An Introduction to Goal-Oriented Error Estimation

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Outline

1) Introduction

2) Estimation and control of discretization errors in quantities of interest

- Linear problems (adjoint and error representation).
- Extension to nonlinear problems.
- Extension to time-dependent problems: Cahn-Hilliard equations.

3) Conclusions

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Introduction

Error estimation is useful for two purposes:

1. To provide a measure of the accuracy in approximations.
2. To control errors in those approximations (for example via mesh adaptation in the case of finite element solutions).

Error estimates have been constructed with respect to:

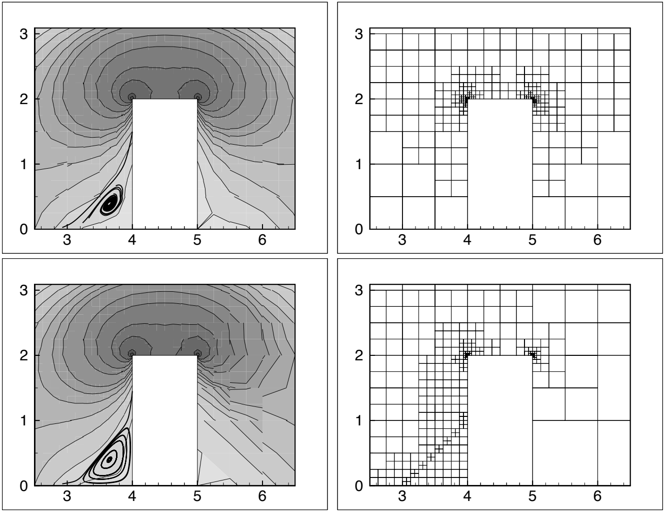
a) Norms associated with the solution function spaces.
b) Quantities of interest $\Rightarrow$ goal-oriented error estimation.

Flow around obstacle (Stokes flow)

Top plots:
Residual-based Error Estimation and adaptivity

Bottom plots:
Goal-Oriented Error Estimation and adaptivity

QoI = averaged vorticity in lower left corner.



Catenary (linearized) model:

$$
\begin{aligned}
-Tu'' &= -\rho g, && \text{in } \Omega = (0,1) \\
u &= u_0, && \text{at } x = 0 \\
u &= u_1, && \text{at } x = 1
\end{aligned}
$$

Exact solution:

$$u(x) = -\frac{\rho g}{2T} x(1-x) + u_0(1-x) + u_1 x$$

Quantity of interest:

Deflection at center point: $Q(u) = u(0.5) = \left[\frac{u_0 + u_1}{2}\right] - \frac{\rho g}{8T}$

Average deflection: $Q(u) = \int_0^1 u(x)dx = \left[\frac{u_0 + u_1}{2}\right] - \frac{\rho g}{12T}$

Slope at origin: $Q(u) = u'(0) = \left[\, u_1 - u_0 \,\right] - \frac{\rho g}{2T}$

Green's function

Suppose that $u_0 = u_1 = 0$, i.e.

$$\begin{aligned} -Tu'' &= -\rho g, \quad \text{in } \Omega = (0,1) \\ u &= 0, \quad \text{at } x = 0 \\ u &= 0, \quad \text{at } x = 1 \end{aligned}$$

Weak formulation:

Given ρg,

Find $u \in V = H_0^1(0,1)$ s.t.

$$B(u,v) = F(v) \quad \forall v \in V$$

where

$$\begin{cases} B(u,v) = \displaystyle\int_0^1 Tu'v'dx \\ F(v) = \displaystyle\int_0^1 -\rho g \, v \, dx \end{cases}$$

Green's function

Let $Q(u) = u(x_0)$.

The Green function is the function $G_0 = G_0(x) \in V$ that satisfies:

$$Q(u) = u(x_0) = \int_0^1 -\rho g \, G_0 \, dx = F(G_0)$$

that is:

$$Q(u) = F(G_0) = B(u, G_0)$$

Note that:

$$Q(u) = u(x_0) = \int_0^1 u(x)\delta(x - x_0)dx$$

Green's function

$$Q(u) = B(u, G_0) = F(G_0)$$

Primal problem:

$$\begin{aligned} -Tu'' &= -\rho g \quad \text{in } (0,1) \\ u &= 0 \quad \text{at } x = 0, 1 \end{aligned}$$

Weak form:

