Multiwavelets and outlier detection for troubled-cell indication

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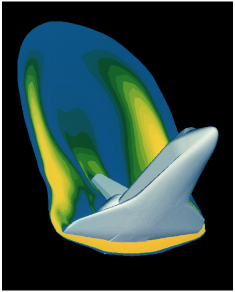
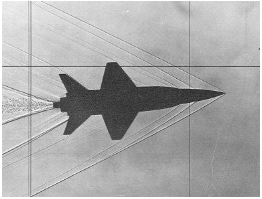
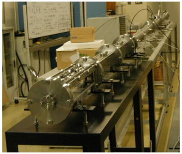
Applied Mathematics seminar
University of East Anglia
May 23, 2016

Motivation

Flow around Space Shuttle | Shock wave | Shock tube

Motivation

Model phenomena using partial differential equation (PDE)

Example:
Tracer concentration q in fluid flowing through pipe:

$$\frac{\partial q}{\partial t} + c\frac{\partial q}{\partial x} = 0$$

c is fluid velocity

Rate of change depends on flux

Motivation

Hyperbolic partial differential equation:

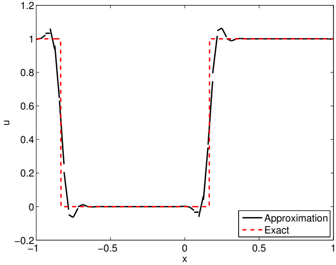
$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, & x \in [-1,1], \quad t > 0, \\ u(x,0) = u_0(x), & x \in [-1,1]. \end{cases}$$

- Exact solution is not known
- Difficult to approximate solution
- Usually, discontinuities arise during time integration

Motivation

Discontinuities → spurious oscillations!

Example: tracer concentration suddenly drops



Remove wiggles by:

- Limiting
- Filtering
- Adding artificial viscosity

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Motivation

Limiters:

- Advantage: approximation no longer oscillatory
- Disadvantage: limits smooth extrema, too diffusive

Troubled-cell indicator: detects discontinuous regions

Motivation

Troubled-cell indicators:

- KXRCF shock detector
  (Krivodonova et al., APNUM 2004)
- Minmod-based TVB indicator
  (Cockburn and Shu, Math. Comp. 1989)

Multiwavelet troubled-cell indicator & outlier detection

Outline

Outline

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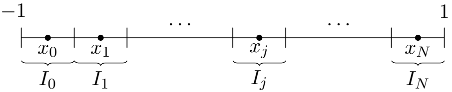
Discontinuous Galerkin method

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

Step 1: Discretize in space:

$$x_j = -1 + (j + \frac{1}{2})\Delta x, \quad j = 0, \dots, N.$$



(Cockburn, Springer, 1998)

Discontinuous Galerkin method

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0$$

Step 2:

- Multiply PDE by test function v
- Integrate over I_j

$$\int_{I_j} \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} \right) v dx = 0$$

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DG approximation

$$\int_{I_j} \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} \right) v dx = 0$$

Step 3: Integrate by parts

Use that

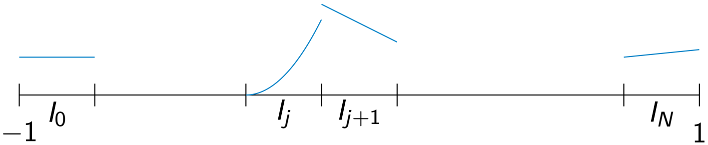
$$\int_{I_j} \frac{\partial uv}{\partial x} dx = \int_{I_j} \frac{\partial u}{\partial x} v dx + \int_{I_j} u \frac{dv}{dx} dx$$

to find

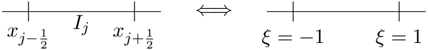
$$\int_{I_j} \frac{\partial u}{\partial t} v dx = \int_{I_j} u \frac{dv}{dx} dx - uv\Big|_{x_{j-1/2}}^{x_{j+1/2}}$$

