# Automated parameters for troubled-cell indicators using outlier detection

Thea Vuik
Delft University of Technology

Collaboration with Jennifer Ryan, University of East Anglia

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# Outline

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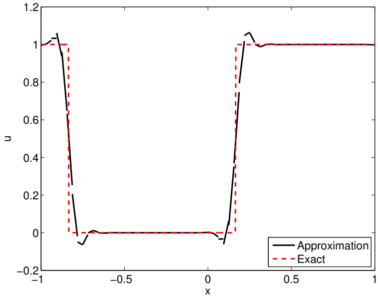
# Introduction: research topic

Nonlinear hyperbolic PDE's:

- Solutions contain shocks or develop discontinuities
- Numerical approximations develop spurious oscillations




How to remove oscillations?

- Filtering
- Adding artificial viscosity
- Limiting

# Introduction: limiters

Limiters: moment limiter, WENO limiter

- Too few elements: oscillatory approximation
- Too many elements: too diffusive, computationally expensive

How to find elements which need limiting?

Troubled-cell indicator: detects discontinuous elements

# Introduction: troubled-cell indicators

Examples of troubled-cell indicators for DG:

- minmod-based TVB indicator
  (Cockburn and Shu, Math. Comput. 1989)
- KXRCF indicator
  (Krivodonova et al., Appl. Numer. Math. 2004)
- multiwavelet troubled-cell indicator
  (V. and Ryan, J. Comput. Phys. 2014)

# Outline



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# Discontinuous Galerkin method

$$\begin{cases} u_t + f(u)_x = 0, & x \in [-1,1], \quad t > 0, \\ u(x,0) = u_0(x), & x \in [-1,1]. \end{cases}$$

- Discretize $[-1,1]$ into $2^n$ elements
- DG approximation: for $x \in I_j$, write,

$$u_h(x) = \sum_{\ell=0}^{k} u_j^{(\ell)} \phi_\ell(\xi_j), \quad \xi_j = \frac{2}{\Delta x}(x - x_j)$$

- Orthonormal Legendre polynomials: $\int_{-1}^{1} \phi_\ell \phi_m dx = \delta_{\ell m}$
- $k$: highest polynomial degree of the approximation

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# Discontinuous Galerkin method

$$u_t + f(u)_x = 0$$

- Approximation space $V_h^k$: $k$th-degree piecewise polynomials
- Approximate $u$ by $u_h \in V_h^k$

- Multiply PDE by $v_h \in V_h^k$, integrate over $I_j$:

$$\int_{I_j} (u_h)_t v_h dx = -\int_{I_j} f(u_h)_x v_h dx$$

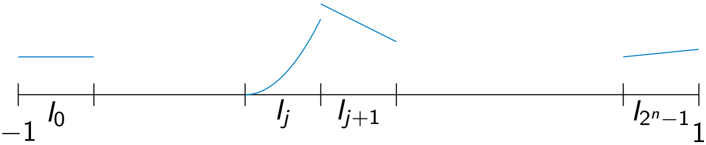
- Integrate by parts:

$$\int_{I_j} (u_h)_t v_h dx = \int_{I_j} f(u_h)(v_h)_x dx + \hat{f}_{j-\frac{1}{2}} (v_h)^+_{j-\frac{1}{2}} - \hat{f}_{j+\frac{1}{2}} (v_h)^-_{j+\frac{1}{2}}$$

# Global DG approximation

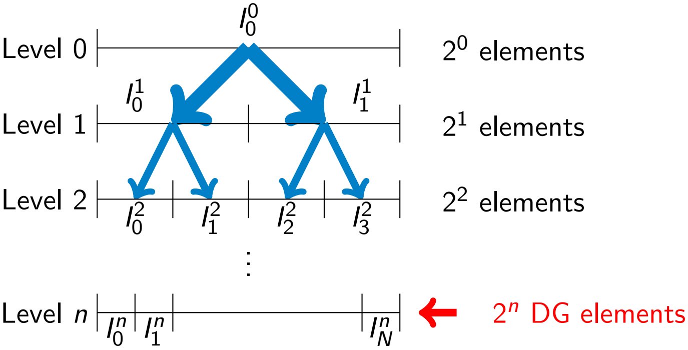
Global DG approximation, $2^n$ elements on $[-1, 1]$:

$$u_h(x) = \sum_{j=0}^{2^n-1} \sum_{\ell=0}^{k} u_j^{(\ell)} \phi_\ell(\xi_j)$$




Discontinuous at element boundaries!