Given ρg, find $u \in V$ s.t.

$$B(u, v) = F(v) \quad \forall v \in V$$

Provide QoI:

$$Q(u) = \int_0^1 u(x)\delta(x - x_0)dx$$

Adjoint problem:

Find $G_0 \in V$ s.t.

$$B(v, G_0) = Q(v) \quad \forall v \in V$$

Strong form:

$$\int_0^1 T v' G_0' dx = \int_0^1 v \delta dx$$

so that

$$\begin{aligned} -TG_0'' &= \delta \quad \text{in } (0,1) \\ G_0 &= 0 \quad \text{at } x = 0, 1 \end{aligned}$$

Generalized Green Function

Abstract linear BVP:

$$\text{Find } u \in V, \quad B(u,v) = F(v), \quad \forall v \in V$$

Quantity of interest:

$$Q(u) = \int_\Omega u(x)k(x)dx$$

Adjoint problem:

$$\text{Find } p \in V, \quad B(v,p) = Q(v), \quad \forall v \in V$$

FE approximation: Let $V^h \subset V$

$$\text{Find } u_h \in V^h, \quad B(u_h,v_h) = F(v_h), \quad \forall v_h \in V^h$$

Error equation:

$$\text{Find } e \in V, \quad B(e,v_h) = \mathcal{R}(u_h;v) \equiv F(v) - B(u_h,v), \quad \forall v \in V$$

Error Representation

Goal is to estimate $\boxed{\mathcal{E} = Q(u) - Q(u_h)}$

$$\begin{aligned}
\mathcal{E} &= B(u,p) - B(u_h,p) && \text{(From adjoint problem)} \\
&= F(p) - B(u_h,p) && \text{(From primal problem)} \\
&= \mathcal{R}(u_h;p) && \text{(From definition of residual)} \\
&= \mathcal{R}(u_h;p-p_h) && \text{(From orthogonality property)}
\end{aligned}$$

$$\begin{aligned}
\mathcal{E} &= Q(u-u_h) = Q(e) && \text{(From linearity of } Q\text{)} \\
&= B(e,p) && \text{(From adjoint problem)} \\
&= \mathcal{B}(e,p-p_h) && \text{(From orthogonality property)} \\
&= \mathcal{R}(u_h;p-p_h) && \text{(From error equation)}
\end{aligned}$$

Adaptive strategies

Let $\tilde{p}$ be a higher-order approximation of the adjoint solution on same mesh as u_h, i.e.

$$\text{Find } \tilde{p} \in V^{h,p+1}, \quad B(v,\tilde{p}) = Q(v), \quad \forall v \in V^{h,p+1}$$

Approach 1: Using only $\tilde{p}$ and $\tilde{p}_h = \Pi^{h,p}\tilde{p}$

$$\mathcal{E} \approx \eta = \mathcal{R}(u_h;\tilde{p}-\tilde{p}_h) = \sum_K \mathcal{R}_K(u_h;\tilde{p}-\tilde{p}_h)$$

Approach 2: Using $\tilde{p}$, but also $\tilde{u} \in V^{h,p+1}$,

$$\mathcal{E} \approx \eta = B(\tilde{u}-u_h,\tilde{p}-\tilde{p}_h) = \sum_K B_K(\tilde{u}-u_h,\tilde{p}-\tilde{p}_h)$$

Strategy favored by Demkowicz et al. in hp-adaptation scheme.

Adaptive Strategies

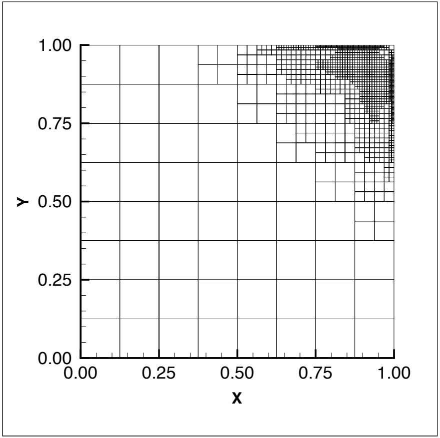
Adaptive scheme (catenary exemple):

