A-posteriori estimators for conservation laws

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Structure of solution

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Scalar non linear conservation law:

Find $u : \mathbb{R}^d \times \mathbb{R}^+ \to \mathbb{R}$ solution of

$$\partial_t u(x,t) \quad + \quad \nabla \cdot f(u(x,t)) = 0 \qquad u(x,0) = u_0(x)$$

with e.g. $f(u) = \frac{1}{2}u^2$

Viscosity limit: let u_ε be a classical solution of the regularized problem:

$$\partial_t u_\varepsilon(x,t) + \nabla \cdot f(u_\varepsilon(x,t)) = \varepsilon \triangle, u_\varepsilon(x,t), \qquad u_\varepsilon(x,0) = u_0(x)$$

There exists $u = \lim_{\varepsilon \to 0} u_\varepsilon$ (a.e.) and u is weak solution.
u is physically relevant weak solution

Equivalent: Entropy Solution

$$-\int_{\mathbb{R}^d}\int_{\mathbb{R}^+} \left(S(u)\partial_t \phi + F_S(u) \cdot \nabla \phi\right)\, dt\, dx - \int_{\mathbb{R}^d} S(u_0)\phi(x,0)\, dx \leq 0$$

for all entropy pairs (S, F_S), i.e., S convex and $F_S' = S'f'$

First order finite-volume scheme

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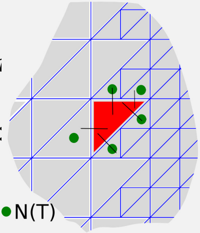
System of conservation law (e.g. Euler Equations):

Find $U : \mathbb{R}^d \times \mathbb{R}^+ \to \mathbb{R}^m$ entropy solution

$$\partial_t U(x,t) \quad + \quad \nabla \cdot F(U(x,t)) = 0 \qquad U(x,0) = U_0(x)$$

Integrate over $T \in \mathbf{T}$ with tessellation $\mathbf{T}$ of Ω:

$$\int_T \partial_t U(\cdot,t) = -\int_T \nabla \cdot F(U(\cdot,t)) = -\int_{\partial T} F(U(\cdot,t)) \cdot n$$



Piecewise constant approximation $U_T(t) \approx \frac{1}{|T|} \int_T U(\cdot,t)$:

$$\frac{d}{dt} U_T(t) = -\frac{1}{|T|} \int_{\partial T} F_h(t)$$

with numerical flux $F_h(t) = F_{T,T'}(U_T(t), U_{T'}(t))$ on intersection between neighboring elements T, T':

$$\frac{d}{dt} U_T(t) = -\frac{1}{|T|} \sum_{T' \in N(T)} F_{T,T'}(U_T(t), U_{T'}(t))$$

$N(T)$ is set of all neighbors of T.

First order finite-volume scheme

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$$\partial_t U(x,t) \quad + \quad \nabla \cdot F(U(x,t)) = 0 \qquad U(x,0) = U_0(x)$$

Semi discrete scheme:

$$\frac{d}{dt} U_T(t) = -\frac{1}{|T|} \sum_{T' \in N(T)} F_{T,T'}(U_T(t), U_{T'}(t))$$

$N(T)$ is set of all neighbors of T.
Forward Euler in time for time steps t^n and $\Delta t^n = t^{n+1} - t^n$:

$$U_T^{n+1} = U_T^n - \frac{\Delta t^n}{|T|} \sum_{T' \in N(T)} F_{T,T'}(U_T^n, U_{T'}^n)$$

First order finite-volume scheme

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System of conservation law (e.g. Euler Equations):

Find $U : \mathbb{R}^d \times \mathbb{R}^+ \to \mathbb{R}^m$ entropy solution

$$\partial_t U(x,t) \quad + \quad \nabla \cdot F(U(x,t)) = 0 \qquad U(x,0) = U_0(x)$$

Fully discrete scheme:

$$U_T^{n+1} = U_T^n - \frac{\Delta t^n}{|T|} \sum_{T' \in N(T)} F_{T,T'}(U_T^n(t), U_{T'}^n(t))$$

Define $U_h(x,t) := U_T^n$ for $x \in T, t \in [t^n, t^{n+1})$.

