

A posteriori error estimation based on potential and flux reconstruction for the heat equation: a unified framework

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Outline

- 1 Introduction
- 2 Setting
 - Continuous setting
 - Discrete setting
- 3 A posteriori error estimates and their efficiency
 - Potential and flux reconstructions
 - A posteriori error estimates
 - Efficiency
- 4 Applications to different numerical methods
 - Discontinuous Galerkin
 - Cell-centered finite volumes
 - Mixed finite elements
 - Vertex-centered finite volumes
 - Face-centered finite volumes
- 5 Numerical experiments
- 6 Conclusions and future work

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What an a posteriori error estimate should fulfill

Guaranteed upper bound (global error upper bound)

- $\|u - u_h\|_{\Omega \times (0, T)}^2 \leq \sum_{n=1}^N \tau^n \sum_{T \in \mathcal{T}^n} \eta_T^n(u_h)^2$
- no undetermined constant: **error control**

Asymptotic exactness

- $\sum_{n=1}^N \tau^n \sum_{T \in \mathcal{T}^n} \eta_T^n(u_h)^2 / \|u - u_h\|_{\Omega \times (0, T)}^2 \rightarrow 1$
- **overestimation factor goes to one** with meshes size

Local efficiency (local error lower bound)

- $\tau^n \eta_T^n(u_h)^2 \leq (C_{\text{eff}, T}^n)^2 \sum_{T' \text{ close to } T} \|u - u_h\|_{T' \times (t^{n-1}, t^n)}^2$
- necessary for **optimal space–time mesh refinement**

Robustness

- $C_{\text{eff}, T}^n$ independent of data, domain, **final time**, meshes, or solution

Negligible evaluation cost

- estimators can be evaluated **locally in space and time**

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Previous results

Continuous finite elements

- Bieterman and Babuška (1982), introduction
- Picasso (1998), no derefinement allowed
- Babuška, Feistauer, and Šolín (2001), continuous-in-time discretization
- Strouboulis, Babuška, and Datta (2003), guaranteed estimates
- Verfürth (2003), efficiency, robustness with respect to the final time
- Makridakis and Nochetto (2003), elliptic reconstruction
- Bergam, Bernardi, and Mghazli (2005), efficiency (not optimal)
- Lakkis and Makridakis (2006), elliptic reconstruction

Previous results

Finite volumes

- Ohlberger (2001), non energy norm estimates
- Amara, Nadau, and Trujillo (2004), energy-norm estimates

Discontinuous Galerkin finite elements

- Sun and Wheeler (2005, 2006), non energy norm estimates
- Georgoulis and Lakkis (2009)

Nonconforming finite elements

- Nicaise and Soualem (2005)

Mixed finite elements

- Cascón, Ferragut, and Asensio (2006)

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The heat equation

The heat equation

$$\begin{aligned}\partial_t u - \Delta u &= f && \text{a.e. in } Q := \Omega \times (0, T), \\ u &= 0 && \text{a.e. on } \partial\Omega \times (0, T), \\ u(\cdot, 0) &= u_0 && \text{a.e. in } \Omega\end{aligned}$$

Assumptions

- $\Omega \subset \mathbb{R}^d$, $d \geq 2$, is a polygonal domain
- $T > 0$ is the final simulation time

Spaces

- $X := L^2(0, T; H_0^1(\Omega))$
- $X' = L^2(0, T, H^{-1}(\Omega))$
- $Y := \{y \in X; \partial_t y \in X'\}$

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The heat equation

Norms

- **energy norm** $\|y\|_X^2 := \int_0^T \|\nabla y\|^2(t) dt$
- **dual norm** $\|y\|_Y := \|y\|_X + \|\partial_t y\|_{X'}$
 $\|\partial_t y\|_{X'} = \left\{ \int_0^T \|\partial_t y\|_{H^{-1}}^2(t) dt \right\}^{1/2}$