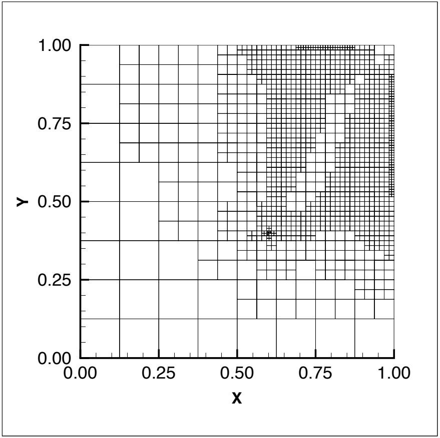
$$\begin{aligned}\eta \approx \mathcal{R}(u_h;\tilde{p}-\tilde{p}_h) &= F(\tilde{p}-\tilde{p}_h) - B(u_h,\tilde{p}-\tilde{p}_h)\\ &= \int_0^1 -\rho g\,(\tilde{p}-\tilde{p}_h)\,dx - \int_0^1 T u_h'\,(\tilde{p}-\tilde{p}_h)'\,dx\\ &= \sum_{K=1}^{N_e}\Big[\int_K -\rho g\,(\tilde{p}-\tilde{p}_h) + T u_h''\,(\tilde{p}-\tilde{p}_h)\,dx - \int_{\partial K} T u_h'(\tilde{p}-\tilde{p}_h)\,ds\Big]\\ &= \sum_{K=1}^{N_e}\underbrace{\Big[\int_K (-\rho g + T u_h'')(\tilde{p}-\tilde{p}_h)\,dx - \sum_{i=1,2}\frac{1}{2}[\![T u_h']\!](\tilde{p}-\tilde{p}_h)|_{x_i^K}\Big]}_{\eta_K}\end{aligned}$$

Refinement criterion:

If $\dfrac{|\eta_K|}{\max_K |\eta_K|} \geq \gamma_{\text{tol}}$, then refine element K

Example: Elliptic problem





Optimal?

Nonlinear Problems

Abstract nonlinear problem:

$$\text{Find } u \in V, \quad B(u; v) = F(v), \quad \forall\, v \in V$$

where V = Banach space and $B(\cdot;\cdot)$ = differentiable semilinear form.
Let $Q(u)$ denote a possibly nonlinear differentiable functional on V.

Linearization (Taylor with exact remainder):

$$B(u + w; v) = B(u; v) + B'(u; w, v) + \Delta_B(u, w, v)$$
$$Q(u + w) = Q(u) + Q'(u; w) + \Delta_Q(u, w)$$

$$\Delta_B(u, w, v) = \int_0^1 B''(u + sw; w, w, v)(1 - s)ds$$
$$\Delta_Q(q, w) = \int_0^1 Q''(u + sw; w, w)(1 - s)ds$$

Secant Form (exact) Representation

$$B(u;v) = B(u_h;v) + \underbrace{\int_0^1 B'(su + (1-s)u_h; e, v)ds}_{\equiv B^s(u,u_h;e,v) = \text{secant form of B}}, \quad \forall v \in V$$

Then

$$\begin{aligned} Q(u) - Q(u_h) = Q(e) &= B^s(u, u_h; e, p) \\ &= B(u;p) - B(u_h;p) \\ &= F(p) - B(u_h;p) \\ &= \mathcal{R}(u_h;p) \end{aligned}$$

where p is the solution of the dual problem:

Find $p \in V$ such that $\quad B^s(u, u_h; v, p) = Q(v), \quad \forall v \in V$

Optimal Approach

Constrained minimization problem*

Find $u \in V$ such that

$$Q(u) = \inf_{v \in M} Q(v)$$

where

$$M = \{v \in V;\ B(v;q) = F(q),\ \forall\, q \in V\}$$

Lagrangian:

$$L(u,p) = Q(u) + F(p) - B(u;p)$$

Here p = influence function (or Lagrange multiplier or adjoint solution) corresponding to the choice Q of the quantity of interest.

*Becker & Rannacher (2001).