A-priori error estimate for scalar case

Let u_h be a first order finite-volume approximation then under suitable conditions on the numerical flux:

$$\max_t \|u_h(\cdot,t) - u(\cdot,t)\|_{L^1(\mathbb{R}^d)} \leq C(u) h^{\frac{1}{4}}$$

Should be $h^{\frac{1}{2}}$, only proven for structured grids.

Euler System of Hydrodynamics

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$$\partial_t \rho + \nabla \cdot (\rho \vec{u}) = 0 \qquad \text{(conservation of mass)},$$
$$\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u}\vec{u}^T + \mathbf{P}) = 0 \qquad \text{(conservation of momentum)},$$
$$\partial_t (\rho e) + \nabla \cdot (\rho e \vec{u} + \mathbf{P}\vec{u}) = 0 \qquad \text{(conservation of energy)},$$

$$e = \varepsilon + \frac{1}{2}|\vec{u}|^2 \qquad \text{(total energy)},$$
$$\mathbf{P} = p(\rho, \varepsilon)\mathbf{I} \qquad \text{(equation of state for pressure)},$$

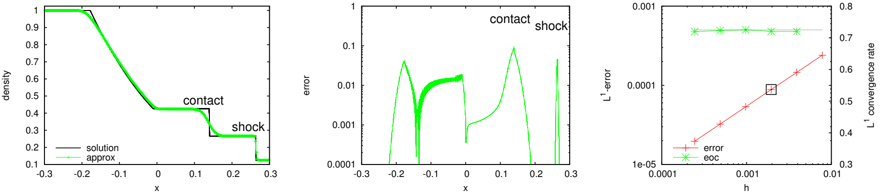
$$(\rho, \rho\vec{u}, \rho e)(\cdot, 0) = (\rho_0, \rho_0\vec{u}_0, \rho_0 e_0) \qquad \text{(initial conditions)}$$

ρ : density, $\rho\vec{u}$: momentum, ρe : total energy density

Numerical results

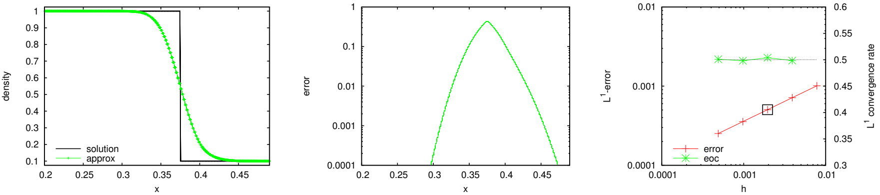
Riemann problem (Euler)

$u_0 = u_L \ (x < 0)$, $u_0 = u_R \ (x > 0)$. Solution: rarefaction, contact, shock



Single contact (Euler)

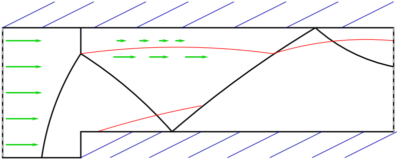
$u_0 = u_L \ (x < 0)$, $u_0 = u_R \ (x > 0)$. Solution: $u(x,t) = u_0(x - at)$



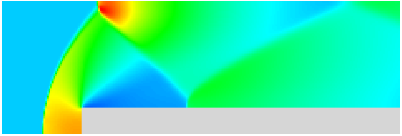
resolution in 3d requires 130.000.000 elements for results shown

Forward facing step (Euler)

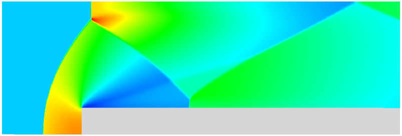
Right moving Mach 3 flow structure:



