UNIVERSITY OF LEEDS

School of Computing
Scientific Computation Group

Runge-Kutta Residual Distribution Schemes

Matthew Hubbard

and

Andrzej Warzyński

HONOM 2013, Bordeaux, 18-22 March 2013

Hyperbolic Conservation Laws

Consider the scalar conservation law

$$\partial_t u + \nabla \cdot \mathbf{f} \ = \ 0 \qquad \text{or} \qquad \partial_t u + \mathbf{a} \cdot \nabla u \ = \ 0$$

on a domain Ω.

- $\mathbf{a} = \frac{\partial \mathrm{f}}{\partial u}$ is the advective velocity of the flow.
- $u(\mathbf{x}, 0)$ is specified.
- $u(\mathbf{x}, t)$ is specified on inflow boundaries.

This work is aiming for high order accurate, oscillation-free approximations to this equation.

The Steady State Case

The residual on a 2D triangular element (E) is given by

$$\phi_E = \int_E \nabla \cdot \mathbf{f} \, \mathrm{d}\Omega = \oint_{\partial E} \mathbf{f} \cdot \mathbf{n} \, \mathrm{d}\Gamma$$

- $\mathbf{n}$ gives the outward pointing normal to the element boundary.
- u varies continuously and is stored at mesh nodes.
- In simple cases ϕ_E can be evaluated exactly using an appropriate (conservative) linearisation.

Residual Distribution Schemes

The aim is to solve the equations given by

$$\nabla \cdot \mathbf{f} \;\equiv\; 0 \qquad \longrightarrow \qquad \sum_{E \in \cup \triangle_i} \beta_i^E \, \phi_E \;=\; 0$$

This can be done iteratively, driving the ϕ_E to zero, by

- distributing each residual ϕ_E to its adjacent nodes,
- carefully choosing the distribution coefficients β_i^E,
- applying a simple pseudo-time-stepping algorithm:

$$S_i \, u_i^{n+1} \;=\; S_i \, u_i^n \;-\; \Delta t \sum_{E \in \cup \triangle_i} \beta_i^E \, \phi_E$$

Scheme Design

Ideally any residual distribution scheme would be

- Conservative – for discontinuity capturing.
- Positive – to prohibit unphysical oscillations.
- Linearity Preserving – for accuracy.
- Continuous – for convergence to steady state.
- Compact – for efficiency.
- Upwind – for physical realism.

Upwind Schemes

- N – linear, positive.
- LDA – linear, linearity preserving.
- PSI – nonlinear, positive and linearity preserving.
- Blended (N,LDA) – nonlinear, (almost) positive and linearity preserving.
  - Precise details depend on the blending.

These schemes, derived from a piecewise linear representation, provide the distribution coefficients β_i^E.

Time-Dependent Problems

UNIVERSITY OF LEEDS

- Simply applying high order pseudo-time-stepping doesn’t improve the accuracy for time-dependent problems beyond first order.

- However, Runge-Kutta time-stepping can be combined with:

  (i) a consistent mass matrix for an equivalent Petrov-Galerkin formulation;

  (ii) a space-time distribution.

The Finite Element Analogy

UNIVERSITY OF LEEDS

Residual distribution schemes:

- Integrate the conservation law over mesh elements.
- Distribute the integrated quantities to update nodes.

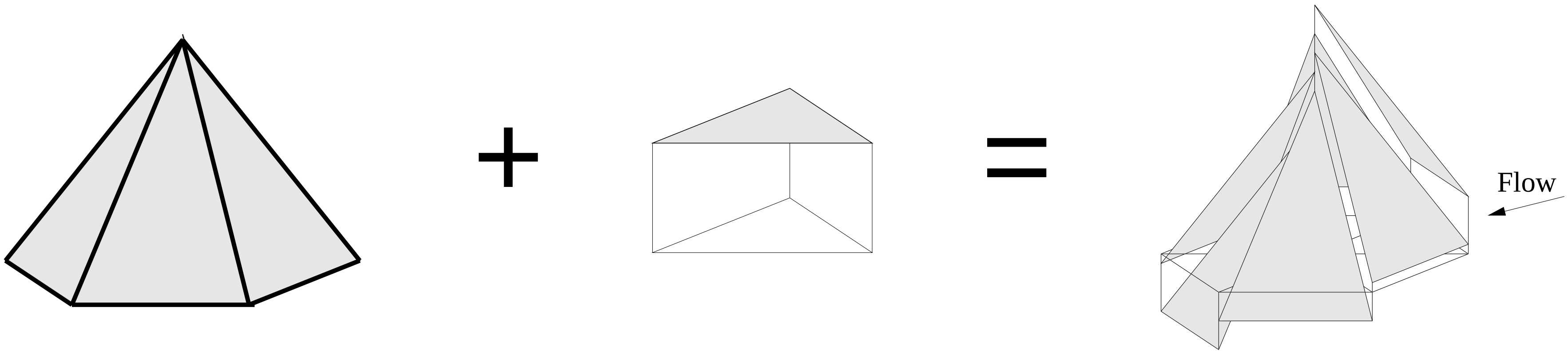
Finite element schemes:

- Integrate a distributed form of the conservation law over mesh elements.
- Assemble the integrated quantities to update nodes.