Optimal Approach

The critical points (u, p) of $L(\cdot, \cdot)$ satisfy:

$$\boxed{L'((u,p);(v,q)) = 0 \qquad \forall\, (v,q) \in V \times V}$$

$$L'((u,p);(v,q)) = \underbrace{Q'(u;v) - B'(u;v,p)}_{\Rightarrow \text{ adjoint}} + \underbrace{F(q) - B(u;q)}_{\Rightarrow \text{ primal}}$$

where

$$\begin{aligned} B'(u;v,p) &= \lim_{\theta \to 0} \theta^{-1} [B(u + \theta v; p) - B(u;p)] \\ Q'(u;v) &= \lim_{\theta \to 0} \theta^{-1} [Q(u + \theta v) - Q(u)] \end{aligned}$$

Primal and adjoint problems:

$$\boxed{\begin{aligned} & B(u;v) = F(v), && \forall\, q \in V \\ & B'(u;v,p) = Q'(u;v), && \forall\, v \in V \end{aligned}}$$

Optimal Approach

Approximation of primal problem:

$$\text{Find } u_h \in V^h \text{ such that } \quad B(u_h; v_h) = F(v_h) \quad \forall\, v_h \in V^h$$

Approximation of adjoint problem:
Define FE space $\tilde{V}^h$ such that $V^h \subset \tilde{V}^h$. Then

$$\text{Find } \tilde{p}_h \in \tilde{V}^h \text{ such that } \quad B'(u_h; v_h, \tilde{p}_h) = Q'(u_h; v_h), \quad \forall\, v_h \in \tilde{V}^h$$

Error Estimation:
Define residual as before, i.e. $\mathcal{R}(u_h; v) = F(v) - B(u_h; v)$. Then:

$$Q(u) - Q(u_h) = \mathcal{R}(u_h; \tilde{p}_h) + \Delta \approx \mathcal{R}(u_h; \tilde{p}_h)$$

where Δ represents higher-order terms in $u - u_h$ and $p - \tilde{p}_h$.

Optimal Approach

Expression for the remainder Δ:

$$\begin{aligned}\Delta = & \frac{1}{2}\int_0^1 B''(u_h + se; e, e, p_h + s\varepsilon)ds \\ & - \frac{1}{2}\int_0^1 Q''(u_h + se; e, e)ds \\ & - \frac{3}{2}\int_0^1 B''(u_h + se; e, e, \varepsilon)(s-1)sds \\ & - \frac{1}{2}\int_0^1 B'''(u_h + se; e, e, p_h + s\varepsilon)(s-1)sds \\ & + \frac{1}{2}\int_0^1 Q'''(u_h + se; e, e, e)(s-1)sds\end{aligned}$$

Linearization approach: Error Equation, Adjoint problem

Error Equation: Let $e = u - u_h$

$$B(u;v) = B(u_h + e; v) = B(u_h; v) + B'(u_h; e, v) + \Delta_B(u_h, e, v) = F(v)$$

So

$$\text{Find } e \in V, \quad B'(u_h; e, v) + \Delta_B(u_h, e, v) = \mathcal{R}(u_h; v), \quad \forall v \in V$$

Dropping higher-order terms, error can be approximated by:

$$\text{Find } \hat{e} \in V, \quad B'(u_h; \hat{e}, v) = \mathcal{R}(u_h; v), \quad \forall v \in V$$

Adjoint problem:

$$\text{Find } p \in V \text{ such that} \quad B'(u_h; v, p) = Q'(u_h; v), \quad \forall v \in V$$

Linearization approach

Representation of the error:

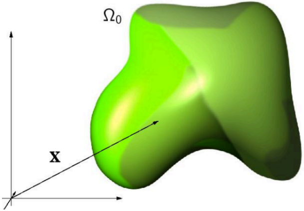
$$
\begin{aligned}
\mathcal{E} = Q(u) - Q(u_h) &= Q'(u_h; e) + \Delta_Q(u_h, e) \\
&= B'(u_h; e, p) + \Delta_Q(u_h, e) \\
&= \mathcal{R}(u_h; p) + \Delta_Q(u_h, e) - \Delta_B(u_h, e, p) \\
&= \underbrace{\mathcal{R}(u_h; p - p_h)}_{\text{Discretization error}} + \underbrace{\Delta_Q(u_h, e) - \Delta_B(u_h, e, p)}_{\text{Linearization error}}
\end{aligned}
$$

with

$$
\boxed{
\begin{aligned}
\Delta_B(u_h, e, p) &= \int_0^1 B''(u_h + se; e, e, p)(1-s)ds \\
\Delta_Q(u_h, e) &= \int_0^1 Q''(u_h + se; e, e)(1-s)ds
\end{aligned}
}
$$

Tumor Growth Model (Cahn-Hilliard)