15.000 elements



230.000 element



High order methods

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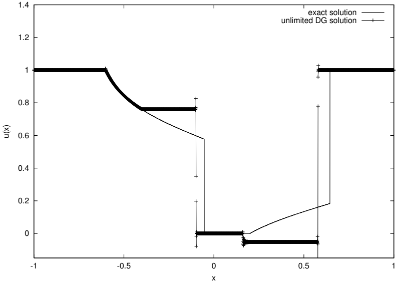
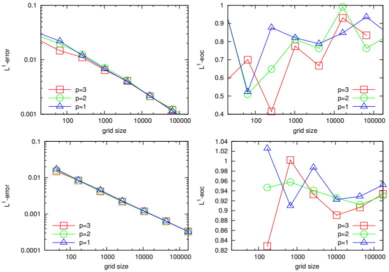
- highly efficient for smooth solution
- Loss of efficiency for non-smooth solution ...
- ... and unstable for non linear discontinuities (shocks)

No stabilization



With simple stabilization



High order methods

- highly efficient for smooth solution
- Loss of efficiency for non-smooth solution ...
- ... and unstable for non linear discontinuities (shocks)

Basis Algorithm:

1. determine troubled cells where the error is high or the scheme is unstable
2. for each troubled cell either increase the order (if solution is smooth) or reduce the order und refine the grid

Determine troubled cells heuristically or by error estimate.

Higher order (Discontinuous Galerkin)

Riemann problem (Euler)

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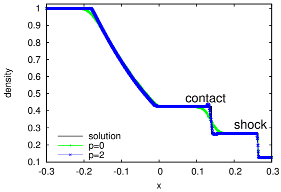

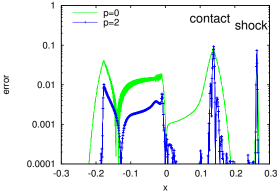

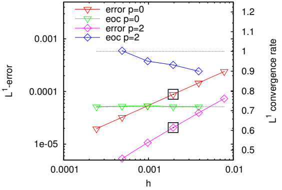

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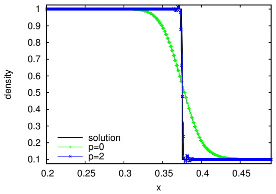

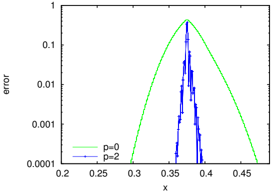

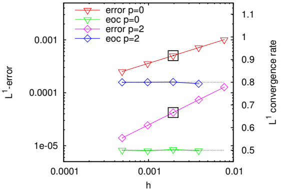

Heuristic strategy for local mesh adaption

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- Find interface between cells where solution has a large jump
- Mark the two elements at that intersection
- Mark a neighborhood of marked elements
- Mark elements for coarsening where the jump is very small

Possibly look at curvature of solution (i.e. jumps between gradients)
Idea: Error is where the discontinueties are
Problems?

- Can not distinguish between contacts and shocks
- Could coarsen wrongly (kinks at ends of rarefactions)
- Indicator does not get smaller with reduction of grid size
- No mathematical proof that it works only many people using successfuly...

Higher order schemes on adaptive grids

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Estimator

Nead indictor η_K for "smoothness" of solution

$$\eta_K = \begin{cases} O(h_K^q) & \text{smooth region} \\ O(h_K^{-1}) & \text{troubled region} \end{cases}$$

A posteriori error estimate
Kruzkov framework (semi implicit)

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D, Makridakis, Ohlberger '06

Structure of a posteriori error estimate:

$$||(u-u_h)(T)||^2_{L^1(B_R(x_0))} \leq K \sum_n \sum_{j \in J^n} \left(h_j + ||\overline{\widetilde{u}_j^n} - \widetilde{u}_j^n||_{L^\infty} \right) \left(\mathbf{R^n_{T,j}} + \mathbf{R^n_{S,jl}} + \mathbf{R^n_{L,j}} \right)$$