# Multiresolution idea

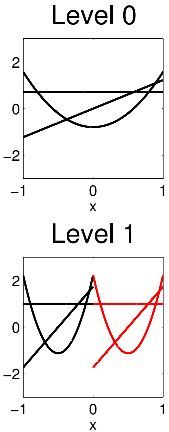



$$V_n^k = \{f : f \in \mathbb{P}^k(I_j^n), j = 0, \ldots, 2^n - 1\}$$

$$V_0^k \subset V_1^k \subset \cdots \subset V_n^k \subset \cdots$$

(Alpert, SIAM J. Math. Anal. 1993)

# Scaling functions and DG basis




DG basis functions:

- Orthonormal Legendre polynomials
- Basis for $V_0^k$ : scaling function basis
- Basis functions for $V_n^k$: dilation and translation

$$\phi_{\ell j}^n(x) = 2^{n/2}\phi_\ell(2^n(x+1) - 2j - 1),$$

$$\ell = 0, \ldots, k,\ j = 0, \ldots, 2^n - 1,\ x \in I_j^n$$

(Archibald et al., Appl. Num. Math. 2011)

# Multiwavelets

$$V_m^k = \{f : f \in \mathbb{P}^k(I_j^m), j = 0, \dots, 2^m - 1\}$$

Multiwavelet space $W_m^k$:

- Orthogonal complement of $V_m^k$ in $V_{m+1}^k$:

$$V_m^k \oplus W_m^k = V_{m+1}^k, \quad W_m^k \perp V_m^k, \quad W_m^k \subset V_{m+1}^k$$

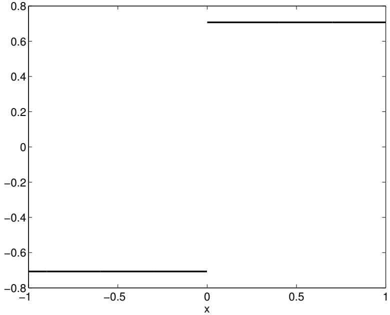
- $V_n^k$ can be split into $n+1$ orthogonal subspaces:

$$V_n^k = V_0^k \oplus W_0^k \oplus W_1^k \oplus \cdots \oplus W_{n-1}^k$$

Split up $f \in V_n^k$ into different levels

# Example: Haar wavelet

$k = 0$: Haar wavelets
Basis: piecewise constants on $I_0^1 = [-1, 0]$ and $I_1^1 = [0, 1]$




Haar wavelets, level 0

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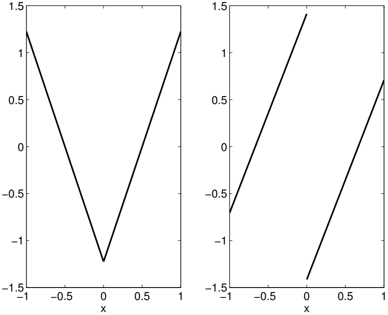
# Multiwavelets




Multiwavelet basis, $k = 1$

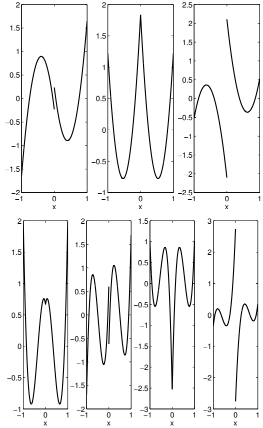
Formulae for $x \in (0,1)$:

$$\psi_0(x) = \sqrt{\frac{3}{2}}(-1+2x), \text{ even in } 0$$

$$\psi_1(x) = \sqrt{\frac{1}{2}}(-2+3x), \text{ odd in } 0$$

(Alpert, SIAM J. Math. Anal. 1993)