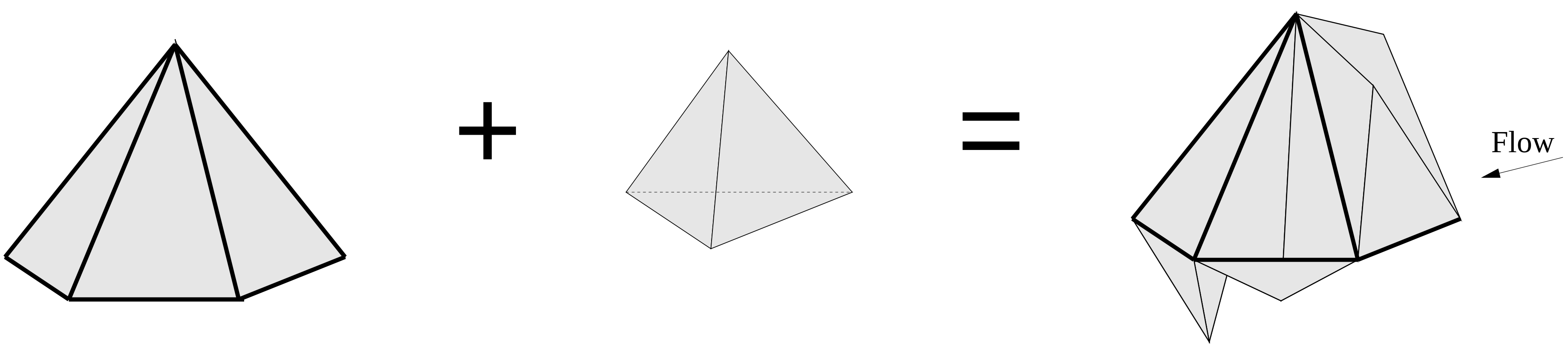
Both methods partition unity for conservation.

Stabilised Finite Elements

Locally constant perturbations, *cf.* SUPG:



Piecewise linear perturbations might be considered:



Consistent Mass Matrix

UNIVERSITY OF LEEDS

The pseudo-time-stepping is replaced by

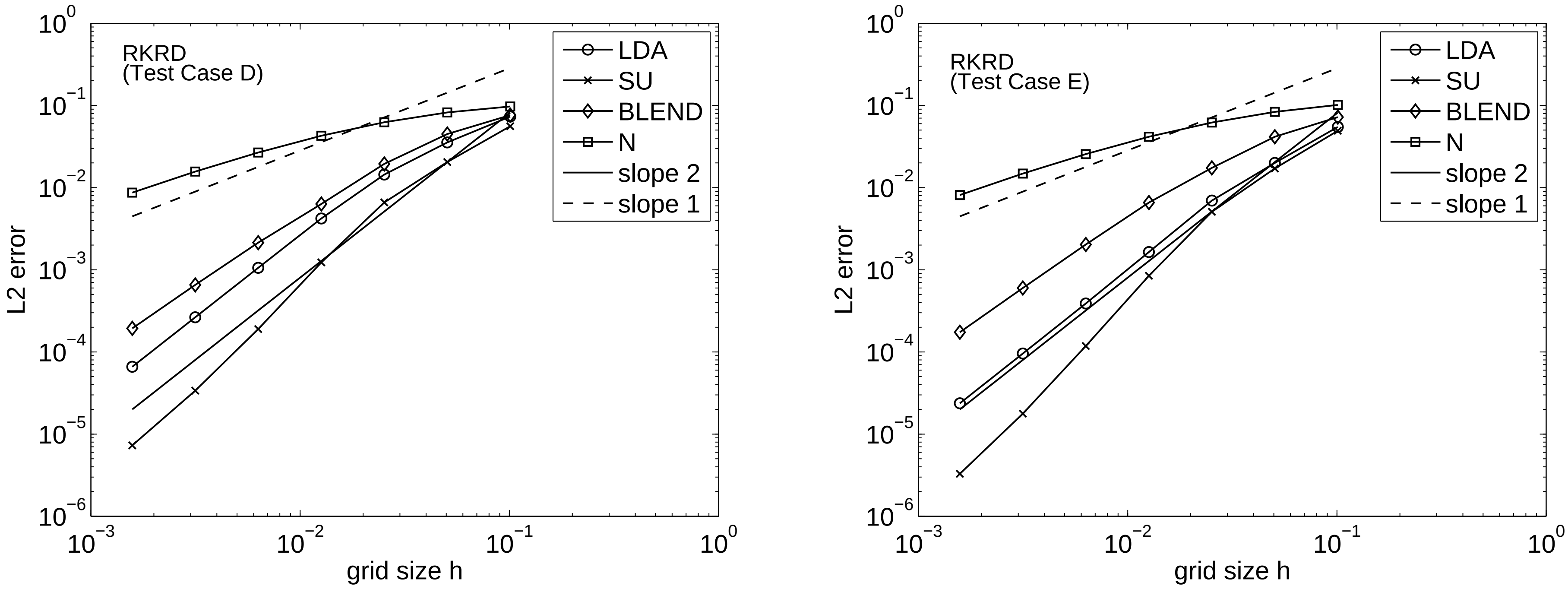
$$\sum_{E \in \cup \triangle_i} \sum_{j \in E} m_{ij}^E \frac{du_i}{dt} + \Delta t \sum_{E \in \cup \triangle_i} \beta_i^E \phi_E = 0$$