- $\mathbf{R^n_{T,j}}$: Element residual
- $\mathbf{R^n_{S,jl}}$: Jump residual (numerical viscosity)
- $\mathbf{R^n_{L,j}}$: Coarsening error
- $||\overline{\widetilde{u}_j^n} - \widetilde{u}_j^n||_{L^\infty}$: difference between aerage and higher order polynomial

Numerical test show:

$$\bar{R}_j^n := \frac{h_j}{|T_j|\Delta t^n} \left(\mathbf{R^n_{T,j}} + \mathbf{R^n_{S,jl}} + \mathbf{R^n_{L,j}} \right) = \begin{cases} O(h_j^{p-1}) & \text{solution is smooth} \\ O(1) & \text{... discontinuous} \end{cases}$$

Strategy for local mesh adaption

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First step:

Define the set of grid cells $\mathbf{I_s}$ with a significant contribution to the overall error indicator η_h.

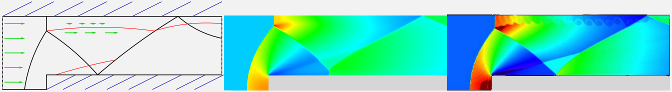
Second step:

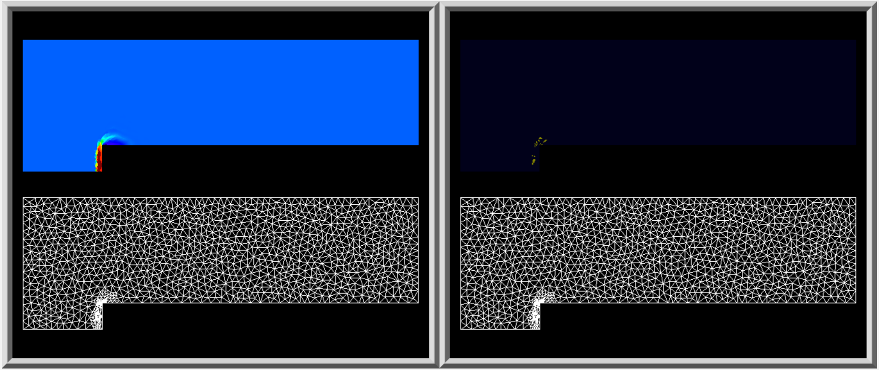
Use an equal distribution strategy to refine or coarsen the elements in $\mathbf{I_s}$ according to the error estimate.

Third step:

For elements that are marked for coarsening, check if the projection error is small enough.

Forward facing step





Approximately 14.000 elements at $t = T$

We now come to a short commercial break...

at University of Warwick 4th to 8th of July, 2016

We now come to a short commercial break...

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uncertainty quantification

inverse problems

biology
engineering
medicine
physics
statistics

model coupling

data assimilation

PDE Software Frameworks 2016

visualization

grid generation

hpc tools

solvers

computer hardware

scripting languages

at University of Warwick 4th to 8th of July, 2016

A very different approach

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Issues with Kruzkov: only works with scalars
Issue with proof: only done for semi discrete scheme

Giesselmann, Makridakis, Pryer: use of relative entropy (RE) framework
Given one convex entropy η then

$$\eta(U \mid V) := \eta(U) - \eta(V) - \eta'(V)(U - V) \approx \|U - V\|_{L^2}$$

and if V is a Lipschitz solution and U a weak solution then

$$\frac{d}{dt}\int \eta(U \mid V) \leq C(V)\int \eta(U \mid V)$$

This can also be used to study perturbed solutions U:
Advantage: works with system of equations (need only one entropy)
Issue with RE: only works in the case that a Lipschitz solution extists
Issue with proof: semi discrete scheme in 1d, very restrictive on flux function