Discontinuous Galerkin method

Step 4: Approximate solution by piecewise polynomial, degree k



$$\xi_j = 2/\Delta x \cdot (x - x_j)$$



Global coordinates Local coordinates

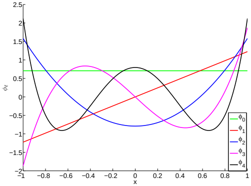
Discontinuous Galerkin method

- Basis of monomials $\{1, x, \ldots, x^k\}$:

$$u_h(x) = a_j^{(0)} + a_j^{(1)}\xi + \cdots + a_j^{(k)}\xi^k$$

- Basis of scaled Legendre polynomials $\{\phi_0, \phi_1, \ldots, \phi_k\}$:

$$u_h(x) = u_j^{(0)}\phi_0(\xi) + u_j^{(1)}\phi_1(\xi) + \cdots + u_j^{(k)}\phi_k(\xi)$$



DG approximation

$$\int_{I_j} \frac{\partial u}{\partial t} v dx = \int_{I_j} u \frac{dv}{dx} dx - uv|_{x_{j-1/2}}^{x_{j+1/2}}$$

Step 5:

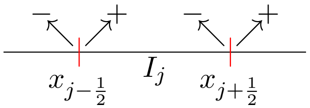
- Replace u (exact solution) by DG approximation
- Replace v by $\phi_m(\xi)$ (Legendre polynomial)
- Use that $\int_{-1}^{1} \phi_\ell(\xi)\phi_m(\xi) d\xi = \delta_{\ell m}$

$$\frac{\Delta x}{2} \frac{du_j^{(m)}(t)}{dt} = \sum_{\ell=0}^{k} u_j^{(\ell)}(t) \int_{-1}^{1} \phi_\ell(\xi)\phi_m'(\xi) d\xi$$
$$- \hat{u}_h(x_{j+\frac{1}{2}}, t)\phi_m(1) + \hat{u}_h(x_{j-\frac{1}{2}}, t)\phi_m(-1)$$

DG approximation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0$$

Step 6: Choose fluxes $\hat{u}_h(x_{j\pm\frac{1}{2}})$



Boundaries of element I_j

Initial condition travels right:

$$\hat{u}_h(x_{j-\frac{1}{2}}) = u_h(x^-_{j-\frac{1}{2}}) \quad \hat{u}_h(x_{j+\frac{1}{2}}) = u_h(x^-_{j+\frac{1}{2}})$$

DG approximation

$$\frac{\Delta x}{2}\frac{du_j^{(m)}(t)}{dt} = \sum_{\ell=0}^{k} u_j^{(\ell)}(t)\int_{-1}^{1}\phi_\ell(\xi)\frac{d}{d\xi}\phi_m(\xi)d\xi$$
$$-\left(\sum_{\ell=0}^{k} u_j^{(\ell)}(t)\phi_\ell(1)\right)\phi_m(1)$$
$$+\left(\sum_{\ell=0}^{k} u_{j-1}^{(\ell)}(t)\phi_\ell(1)\right)\phi_m(-1)$$

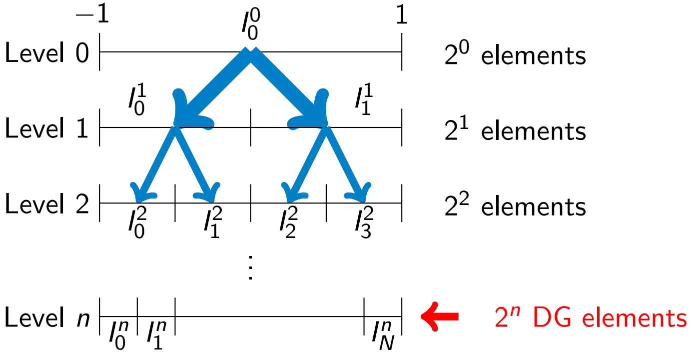
Step 7: Use time-integration method to find $u_j^{(\ell)}(t)$

DG approximation

1. Discretize in space
2. Multiply PDE by test function and integrate
3. Integrate by parts
4. Define DG approximation space
5. Replace solution by DG approximation
6. Choose fluxes
7. Integrate ODE in time