One possible form, for piecewise linears, gives

$$m_{ij}^E = \frac{|E|}{36}(3\delta_{ij} + 12\beta_i^E - 1)$$

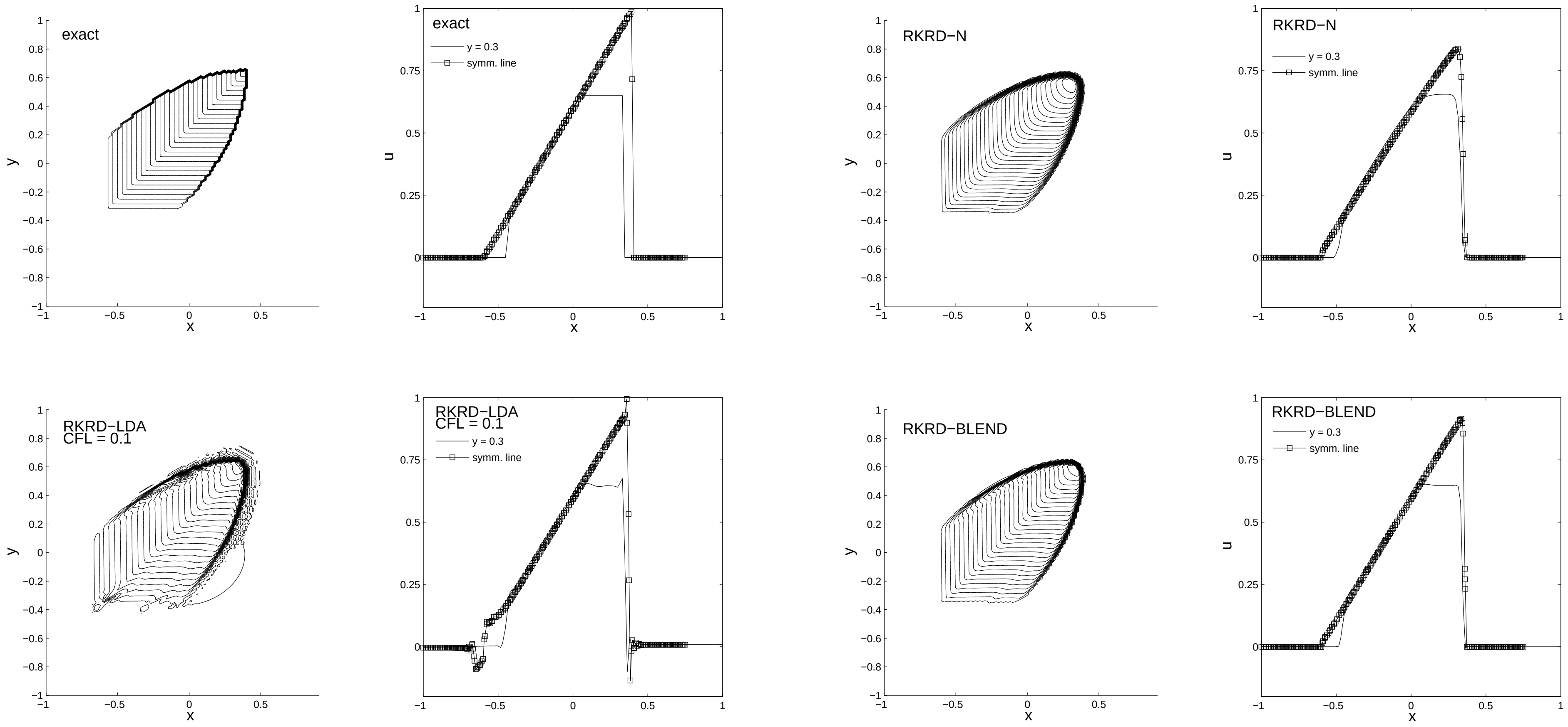
- The β_i^E can be evaluated at the old time level.
- Even with TVD RK time-stepping, positivity is lost.

