Goal-oriented error estimates and mesh adaptation for flux-limited Galerkin schemes

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Overview

1. Flux-limited Galerkin schemes
   - Algebraic flux correction
2. Goal-oriented error estimation
   - A general review of the duality argument
   - Error estimates for steady transport problems
3. Mesh adaptation algorithm
   - Refinement, recoarsening, data structures
4. Conclusions

Algebraic flux correction

High-order scheme

$$M_C \frac{\mathrm{d}u}{\mathrm{d}t} = Ku, \quad \exists j \neq i : k_{ij} < 0$$

Algebraic flux correction

High-order scheme

$$M_C \frac{\mathrm{d}u}{\mathrm{d}t} = Ku, \quad \exists j \neq i : k_{ij} < 0$$

Low-order scheme

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = Lu, \quad l_{ij} \geq 0, \ \forall j \neq i$$

Algebraic flux correction

High-order scheme

$M_C \frac{\mathrm{d}u}{\mathrm{d}t} = Ku, \quad \exists j \neq i : k_{ij} < 0$

artificial diffusion

$L = K + D$

Low-order scheme

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Algebraic flux correction

High-order scheme

$$M_C \frac{\mathrm{d}u}{\mathrm{d}t} = Ku, \quad \exists j \neq i : k_{ij} < 0$$

mass-lumping

$$M_L = \text{diag}\{\textstyle\sum_j m_{ij}\}$$

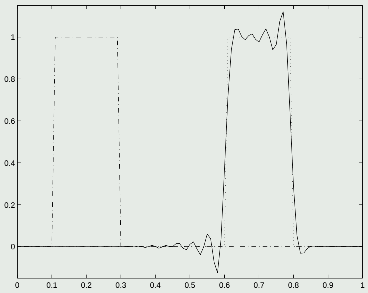
artificial diffusion

$$L = K + D$$

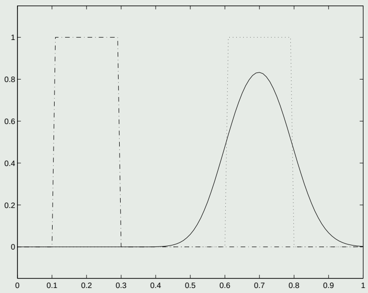
Low-order scheme

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = Lu, \quad l_{ij} \geq 0, \ \forall j \neq i$$

Algebraic flux correction



high-order scheme



low-order scheme

Algebraic flux correction

High-order scheme

$$M_C \frac{\mathrm{d}u}{\mathrm{d}t} = Ku$$

Residual difference

$$f = (M_L - M_C)\frac{\mathrm{d}u}{\mathrm{d}t} - Du$$

Low-order scheme

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = Lu$$

Algebraic flux correction

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High-order scheme

$$M_C \frac{\mathrm{d}u}{\mathrm{d}t} = Ku$$

$$=$$

Residual difference

$$f = (M_L - M_C)\frac{\mathrm{d}u}{\mathrm{d}t} - Du$$

$$+$$

Low-order scheme

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = Lu$$

High-resolution scheme

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = Lu + \bar{f}(u)$$

$=$

Residual difference

$$f = (M_L - M_C)\frac{\mathrm{d}u}{\mathrm{d}t} - Du$$

$+$ limited antidiffusion

Low-order scheme

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Low-order scheme

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = Lu$$

Approximate solution $u_h \approx u$ may lack Galerkin orthogonality!