# Multiwavelets




Multiwavelets, $k = 2$ (top) and $k = 3$ (bottom)

$$\psi_0(x) = \frac{1}{3}\sqrt{\frac{1}{2}}(1 - 24x + 30x^2)$$

$$\psi_1(x) = \frac{1}{2}\sqrt{\frac{3}{2}}(3 - 16x + 15x^2)$$

$$\psi_2(x) = \frac{1}{3}\sqrt{\frac{5}{2}}(4 - 15x + 12x^2)$$

$$\psi_0(x) = \sqrt{\frac{15}{34}}(1 + 4x - 30x^2 + 28x^3)$$

$$\psi_1(x) = \sqrt{\frac{1}{42}}(-4 + 105x - 300x^2 + 210x^3)$$

$$\psi_2(x) = \frac{1}{2}\sqrt{\frac{35}{34}}(-5 + 48x - 105x^2 + 64x^3)$$

$$\psi_3(x) = \frac{1}{2}\sqrt{\frac{5}{42}}(-16 + 105x - 192x^2 + 105x^3)$$

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# Multiwavelets and DG

$$V_n^k = V_0^k \oplus W_0^k \oplus W_1^k \oplus \cdots \oplus W_{n-1}^k$$

Relation between DG and multiwavelets ($2^n$ elements):

$$\begin{aligned} u_h(x) &= \sum_{j=0}^{2^n-1} \sum_{\ell=0}^{k} u_j^{(\ell)} \phi_\ell(\xi_j) \\ &= \underbrace{\sum_{\ell=0}^{k} s_{\ell 0}^{0} \phi_\ell(x)}_{\substack{\text{global average} \\ \in V_0^k}} + \underbrace{\sum_{m=0}^{n-1} \sum_{j=0}^{2^m-1} \sum_{\ell=0}^{k} d_{\ell j}^{m} \psi_{\ell j}^{m}(x)}_{\substack{\text{finer details} \\ \in W_m^k}} \end{aligned}$$

Coefficients computed by decomposition method

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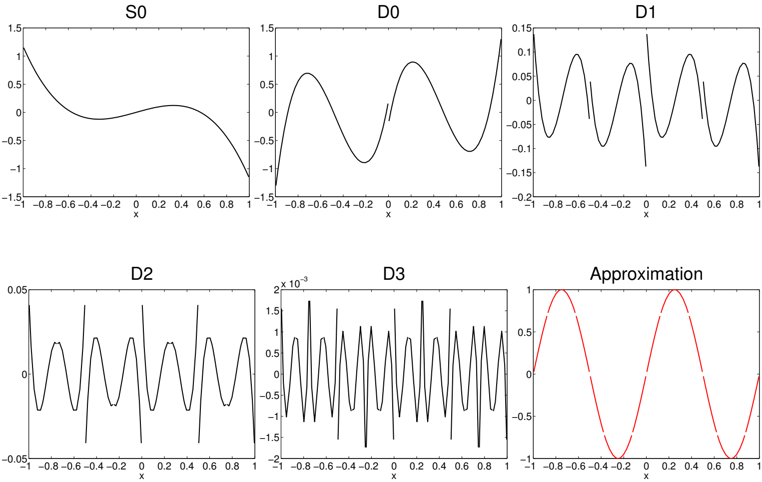
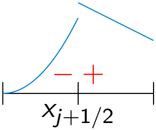
# Example: $\sin(2\pi x), n = 4, k = 3$

Projection on DG basis, multiwavelet decomposition



# Jumps in DG approximations

$$u_h(x) = \sum_{\ell=0}^{k} s_{\ell 0}^{0} \phi_\ell(x) + \sum_{m=0}^{n-1} \sum_{j=0}^{2^m-1} \sum_{\ell=0}^{k} d_{\ell j}^{m} \psi_{\ell j}^{m}(x)$$




