Exact bounds for functional outputs of parabolic problems: application to the transient convection-diffusion-reaction equation

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Outline of the presentation

- Introduction: certification for PDE's
- Review of output bounds for steady problems
- Bounds for transient problems
  - Model problem: transient convection-reaction-diffusion (discontinuous Galerkin discretization)
  - Bounds guaranteed with respect to space
  - Bounds guaranteed with respect to space and time
- Numerical examples

Objectives

- Engineering decisions are based on approximations of quantities of interest
- Can we trust the results of our simulations?

1. Provide guaranteed upper and lower bounds (for any level of refinement, not just asymptotically)
2. Provide certificates that guarantee the bounds

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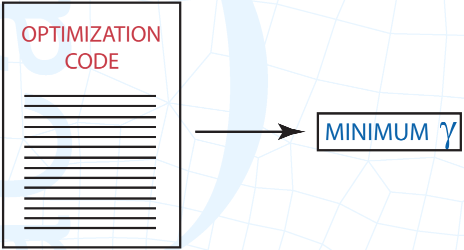
  2. Provide certificates that guarantee the bounds

- "The output lies between the bounds" is guaranteed by a certificate

  - This certificate is a list of numbers (data set)
  - Can be used to prove the correctness of the claim, without access to the original code/method used to compute it

Objectives

Lower bound of a function: $F(x) \geq \gamma, \quad \forall x \in \mathbb{R}$



Objectives

Lower bound of a function: $F(x) \geq \gamma, \quad \forall x \in \mathbb{R}$

OPTIMIZATION CODE

+

SOS CODE

→ MINIMUM γ

+

Polynomials p_i, i=1…m

such that

$$F(x) - \gamma = \sum_{i=1}^{m} p_i^2(x)$$

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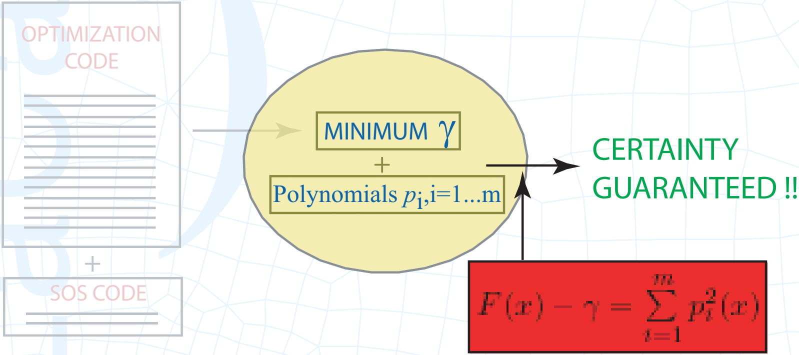

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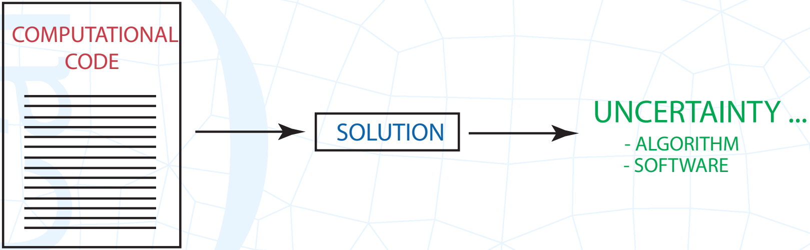
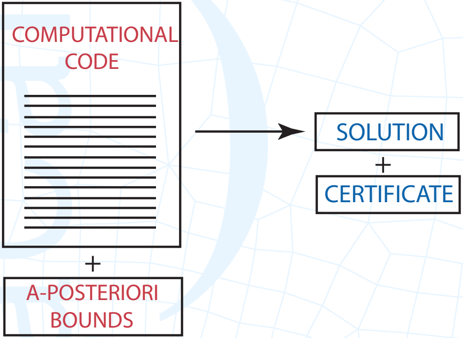

COMPUTATIONAL CODE
SOLUTION
UNCERTAINTY ...
- ALGORITHM
- SOFTWARE

Objectives


COMPUTATIONAL
CODE
+
A-POSTERIORI
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CERTIFICATE

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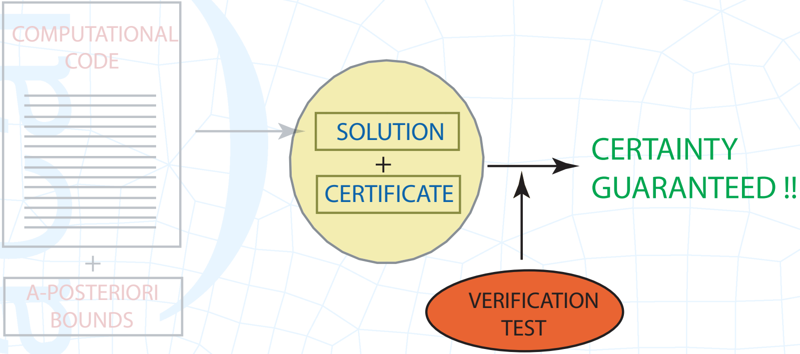
COMPUTATIONAL CODE
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CERTIFICATE
CERTAINTY GUARANTEED !!
VERIFICATION TEST