Weak solution

Find $u \in Y$ such that, for a.e. $t \in (0, T)$ and for all $v \in H_0^1(\Omega)$,

$$\langle \partial_t u, v \rangle(t) + (\nabla u, \nabla v)(t) = (f, v)(t)$$

The heat equation

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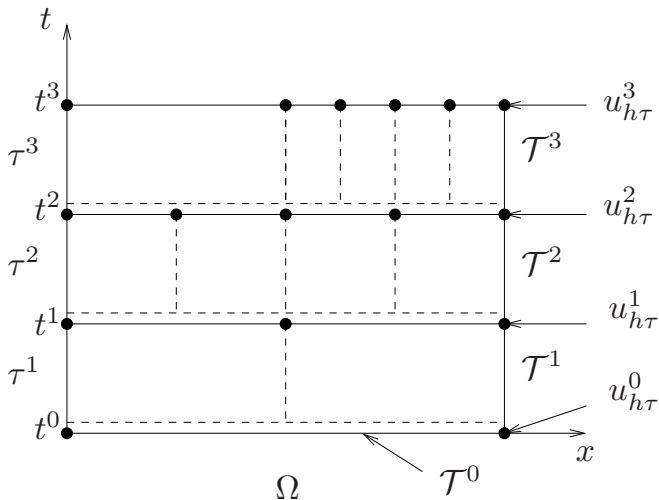
Time-dependent meshes and discrete solutions

Approximate solutions

- discrete times $\{t^n\}_{0 \leq n \leq N}$, $t^0 = 0$ and $t^N = T$
- $I_n := (t^{n-1}, t^n]$, $\tau^n := t^n - t^{n-1}$, $1 \leq n \leq N$
- a different simplicial mesh \mathcal{T}^n on all $0 \leq n \leq N$
- $u_{h\tau}^n \in V_h^n := V_h(\mathcal{T}^n)$, $0 \leq n \leq N$
- $u_{h\tau}^n$ possibly nonconforming, not included in $H_0^1(\Omega)$
- $u_{h\tau} : Q \rightarrow \mathbb{R}$ continuous and piecewise affine in time

$$u_{h\tau}(\cdot, t) := (1 - \varrho)u_{h\tau}^{n-1} + \varrho u_{h\tau}^n, \quad \varrho = \frac{1}{\tau^n}(t - t^{n-1})$$

Time-dependent meshes and discrete solutions

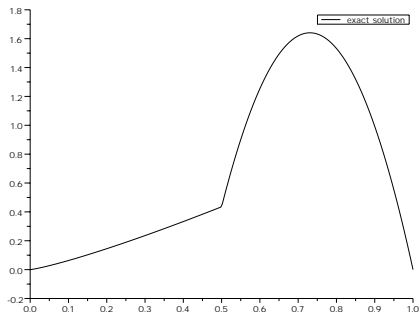


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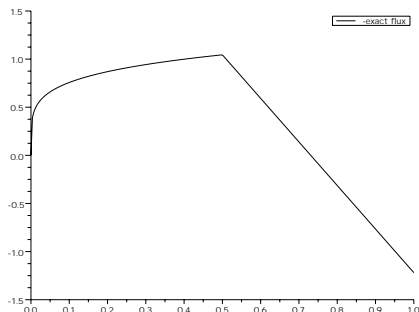
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Properties of the weak solution

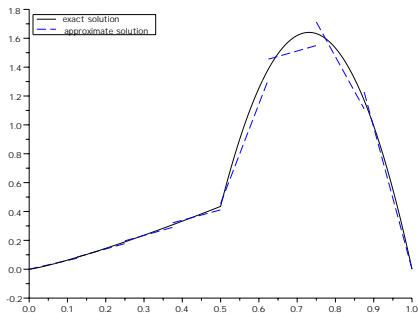


Potential u^n is in $H_0^1(\Omega)$

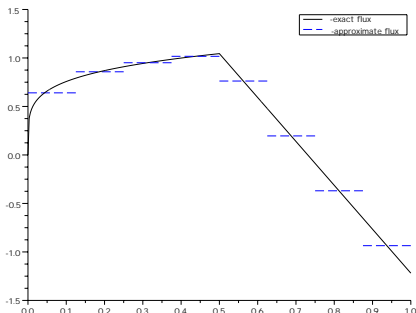


Flux $-\nabla u^n$ is in $\mathbf{H}(\text{div}, \Omega)$

Approximate potential and approximate flux



Approximate potential u_h^n is not
in $H_0^1(\Omega)$



Approximate flux $-\nabla u_h^n$ is not
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Potential and flux reconstructions