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A-posteriori estimator based on RE (semi discrete version in 1d)

- Construct semi discrete solution $U(t)$ in the DG space of order p
- Use a spacial reconstruction $U^s(t)$ in a Lagrange space of order $p+1$: construct solution on each element
  - local L^2 projection on polynomial space of order $p-1$
  - use $U^* = U^*(U^+, U^-)$ for continuety at the vertices of the grid
- Compute pointwise residual using $U^s(t)$:

$$R^s = \partial_t U^s + \nabla \cdot F(U^s)$$

Assumption:

- Have good choice for U^* (get to that later)
- existence of smooth solutions (we are stuck with that)

Reconstruction in time (ODE case)

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Problem: General ODE

$$\frac{d}{dt}U(t) = F(U(t))$$

Assume: some time stepping method of order q giving approximations

$$(t^0, U^0), (t^1, U^1), \dots, (t^n, U^n), (t^{n+1}, U^{n+1})$$

Reconstruction: Choose s and d with $(d+1)s - 1 := r \geq q$ and assume given approximations

$$U_{ij} \approx \frac{d^i}{dt^i}U(t^{n-j})$$

for $i = 0, \dots, d$ and $j = -1, \dots, s$ (could be more general).
Using these values construct polynomial $U^t := H^{s,d}$ of order r on (t^n, t^{n+1}) through Hermite interpolation.
Easiest example is $d = 1, s \geq 0$ since we can take $U_{1j} = F(U(t^{n-j}))$
Otherwise can use finite difference approximation to approximate higher order derivatives

A-posteriori estimate (ODE case)

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Lemma: Stability of Hermite interpolation:
we can replace exact derivatives with approximations (of the right order)

Estimate

Define residual $R := \frac{d}{dt}U^t(t) - F(U^t(t))$ then

$$\|u - u^t\|_\infty \leq \|R\|_{L^1} e^{LT}$$

Note: $U^t \in C^1(0,T)$ and locally computable

Optimality

Assume L^k is the Lipschitz constant of kth derivative of rhs F then

$$\|R\|_\infty \leq \sum_{k=0}^{q+1} L^k \mathcal{O}(\tau^{q+k}).$$

So we can have $L = \mathcal{O}(\tau^{-1})$ for residual to be order q

A-posteriori estimate for fully discrete scheme

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1. Compute DG solution U^{n+1}
2. Use U^{n-j} to compute Hermite reconstruction U^t (in DG space)
3. Use spatial reconstruction (given U^*) to construct U^{ts} in Lagrange space
4. Compute pointwise Residual R

Estimate:

$$\|U(t^n,\cdot) - U^n(\cdot)\|_{L^2}^2 \leq \|u^{st}(t^n,\cdot) - U^n(\cdot)\|_{L^2}^2 + \|R\|_{L^2((0,t^n)\times\Omega}^2 \exp(\dots)$$

Optimality of the estimate

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Condition on the numerical flux

There exists $\mathbf{U}^* : \mathcal{U} \times \mathcal{U} \to \mathcal{U}$ so that

$$\mathbf{F}_{\mathbf{T},\mathbf{T}'}(\mathbf{a},\mathbf{b}) = \mathbf{F}(\mathbf{U}^*(\mathbf{a},\mathbf{b})) - \mu(\mathbf{a},\mathbf{b};h)h^\nu(\mathbf{b}-\mathbf{a}) \quad \forall\, \mathbf{a},\mathbf{b} \in \mathcal{U}$$

with $\nu \in \mathbb{N}_0$, matrix-valued μ with $|\mu(\mathbf{a},\mathbf{b};h)| \le \mu_K \left(1 + \frac{|\mathbf{b}-\mathbf{a}|}{h}\right)$.