Mixture theory: diffuse-interface phase-field model

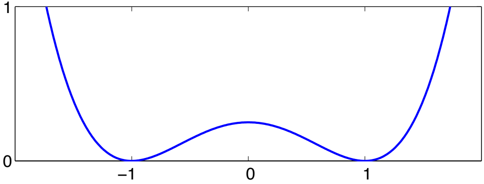


The tumor cell concentration u satisfies

$$\begin{aligned} u_t &= \Delta\mu(u) + g(\sigma, u) && \text{in } \Omega \\ \mu(u) &= f'(u) - \epsilon^2 \Delta u && \text{in } \Omega \\ \partial_n u = \partial_n \mu &= 0 && \text{on } \partial\Omega \\ u(0) &= u_0 && \text{in } \Omega \end{aligned}$$

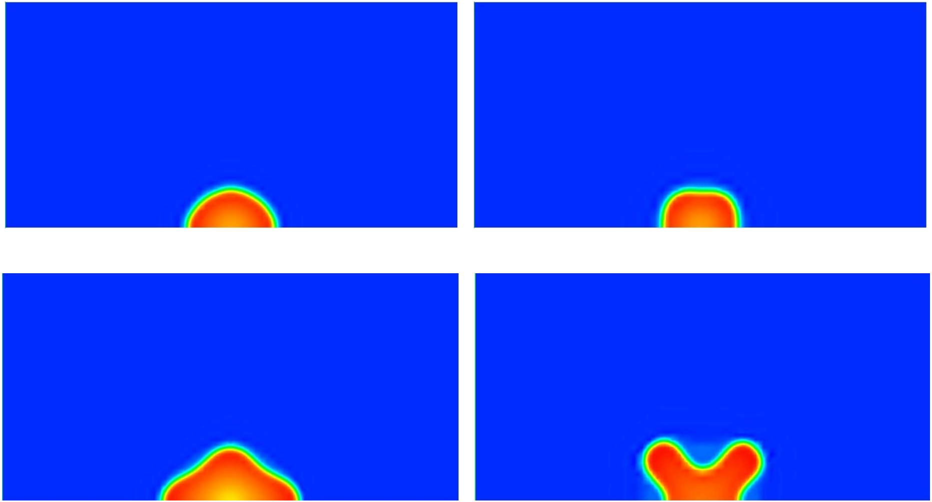
Nonlinear free energy density $f(u)$ drives phase separation

$$f(u) = \frac{1}{4}(u^2 - 1)^2$$

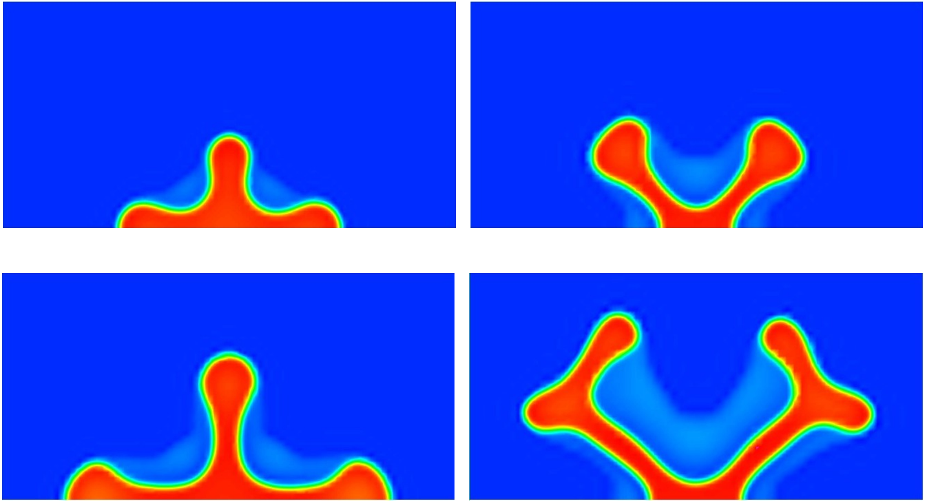


Lowengrub et al., NL (2010), Cristini et al., JMB (2009), Oden et al, M3AS (2010)

Model is sensitive!



Model is sensitive!