Objectives

Guaranteed bounds for steady problems:

- scalar equation
  (Sauer-Budge, Bonet, Huerta, Peraire, SINUM 2004)
- linear elasticity
  (Parés, Bonet, Huerta, Peraire, CMAME 2005)
- energy realease rates in linear elasticity (quadratic output)
  (Xuan, Parés, Peraire, CMAME 2005)
- convection-reaction-diffusion equation
  (Sauer-Budge, Peraire, SSC 2004)

Is it possible to obtain bounds for transient convection-reaction-diffusion equation?

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Is it possible to obtain bounds for transient convection-reaction-diffusion equation?

Steady convection-reaction-diffusion

Weak form: find $u \in \mathcal{V}$ such that

$$\underbrace{\int_\Omega \Big(\nu \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v + \sigma u v + (\boldsymbol{a} \cdot \boldsymbol{\nabla} u) v\Big) d\Omega}_{a(u,v)} = \underbrace{\int_\Omega f v d\Omega}_{\ell(v)} \quad \text{for all } v \in \mathcal{V},$$

$a(\cdot,\cdot)$ bilinear coercive *non-symmetric* form.

Output: $\ell^{\mathcal{O}}(u)$, where $\ell^{\mathcal{O}} : \mathcal{V} \to \mathbb{R}$ is a *linear* functional

Finite element approximation: $u_H \in \mathcal{V}^H$

Approximation of the Output: $\ell^{\mathcal{O}}(u_H)$

Goal: find bounds for the error in the output $\qquad e = u - u_H$

$\ell^{\mathcal{O}}(u) - \ell^{\mathcal{O}}(u_H) = \ell^{\mathcal{O}}(e)$

$$s_e^{lb} \leq s := \ell^{\mathcal{O}}(e) \leq s_e^{ub}.$$

Steady convection-reaction-diffusion

Adjoint weak problem: find $\psi \in \mathcal{V}$ such that

$$a(v, \psi) = \ell^{\mathcal{O}}(v) \quad \text{for all } v \in \mathcal{V}.$$

Finite element approximation of the adjoint problem:
$\psi_H \in \mathcal{V}^H$

Adjoint error: $\varepsilon = \psi - \psi_H$

Symmetrization: introduce the symmetric bilinear form

$$a^{\mathrm{s}}(w, v) = \frac{1}{2}\Big(a(w, v) + a(v, w)\Big),$$

where $a^{\mathrm{s}}(w, v) = \int_\Omega \Big(\nu \boldsymbol{\nabla} w \cdot \boldsymbol{\nabla} v + \sigma w v\Big) d\Omega.$

Steady convection-reaction-diffusion

Symmetrized error equations: e^{s} and $\varepsilon^{\mathrm{s}} \in \mathcal{V}$ verifying

$$a^{\mathrm{s}}(e^{\mathrm{s}}, v) = \ell(v) - a(u_H, v) =: R^{\mathrm{P}}(v) \quad \forall v \in \mathcal{V},$$

and

$$a^{\mathrm{s}}(v, \varepsilon^{\mathrm{s}}) = \ell^{\mathcal{O}}(v) - a(v, \psi_H) =: R^{\mathrm{D}}(v) \quad \forall v \in \mathcal{V}.$$

Norm: consider $\|v\|^2 = a^{\mathrm{s}}(v, v) = a(v, v)$

Bounds for the error in the output:

$$-\frac{1}{4}\|\kappa e^{\mathrm{s}} - \frac{1}{\kappa}\varepsilon^{\mathrm{s}}\|^2 \quad \leq \ell^{\mathcal{O}}(e) \leq \frac{1}{4}\|\kappa e^{\mathrm{s}} + \frac{1}{\kappa}\varepsilon^{\mathrm{s}}\|^2$$

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Guaranteed bounds: **using only local computations**
(local complementary energy approach)

Sauer-Budge, Peraire, SSC 2004

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Sketch of the computation of $\boldsymbol{p}_{e^{\mathrm{s}}}, r_{e^{\mathrm{s}}}$