General form

- potential reconstruction s is **continuous** and **piecewise affine in time** with $s^n \in H_0^1(\Omega)$ for all $0 \leq n \leq N$ (s^n are in the correct space)
- flux reconstruction θ is **piecewise constant in time** with $\theta|_{I_n} \in \mathbf{H}(\text{div}, \Omega)$ for all $1 \leq n \leq N$ ($\theta|_{I_n}$ are in the correct space)

Two additional assumptions

- s^n **preserves the mean values** of $u_{h\tau}^n$ on $\mathcal{T}^{n,n+1}$, a common refinement of \mathcal{T}^n and \mathcal{T}^{n+1}

$$(s^n, 1)_{T'} = (u_{h\tau}^n, 1)_{T'} \quad \forall T' \in \mathcal{T}^{n,n+1}$$

- θ^n satisfies a **local conservation property**

$$(\tilde{f}^n - \partial_t u_{h\tau}^n - \nabla \cdot \theta^n, 1)_T = 0 \quad \forall T \in \mathcal{T}^n$$

Potential and flux reconstructions

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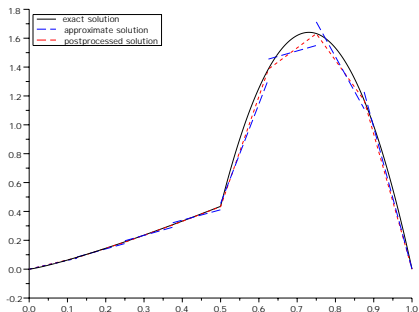
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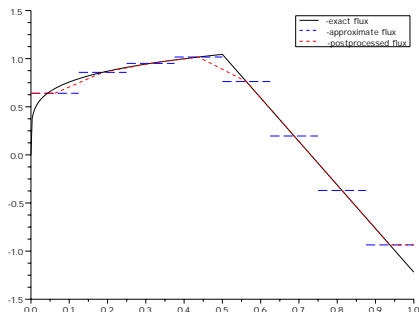
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Potential and flux reconstructions



A postprocessed potential s_h^n is
in $H_0^1(\Omega)$



A postprocessed flux θ^n is in
 $\mathbf{H}(\text{div}, \Omega)$

Practical construction of s and θ

Construction of s^n

$$s^n := \mathcal{I}_{\text{av}}^n(u_{h\tau}^n) + \sum_{T' \in \mathcal{T}^{n,n+1}} \alpha_{T'}^n b_{T'},$$

$$\alpha_{T'}^n := \frac{1}{(b_{T'}, \mathbf{1})_{T'}} (u_{h\tau}^n - \mathcal{I}_{\text{av}}^n(u_{h\tau}^n), \mathbf{1})_{T'}$$

- $\mathcal{I}_{\text{av}}^n$: the averaging interpolate on the mesh \mathcal{T}^n
- $b_{T'}$ standard (time-independent) bubble function supported on T'
- the mean value is preserved on all $T' \in \mathcal{T}^{n,n+1}$
- specificity of the parabolic case
- independent of the numerical scheme

Construction of θ^n

- inspired from the elliptic case
- depends on the numerical scheme

Practical construction of s and θ

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A posteriori error estimate

Theorem (A posteriori error estimate)

There holds

$$\begin{aligned} \|u - u_{h\tau}\|_Y \leq & 3 \left\{ \sum_{n=1}^N \int_{I_n} \sum_{T \in \mathcal{T}^n} (\eta_{R,T}^n + \eta_{DF,T}^n(t))^2 dt \right\}^{1/2} \\ & + \left\{ \sum_{n=1}^N \int_{I_n} \sum_{T \in \mathcal{T}^n} (\eta_{NC1,T}^n)^2(t) dt \right\}^{1/2} \\ & + \left\{ \sum_{n=1}^N \tau^n \sum_{T \in \mathcal{T}^n} (\eta_{NC2,T}^n)^2 \right\}^{1/2} + \eta_{IC} + 3\|f - \tilde{f}\|_{X'}. \end{aligned}$$

- **unified setting**: no specification of the numerical scheme
- only mean values-preserving **potential reconstruction** s and locally conservative **flux reconstruction** θ needed

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Estimators

Estimators

- *diffusive flux estimator*

- $\eta_{\text{DF},T}^n(t) := \|\nabla s(t) + \theta^n\|_T, \quad t \in I_n$
- penalizes the fact that $-\nabla u_{h_T}^n \notin \mathbf{H}(\text{div}, \Omega)$