Coefficient $d_{\ell j}^{n-1}$: measures jump in (derivatives) approximation

$$d_{\ell j}^{n-1} = \sum_{m=0}^{k} c_{m\ell}^{n} \left( u_h^{(m)}(x_{j+1/2}^{+}) - u_h^{(m)}(x_{j+1/2}^{-}) \right),$$

where

$$c_{m\ell}^{n} = \frac{2^{(-n+1)m}}{m!} \cdot \int_0^1 x^m \psi_\ell(x)\, dx.$$

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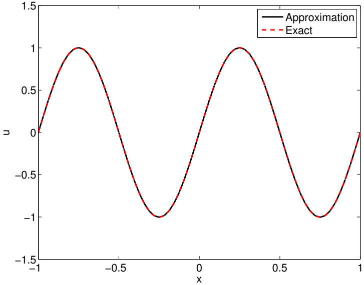
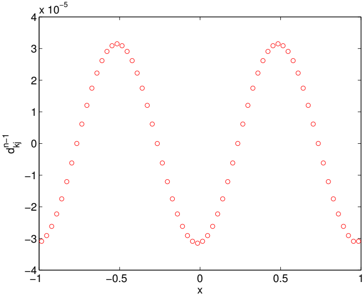
# Example: sine



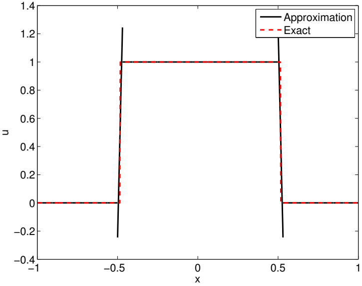

Approximation



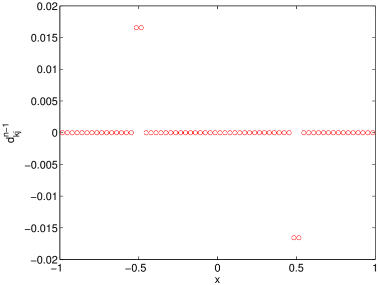

$d_{kj}^{n-1}$

64 elements, $k = 1$

# Example: square wave




Approximation




$d_{kj}^{n-1}$

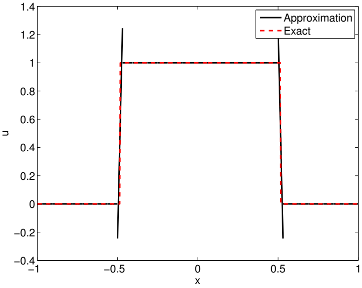
64 elements, $k = 1$

# Outline

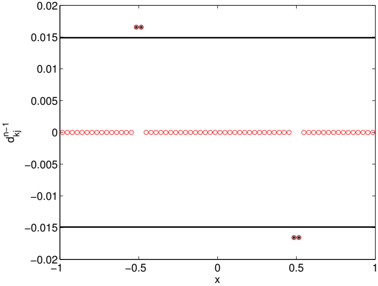
# Original approach

Detect elements $I_j$ and $I_{j+1}$ if

$$|d_{kj}^{n-1}| > C \cdot \max_j |d_{kj}^{n-1}|, C \in [0, 1].$$



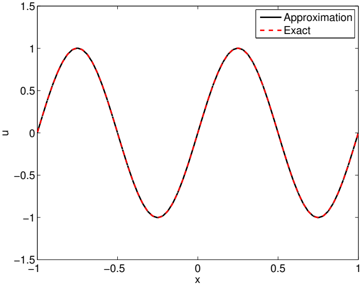

Approximation

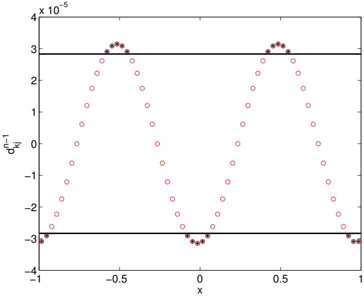



Detected, $C = 0.9$

64 elements, $k = 1$

# Problem I: continuous function



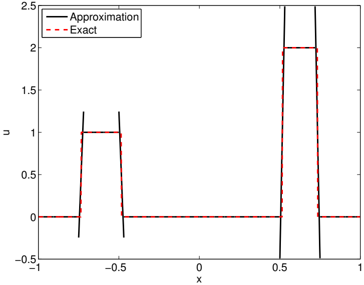




Approximation

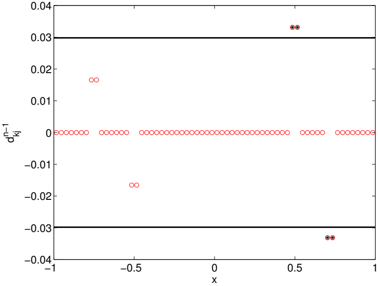
Detected, $C = 0.9$

64 elements, $k = 1$

# Problem II: different discontinuities




Approximation




Detected, $C = 0.9$

64 elements, $k = 1$

How to choose $C$?