Duality argument

Primal problem $\qquad a(w,u) = b(w), \qquad \forall w \in V$

$$u_h \approx u, \qquad \rho(w,u_h) = b(w) - a(w,u_h), \qquad \rho(w,u) = 0$$

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- Galerkin orthogonality $\qquad \rho(w_h,u_h) = 0, \qquad \forall w_h \in V_h$

Duality argument

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- Linear target functional $j(u)$, mean/point value, boundary flux

Dual problem $a(z,e) = j(e), \qquad \forall e \in V$

$$e = u - u_h, \qquad j(e) = a(z,u) - a(z,u_h) = \rho(z,u_h)$$

Duality argument

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- Error representation $\quad j(e) = \rho(z - z_h, u_h) + \underbrace{\rho(z_h, u_h)}_{\text{computable}}, \quad z_h \approx z$

Duality argument

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Primal problem $a(w,u) = b(w), \qquad \forall w \in V$

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- Error representation $j(e) \approx \underbrace{\rho(\hat{z} - z_h, u_h)}_{\text{small !?}} + \underbrace{\rho(z_h,u_h)}_{\text{computable}}, \qquad \hat{z} \approx z$

Steady convection

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Primal problem

$$\begin{aligned} \nabla \cdot (\mathbf{v}u) &= s \quad \text{in } \Omega \\ u &= g \quad \text{on } \Gamma_- \end{aligned}$$

Dual problem

$$\begin{aligned} -\mathbf{v} \cdot \nabla z &= j \quad \text{in } \Omega \\ z &= h \quad \text{on } \Gamma_+ \end{aligned}$$

Steady convection

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$$\int_\Omega w \nabla \cdot (\mathbf{v}u) \,\mathrm{d}\mathbf{x} - \int_{\Gamma_-} wu\,\mathbf{v} \cdot \mathbf{n} \,\mathrm{d}s = \int_\Omega ws \,\mathrm{d}\mathbf{x} - \int_{\Gamma_-} wg\,\mathbf{v} \cdot \mathbf{n} \,\mathrm{d}s$$

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- Functional $j(u) = \int_\Omega hu\,\mathrm{d}\mathbf{x} + \int_{\Gamma_+} hu\,\mathbf{v} \cdot \mathbf{n}\,\mathrm{d}s, \quad h(\mathbf{x}) \in \{0,1\}$

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Dual problem $\quad a(z,w) = a^*(w,z) = j(w), \qquad \forall w \in V$

$$-\int_\Omega w\mathbf{v}\cdot\nabla z\,\mathrm{d}\mathbf{x} + \int_{\Gamma_+} wz\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}s = \int_\Omega hw\,\mathrm{d}\mathbf{x} + \int_{\Gamma_+} hw\,\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}s$$

Global error estimates

- Finite element solutions $\quad u_h \approx u, \quad z_h \approx z, \quad \hat{z} \approx z$
- Error representation $\quad j(u - u_h) \approx \rho(\hat{z} - z_h, u_h) + \rho(z_h, u_h)$

Computable error bounds $\quad |j(u - u_h)| \leq \eta$

$$\eta = \Phi + \Psi, \qquad |\rho(\hat{z} - z_h, u_h)| \leq \Phi, \qquad |\rho(z_h, u_h)| \leq \Psi$$

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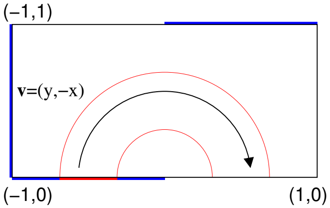
- Effectivity indices

$$I_{\text{eff}} = \frac{\eta}{|j(u-u_h)|}, \qquad I_{\text{rel}} = \left| \frac{|j(u-u_h)| - \eta}{|j(u)|} \right|$$

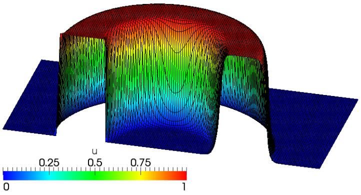
Steady convection in 2D

Circular convection $\nabla \cdot (\mathbf{v}u) = 0$ in $\Omega = (-1,1) \times (0,1)$

$$u(x,y) = \begin{cases} 1, & 0.35 \le r \le 0.65 \\ 0, & \text{otherwise} \end{cases} \qquad r(x,y) = \sqrt{x^2 + y^2}$$



domain and velocity



FEM-TVD, $h = 1/80$

Steady convection in 2D, contd.