- *residual estimator*

- $\eta_{\text{R},T}^n := C_P h_T \|\tilde{f}^n - \partial_t s^n - \nabla \cdot \theta^n\|_T$
- residue evaluated for θ^n
- $C_P = 1/\pi$

- *nonconformity estimators*

- $\eta_{\text{NC1},T}^n(t) := \|\nabla^{n-1,n}(s - u_{h_T})(t)\|_T, \quad t \in I_n$
- $\eta_{\text{NC2},T}^n := C_P h_T \|\partial_t (s - u_{h_T})^n\|_T$
- penalize the fact that $u_{h_T}^n \notin H_0^1(\Omega)$

- *initial condition estimator*

- $\eta_{\text{IC}} := 2^{1/2} \|s^0 - u^0\|$

- *data oscillation estimator*

- $\|f - \tilde{f}\|_{X'}$

Estimators

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- *diffusive flux estimator*

- $\eta_{\text{DF},T}^n(t) := \|\nabla s(t) + \theta^n\|_T, \quad t \in I_n$
- penalizes the fact that $-\nabla u_{h_T}^n \notin \mathbf{H}(\text{div}, \Omega)$

- *residual estimator*

- $\eta_{\text{R},T}^n := C_P h_T \|\tilde{f}^n - \partial_t s^n - \nabla \cdot \theta^n\|_T$
- **residue** evaluated for θ^n
- $C_P = 1/\pi$

- *nonconformity estimators*

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Conforming methods

- in **conforming methods** (FEs, VCFVs) $u_{h\tau}^n \in H_0^1(\Omega)$
- set $s^n := u_{h\tau}^n$
- \Rightarrow **nonconformity estimators** $\eta_{\text{NC}1,T}^n$ and $\eta_{\text{NC}2,T}^n$ **vanish**

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- notice that $\int_{I_n} (\eta_{\text{DF},T}^n)^2 \leq (\eta_{\text{DF},T,1}^n)^2 + (\eta_{\text{DF},T,2}^n)^2$, where

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A space-time adaptive time-marching algorithm

Algorithm for achieving a given relative precision ε

$$\frac{\sum_{n=1}^N \{(\eta_{\text{sp}}^n)^2 + (\eta_{\text{tm}}^n)^2\}}{\sum_{n=1}^N \|u_{h\tau}\|_{Z(I_n)}^2} \leq \varepsilon^2$$

1 Initialization

- 1 choose an initial mesh \mathcal{T}^0 ;
- 2 select an initial time step τ^0 and set $n := 1$;

2 Loop in time: while $\sum_j \tau^j < T$,

- 1 set $\mathcal{T}^{n*} := \mathcal{T}^{n-1}$ and $\tau^{n*} := \tau^{n-1}$;
- 2 solve $u_{h\tau}^{n*} := \text{Sol}(u_{h\tau}^{n-1}, \tau^{n*}, \mathcal{T}^{n*})$;
- 3 estimate the space and time errors by η_{sp}^n and η_{tm}^n ;
- 4 when η_{sp}^n or η_{tm}^n are too much above or below $\varepsilon \|u_{h\tau}\|_{Z(I_n)} / \sqrt{2}$ or not of similar size, refine or derefine the time step τ^{n*} and the space mesh \mathcal{T}^{n*} and return to step (2-2), otherwise save approximate solution, mesh, and time step as $u_{h\tau}^n$, \mathcal{T}^n , and τ^n and set $n := n + 1$.

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Efficiency

Theorem (Efficiency)

There holds

$$\eta_{\text{sp}}^n + \eta_{\text{tm}}^n \lesssim \|u - u_{h\tau}\|_{Y(I_n)} + \mathcal{J}^n(u_{h\tau}) + \mathcal{E}_f^n$$

Notation

- $\mathcal{J}^n(u_{h\tau})^2 := \tau^n \sum_{T \in \mathcal{T}^{n-1}} \|\llbracket u_{h\tau}^{n-1} \rrbracket\|_{-\frac{1}{2}, \mathfrak{F}_T^{n-1}}^2 + \tau^n \sum_{T \in \mathcal{T}^n} \|\llbracket u_{h\tau}^n \rrbracket\|_{-\frac{1}{2}, \mathfrak{F}_T^n}^2$
- (\mathcal{E}_f^n) is space-time data oscillation term