1. Starting point: $a^{\mathrm{s}}(e^{\mathrm{s}}, v) = R^{\mathrm{P}}(v) \quad \forall v \in \mathcal{V} \Longrightarrow \boxed{\|e^{\mathrm{s}}\|^2_{\mathrm{UB}}}$

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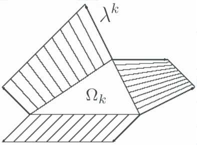
2. Domain decomposition: global problem not affordable / elemental decomposition $\Longrightarrow$ compute equilibrated fluxes

$$a^{\mathrm{s}}_k(e^{\mathrm{s}}_k, v) = R^{\mathrm{P}}_k(v) - \int_{\partial\Omega_k} \tau_k \lambda_k v \, d\Gamma \quad \forall v \in \mathcal{V}(\Omega_k)$$



Hybrid fluxes - unknown local Neumann BC

Solvability - $R^{\mathrm{P}}_k(v) - \int_{\partial\Omega_k} \tau_k \lambda_k v \, d\Gamma$ for $v = 1$

Steady convection-reaction-diffusion

Sketch of the computation of $\boldsymbol{p}_{e^{\rm s}}, r_{e^{\rm s}}$

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$$\int_{\Omega_k} \nu \underbrace{\boldsymbol{\nabla} e^{\mathrm{s}}_k}_{\approx\, \boldsymbol{p}^k_{e^{\mathrm{s}}}} \cdot \boldsymbol{\nabla} v + \sigma \underbrace{e^{\mathrm{s}}_k}_{\approx\, r^k_{e^{\mathrm{s}}}} v \, d\Omega = \int_{\Omega_k} f_k v d\Omega - \int_{\partial\Omega_k} g_k v d\Gamma \quad \forall v \in \mathcal{V}(\Omega_k)$$

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$$\begin{cases} \nu \boldsymbol{\nabla} \cdot \boldsymbol{p}^k_{e^{\mathrm{s}}} + \sigma r^k_{e^{\mathrm{s}}} = f_k & \text{in } \Omega_k \\ \nu \boldsymbol{p}^k_{e^{\mathrm{s}}} \cdot \boldsymbol{n} = g_k & \text{on } \partial\Omega_k \end{cases}$$

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polynomial f_k, g_k — *Sauer-Budge, Peraire, SSC 2004*

general f_k, g_k — *Vejchodský, IMAJNA 2006*

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4. Recover the global UB for $\|e^{\mathrm{s}}\|^2$

$$\|e^{\mathrm{s}}\|^2 \leq \sum_k \|e^{\mathrm{s}}_k\|^2_k \leq \sum_k \int_{\Omega_k} \nu\, \boldsymbol{p}^k_{e^{\mathrm{s}}} \cdot \boldsymbol{p}^k_{e^{\mathrm{s}}} + \sigma(r^k_{e^{\mathrm{s}}})^2 d\Omega$$

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Transient convection-reaction-diffusion

Strong form:

$$\begin{aligned} \dot{u} + \boldsymbol{a}\cdot\boldsymbol{\nabla} u - \boldsymbol{\nabla}\cdot(\nu\boldsymbol{\nabla} u) + \sigma u &= f && \text{in } \Omega\times[0,T] \\ u(\boldsymbol{x},0) &= u_0(\boldsymbol{x}) && \text{for } \boldsymbol{x}\in\Omega \\ \text{(homogeneous) Dirichlet b.c. on } \partial\Omega & && \text{for } t\in[0,T] \end{aligned}$$

Weak form (in space and time): find $u(\boldsymbol{x},t)$, $u\in\mathcal{W}$, s.t.

$$\underbrace{\int_0^T \Big[(\dot{u},v) + a(u,v)\Big]\,\mathrm{d}t + (u^+(0),v^+(0))}_{A(u,v)} = \underbrace{\int_0^T \ell(v)\,\mathrm{d}t + (u_0,v^+(0))}_{L(v)}$$

for $v^{\pm}(t) = \lim_{s\to 0^{\pm}} v(t+s)$.

Transient convection-reaction-diffusion

Time grid: $0 = t^0 < t^1 < \ldots < t^n < \ldots < t^N = T$

Time slabs: $I_n = (t^{n-1}, t^n]$

Functional space (continuous in space, discontinuous in time):

$$\mathcal{W}^{\mathrm{DG}} := \left\{ v(\boldsymbol{x}, t) \;\middle|\; v(\cdot, t) \in \mathcal{V},\, v(\boldsymbol{x}, \cdot)|_{I_n} \in \mathbb{P}_q(I_n) \right\},$$

where $\mathbb{P}_q(I_n)$ are polynomials of degree q in I_n.