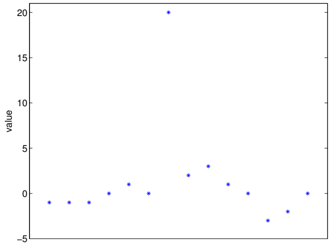
# Outline

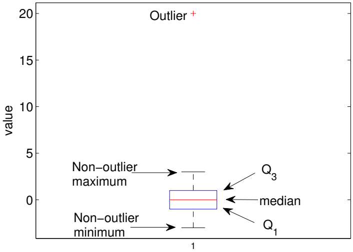
# Outlier detection

$d_{kj}^{n-1}$:

- vector containing jumps over element boundaries
- coefficient big compared to neighbors: detect

$\Rightarrow$ Boxplot approach




(Tukey, 1977)

# Outlier-detection algorithm

1. Send in troubled-cell indication vector **d**
2. Sort **d** to obtain $\mathbf{d}^s$
3. Compute quartiles of $\mathbf{d}^s$: $Q_1$ and $Q_3$
4. Construct outer fences:

$$Q_1 - 3(Q_3 - Q_1) \text{ and } Q_3 + 3(Q_3 - Q_1)$$

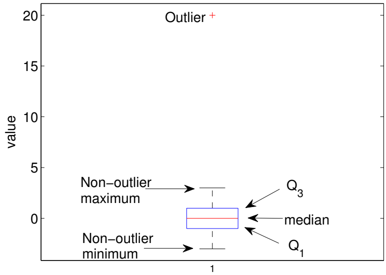
5. Determine outliers:

$$d_j < Q_1 - 3(Q_3 - Q_1) \text{ or } d_j > Q_3 + 3(Q_3 - Q_1)$$

# Boxplot

$$\mathbf{d} = \begin{pmatrix} -1 \\ -1 \\ -1 \\ 0 \\ 1 \\ 0 \\ 20 \\ 2 \\ 3 \\ 1 \\ 0 \\ -3 \\ -2 \\ 0 \end{pmatrix}, \quad \mathbf{d}^s = \begin{pmatrix} -3 \\ -2 \\ -1 \\ -1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 2 \\ 3 \\ 20 \end{pmatrix}$$

- 25th and 75th percentiles:
  $Q_1 = -1, \quad Q_3 = 1$
- Lower bound:
  $Q_1 - 3(Q_3 - Q_1) = -7$
- Upper bound:
  $Q_3 + 3(Q_3 - Q_1) = 7$



# Whisker length

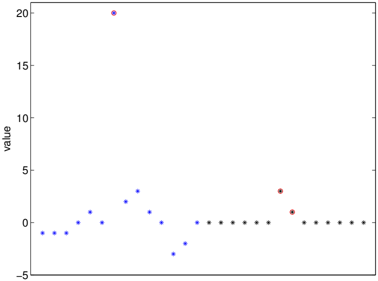
$$d_j < Q_1 - W \cdot (Q_3 - Q_1) \text{ or } d_j > Q_3 + W \cdot (Q_3 - Q_1)$$

Whisker length 3:

- Coverage of 99.9998%
- Normally distributed: 0.0002% detected asymptotically
- Few false positives if data well behaved
- Continuous function: no elements are detected!

(Hoaglin et al., J. Amer. Statist. Assoc. (1986))

# Local information




- Divide global vector in local vectors
- Apply boxplot approach for each local vector
- Ignore 'outliers' near split boundaries