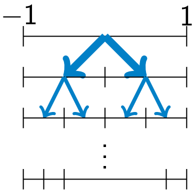
Outline

Multiresolution idea



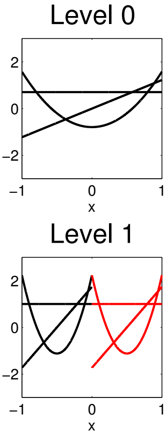
(Alpert, SIAM J. Math. Anal. 1993)

Approximation space



- Level 0: $V_0^{k+1} = \{f : f \in \mathbb{P}^k[-1,1]\}$,
- Level 1: $V_1^{k+1} = \{f : f \in \mathbb{P}^k[-1,0) \cup \mathbb{P}^k[0,1)\}$,
- Level n: V_n^{k+1} is DG approximation space.

Scaling functions



$k = 2$

- Basis multiresolution space: start from level 0
- Orthonormal Legendre polynomials $\phi_0, \ldots, \phi_k$
- Basis functions higher levels: dilation and translation

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

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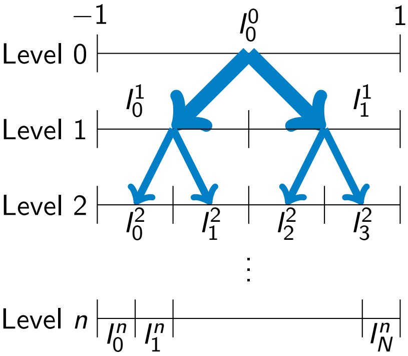
Multiresolution idea

Find basis next level using multiwavelet space!



$$V_0^{k+1}$$

$$V_1^{k+1} = V_0^{k+1} \oplus W_0^{k+1}$$

$$V_2^{k+1} = V_1^{k+1} \oplus W_1^{k+1}$$

$$V_n^{k+1} = V_{n-1}^{k+1} \oplus W_{n-1}^{k+1}$$

Multiwavelets

Multiwavelet space W_m^{k+1}:
Orthogonal complement of V_m^{k+1} in V_{m+1}^{k+1}:

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

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

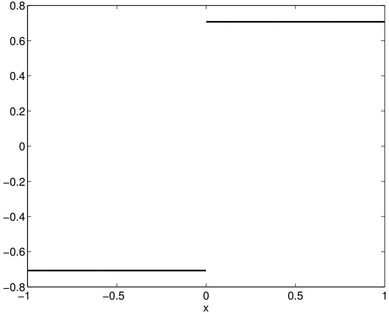
$$\begin{aligned} V_n^{k+1} &= V_{n-1}^{k+1} \oplus W_{n-1}^{k+1} = V_{n-2}^{k+1} \oplus W_{n-2}^{k+1} \oplus W_{n-1}^{k+1} \\ &= V_0^{k+1} \oplus W_0^{k+1} \oplus W_1^{k+1} \oplus \cdots \oplus W_{n-1}^{k+1} \end{aligned}$$

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

Example: Haar wavelet

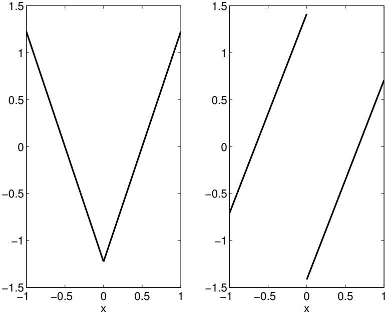
$k = 0$: Haar wavelet

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



Haar wavelets, level 0

Multiwavelets



Multiwavelet basis, $k = 1$

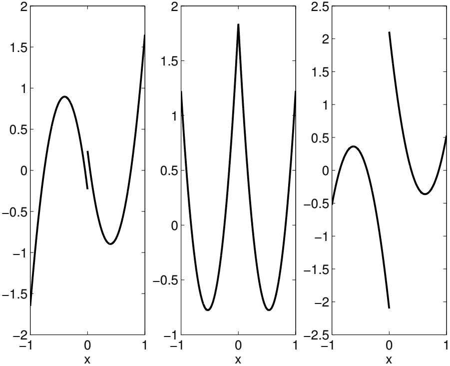
Formulae for $x \in (0, 1)$:

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

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

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

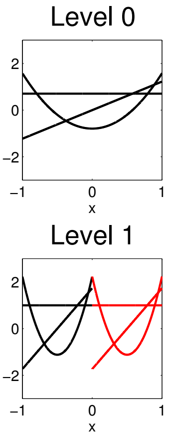
Multiwavelets, $k = 2$



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

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

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



Scaling functions, $k = 2$

Multiwavelets on higher levels

Multiwavelets on higher levels: dilation and translation

$$\psi_{\ell j}^{m}(x) = \sqrt{\frac{2}{\Delta x^m}}\psi_\ell\left(\frac{2}{\Delta x^m}(x - x_j^m)\right),$$

Δx^m is mesh width on level m
$\ell = 0, \ldots, k, \ j = 0, \ldots, 2^m - 1$

Outline

Multiwavelets and DG

- V_n^{k+1} (multiresolution scheme) equals V_h (DG scheme)!
- Decompose DG space using multiwavelets:

$$
\begin{aligned}
V_h = V_n^{k+1} &= V_{n-1}^{k+1} \oplus W_{n-1}^{k+1} \\
&= V_0^{k+1} \oplus W_0^{k+1} \oplus W_1^{k+1} \oplus \cdots \oplus W_{n-1}^{k+1}
\end{aligned}
$$

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Multiwavelets and DG

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

This means that:

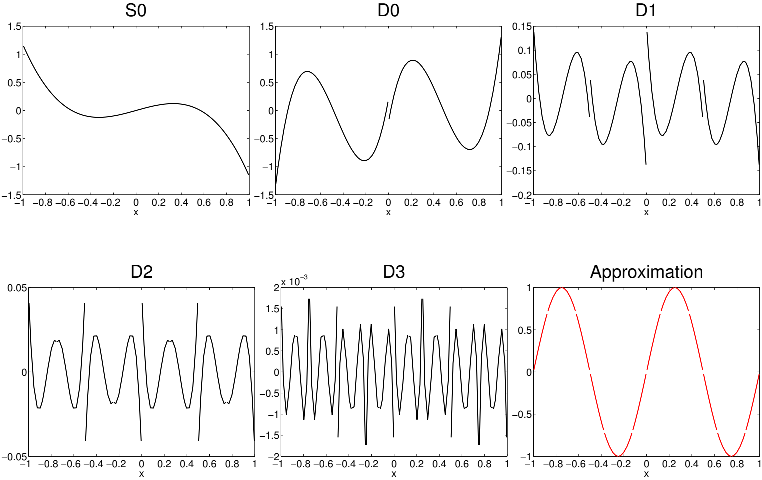
$$u_h(x) = \sum_{j=0}^{2^n-1} \sum_{\ell=0}^{k} u_j^{(\ell)} \phi_\ell(\xi_j)$$

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

Coefficients efficiently computed by decomposition method

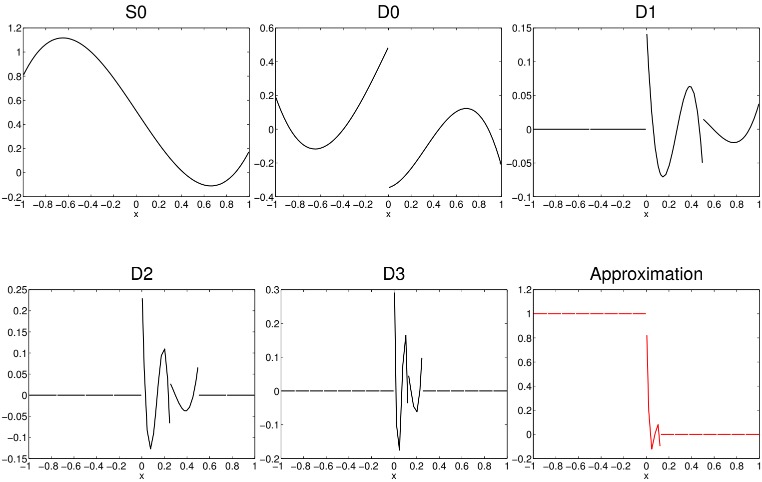
Continuous example

Projection on DG basis, multiwavelet decomposition



Square wave

Projection on DG basis, multiwavelet decomposition



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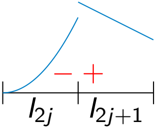
Jumps in DG approximations