DG solution (piecewise-polynomial in time): find $u_{\mathrm{DG}} \in \mathcal{W}^{\mathrm{DG}}$ s.t.

$$A_{\mathrm{DG}}(u_{\mathrm{DG}}, v) := A(u_{\mathrm{DG}}, v) + \sum_{n=1}^{N-1} ([\![u_{\mathrm{DG}}]\!]_n, v^+(t^n)) = L(v) \; \forall v \in \mathcal{W}^{\mathrm{DG}}$$

u_{DG} is discontinuous at $t^n, n = 1 \ldots N-1$.

The time marching decouples every I_n.

Transient convection-reaction-diffusion

Interpolation space cG(p)dG(q): $\mathcal{W}^{\mathrm{DG},H}$

- SPACE: standard continuous FE interpolation of degree p
- TIME: discontinuous Galerkin approximation of degree q

cG(p)dG(q) approximation: find $u_H \in \mathcal{W}^{\mathrm{DG},H}$ s.t.

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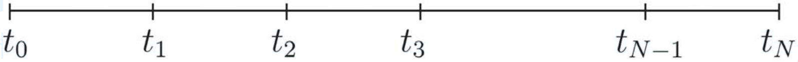

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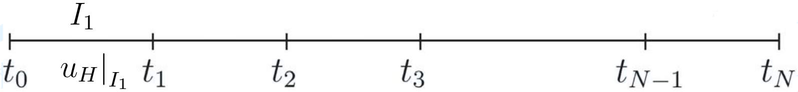

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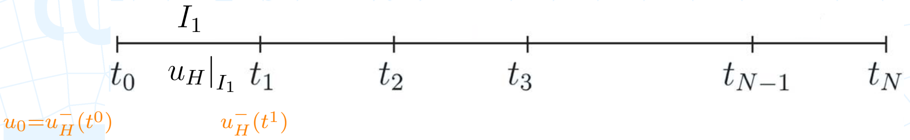

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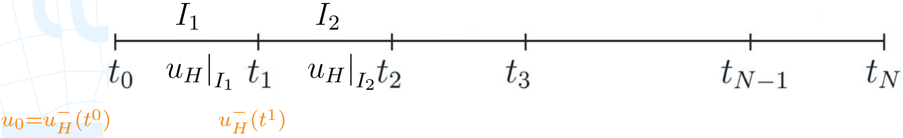


Transient convection-reaction-diffusion

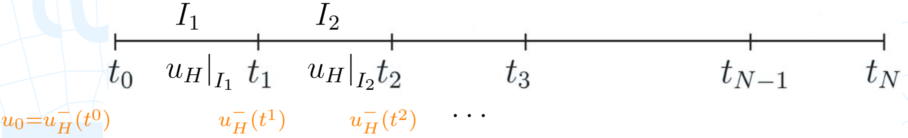
Interpolation space cG(p)dG(q): $\mathcal{W}^{\mathrm{DG},H}$

- SPACE: standard continuous FE interpolation of degree p
- TIME: discontinuous Galerkin approximation of degree q

cG(p)dG(q) approximation: find $u_H \in \mathcal{W}^{\mathrm{DG},H}$ s.t.

$$A_{\mathrm{DG}}(u_H, v) = L(v) \quad \forall v \in \mathcal{W}^{\mathrm{DG},H}.$$

The time marching decouples every I_n:
for $n = 1, \ldots, N$ compute $u_H|_{I_n} \in \mathbb{P}^q(I_n; \mathcal{V}^H)$



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Output of interest:

$$s = L^{\mathcal{O}}(u) = \underbrace{\int_0^T \ell^{\mathcal{O}}(u)\,\mathrm{d}t}_{\text{solution along the time}} + \underbrace{(u_T^{\mathcal{O}}, u(T))}_{\text{solution at the last instant}}$$

FE approximation: $u_H \in \mathcal{W}^{\mathrm{DG},H} \Longrightarrow L^{\mathcal{O}}(u_H)$

GOAL: bound the error in the output $L^{\mathcal{O}}(u) - L^{\mathcal{O}}(u_H) = L^{\mathcal{O}}(e)$

ASSUMPTION: the error introduced by the time discretization can be neglected in front of the error introduced by the mesh, $u_{\mathrm{DG}} \approx u$.