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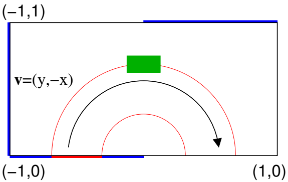
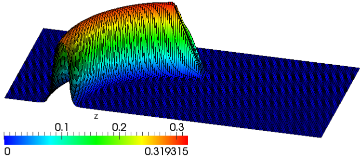
Target functional

$$j(u) = \int_\Omega hu\,\mathrm{d}\mathbf{x}, \quad h(\mathbf{x}) \in \{0,1\}$$

$$h \equiv 1 \text{ in } (-0.1, 0.1) \times (0.6, 0.7)$$



L	$j(e)$	Ψ	$I_{\rm eff}$	$I_{\rm rel}$
1	4.97e-4	2.86e-3	5.75	2.49e-1
2	2.67e-3	2.53e-3	0.95	1.40e-2
3	1.91e-3	2.47e-3	1.29	5.91e-2
4	1.22e-3	2.19e-3	1.79	1.02e-1



FEM-TVD, $h = 1/80$

- Error estimation based on $\eta = \Psi(z_h, u_h)$ neglecting $\Phi(\hat{z} - z_h, u_h)$

Local error estimates

- Error representation $j(u - u_h) \approx \rho(\hat{z} - z_h, u_h) + \rho(z_h, u_h)$

$$|\rho(\hat{z} - z_h, u_h)| \leq \Phi = \sum_i \Phi_i, \qquad |\rho(z_h, u_h)| \leq \Psi = \sum_i \Psi_i$$

Local error estimates

- Error representation $\qquad j(u-u_h) \approx \rho(\hat{z}-z_h, u_h) + \rho(z_h, u_h)$

$$|\rho(\hat{z}-z_h, u_h)| \leq \Phi = \sum_i \Phi_i, \qquad |\rho(z_h, u_h)| \leq \Psi = \sum_i \Psi_i$$

- Nodal localization $\qquad z_h = \sum_i z_i \varphi_i, \qquad \Psi_i = |\rho(z_i \varphi_i, u_h)|$

$$\hat{z}-z_h = \sum_i w_i, \qquad w_i = \varphi_i(\hat{z}-z_h), \qquad \Phi_i = |\rho(w_i, u_h)|$$

Local error estimates

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Conversion to element contributions $\quad \eta = \sum_k \eta_k = \Phi + \Psi$

$$\xi = \sum_i \xi_i\varphi_i, \qquad \xi_i = \frac{\Phi_i+\Psi_i}{\int_\Omega \varphi_i \, \mathrm{d}\mathbf{x}}, \qquad \eta_k = \int_{\Omega_k} \xi \, \mathrm{d}\mathbf{x}$$

Local error estimates

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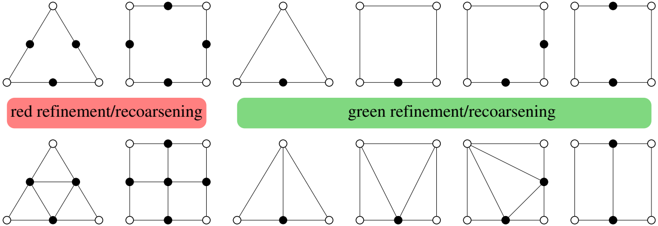
Mesh adaptation algorithm

Conformal refinement algorithm *Bank, et al. '83*

1. subdivide marked elements regularly (red rule)
2. eliminate 'hanging nodes' by transition cells (green rule)



Mesh adaptation, contd.

- Vertex-locking algorithm is used to reverse mesh refinement
- Nodal generation function provides all necessary information: *element type, inter-element relationship, refinement level, ...*

Mesh adaptation, contd.