Approaches for error estimation

- Ignore $\Delta = \Delta_Q - \Delta_B$. Compute $\tilde{p}$ and $\tilde{p}_h = \Pi^{h,p}\tilde{p}$ such that:

$$\boxed{\text{Find } \tilde{p} \in V^{h,p+1}, \quad B'(u_h; v, \tilde{p}) = Q'(u_h; v), \quad \forall v \in V^{h,p+1}}$$

$$\Rightarrow \eta = \mathcal{R}(u_h; \tilde{p} - \tilde{p}_h)$$

- Estimate Δ:
  - From linear case: $Q(u_h) = F(p_h)$. In nonlinear case, is $Q(u_h) - F(p_h)$ related to Δ?
  - Approximate error e , i.e. $\hat{e}$, using the linearized error equation:

$$\text{Find } \tilde{e} \in V^{h,p+1}, \quad B'(u_h; \tilde{e}, v) = \mathcal{R}(u_h; v), \quad \forall v \in V^{h,p+1}$$

Estimate $\Delta \approx \Delta_Q(u_h, \tilde{e}) - \Delta_B(u_h, \tilde{e}, \tilde{p})$. Relatively cheap but ignores linearization error in error equation.

Approaches for estimation

- Approximate iteratively error $\tilde{e}_i$ from $\tilde{e}_{i-1}$

$$\boxed{\tilde{e}_i \in V^{h,p+1}, \quad B'(u_h + \tilde{e}_{i-1}; v) = \mathcal{R}(u_h + \tilde{e}_{i-1}; v), \quad v \in V^{h,p+1}}$$

- Compute:

$$\Delta_i \approx \Delta_Q(u_h, \tilde{e}_i) - \Delta_B(u_h, \tilde{e}_i, \tilde{p})$$

  or simply:

$$\Delta_i \approx Q(u_h + \tilde{e}_i) - Q(u_h) - \mathcal{R}(u_h; \tilde{p} - \tilde{p}_h)$$

- Stop iterative process if

$$|\mathcal{R}(u_h; \tilde{p} - \tilde{p}_h)| \gg |\Delta_i - \Delta_{i-1}|$$

Mesh adaptivity

- If $|\Delta| \ll |\mathcal{R}(u_h; \tilde{p} - \tilde{p}_h)|$, adapt mesh as usual based on the element-wise contributions to

$$\eta = \mathcal{R}(u_h; \tilde{p} - \tilde{p}_h) = \sum_K \mathcal{R}_K(u_h; \tilde{p} - \tilde{p}_h)$$

- Otherwise, consider

$$\eta = \mathcal{R}(u_h; \tilde{p} - \tilde{p}_h) + \Delta_Q(u_h, \tilde{e}) - \Delta_B(u_h, \tilde{e}, \tilde{p})$$

Note that Δ_Q and Δ_B are integrals defined over the whole domain that can be decomposed into element-wise contributions.

Question: should we refine linearization errors based on Δ_Q and Δ_B or simply on $\|\tilde{e}\|^2$?

1D Example

$$-\nabla \cdot \epsilon(u)\nabla u = f, \qquad \text{in } \Omega = (0,1)$$
$$u = 0, \qquad \text{at } x = 0,1$$

where $\epsilon(u) = 3|u|^2 + \epsilon_0$, with $\epsilon_0 = 10^{-1}$.

Choose f s.t. $u = \sin x$ and Q s.t. $p = x(1-x)$.

Mesh	$\mathcal{R}(u_h;p)/\|e\|$	$\Delta/\|e\|$	$Q(e)/\|e\|$
64	3.4509	−4.4734	−1.0224
128	3.4516	−4.1813	−0.7297
256	3.4518	−4.2736	−0.8218
1024	3.4519	−5.6702	−2.2183
5096	3.4211	−3.8791	−0.4580