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



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

$u_h^{(m)}$: mth derivative of u_h

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

(Vuik and Ryan, Proc. ICOSAHOM 2015)

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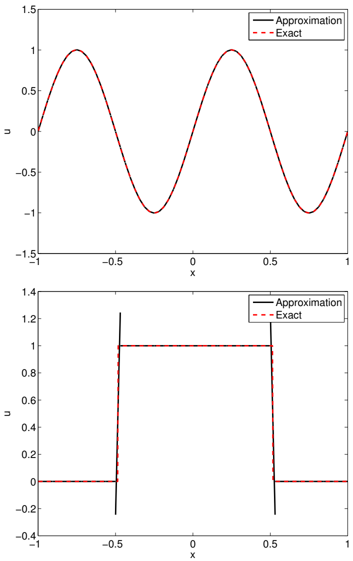
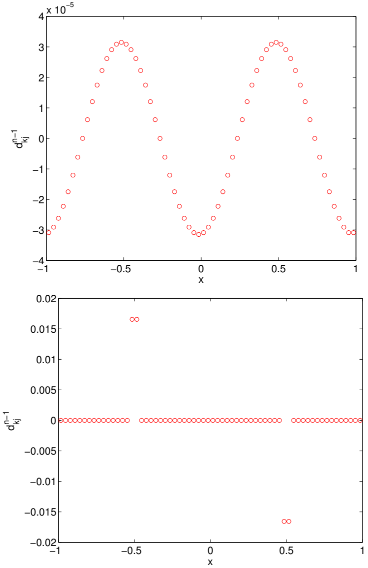


Approximation



d_{kj}^{n-1}

Outline

Highest level

This means that $d_{\ell j}^{n-1}$:

- Measures element-boundary jumps
- Can be used for discontinuity detection

- Cancellation property for decay rate:

$$|d_{\ell j}^{n-1}| \lesssim 2^{-(n-1)(\ell+k)} ||u_h||_{W^{1,\ell+k}(I_j^{n-1})}$$

(Vuik and Ryan, JCP 2014)
(Gerhard and Müller, CAM 2014)

Multiwavelet troubled-cell indicator

Detect an element as being troubled if

$$|d_{kj}^{n-1}| > C \cdot \max\{|d_{kj}^{n-1}|,\ j = 0, \ldots, 2^n - 1\}$$

C prescribes strictness of indicator:

- $C = 0$: all elements are detected
- $C = 1$: no elements are detected

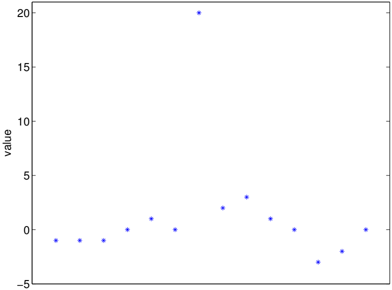
Parameter choice

Troubled-cell indication methods rely on parameters

How should we choose the parameters?

Outline

Indication vector



- Troubled-cell indication vector: $\mathbf{d} = (d_0, \ldots, d_N)^\top$
- Detect sudden changes compared to neighboring values
- No problem-dependent parameters

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Outlier detection algorithm

1. Sort $\mathbf{d}$ to obtain $\mathbf{d}^s = (d_0^s, d_1^s, \ldots, d_N^s)$
2. Compute quartiles $Q_1,\ Q_2,\ Q_3$ of $\mathbf{d}$
3. Construct inner and outer fences
4. Determine outliers (Tukey, 1977)

Quartile computation

- Median Q_2:

$$Q_2 = \begin{cases} d^s_{N/2}, & \text{if \# elements is odd,} \\ \frac{1}{2}\left(d^s_{(N-1)/2} + d^s_{(N+1)/2}\right), & \text{if \# elements is even.} \end{cases}$$