Linear, Scalar



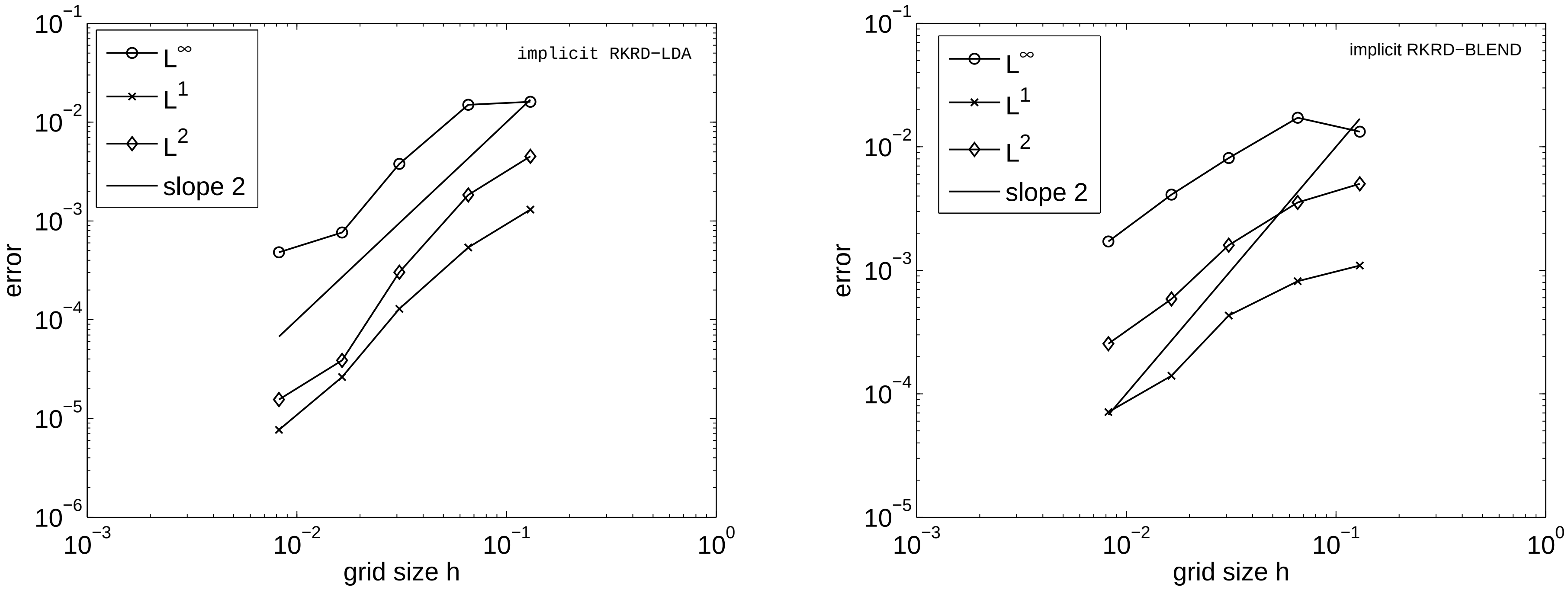
Smooth cone: constant (left) and rotational (right) advection.

Nonlinear, Scalar



Inviscid Burgers’ equation: Exact + N, LDA and Blend schemes.

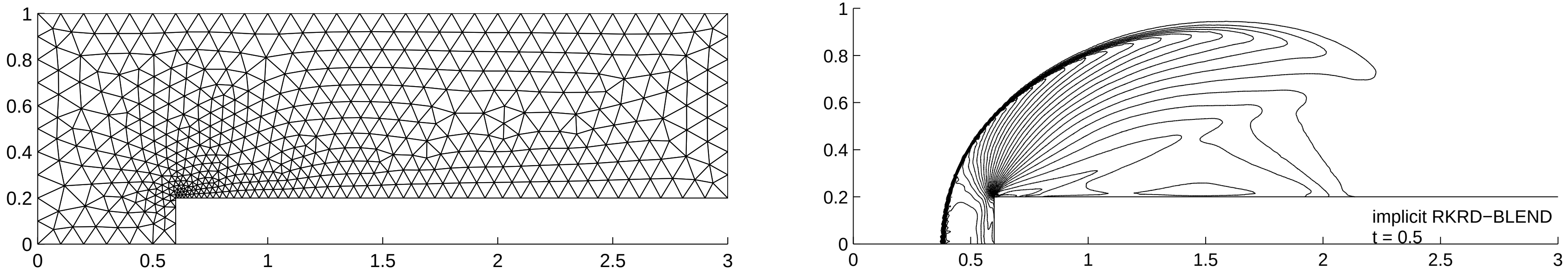
Nonlinear, System



Euler equations, travelling vortex: pressure errors, LDA (left) and blended (right) schemes.

