Automated parameters for troubled-cell indicators using outlier detection

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April 15, 2015
Outline

1. Introduction
2. Building blocks: DG and multiwavelets
3. Multiwavelet troubled-cell indicator (with parameter)
4. Outlier detection
5. Results
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1. Introduction
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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

- KXRCF indicator

- multiwavelet troubled-cell indicator
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Discontinuous Galerkin method

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

- 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
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

\[ V_n^k = \{ f : f \in \mathbb{P}_k(I^n_j), j = 0, \ldots, 2^n - 1 \} \]

\[ V_0^k \subset V_1^k \subset \cdots \subset V_n^k \subset \cdots \]

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

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

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

Multiwavelets

\[ V^k_m = \{ f : f \in \mathbb{P}^k(I^m_j), j = 0, \ldots, 2^m - 1 \} \]

Multiwavelet space \( W^k_m \):
- Orthogonal complement of \( V^k_m \) in \( V^k_{m+1} \):
  \[ V^k_m \oplus W^k_m = V^k_{m+1}, \quad W^k_m \perp V^k_m, \quad W^k_m \subset V^k_{m+1} \]
- \( V^k_n \) can be split into \( n + 1 \) orthogonal subspaces:
  \[ V^k_n = V^k_0 \oplus W^k_0 \oplus W^k_1 \oplus \cdots \oplus W^k_{n-1} \]

Split up \( f \in V^k_n \) into different levels
Example: Haar wavelet

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

Multiwavelet basis, $k = 1$

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

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

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

Multiwavelets

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

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

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

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

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

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

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

\[
u_h(x) = \sum_{j=0}^{2^n-1} \sum_{\ell=0}^k u_j^{(\ell)} \phi_\ell(\xi_j) = \sum_{\ell=0}^k s_{\ell0}^0 \phi_\ell(x) + \sum_{m=0}^{n-1} \sum_{j=0}^{2^m-1} \sum_{\ell=0}^k d_{\ell j}^m \psi_{\ell j}^m(x)
\]

Coefficients computed by decomposition method
Example: $\sin(2\pi x)$, $n = 4$, $k = 3$

Projection on DG basis, multiwavelet decomposition

- $S_0$
- $D_0$
- $D_1$
- $D_2$
- $D_3$
- Approximation
Jumps in DG approximations

\[ u_h(x) = \sum_{\ell=0}^{k} s_0^{\ell} \phi_\ell(x) + \sum_{m=0}^{n-1} \sum_{j=0}^{2^m-1} \sum_{\ell=0}^{k} d_{\ell j}^m \psi_{\ell j}^m(x) \]

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

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

Approximation

64 elements, $k = 1$
Example: square wave

Approximation

64 elements, $k = 1$
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Original approach

Detect elements $l_j$ and $l_{j+1}$ if

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

Approximation

64 elements, $k = 1$

Detected, $C = 0.9$
Problem I: continuous function

Approximation

64 elements, $k = 1$

Detected, $C = 0.9$
Problem II: different discontinuities

Approximation

64 elements, $k = 1$

Detected, $C = 0.9$

How to choose $C$?
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Outlier detection

$d_{kj}^{n-1}$:
- vector containing jumps over element boundaries
- coefficient big compared to neighbors: detect

⇒ Boxplot approach

(Tukey, 1977)
Outlier-detection algorithm

1. Send in troubled-cell indication vector \( \mathbf{d} \)
2. Sort \( \mathbf{d} \) to obtain \( \mathbf{d}^s \)
3. Compute quartiles of \( \mathbf{d}^s \): \( Q_1 \) and \( Q_3 \)
4. Construct outer fences:
   \[
   Q_1 - 3(Q_3 - Q_1) \quad \text{and} \quad Q_3 + 3(Q_3 - Q_1)
   \]
5. Determine outliers:
   \[
   d_j < Q_1 - 3(Q_3 - Q_1) \quad \text{or} \quad d_j > Q_3 + 3(Q_3 - Q_1)
   \]
Boxplot

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

- 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
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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
Minmod-based TVB indicator

\[ u_{j+\frac{1}{2}}^- = \bar{u}_j + \tilde{u}_j, \quad \tilde{u}_j = \sum_{\ell=1}^{k} u_{j}^{(\ell)} \phi_{\ell}(1) \]

\[ u_{j-\frac{1}{2}}^+ = \bar{u}_j - \tilde{u}_j, \quad \tilde{u}_j = -\sum_{\ell=1}^{k} u_{j}^{(\ell)} \phi_{\ell}(-1) \]

\[ M = 100 \]

Outlier
KXRCF detector

Jump across inflow edge:

\[ I_j = \left| \int_{\partial I_j^-} (u_h|_{I_j} - u_h|_{I_{nj}}) \, ds \right| \]

Threshold equal to 1

Outlier
Double Mach reflection: contour plots

Original

$C = 0.05$

Outlier
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