# Outline

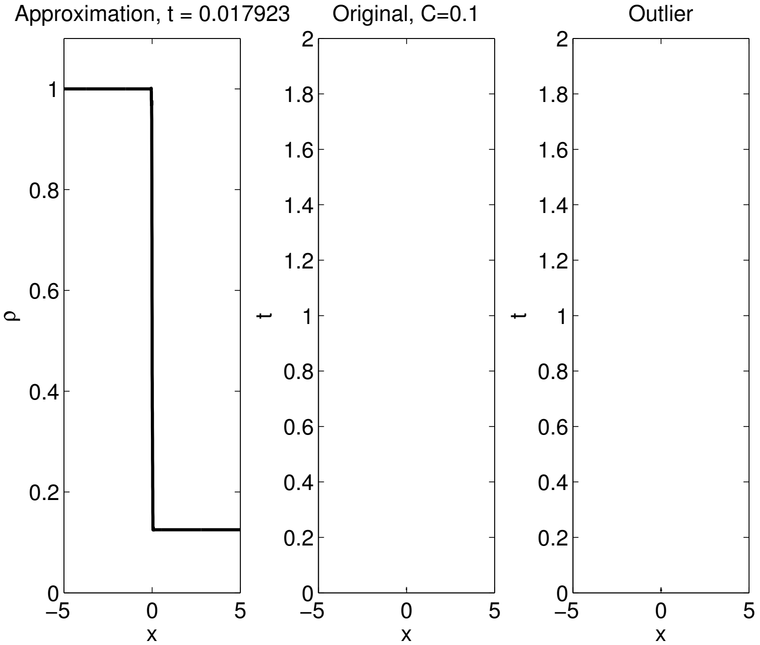
# Applications

Applications:

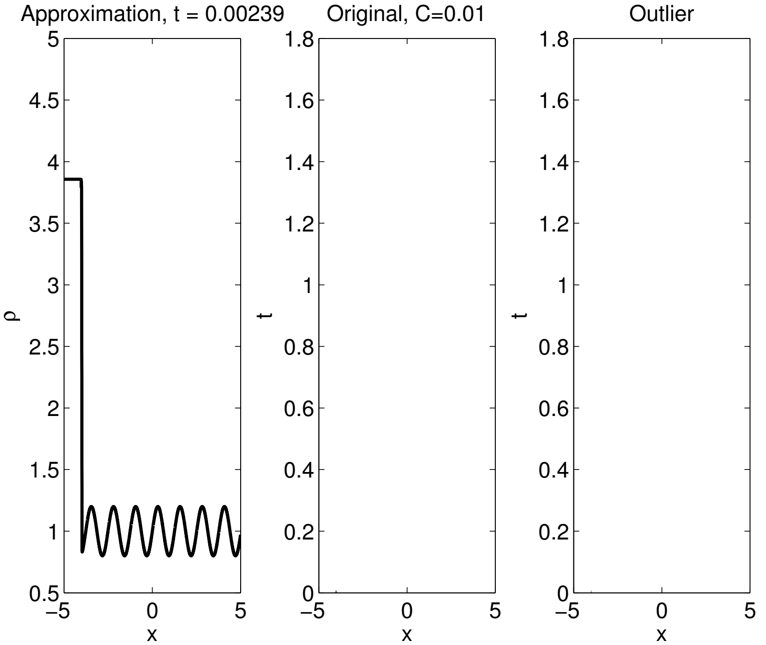
- Apply original indicator with optimal parameter $C$
- Compare with outlier-detected results (no parameter)

Euler equations:

- 1d: Sod's shock tube, sine-entropy wave
- 2d: double Mach reflection problem



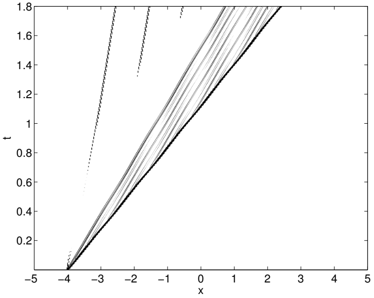
Approximation, t = 0.017923
Original, C=0.1
Outlier
ρ
t
t
x
x
x


Approximation, t = 0.00239
Original, C=0.01
Outlier
ρ
t
t
x
x
x
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
–5
0
5