Comments on \mathcal{J}^n

- \mathcal{J}^n is a typical jump seminorm
- it can be bounded by the energy error if the jumps in $u_{h\tau}$ have zero mean values (MFEs, FCFVs, NCFEs); it can also be bounded in DGs, using the scheme
- it can alternatively be added to the error measure (note that $\mathcal{J}^n(u_{h\tau}) = \mathcal{J}^n(u - u_{h\tau})$)

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Assumptions for the lower bound proof

Main assumption: approximation property of the flux reconstruction

$$\|\nabla u_{h\tau}^n + \theta^n\|_T \lesssim \left\{ \sum_{T' \in \mathfrak{T}_T} h_{T'}^2 \|\tilde{f}^n - \partial_t u_{h\tau}^n + \Delta u_{h\tau}^n\|_{T'}^2 \right\}^{1/2} + |\mathbf{n} \cdot \llbracket \nabla^n u_{h\tau}^n \rrbracket|_{+\frac{1}{2}, \mathfrak{F}_T^{i,n}} + \|\llbracket u_{h\tau}^n \rrbracket\|_{-\frac{1}{2}, \mathfrak{F}_T^n}$$

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Other assumptions

- the meshes $\{\mathcal{T}^n\}_{0 \leq n \leq N}$ are shape regular uniformly in n ;
- the meshes cannot be refined or coarsened too quickly;
- for nonconforming methods on time-varying meshes, $(h^n)^2 \lesssim \tau^n$ (mild inverse parabolic CFL on time step)

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General concept

Upper bound

- for $0 \leq n \leq N$, we only have to **construct $\theta^n \in \mathbf{H}(\text{div}, \Omega)$ which is locally conservative**, i.e., such that

$$(\tilde{f}^n - \partial_t u_{h\tau}^n - \nabla \cdot \theta^n, 1)_T = 0, \quad \forall T \in \mathcal{T}^n$$

- we construct θ^n in some mixed finite element space;
example: Raviart–Thomas–Nédélec spaces

$$\mathbf{RTN}_l(\mathcal{T}^n) := \{ \mathbf{v}_h \in \mathbf{H}(\text{div}, \Omega); \mathbf{v}_h|_T \in \mathbf{RTN}_l(T) \quad \forall T \in \mathcal{T}^n \}$$

Lower bound

- we only have to **verify the flux approximation property**

We achieve this by a straightforward generalization of the elliptic case (previous works)

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Discontinuous Galerkin method

Definition (DG method)

On $I_n, \mathcal{T}^n, 1 \leq n \leq N$, find $u_{h\tau}^n \in V_h^n := \mathbb{P}_k(\mathcal{T}^n), k \geq 1$, such that

$$\begin{aligned}
 & (\partial_t u_{h\tau}^n, v_h) - \sum_{F \in \mathcal{F}^n} \{(\mathbf{n}_F \cdot \{\{\nabla^n u_{h\tau}^n\}\}, [\![v_h]\!])_F + \theta(\mathbf{n}_F \cdot \{\{\nabla^n v_h\}\}, [\![u_{h\tau}^n]\!])_F\} \\
 & + (\nabla^n u_{h\tau}^n, \nabla^n v_h) + \sum_{F \in \mathcal{F}^n} (\alpha_F h_F^{-1} [\![u_{h\tau}^n]\!], [\![v_h]\!])_F = (\tilde{f}^n, v_h) \quad \forall v_h \in V_h^n.
 \end{aligned}$$

Flux $\theta^n \in \text{RTN}_l(\mathcal{T}^n), l \in \{k-1, k\}$

For all $T \in \mathcal{T}^n$, all $F \in \mathcal{F}_T^n$, all $q_h \in \mathbb{P}_l(F)$ (**face normal comp.**),

$$(\theta^n \cdot \mathbf{n}_F, q_h)_F = (-\mathbf{n}_F \cdot \{\{\nabla^n u_{h\tau}^n\}\} + \alpha_F h_F^{-1} [\![u_{h\tau}^n]\!], q_h)_F,$$

and for all $\mathbf{r}_h \in \mathbb{P}_{l-1}^d(T)$ (**element components**),

$$(\theta^n, \mathbf{r}_h)_T = -(\nabla^n u_{h\tau}^n, \mathbf{r}_h)_T + \theta \sum_{F \in \mathcal{F}_T^n} \omega_F (\mathbf{n}_F \cdot \mathbf{r}_h, [\![u_{h\tau}^n]\!])_F.$$