ALTERNATIVE GOAL: bound $L^{\mathcal{O}}(u_{\mathrm{DG}}) - L^{\mathcal{O}}(u_H) = L^{\mathcal{O}}(e_{\mathrm{DG}})$

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Adjoint weak problem: find $\psi_{\mathrm{DG}} \in \mathcal{W}^{\mathrm{DG}}$ such that

$$A_{\mathrm{DG}}(v, \psi_{\mathrm{DG}}) = L^{\mathcal{O}}(v) \quad \text{for all } v \in \mathcal{W}^{\mathrm{DG}}.$$

Finite element approximation: $\psi_H \in \mathcal{W}^{\mathrm{DG},H}$

Adjoint error: $\varepsilon_{\mathrm{DG}} = \psi_{\mathrm{DG}} - \psi_H$

Symmetrization: natural symmetric bilinear form $A^{\mathrm{s}}_{\mathrm{DG}}(w, v)$

$$\int_0^T a^{\mathrm{s}}(w,v)\,\mathrm{d}t + \frac{1}{2}\Big[(w_N^-, v_N^-) + (w_0^+, v_0^+)\Big] + \frac{1}{2}\sum_{n=1}^{N-1} ([\![w]\!]_n, [\![v]\!]_n)$$

yield to non-time-decoupled problems for the estimates.

Alternative symmetrization and associated norm:

$$B^{\mathrm{s}}(w,v) = \int_0^T a^{\mathrm{s}}(w,v)\,\mathrm{d}t \Longrightarrow |||v|||^2 = B^{\mathrm{s}}(v,v) = \int_0^T \|v\|^2\,\mathrm{d}t$$

Transient convection-reaction-diffusion

Symmetrized error equations: $e^{\rm s}_{\rm DG}$ and $\varepsilon^{\rm s}_{\rm DG} \in \mathcal{W}^{\rm DG}$ verifying

$$B^{\rm s}(e^{\rm s}_{\rm DG}, v) = L(v) - A_{\rm DG}(u_H, v) =: R^{\rm P}(v) \; \forall v \in \mathcal{W}^{\rm DG}$$

and

$$B^{\rm s}(\varepsilon^{\rm s}_{\rm DG}, v) = L^{\mathcal{O}}(v) - A_{\rm DG}(v, \psi_H) =: R^{\rm D}(v) \; \forall v \in \mathcal{W}^{\rm DG}$$

Bounds for the error in the output:

$$-\frac{1}{4}\int_0^T \|\kappa e^{\rm s}_{\rm DG} - \frac{1}{\kappa}\varepsilon^{\rm s}_{\rm DG}\|^2 \; dt \leq L^{\mathcal{O}}(e_{\rm DG}) \leq \frac{1}{4}\int_0^T \|\kappa e^{\rm s}_{\rm DG} + \frac{1}{\kappa}\varepsilon^{\rm s}_{\rm DG}\|^2 \; dt$$

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Symmetrized error equations: $e^{\mathrm{s}}_{\mathrm{DG}}$ and $\varepsilon^{\mathrm{s}}_{\mathrm{DG}} \in \mathcal{W}^{\mathrm{DG}}$ verifying

$$B^{\mathrm{s}}(e^{\mathrm{s}}_{\mathrm{DG}}, v) = L(v) - A_{\mathrm{DG}}(u_H, v) =: R^{\mathrm{P}}(v) \; \forall v \in \mathcal{W}^{\mathrm{DG}}$$

and

$$B^{\mathrm{s}}(\varepsilon^{\mathrm{s}}_{\mathrm{DG}}, v) = L^{\mathcal{O}}(v) - A_{\mathrm{DG}}(v, \psi_H) =: R^{\mathrm{D}}(v) \; \forall v \in \mathcal{W}^{\mathrm{DG}}$$

Bounds for the error in the output:

$$-\frac{1}{4}\int_0^T \|\kappa e^{\mathrm{s}}_{\mathrm{DG}} - \frac{1}{\kappa}\varepsilon^{\mathrm{s}}_{\mathrm{DG}}\|^2_{\mathrm{UB}} dt \leq L^{\mathcal{O}}(e_{\mathrm{DG}}) \leq \frac{1}{4}\int_0^T \|\kappa e^{\mathrm{s}}_{\mathrm{DG}} + \frac{1}{\kappa}\varepsilon^{\mathrm{s}}_{\mathrm{DG}}\|^2_{\mathrm{UB}} dt$$

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Symmetrized error equations: $e^{\rm s}_{\rm DG}$ and $\varepsilon^{\rm s}_{\rm DG} \in \mathcal{W}^{\rm DG}$ verifying

$$B^{\rm s}(e^{\rm s}_{\rm DG}, v) = L(v) - A_{\rm DG}(u_H, v) =: R^{\rm P}(v)\ \forall v \in \mathcal{W}^{\rm DG} \longrightarrow \boldsymbol{p}_{e^{\rm s}_{\rm DG}}(t)$$

and

$$B^{\rm s}(\varepsilon^{\rm s}_{\rm DG}, v) = L^{\mathcal{O}}(v) - A_{\rm DG}(v, \psi_H) =: R^{\rm D}(v)\ \forall v \in \mathcal{W}^{\rm DG} \longrightarrow \boldsymbol{p}_{\varepsilon^{\rm s}_{\rm DG}}(t)$$