  Separates higher half from lower half

- Q_1: value below which 25% data falls

- Q_3: value below which 75% data falls

Constructing fences

- **Inner fence:** detect soft outliers

$$[Q_1 - 1.5(Q_3 - Q_1), Q_3 + 1.5(Q_3 - Q_1)]$$

Normal distribution: 0.7% identified as soft outlier

- **Outer fence:** detect extreme outliers outside interval

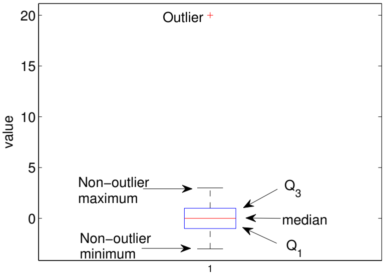
$$[Q_1 - 3(Q_3 - Q_1), Q_3 + 3(Q_3 - Q_1)]$$

Normal distribution: 0.0002% identified as extreme outlier

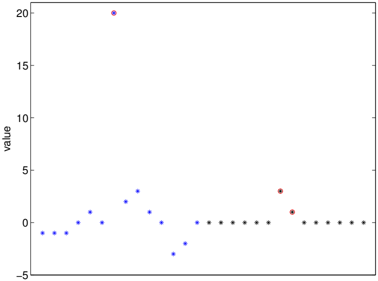
Boxplot

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

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



Local information



- Divide global vector in locals
- Apply boxplot approach for each local vector
- Ignore 'outliers' near split boundaries
- Local vectors: size 16

Outline

Euler equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) &= 0\\
\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x}(\rho u^2 + p) &= 0\\
\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}((E + p)u) &= 0
\end{aligned}
$$

where,

$$
E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u^2.
$$

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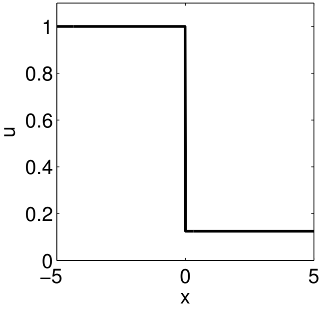
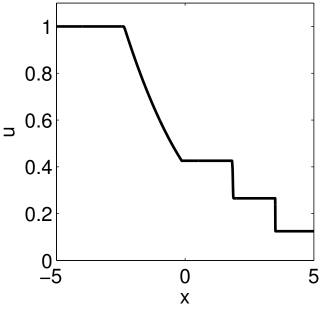
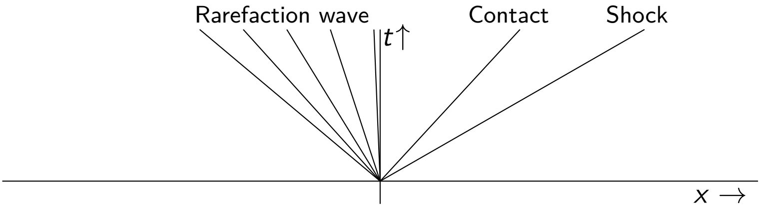
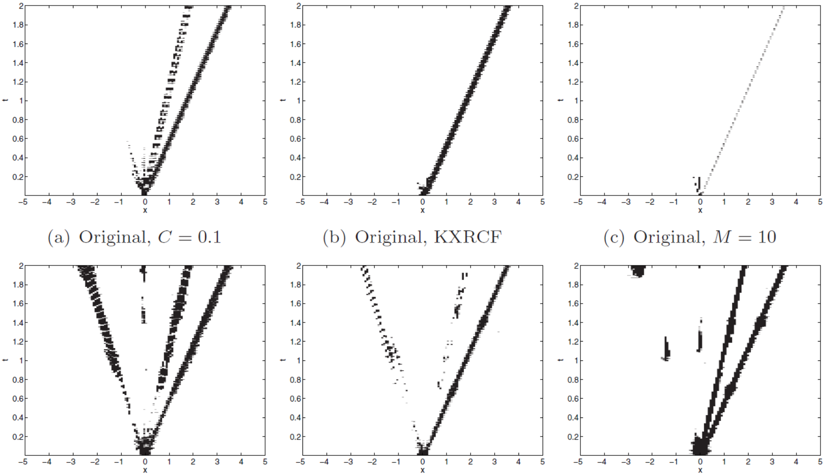
Sod's shock tube