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On I_n , \mathcal{T}^n , $1 \leq n \leq N$, find $u_{h\mathcal{T}}^n \in V_h^n := \mathbb{P}_k(\mathcal{T}^n)$, $k \geq 1$, such that

$$\begin{aligned}
 & (\partial_t u_{h\mathcal{T}}^n, v_h) - \sum_{F \in \mathcal{F}^n} \{(\mathbf{n}_F \cdot \{\{\nabla^n u_{h\mathcal{T}}^n\}\}, \llbracket v_h \rrbracket)_F + \theta(\mathbf{n}_F \cdot \{\{\nabla^n v_h\}\}, \llbracket u_{h\mathcal{T}}^n \rrbracket)_F\} \\
 & + (\nabla^n u_{h\mathcal{T}}^n, \nabla^n v_h) + \sum_{F \in \mathcal{F}^n} (\alpha_F h_F^{-1} \llbracket u_{h\mathcal{T}}^n \rrbracket, \llbracket v_h \rrbracket)_F = (\tilde{f}^n, v_h) \quad \forall v_h \in V_h^n.
 \end{aligned}$$

Flux $\theta^n \in \mathbf{RTN}_l(\mathcal{T}^n)$, $l \in \{k-1, k\}$

For all $T \in \mathcal{T}^n$, all $F \in \mathcal{F}_T^n$, all $q_h \in \mathbb{P}_l(F)$ (**face normal comp.**),

$$(\theta^n \cdot \mathbf{n}_F, q_h)_F = (-\mathbf{n}_F \cdot \{\{\nabla^n u_{h\mathcal{T}}^n\}\} + \alpha_F h_F^{-1} \llbracket u_{h\mathcal{T}}^n \rrbracket, q_h)_F,$$

and for all $\mathbf{r}_h \in \mathbb{P}_{l-1}^d(T)$ (**element components**),

$$(\theta^n, \mathbf{r}_h)_T = -(\nabla^n u_{h\mathcal{T}}^n, \mathbf{r}_h)_T + \theta \sum_{F \in \mathcal{F}_T^n} \omega_F (\mathbf{n}_F \cdot \mathbf{r}_h, \llbracket u_{h\mathcal{T}}^n \rrbracket)_F.$$

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Cell-centered finite volume method

Definition (CCFV method)

On I_n , \mathcal{T}^n , $1 \leq n \leq N$, find $\bar{u}_{h\tau}^n \in \bar{V}_h^n := \mathbb{P}_0(\mathcal{T}^n)$ such that

$$\frac{1}{\tau^n} (\bar{u}_{h\tau}^n - u_{h\tau}^{n-1}, \mathbf{1})_T + \sum_{F \in \mathcal{F}_T^n} S_{T,F}^n = (\tilde{f}^n, \mathbf{1})_T \quad \forall T \in \mathcal{T}^n.$$

Flux $\theta^n \in \text{RTN}_0(\mathcal{T}^n)$

$$(\theta^n \cdot \mathbf{n}, \mathbf{1})_F := S_{T,F}^n$$

Postprocessing of the potential

- $\bar{u}_{h\tau}^n \in \bar{V}_h^n$ not suitable for energy error estimates ($\nabla \bar{u}_{h\tau}^n = 0$)
- $u_{h\tau}^n \in V_h^n$, V_h^n is $\mathbb{P}_1(\mathcal{T}^n)$ enriched elementwise by the parabolas $\sum_{i=1}^d x_i^2$
- $$-\nabla u_{h\tau}^n = \theta^n,$$

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Mixed finite element method

Definition (MFE method)

On I_n , \mathcal{T}^n , $1 \leq n \leq N$, find $\sigma_{h\tau}^n \in \mathbf{W}_h^n$ and $\bar{u}_{h\tau}^n \in \bar{V}_h^n$ such that

$$(\sigma_{h\tau}^n, \mathbf{w}_h) - (\bar{u}_{h\tau}^n, \nabla \cdot \mathbf{w}_h) = 0 \quad \forall \mathbf{w}_h \in \mathbf{W}_h^n,$$

$$(\nabla \cdot \sigma_{h\tau}^n, v_h) + \frac{1}{\tau^n} (\bar{u}_{h\tau}^n - u_{h\tau}^{n-1}, v_h) = (\tilde{f}^n, v_h) \quad \forall v_h \in \bar{V}_h^n.$$