$$Q(e) = \mathcal{R}(u_h;p) + \Delta$$

1D Example

$$\epsilon(u) = \frac{1}{\epsilon_0 + a u_x^2}$$

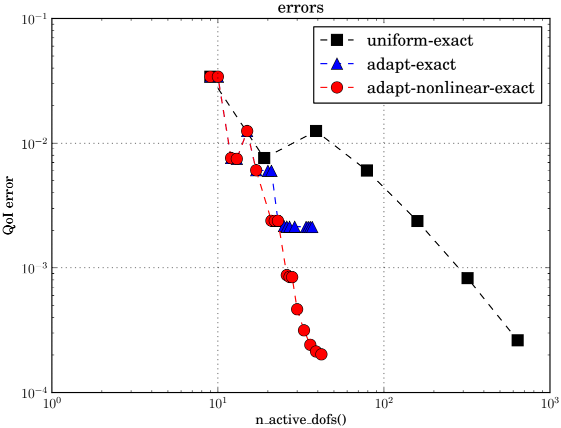
$$\epsilon_0 = 10$$

$$a = 0.001$$

$$Q(u) = |u(x_0)|^\alpha$$

$$x_0 = 0.8$$

$$\alpha = 12$$



$u = (1 - |1 - x|^p)(1 - |x|^q),$ with $p = 100$, $q = 6$

Extension to Time-dependent Problems: Cahn-Hilliard

$$\left.\begin{aligned} u_t &= \Delta\mu \\ \mu &= f'(u) - \epsilon^2 \Delta u \end{aligned}\right\} \quad \text{in } \Omega \text{ + BCs}$$

Weak formulation:

$$\boxed{\text{Find } (u,\mu) \in W_0 \times V \text{ s.t. } \quad \mathcal{B}\big((u,\mu);(v,\eta)\big) = 0 \quad \forall (v,\eta) \in V \times V}$$

$$\mathcal{B}\big(U,V\big) = \int_0^T \Big(\langle u_t, v\rangle + (\nabla\mu, \nabla v)\Big) + \Big((\mu,\eta) - (f'(u),\eta) - \epsilon^2(\nabla u, \nabla\eta)\Big)\, dt$$

$$W_0 = \big\{u \in V;\ u_t \in V^*,\ u(0) = u_0\big\}$$

$$V = L^2(0,T;H^1(\Omega))$$

Adjoint of the Cahn-Hilliard problem

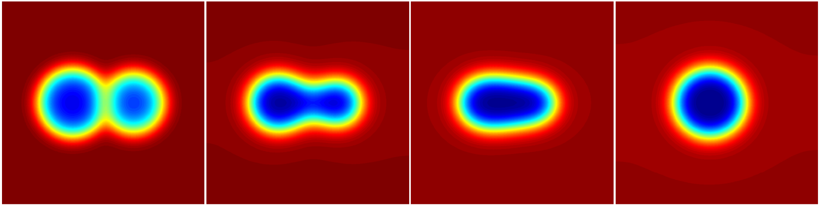
Goal:

$$Q(u, \mu) = \big(k_T, u(T)\big) + \int_0^T \Big((k_u, u) + (k_\mu, \mu) \Big)\, dt$$

Adjoint: (Backward-in-time linearized-adjoint problem)

$$\begin{aligned} -\partial_t p_u + \epsilon^2 \Delta p_\mu - f''(u^h)\, p_\mu &= k_u && \text{in } \Omega \\ p_\mu - \Delta p_u &= k_\mu && \text{in } \Omega \\ p_u(T) &= k_T && \text{(Final condition) + [Natural BCs]} \end{aligned}$$

Example: merging bubbles



Time steps	$Q(u,\mu) - Q(\hat{u},\hat{\mu})$ 64	256	1,024	$\mathrm{Est}(\hat{u},\hat{\mu};\hat{p},\hat{\chi})$ 64	256	1,024	Effectivity 64	256	1,024
Elements 64	-0.01183	-0.02205	-0.02306	-0.26392	-1.78933	-7.76063	22.311	81.162	336.469
256	0.00946	0.01751	0.01982	0.02108	0.12233	0.38726	2.229	6.985	19.537
1,024	0.00199	0.00104	0.00073	0.00322	0.00362	0.00315	1.620	3.484	4.308
4,096	0.00165	0.00049	0.00012	0.00173	0.00077	0.00021	1.045	1.572	1.774
16,384	0.00162	0.00048	0.00011	0.00144	0.00055	0.00013	0.886	1.146	1.159

van der Zee, Oden, Prudhomme, Hawkins, NMPDE 2011

Conclusions

- Goal-oriented error estimation is based on the notion of the adjoint/dual problem.
- The adjoint problem is “straightforwardly” derived from the weak formulation of the primal problem.
- The error in the quantity of interest is represented as the product of the residual by the adjoint solution.
- Error estimates and refinement indicators are obtained by solving for approximations to the adjoint problem.
- Approach is generic!
- Goal-oriented error estimates can be applied to other discretization methods (FD, FV, DGM, spectral methods, meshless methods, etc.).