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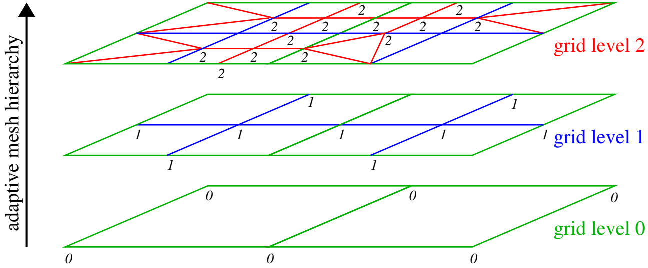

Steady convection in 2D, revisited

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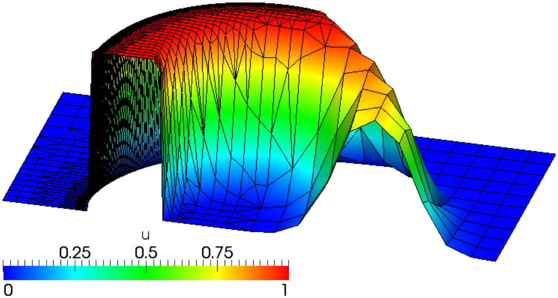
Adaptive mesh refinement $tol = 1\text{e-}8, \quad L_{\max} = 5$

$j(e) = 6.08\text{e-}4, \quad \Psi = 1.47\text{e-}3, \quad I_{\text{eff}} = 2.42, \quad I_{\text{rel}} = 9.16\text{e-}2$



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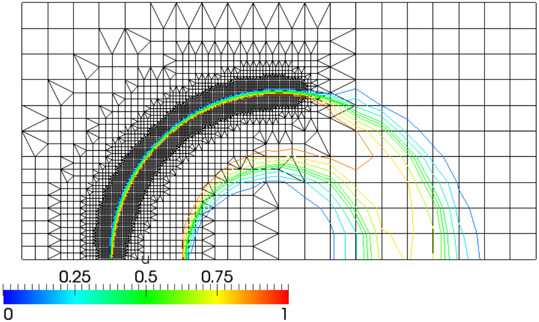

Primal problem $\nabla \cdot (\mathbf{v}u - \epsilon \nabla u) = s \quad + \quad$ b.c.

$$\int_\Omega w \nabla \cdot (\mathbf{v}u)\, \mathrm{d}\mathbf{x} + \int_\Omega \epsilon \nabla w \cdot \nabla u \, \mathrm{d}\mathbf{x} = \int_\Omega ws \, \mathrm{d}\mathbf{x}$$

Steady convection-diffusion

Primal problem $\nabla \cdot (\mathbf{v}u - \epsilon \nabla u) = s$ + b.c.

$$\int_\Omega w \nabla \cdot (\mathbf{v}u)\, \mathrm{d}\mathbf{x} + \int_\Omega \epsilon \nabla w \cdot \nabla u \, \mathrm{d}\mathbf{x} = \int_\Omega ws \, \mathrm{d}\mathbf{x}$$

- Residual weighted by the dual error $w = \hat{z} - z_h = \sum_i w_i$

$$\rho(w, u_h) = \int_\Omega w \left(s - \nabla \cdot (\mathbf{v}u_h)\right) \mathrm{d}\mathbf{x} - \epsilon \int_\Omega \nabla w \cdot \nabla u_h \, \mathrm{d}\mathbf{x}$$

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- Approximation $\quad \mathbf{g}_h \approx \nabla u, \qquad \int_\Omega w \nabla \cdot \mathbf{g}_h\,\mathrm{d}\mathbf{x} + \int_\Omega \nabla w \cdot \mathbf{g}_h\,\mathrm{d}\mathbf{x} = 0$

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- Residual weighted by the dual error $\quad w = \hat{z} - z_h = \sum_i w_i$

$$\rho(w, u_h) = \int_\Omega w\,(s - \nabla \cdot (\mathbf{v}u_h - \epsilon \mathbf{g}_h))\,\mathrm{d}\mathbf{x} \qquad \textit{residual error}$$

$$+\,\varepsilon \int_\Omega \nabla w \cdot (\mathbf{g}_h - \nabla u_h)\,\mathrm{d}\mathbf{x} \qquad \textit{diffusive flux error}$$