Nonlinear, System

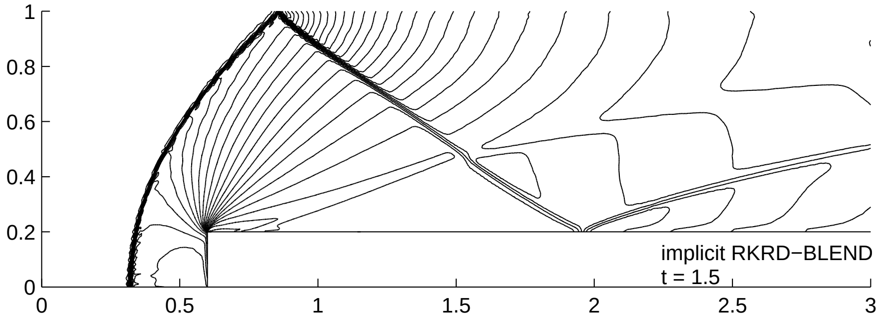
UNIVERSITY OF LEEDS

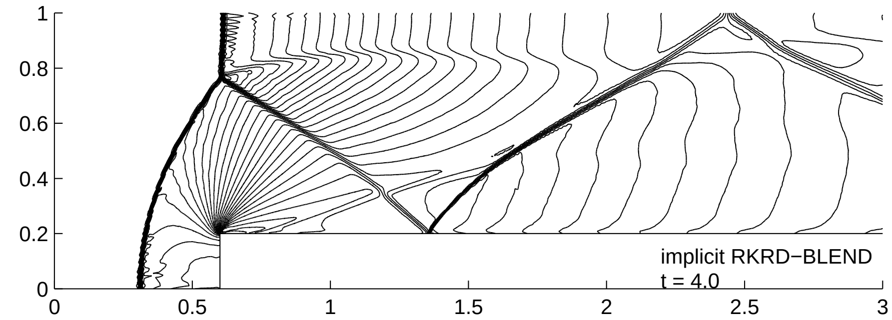


Euler equations, flow over a step: density contours.

Nonlinear, System

UNIVERSITY OF LEEDS





Euler equations, flow over a step: density contours.

Higher Order Accuracy

UNIVERSITY OF LEEDS

The order of accuracy of a linearity preserving scheme corresponds to the order of accuracy of the representation of the residual (Abgrall, 2001).

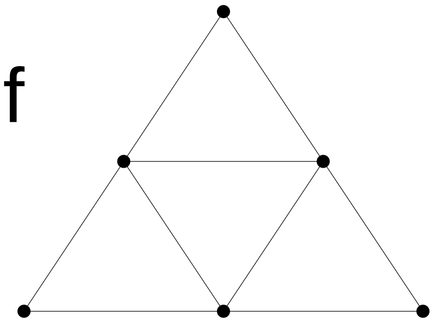
Therefore, to get a higher order scheme,

- create a higher order representation of u,
- use this to evaluate the residual,
- distribute this residual in a linearity preserving manner.

High Order Accuracy

UNIVERSITY OF LEEDS

- Cell subdivision (Abgrall & Roe, 2003),
  e.g. 4 subelements give 6 degrees of freedom, enough for piecewise continuous quadratics.



- Local derivative recovery (Caraeni *et al.*, 2001),
  e.g. gradient recovery at the nodes also gives enough for piecewise continuous quadratics.
- Extending the stencil (Hubbard & Mebrate, 2006),
  e.g. 6 nodes per element/edge is enough for piecewise continuous quadratics.