Sod, $k = 2$

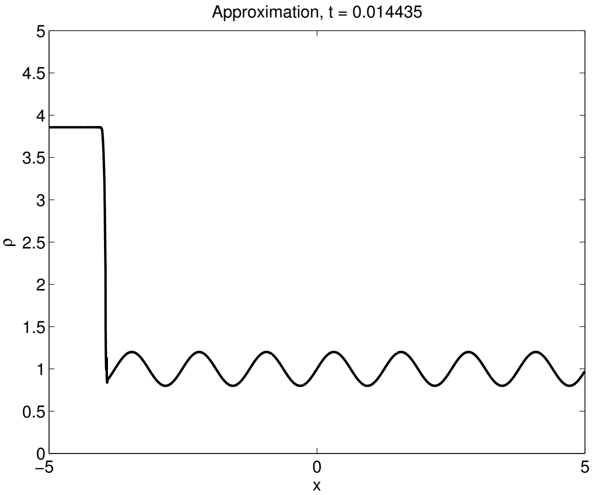


(a) Original, $C = 0.1$ (b) Original, KXRCF (c) Original, $M = 10$

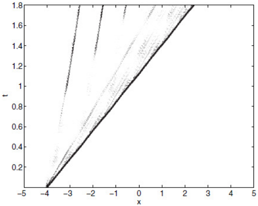
(d) Outlier, multiwavelets (e) Outlier, KXRCF value (f) Outlier, minmod-based TVB

(Vuik and Ryan, SISC 2016)

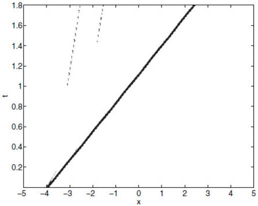
Sine-entropy wave



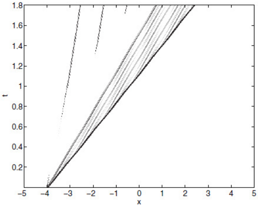
Sine-entropy wave, $k = 2$



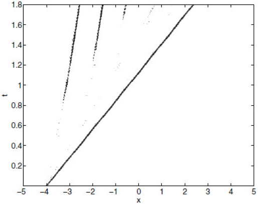
(a) Original, $C = 0.01$



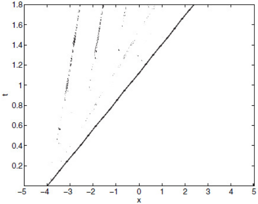
(b) Original, KXRCF



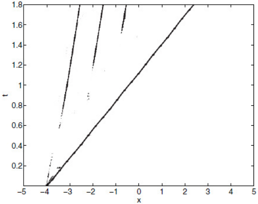
(c) Original, $M = 100$



(d) Outlier, multiwavelets

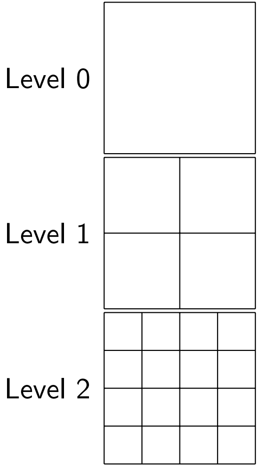


(e) Outlier, KXRCF value



(f) Outlier, minmod-TVB

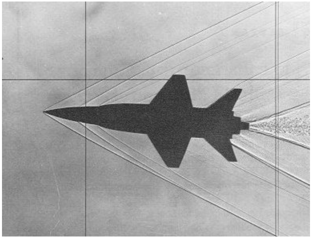
Two dimensions: rectangular mesh (tensor)