Flux $\theta^n \in \mathbf{W}_h^n$

$\theta^n := \sigma_{h\tau}^n$ directly

Postprocessing of the potential

- $u_{h\tau}^n \in V_h^n$, V_h^n is $\mathbb{P}_{l+1}(\mathcal{T}^n)$ enriched by bubbles (Arbogast and Chen, 1995)

-

$$\Pi_{\mathbf{W}_h^n}(-\nabla^n u_{h\tau}^n) = \sigma_{h\tau}^n,$$

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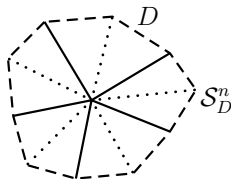
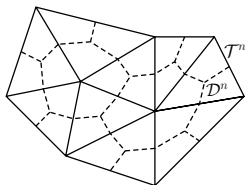
Vertex-centered finite volume method

Definition (VCFV method)

On I_n , \mathcal{T}^n , $1 \leq n \leq N$, find $u_{h\mathcal{T}}^n \in V_h^n := \mathbb{P}_1(\mathcal{T}^n) \cap H_0^1(\Omega)$ s. t.

$$(\partial_t u_{h\mathcal{T}}^n, 1)_D - (\nabla u_{h\mathcal{T}}^n \cdot \mathbf{n}_D, 1)_{\partial D} = (\tilde{f}^n, 1)_D \quad \forall D \in \mathcal{D}^{i,n}.$$

Setting



- triangulation \mathcal{T}^n , dual mesh \mathcal{D}^n , simplicial submesh \mathcal{S}^n

Flux $\theta^n \in \mathbf{RTN}_0(\mathcal{S}^n)$

- by prescription: $\theta^n \cdot \mathbf{n}_F|_F := -\{\{\nabla u_{h\mathcal{T}}^n \cdot \mathbf{n}_F\}\}$ on faces F of \mathcal{S}^n
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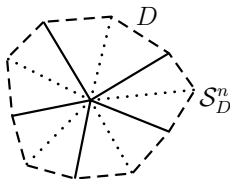
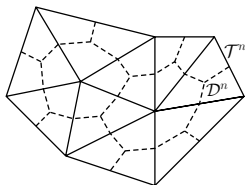
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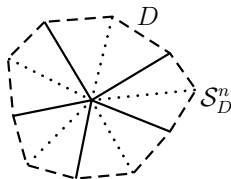
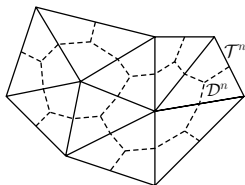
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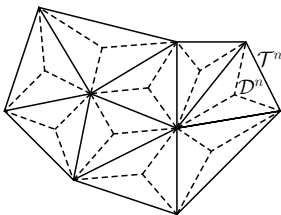
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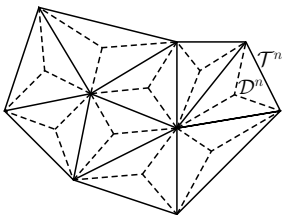
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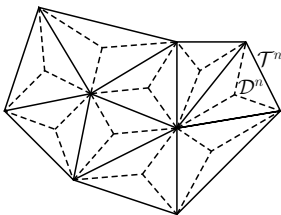
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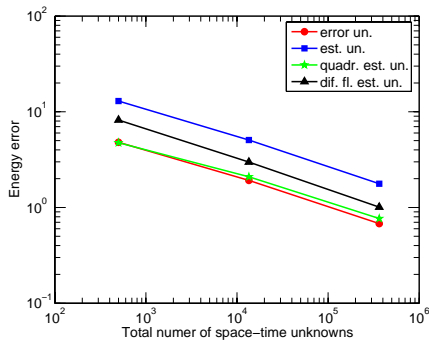
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Numerical experiment