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$$\Phi_i = \int_\Omega |w_i(s - \nabla \cdot (\mathbf{v}u_h - \varepsilon \mathbf{g}_h))|\mathrm{d}\mathbf{x} + \varepsilon \int_\Omega |\nabla w_i \cdot (\mathbf{g}_h - \nabla u_h)|\mathrm{d}\mathbf{x}$$

Steady convection-diffusion in 1D

Estimates for $\mathrm{Pe}\,\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = 0$ in $(0,1)$, $u(0) = 0$, $u(1) = 1$

$$u(x) = \frac{e^{\mathrm{Pe}\,x} - 1}{e^{\mathrm{Pe}} - 1}, \qquad j(u) = \int_0^1 u \,\mathrm{d}x, \qquad z(x) = \frac{e^{\mathrm{Pe}\,(1-x)} + x(e^{\mathrm{Pe}} - 1) - e^{\mathrm{Pe}}}{\mathrm{Pe}\,(1 - e^{\mathrm{Pe}})}$$

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Discretization: central difference scheme, $\quad h = 1/10$

Pe	$\lvert j(u-u_h)\rvert$	Φ	Ψ	η	I_{rel}
1	7.67e-04	7.80e-04	4.09e-16	7.80e-04	3.05e-05
10	2.84e-05	4.10e-05	3.56e-18	4.10e-05	1.25e-04
100	–	–	–	–	–

Estimates for $\quad \mathrm{Pe}\,\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = 0$ in $(0,1)$, $\quad u(0) = 0, \quad u(1) = 1$

$$u(x) = \frac{e^{\mathrm{Pe}\,x} - 1}{e^{\mathrm{Pe}} - 1}, \qquad j(u) = \int_0^1 u\,\mathrm{d}x, \qquad z(x) = \frac{e^{\mathrm{Pe}\,(1-x)} + x(e^{\mathrm{Pe}} - 1) - e^{\mathrm{Pe}}}{\mathrm{Pe}\,(1 - e^{\mathrm{Pe}})}$$

Discretization: upwind difference scheme, $\quad h = 1/10$

Pe	$\lvert j(u-u_h)\rvert$	Φ	Ψ	η	I_{rel}
1	4.52e-03	7.38e-04	3.58e-03	4.32e-03	4.79e-04
10	4.91e-02	3.06e-04	4.76e-02	4.79e-02	1.21e-02
100	5.00e-02	1.59e-09	5.00e-02	5.00e-02	1.21e-08

Estimates for $\mathrm{Pe}\,\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = 0$ in $(0,1)$, $u(0) = 0$, $u(1) = 1$

$$u(x) = \frac{e^{\mathrm{Pe}\,x} - 1}{e^{\mathrm{Pe}} - 1}, \qquad j(u) = \int_0^1 u\,\mathrm{d}x, \qquad z(x) = \frac{e^{\mathrm{Pe}\,(1-x)} + x(e^{\mathrm{Pe}} - 1) - e^{\mathrm{Pe}}}{\mathrm{Pe}\,(1 - e^{\mathrm{Pe}})}$$

Discretization: TVD scheme, MC limiter $h = 1/10$

Pe	$\lvert j(u - u_h)\rvert$	Φ	Ψ	η	I_{rel}
1	1.03e-03	7.74e-04	2.60e-04	1.03e-03	1.34e-05
10	1.51e-02	9.12e-05	1.50e-02	1.51e-02	3.81e-05
100	4.51e-02	4.23e-09	4.51e-02	4.51e-02	1.97e-07

Galerkin orthogonality errors $(\hat{z} = z_h)$ may be all you need *in practice*

Conclusions

- Flux-limited Galerkin discretizations of AFC type
  - high resolution, violation of the Galerkin orthogonality
  - flux correction provides feedback for mesh adaptation
- Goal-oriented error estimation for transport problems
  - no dubious constants, control of local and transmitted errors
  - nodal decomposition of the error in the target functional
  - Galerkin orthogonality error is a handy criterion for refinement
  - Stabilization of diffusive fluxes using gradient recovery