- Richtmyer flux ($\mu = 0$):

$$U^*(V,W) = \frac{1}{2}(V+W) - \frac{\Delta t}{2h}(F(W) - F(V))$$

- Richtmyer flux with artificial viscosity of the form $h^2\partial_x^h(|\partial_x^h u|\partial_x^h u)$ ($\nu = 1$)
- The Lax Friedrichs flux

$$\mathbf{F}_{\mathbf{T},\mathbf{T}'}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\Big(\mathbf{F}(\mathbf{a}) + \mathbf{F}(\mathbf{b})\Big) - \lambda(\mathbf{b}-\mathbf{a})$$

with $\mathbf{U}^*(\mathbf{a},\mathbf{b}) = \frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\nu = 0$, and

$$\mu(\mathbf{a},\mathbf{b},h) = \frac{\mathbf{F}(\mathbf{a}) - 2\mathbf{F}(\mathbf{U}^*(\mathbf{a},\mathbf{b})) + \mathbf{F}(\mathbf{b})}{2\|\mathbf{b}-\mathbf{a}\|^2} \otimes (\mathbf{b}-\mathbf{a}) - \lambda\,.$$

Optimality of the estimate

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Condition on the numerical flux

There exists $\mathbf{U}^* : \mathcal{U} \times \mathcal{U} \to \mathcal{U}$ so that

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with $\nu \in \mathbb{N}_0$, matrix-valued μ with $|\mu(\mathbf{a},\mathbf{b};h)| \leq \mu_K \left(1 + \frac{|\mathbf{b}-\mathbf{a}|}{h}\right)$.

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Lemma (Conditional optimality of residuals)

Consider fully discrete DG scheme of order $q+1$ in time, q-th order polynomials in space, and a numerical flux satisfying previous Assumption. Let the exact error be of order $\mathcal{O}(h^{q+\gamma})$ with $\gamma \in \{\frac{1}{2}, 1\}$. Then, the residual $\mathbf{R}$ is of order $\mathcal{O}(h^{q+\gamma} + h^{q+\gamma+\nu-1})$ under CFL conditions.

So for optimality we need

- CFL condition
  (gives $O(\tau^{-1})$ for Lipschitz constant in time reconstruction error)
- numerical flux with $\nu = 1$ (or $\mu = 0$)

Lemma (Suboptimality)

Consider a numerical flux satisfying our Assumption with $\nu = 0$ and $\mu(a, b; h) = \mu_0 > 0$ and $\tau = \mathcal{O}(h)$. Then, for a linear DG scheme the norm of the residualx $\mathbf{R}$ is bounded from below by terms of order h^γ even if the error of the method is $\mathcal{O}(h^{1+\gamma})$.

D, Giesselmann: A posteriori analysis of fully discrete method of lines DG schemes for systems of conservation laws, submitted

Lemma (Conditional optimality of residuals)

Consider fully discrete DG scheme of order $q+1$ *in time,* q*-th order polynomials in space, and a numerical flux satisfying previous Assumption. Let the exact error be of order* $\mathcal{O}(h^{q+\gamma})$ *with* $\gamma \in \{\frac{1}{2}, 1\}$*.*
Then, the residual $\mathbf{R}$ *is of order* $\mathcal{O}(h^{q+\gamma} + h^{q+\gamma+\nu-1})$ *under CFL conditions.*