Bounds for the error in the output:

$$-\frac{1}{4}\int_0^T \|\kappa e^{\rm s}_{\rm DG} - \frac{1}{\kappa}\varepsilon^{\rm s}_{\rm DG}\|^2_{\rm UB} dt \le L^{\mathcal{O}}(e_{\rm DG}) \le \frac{1}{4}\int_0^T \|\kappa e^{\rm s}_{\rm DG} + \frac{1}{\kappa}\varepsilon^{\rm s}_{\rm DG}\|^2_{\rm UB} dt$$

$\boldsymbol{p}_{e^{\rm s}_{\rm DG}}(t)$ and $\boldsymbol{p}_{\varepsilon^{\rm s}_{\rm DG}}(t)$ are computed applying $q+1$ times the steady approach in each slab I_n

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Transient convection-reaction-diffusion

Steps to compute the bounds:

- Loop forward in time: For each $I_n, n = 1 \ldots N$
  - compute and store $u_H|_{I_n}$
- Loop backward in time: For each $I_n, n = N \ldots 1$
  - compute $\psi_H|_{I_n}$
  - apply $q+1$ times the error estimation technique for steady problems to compute $\boldsymbol{p}_{e^{\mathrm{s}}_{\mathrm{DG}}}(t)\Big|_{I_n}$ and $\boldsymbol{p}_{\varepsilon^{\mathrm{s}}_{\mathrm{DG}}}(t)\Big|_{I_n}$
- Compute the bounds for $L^{\mathcal{O}}(e_{\mathrm{DG}})$

$$-\frac{1}{4}\int_0^T \|\kappa \boldsymbol{p}_{e^{\mathrm{s}}_{\mathrm{DG}}} - \frac{1}{\kappa}\boldsymbol{p}_{\varepsilon^{\mathrm{s}}_{\mathrm{DG}}}\|^2 dt \leq L^{\mathcal{O}}(e_{\mathrm{DG}}) \leq \frac{1}{4}\int_0^T \|\kappa \boldsymbol{p}_{e^{\mathrm{s}}_{\mathrm{DG}}} + \frac{1}{\kappa}\boldsymbol{p}_{\varepsilon^{\mathrm{s}}_{\mathrm{DG}}}\|^2 dt$$

Transient convection-reaction-diffusion

Goal: compute an interval of certainty

$$L^{\mathcal{O}}(u) \in [s^{lb}, s^{ub}]$$

and provide certificates that prove the correctness of the claim.

Computation of the bounds:

- compute an approximation of u, u^* $\Longrightarrow$ $L^{\mathcal{O}}(u^*) \approx s$
- compute bounds for $s - L^{\mathcal{O}}(u^*) = L^{\mathcal{O}}(e)$

$$s_e^{lb} \leq L^{\mathcal{O}}(e) \leq s_e^{ub} \Longrightarrow L^{\mathcal{O}}(u^*) + s_e^{lb} \leq s \leq L^{\mathcal{O}}(u^*) + s_e^{ub}$$

Approximation of u $\longrightarrow$ discontinuous Galerkin discretization

Transient convection-reaction-diffusion

Two choices:

	ADVANTAGE	DISADVANTAGE
▶ take $u^* = u_H$ discont. in time	natural choice galerkin orthogonality	no strict bounds (only w.r.t. space)
▶ take $u^* = u_H^{\mathrm{sm}}$ cont. in time	choice of u_H^{sm} loss of orthogonality	strict bounds w.r.t. space and time

Transient convection-reaction-diffusion

Symmetrized error equations: $e^{\rm s}$ and $\varepsilon^{\rm s} \in \mathcal{W}$ verifying

$$B^{\rm s}(e^{\rm s}, v) = L(v) - A_{\rm DG}(u_H^{\rm sm}, v) =: R^{\rm P}(v) \quad \forall v \in \mathcal{W}$$

and

$$B^{\rm s}(\varepsilon^{\rm s}, v) = L^{\mathcal{O}}(v) - A_{\rm DG}(v, \psi_H^{\rm sm}) =: R^{\rm D}(v) \quad \forall v \in \mathcal{W}$$

Bounds for the error in the output:

$$-\frac{1}{4}\int_0^T \|\kappa e^{\rm s} - \frac{1}{\kappa}\varepsilon^{\rm s}\|^2 \;\; dt \leq L^{\mathcal{O}}(e) - R^{\rm P}(\psi_H^{\rm sm}) \leq \frac{1}{4}\int_0^T \|\kappa e^{\rm s} + \frac{1}{\kappa}\varepsilon^{\rm s}\|^2 \;\; d$$