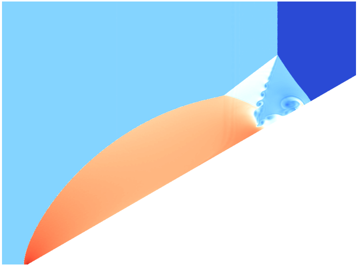


- Scaling functions: $\phi_{\ell_x}(x)\phi_{\ell_y}(y)$
- Multiwavelets:
  - α mode: $\phi_{\ell_x}(x)\psi_{\ell_y}(y)$
  - β mode: $\psi_{\ell_x}(x)\phi_{\ell_y}(y)$
  - γ mode: $\psi_{\ell_x}(x)\psi_{\ell_y}(y)$
- Compute outliers in each direction separately

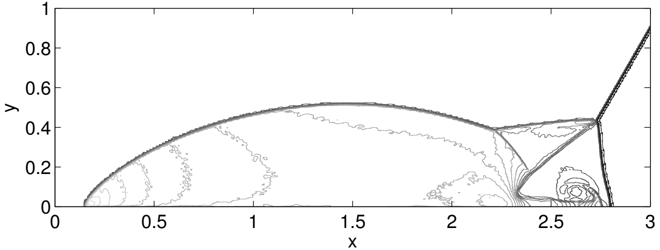
TU Delft

Double Mach reflection

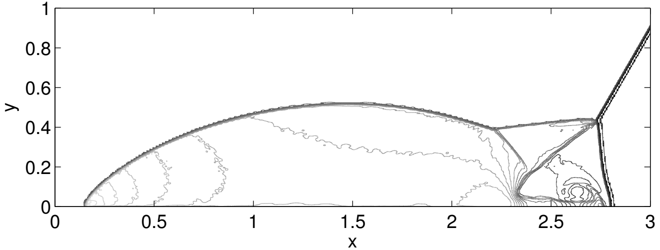




Double Mach reflection: contour plots

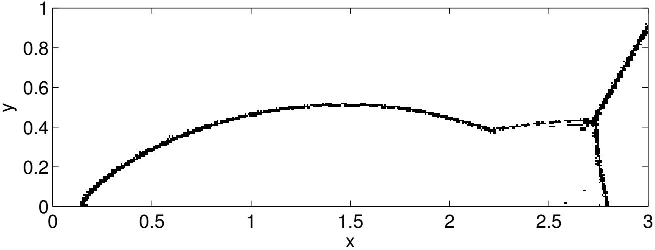


Original
$C = 0.05$

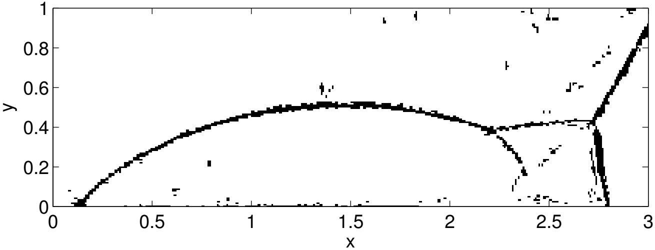


Outlier

Double Mach reflection: troubled cells



Original
$C = 0.05$



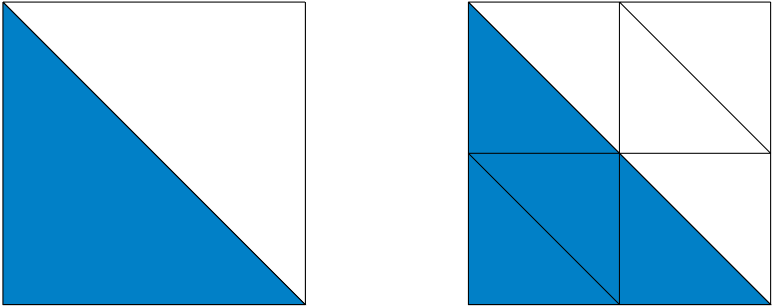
Outlier

Conclusion and future research

- Relation DG and multiwavelets
- Multiwavelet coefficients for troubled-cell indication
- Originally: problem-dependent parameter
- Outlier-detection technique using boxplots
- Problem-dependent parameters no longer needed!

- Non-uniform Cartesian meshes
- Triangular meshes

Two dimensions: triangular mesh



- No tensor product, but genuinely two dimensional!
- Multiwavelets: theory of Yu et al. (1997)
  - Based on Alpert's algorithm
  - Efficient coefficient computation still possible
  - Relation with DG coefficients