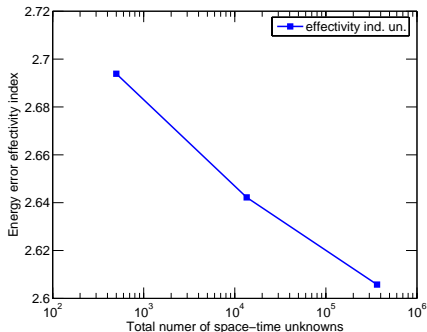
Numerical experiment

- exact solution $u = e^{x+y+t-3}$ on square domain $\Omega = (0, 3) \times (0, 3)$, $T = 1.5$ or $T = 3$
- square meshes: 10×10 , 30×30 , 90×90
- time steps: 0.3, 0.1, 0.3333
- vertex-centered finite volumes
- additional quadrature/mass lumping estimator

Energy norm results, $T = 1.5$

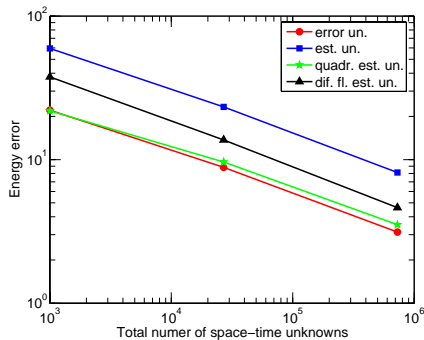


Energy error and estimators

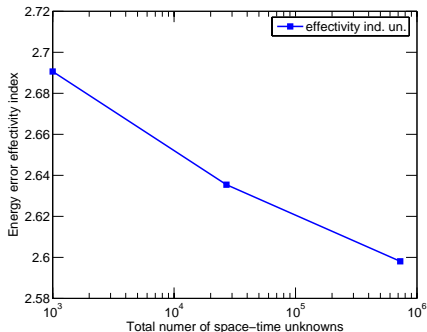


Effectivity index

Energy norm results, $T = 3$

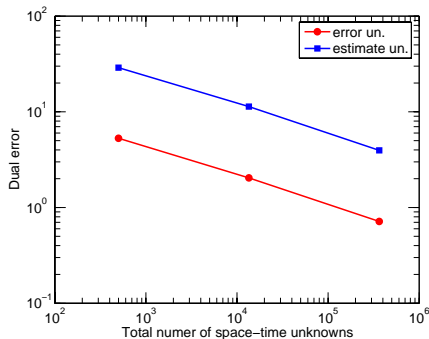


Energy error and estimators

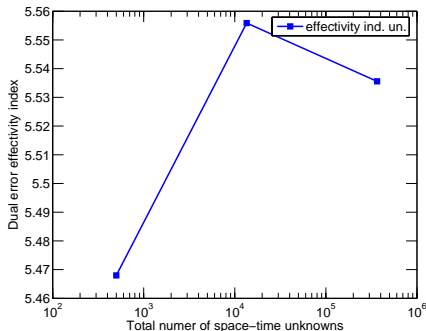


Effectivity index

Dual norm results, $T = 1.5$

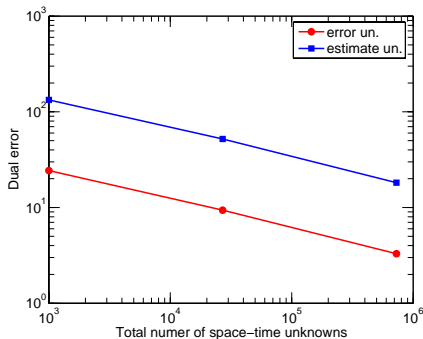


Dual error and estimators

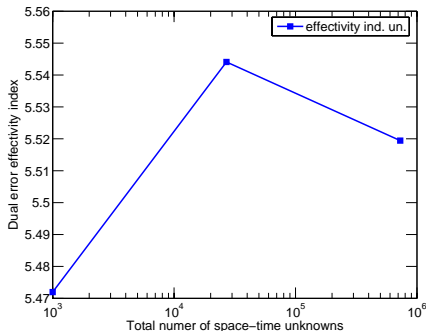


Effectivity index

Dual norm results, $T = 3$



Dual error and estimators



Effectivity index

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- **unified framework** for the heat equation (works for **all** major **numerical schemes**)
- directly and **locally computable** estimates
- global-in-space and local-in-time **efficiency** and **robustness with respect to the final time** as in Verfürth (2003)

Future work

- nonlinear problems
- extensions to other types of problems

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Thanks for your attention!