Transient convection-reaction-diffusion

Symmetrized error equations: e^{s} and $\varepsilon^{\mathrm{s}} \in \mathcal{W}$ verifying

$$B^{\mathrm{s}}(e^{\mathrm{s}}, v) = L(v) - A_{\mathrm{DG}}(u_H^{\mathrm{sm}}, v) =: R^{\mathrm{P}}(v) \quad \forall v \in \mathcal{W} \longrightarrow \boldsymbol{p}_{e^{\mathrm{s}}}(t)$$

and

$$B^{\mathrm{s}}(\varepsilon^{\mathrm{s}}, v) = L^{\mathcal{O}}(v) - A_{\mathrm{DG}}(v, \psi_H^{\mathrm{sm}}) =: R^{\mathrm{D}}(v) \quad \forall v \in \mathcal{W} \longrightarrow \boldsymbol{p}_{\varepsilon^{\mathrm{s}}}(t)$$

Bounds for the error in the output:

$$-\frac{1}{4}\int_0^T \|\kappa e^{\mathrm{s}} - \frac{1}{\kappa}\varepsilon^{\mathrm{s}}\|_{\mathrm{UB}}^2 dt \leq L^{\mathcal{O}}(e) - R^{\mathrm{P}}(\psi_H^{\mathrm{sm}}) \leq \frac{1}{4}\int_0^T \|\kappa e^{\mathrm{s}} + \frac{1}{\kappa}\varepsilon^{\mathrm{s}}\|_{\mathrm{UB}}^2 d$$

$\boldsymbol{p}_{e^{\mathrm{s}}}(t)$ and $\boldsymbol{p}_{\varepsilon^{\mathrm{s}}}(t)$ are computed applying $q+1$ times the steady approach in each slab I_n

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Symmetrized error equations: e^{s} and $\varepsilon^{\mathrm{s}} \in \mathcal{W}$ verifying

$$B^{\mathrm{s}}(e^{\mathrm{s}}, v) = L(v) - A_{\mathrm{DG}}(u_H^{\mathrm{sm}}, v) =: R^{\mathrm{P}}(v) \quad \forall v \in \mathcal{W} \longrightarrow \boldsymbol{p}_{e^{\mathrm{s}}}(t)$$

and

$$B^{\mathrm{s}}(\varepsilon^{\mathrm{s}}, v) = L^{\mathcal{O}}(v) - A_{\mathrm{DG}}(v, \psi_H^{\mathrm{sm}}) =: R^{\mathrm{D}}(v) \quad \forall v \in \mathcal{W} \longrightarrow \boldsymbol{p}_{\varepsilon^{\mathrm{s}}}(t)$$

Bounds for the error in the output:

$$-\frac{1}{4}\int_0^T \|\kappa e^{\mathrm{s}} - \frac{1}{\kappa}\varepsilon^{\mathrm{s}}\|^2_{\mathrm{UB}} dt \leq L^{\mathcal{O}}(e) - R^{\mathrm{P}}(\psi_H^{\mathrm{sm}}) \leq \frac{1}{4}\int_0^T \|\kappa e^{\mathrm{s}} + \frac{1}{\kappa}\varepsilon^{\mathrm{s}}\|^2_{\mathrm{UB}} d$$

$\boldsymbol{p}_{e^{\mathrm{s}}}(t)$ and $\boldsymbol{p}_{\varepsilon^{\mathrm{s}}}(t)$ are computed applying $q+1$ times the steady approach in each slab I_n

EXTRA COST: recovery of the orthogonality of the residual (solve a global problem on the coarse mesh $\mathcal{V}^H$)

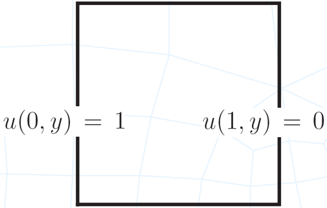
Numerical examples

$$\frac{\partial u}{\partial t} - \Delta u + \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} u + u = 0$$

$$u(x,y,0) = 1 - x$$

$$\boldsymbol{\alpha} = (\alpha, 0) \quad T = 1$$

$$L^{\mathcal{O}}(u) = \int_0^T \int_\Omega u(x,y,t)\, \mathrm{d}\Omega\, \mathrm{d}t$$



NOTATION:

