \mathcal{M}(v) \quad \forall\, v \in V_h$$

can be generated and solved automatically.

Problem

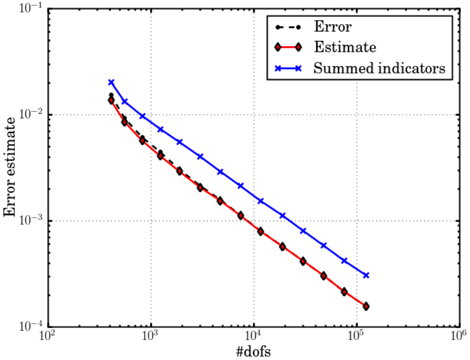
With same discretization as primal: $\eta_h = r(z_h) = 0$.

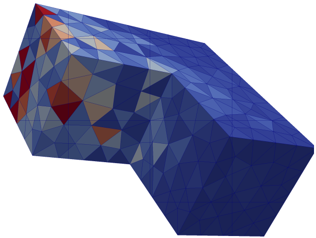
Suggested solution

Let $W_h \supset V_h$. Improve approximation by a patch-based least-squares curve fitting procedure:

$$z_h \mapsto \tilde{z}_h = E_h z_h, \quad E_h : V_h \to W_h$$

The error estimates are virtually perfect for Poisson on a 3D L-shape

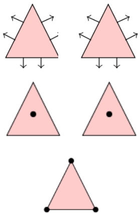


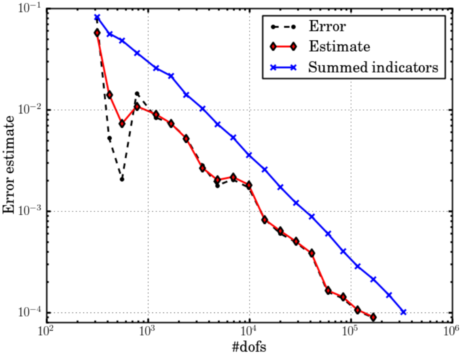


$$a(v, u) = \langle \nabla v, \nabla u \rangle,$$

$$\mathcal{M}(u) = \int_\Gamma u \,\mathrm{d}s, \quad \Gamma \subset \partial\Omega.$$

The error estimates are highly satisfactory for a three-field mixed elasticity formulation also

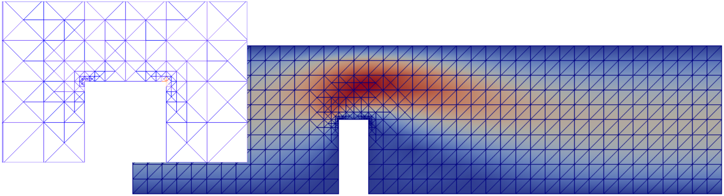




$$a((\tau, v, \eta), (\sigma, u, \gamma)) = \langle \tau, A\sigma \rangle + \langle \operatorname{div} \tau, u \rangle + \langle v, \operatorname{div} \sigma \rangle + \langle \tau, \gamma \rangle + \langle \eta, \sigma \rangle$$

$$\mathcal{M}((\sigma, u, \eta)) = \int_\Gamma g\, \sigma \cdot n \cdot t \,\mathrm{d}s$$

Goal-oriented adaptivity is worth it



$\text{Outflux} \approx 0.4087 \pm 10^{-4}$

Uniform

1.000.000 dofs, > 3 hours

Adaptive

5.200 dofs, 127 seconds

```python
from dolfin import *

class Noslip(SubDomain): ...

mesh = Mesh("channel-with-flap.xml.gz"
V = VectorFunctionSpace(mesh, "CG", 2)
Q = FunctionSpace(mesh, "CG", 1)

# Define test functions and unknown(s)
(v, q) = TestFunctions(V * Q)
w = Function(V * Q)
(u, p) = (as_vector((w[0], w[1])), w[2])

# Define (non-linear) form
n = FacetNormal(mesh)
p0 = Expression("(4.0 - x[0])/4.0")
F = (0.02*inner(grad(v), grad(u)) + inner(v, grad(u)*u))*dx
    - div(v)*p + q*div(u)  + p0*dot(v, n)*ds

# Define goal and pde
M = u[0]*ds(0)
pde = AdaptiveVariationalProblem(F, bcs=[...], M, u=w, ...)

# Compute solution
(u, p) = pde.solve(1.e-4).split()
```