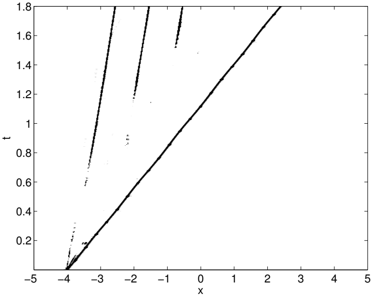
# Minmod-based TVB indicator

$$u^-_{j+\frac{1}{2}} = \bar{u}_j + \tilde{u}_j, \quad \tilde{u}_j = \sum_{\ell=1}^{k} u_j^{(\ell)} \phi_\ell(1)$$

$$u^+_{j-\frac{1}{2}} = \bar{u}_j - \tilde{\tilde{u}}_j, \quad \tilde{\tilde{u}}_j = -\sum_{\ell=1}^{k} u_j^{(\ell)} \phi_\ell(-1)$$




$M = 100$




Outlier

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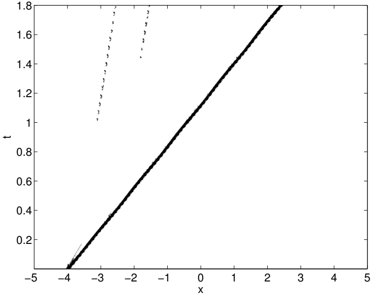
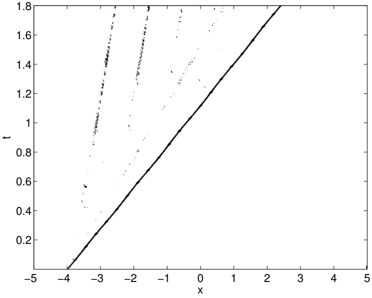
# KXRCF detector

Jump across inflow edge:

$$\mathcal{I}_j = \left| \int_{\partial I_j^-} (u_h|_{I_j} - u_h|_{I_{n_j}}) ds \right|$$

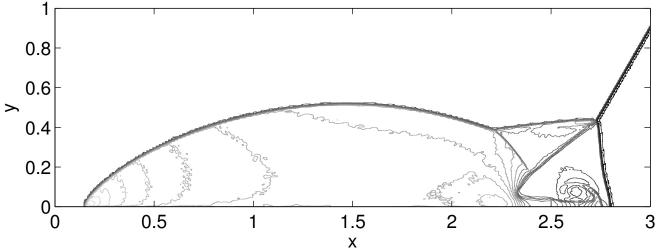



Threshold equal to 1

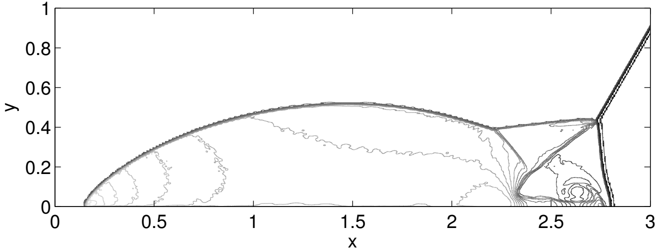



Outlier

# Double Mach reflection: contour plots




Original
$C = 0.05$




Outlier

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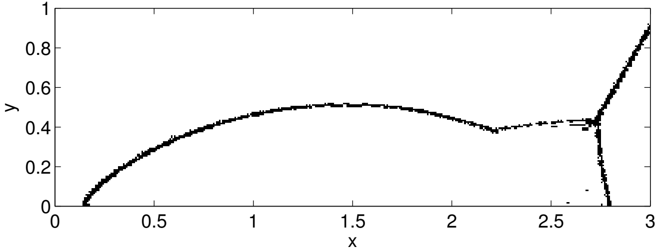
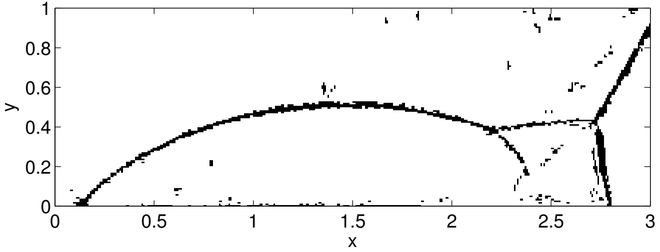
# Double Mach reflection: troubled cells




Original
$C = 0.05$




Outlier

# Conclusion and future research

- Original troubled-cell indicators: problem-dependent parameter
- Outlier-detection technique using boxplots
- Local-vector approach
- Parameters no longer needed!

- Proof on smooth functions
- General meshes