Lower bound: s^{lb}

Upper bound: s^{ub}

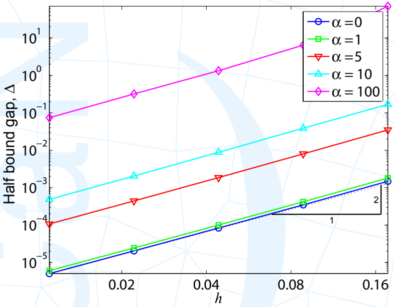
Bound average: $s^{\text{ave}} := (s^{ub} + s^{lb})/2$

Half bound gap: $\Delta = (s^{ub} - s^{lb})/2$

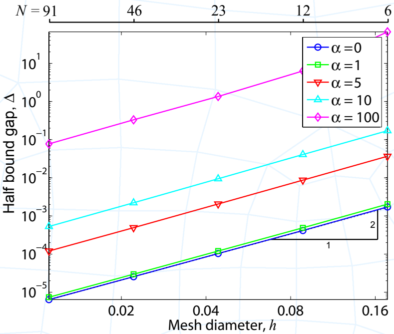
$$L^{\mathcal{O}}(u) \in [s^{lb}, s^{ub}]$$

$$|L^{\mathcal{O}}(u) - s^{\text{ave}}| \leq \Delta$$

Numerical examples



$N = 20$



$\Delta t \propto h$

- the bounds deteriorate as the convection parameter is increased
- the bounds taking into account the error in time do not properly converge if the time step is not adjusted

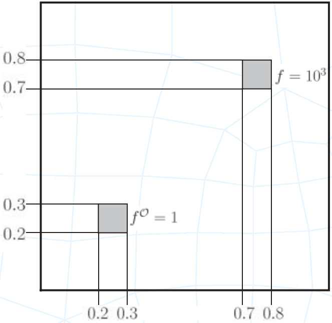
Numerical examples

$$\frac{\partial u}{\partial t} - \Delta u + \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} u + 10u = f$$

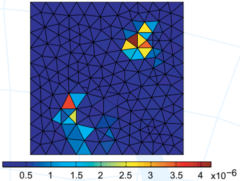
Dirichlet homogeneous BC

$$\boldsymbol{\alpha} = 250(y - 0.5)(0.5 - x)$$

$$L^{\mathcal{O}}(u) = \int_0^T \int_{[0,1]^2} f^{\mathcal{O}} u \, \mathrm{d}\Omega \, \mathrm{d}t$$

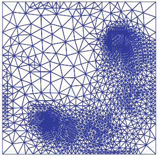


Numerical examples



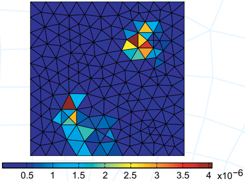
$$L^{\mathcal{O}}(u_{\mathrm{DG}}) = (3.769 \pm 7.747) \cdot 10^{-5}$$

$$n_{\mathrm{el}} = 322, N = 30$$



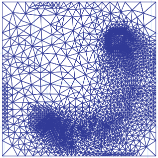
$$(3.795 \pm 0.715) \cdot 10^{-5}$$

$$n_{\mathrm{el}} = 4238, N = 30$$



$$L^{\mathcal{O}}(u) = (3.773 \pm 9.4545) \cdot 10^{-5}$$

$$n_{\mathrm{el}} = 322, N = 6$$

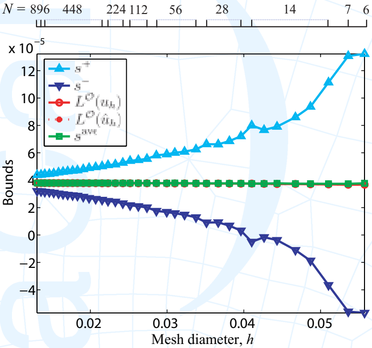


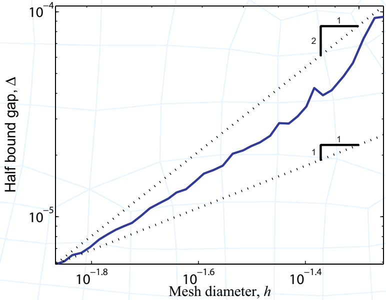
$$(3.796 \pm 0.587) \cdot 10^{-5}$$

$$n_{\mathrm{el}} = 5855, N = 896$$

Numerical examples

Strict bounds and its convergence





Conclusions

Summary

- upper and lower bounds for outputs of transient problems guaranteed in space (asymptotic in time)
- upper and lower bounds for outputs of transient problems guaranteed in space and time
- local indicators for adaptivity for both cases
- the local indicators may be also used to derive adaptive strategies that use time-dependent meshes – different in each time slab – and also to adapt the time spacing

References

Parés, Díez, Huerta, CMAME - PART I (accepted)
Parés, Díez, Huerta, CMAME - PART II (accepted)