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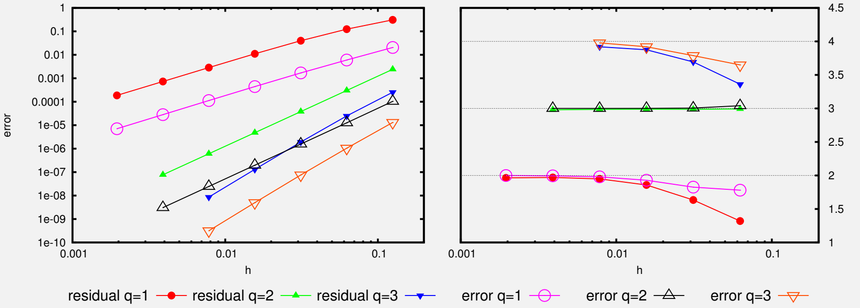
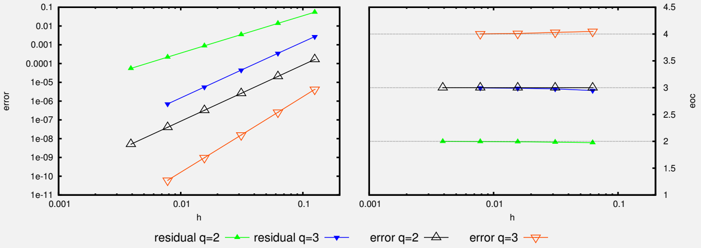
Linear Advection with optimal flux

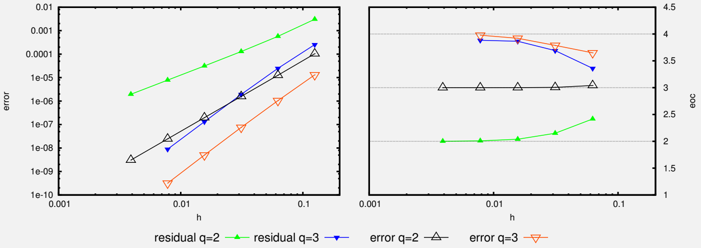


Linear Advection with ...

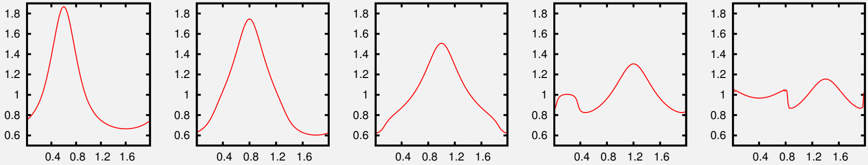
... sub optimal flux



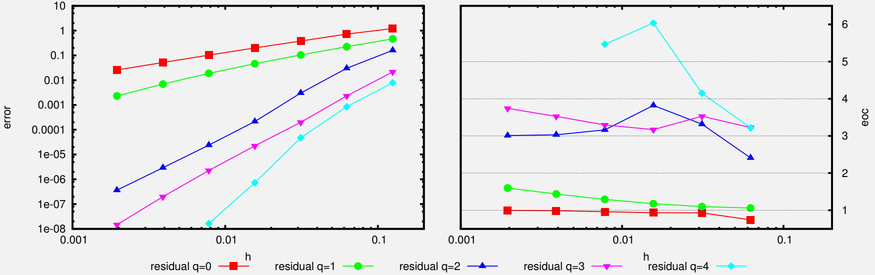
... optimal flux but lower temporal reconstruction



Euler Equations



Density evolution: $t = 0.6, 0.8, \mathbf{1.0}, 1.2, 1.4$.



Results

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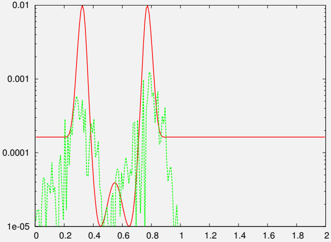

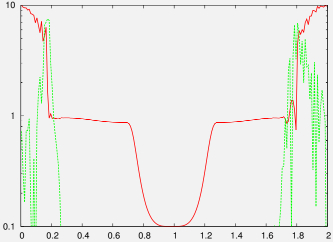

A-posteriori estimator based on RE: Some remarks

WARWICK

- works now for fully discrete scheme
- we are working on extending it to higher dimensions
- only works with smooth solutions:
  For grid adaptivity and stabilization this is not really an issue?
- needs very specific flux function:
  We can show that this is required
  With general flux the Residual is not optimal
- expensive to compute:
  using a simpler spatial reconstruction again lowers the order by one
  For grid adaptivity and stabilization this is not really an issue?