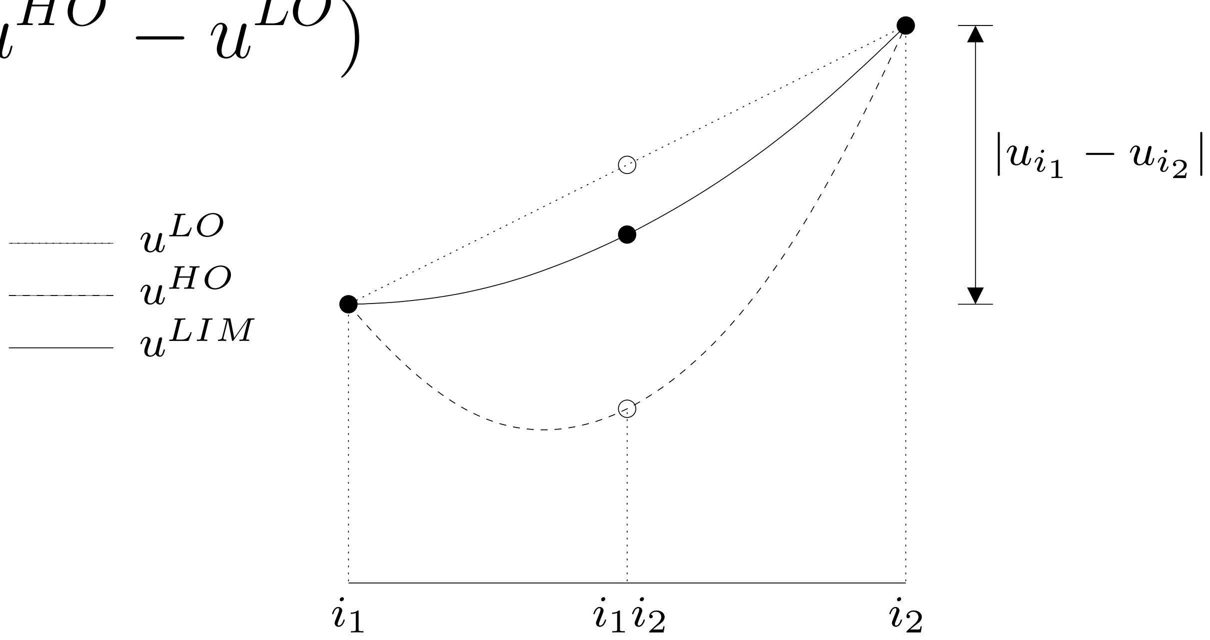
Combining With Positivity

The desired properties are all straightforward to achieve, except positivity.

Along each (sub)element edge take

$$u^{LIM} = u^{LO} + \gamma(u^{HO} - u^{LO})$$

where γ must be chosen appropriately for each edge.



Restricting the Interpolant

As long as $u^{LIM} - u^{LO}$ is bounded by $C\,\delta u_{edge}$ the affected residuals can always be distributed to the vertices of their own (sub)elements in a positive manner.

- Edge-based limiting guarantees conservation.
- The time-step must be restricted, but not by much.
- To guarantee positivity, upwinding is sacrificed.
- The γ can be chosen to give locally monotonic u.

(Hubbard, 2007)

A Space-Time Approach

The residual on a prismatic space-time element is

$$\phi_{E_t} \; = \; \int_{t^n}^{t^{n+1}} \int_E \left(\partial_t u + \nabla \cdot \mathbf{f}\right) \, \mathrm{d}\Omega$$

and should be evaluated exactly once supplied with u_h.

The aim is now to solve equations of the form

$$\partial_t u + \nabla \cdot \mathbf{f} \; \equiv \; 0 \qquad \longrightarrow \qquad \sum_{E \in \cup \triangle_i} \beta_i^{E_t} \, \phi_{E_t} \; = \; 0$$

with new distribution coefficients $\beta_i^{E_t}$.

Comments

UNIVERSITY OF LEEDS

- The temporal derivative term must be integrated consistently for full accuracy.
- Signals should only be sent forward in time.
- A PSI-like limiting procedure can create a linearity preserving scheme from a positive one, *i.e.*

$$(\beta_i^{E_t})^{LIM} = \frac{[(\beta_i^{E_t})^{LO}]^+}{\sum_{k \in E_t} [(\beta_k^{E_t})^{LO}]^+}$$

- Pseudo-time-stepping can still be applied:

$$S_i\, u_i^{(m+1)} = S_i\, u_i^{(m)} - \Delta\tau \sum_{E_t \in \cup \triangle_i} \beta_i^{E_t}\, \phi_{E_t}$$

A Second Order Scheme

UNIVERSITY OF LEEDS

Given a positive distribution of the spatial derivative terms, local updates take the form

$$\frac{|E|}{3}\begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^* \to \frac{|E|}{3}\begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^* - \Delta\tau\left[\frac{|E|}{3}\begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^* - \frac{|E|}{3}\begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^n + \Delta t\begin{pmatrix} \text{distribution} \\ \text{of Runge-Kutta} \\ \text{spatial terms} \end{pmatrix}\right]$$

and lead to a positive iteration. When u is linear

- The terms in the square brackets lead to low order distribution coefficients, β_i^{LO}.
- These can be limited for second order accuracy (Abgrall & Mezine, 2003).

Higher Than Second Order

UNIVERSITY OF LEEDS

Limiting the quadratic interpolant allows an element's "mass" to be written as a weighted sum of its vertex values, so a single element update can be written

$$\begin{pmatrix} D_i & 0 & 0 \\ 0 & D_j & 0 \\ 0 & 0 & D_k \end{pmatrix}^* \begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^* - \begin{pmatrix} D_i & 0 & 0 \\ 0 & D_j & 0 \\ 0 & 0 & D_k \end{pmatrix}^n \begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^n + \Delta t \begin{pmatrix} \text{distribution} \\ \text{of Runge-Kutta} \\ \text{spatial terms} \end{pmatrix}$$

- In the piecewise linear case, $\mathbf{D} = |E|\,\mathbf{I}/3$, is independent of the data.
- In the high order case $\mathbf{D}$ is a diagonal matrix which depends on the data, specifically

$$D_i = |E|(1 + \gamma'_{ki} - \gamma'_{ij})/3 \qquad \text{etc.}$$

Notes

- If the interpolant wasn't limited, the elements of $\mathbf{D}$ could become unbounded.
- If $C \leq 0.5$ in the limiting of the interpolant along each edge then the elements of $\mathbf{D}$ are guaranteed to be positive.
- In general $\mathbf{D}^* \neq \mathbf{D}^n$, even when they are bounded and positive, so a positive discretisation of the spatial terms does not guarantee a maximum principle overall because

$$u_i^{n+1} = \sum_{\text{nodes}} w_j u_j^n \quad \text{where} \quad w_j \geq 0 \quad \text{but} \quad \sum_{\text{nodes}} w_j \neq 1$$

Limiting the Mass Matrix

The mass at the new time level can be related to the mass at the old time level, *i.e.*

$$\begin{pmatrix} D_i^* & 0 & 0 \\ 0 & D_j^* & 0 \\ 0 & 0 & D_k^* \end{pmatrix} = \begin{pmatrix} D_i^n - \psi_{ij} + \psi_{ki} & 0 & 0 \\ 0 & D_j^n - \psi_{jk} + \psi_{ij} & 0 \\ 0 & 0 & D_k^n - \psi_{ki} + \psi_{jk} \end{pmatrix}$$

where the $\psi = \frac{|E|}{3}(\gamma'^* - \gamma'^n)$.

- It is also possible to write D^n in terms of D^* and follow a similar process.

Limiting the Mass Matrix

UNIVERSITY OF LEEDS

The element's "mass" can be redistributed locally, *i.e.*

$$\mathbf{D}^* \rightarrow \begin{pmatrix} D_i^n - \psi_{ij}^- + \psi_{ki}^+ & \psi_{ij}^- & -\psi_{ki}^+ \\ -\psi_{ij}^+ & D_j^n - \psi_{jk}^- + \psi_{ij}^+ & \psi_{jk}^- \\ \psi_{ki}^- & -\psi_{jk}^+ & D_k^n - \psi_{ki}^- + \psi_{jk}^+ \end{pmatrix}$$

- This leads to a conservative method because each column sums to $D_\cdot^*$.
- This is an M-matrix when $C \leq 0.25$ in the limiting of the interpolant along each edge.

Solving the New System

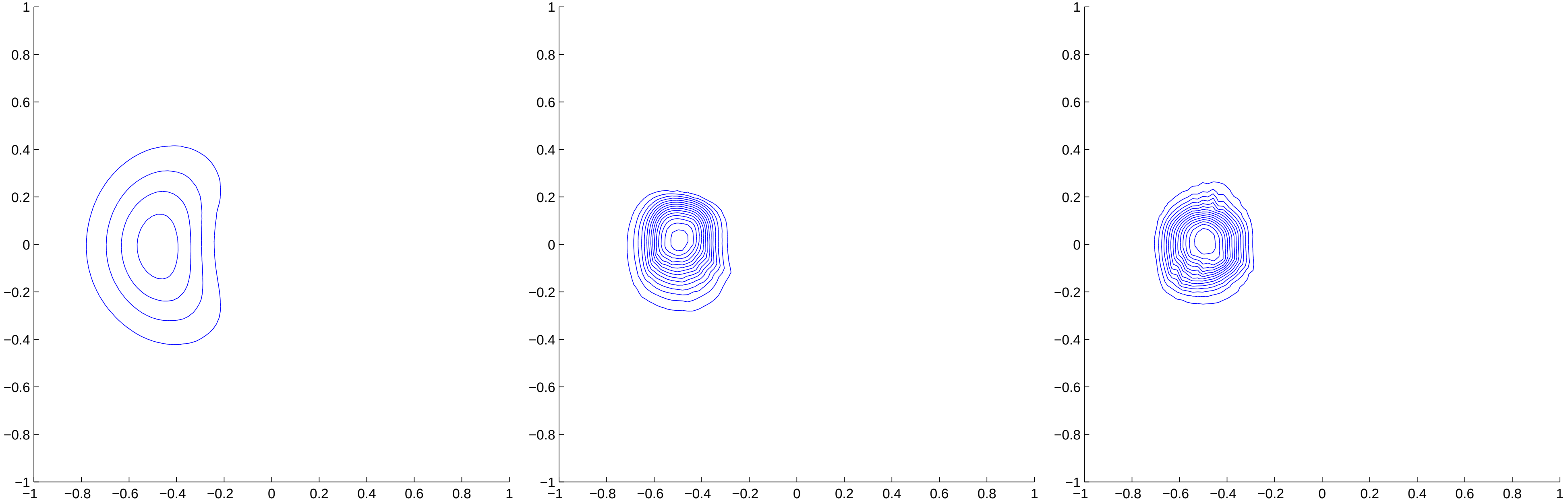
UNIVERSITY OF LEEDS

For each mesh element, assemble the following:

$$
\begin{aligned}
\frac{|E|}{3}\begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^* \rightarrow \frac{|E|}{3}\begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^* \\
- \Delta\tau \left[\begin{pmatrix} D_i^n - \psi_{ij}^- + \psi_{ki}^+ & \psi_{ij}^- & -\psi_{ki}^+ \\ -\psi_{ij}^+ & D_j^n - \psi_{jk}^- + \psi_{ij}^+ & \psi_{jk}^- \\ \psi_{ki}^- & -\psi_{jk}^+ & D_k^n - \psi_{ki}^- + \psi_{jk}^+ \end{pmatrix} \begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^* \right. \\
\left. - \begin{pmatrix} D_i & 0 & 0 \\ 0 & D_j & 0 \\ 0 & 0 & D_k \end{pmatrix}^n \begin{pmatrix} u_i \\ u_j \\ u_k \end{pmatrix}^n + \Delta t \begin{pmatrix} \text{distribution} \\ \text{of Runge-Kutta} \\ \text{spatial terms} \end{pmatrix} \right]
\end{aligned}
$$

This leads to a positive iteration as long as the discretisation of the spatial terms is positive and $\Delta\tau$ is small enough.

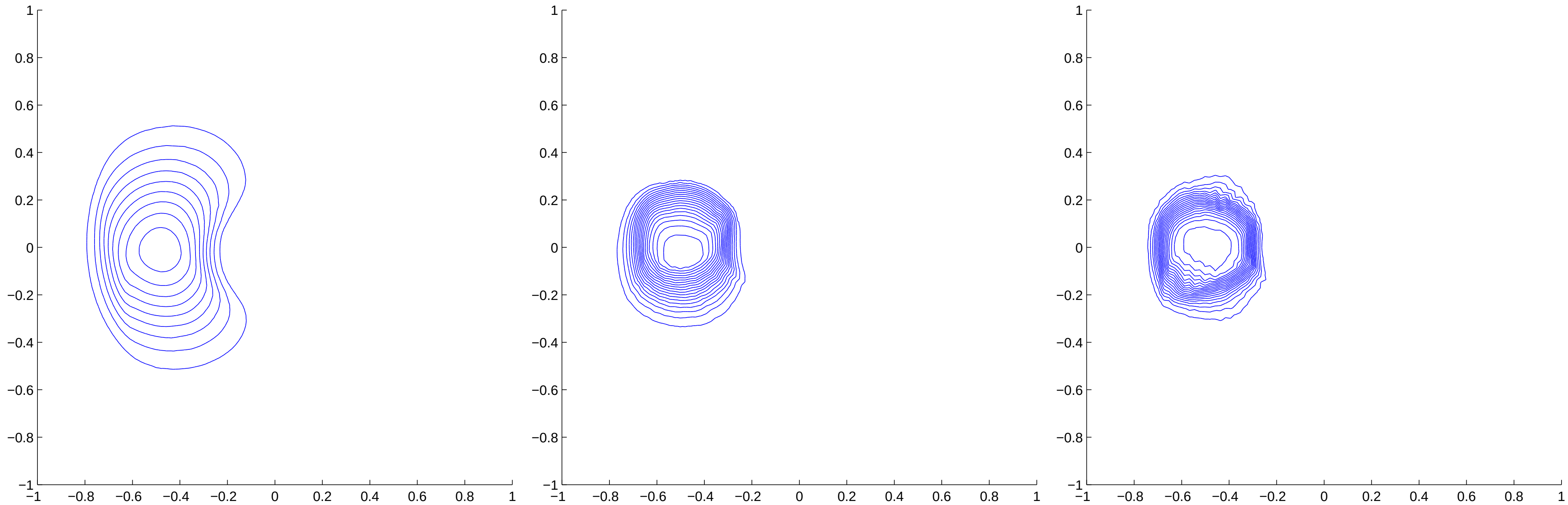
Comparison of Results



Rotating cone after one revolution for first order (left), second order (middle) and third order (right) positive methods. Maximum values of u are 0.2577, 0.7702 and 0.7760, respectively.

Comparison of Results

UNIVERSITY OF LEEDS



Rotating cylinder after one revolution for first order (left), second order (middle) and third order (right) positive methods. Maximum values of u are 0.4828, 0.9844 and 0.9752, respectively.

Summary

UNIVERSITY OF LEEDS

- For time-dependent problems, higher order accuracy requires consistent spatial integration of the time derivative.
- This can be done by introducing a mass matrix, at the expense of positivity.
- It is simpler to avoid oscillations in a space-time framework.
- With careful limiting, it may be possible to combine higher than second order accuracy with positivity.