High-order methods for computational fluid dynamics

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Outline

1. Why high-order in CFD?

2. On a discontinuous hybrid CV & FE algorithm
   - The idea: motivations and features
   - Governing equations
   - Fourier analysis
   - Numerical results
   - Conclusions I

3. Finite-difference high-order MWCS (WCS+WENO)
   - Weighted schemes: insight
   - Motivations and objectives
   - Numerical results
   - Conclusions II

4. General concluding remarks
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Why high-order in CFD?

1. **Low-order methods (1\textsuperscript{st} and 2\textsuperscript{nd} order)**
   - simplicity and robustness
   - satisfactory solution with "little" effort
   - may be inaccurate

2. **High-order methods (3\textsuperscript{rd} and above)**
   - shocks, high gradients
   - complex smooth flow features (small-length scales)
   - long time evolution
   - **Advantages:**
     - fast convergence
     - low dispersion and dissipation
     - smaller amount of data
     - higher accuracy
   - **Disadvantages:**
     - elevated computational cost per degree of freedom
     - implementation and stability
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Why high-order in CFD?

Computational work (\# floating-point operations) required to integrate a linear advection for \( M \) periods maintaining a constant cumulative phase error \( \epsilon = 10\% \) [Karniadakis-Sherwin 2005]
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Discontinuous approach: insight

Sketch of the discontinuous approach: the generic quadrilateral elements communicate only through *numerical fluxes*
Canonical element and control volumes

Canonical element of order $P = 2$ in the transformed space. For better conditioning the control volumes’ faces (dashed blue) are placed at Gauss-Legendre points.
Motivations and features

1. Hybrid CV and FE merges the advantages of both
   - Control Volume: integral method conservative at CV level
   - Geometric flexibility

2. Discontinuous methods:
   - local $P$-adaptivity for high-order accuracy
   - extremely local data structure: high-efficiency parallelization
   - used for hyperbolic problems (discontinuities) or advection-dominated problems (high-Reynolds numbers)

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4. General concluding remarks
The advection-diffusion equation is solved.

**Fundamental formulation:**

\[
\frac{\partial}{\partial t} (C T) - \nabla \cdot (D \nabla T) + \nabla \cdot (C T u) = Q
\]

**Mixed formulation:** constitutive and conservation equations

\[
\begin{aligned}
q_d + D \nabla T &= 0 \\
\frac{\partial}{\partial t} (C T) + \nabla \cdot q &= Q \\
q &= q_d + q_a \\
q_a &= C T u
\end{aligned}
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Governing equations

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Fourier analysis

Stability and resolution characteristics:

1. The resolution is significantly better if compared to the finite-difference and continuous Galerkin FEM

2. The specific choice of numerical flux strongly affects the method’s stability and resolution characteristics

3. The order of convergence is $P + 1$ for $T$, and $P$ for $q$ (depending on the choice of numerical flux)

\[
\hat{T} = \{ T \} \\
\hat{q} = \{ q \} + C_{11} [ T ] \quad \text{where} \quad \{ T \} \equiv \frac{1}{2} (T^+ + T^-) \\
[ T ] \equiv (T^- n^- + T^+ n^+) \]

4. There exist more complex formulations for the numerical flux; accuracy may be affected (verified by preliminary results)
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Diffusive term: *dissipation*

\[
P = 2, \text{ symbol } \Box, \circ: \text{DCVFEM}; \text{ symbol } \triangle: \text{FD4}; \text{ symbol } \triangledown: \text{GFEM2}
\]

\[
P = 3, \text{ symbol } \Box, \circ: \text{DCVFEM}
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Numerical results
1D steady advection-diffusion: the Hemker problem

The Hemker problem is defined as:

\[
\begin{aligned}
\frac{d}{dx} (u \, T) - D \frac{d^2 T}{dx^2} &= Q(x), \quad x \in (-1, 1) \\
T(-1) &= -2; \quad T(1) = 0
\end{aligned}
\]

\[
\begin{aligned}
u(x) &= x; \quad D = 10^{-10} \\
Q(x) &= -D \pi^2 \cos(\pi x) - \pi x \sin(\pi x) \\
&\quad + \cos(\pi x) + \frac{\text{erf} \left( \frac{x}{\sqrt{2D}} \right)}{\sqrt{2D}} \\
&\quad + \frac{\text{erf} \left( \frac{1}{\sqrt{2D}} \right)}{\sqrt{2D}}
\end{aligned}
\]
1D steady advection-diffusion: the Hemker problem
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DCVFEM (○) and DGFEM (●) with $P = 2$
2D practical application to a Tuned Liquid Damper (TLD)
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**Tuned Liquid Dampers:**
- Stabilization of tall buildings from wind action and earthquakes
- Low cost of maintenance and easiness of adjusting the natural frequency
- Possibility for temporary use
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*Tuned Liquid Dampers:*
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Mathematical model

- From the *linear potential theory*:

\[
\begin{aligned}
\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} &= 0, \quad \nabla \phi = \mathbf{V} \\
\frac{\partial \phi}{\partial n} &= \mathbf{V}_r \cdot \mathbf{n}, \quad \text{on } \partial \Omega_{r.b.} \\
\frac{\partial^2 \phi}{\partial t^2} &= -g \frac{\partial \phi}{\partial y} - \mu \frac{\partial \phi}{\partial t}, \quad \text{on } \partial \Omega_{f.s.}
\end{aligned}
\]

- The solution is obtained in *frequency domain*

- The artificial damping: \( \mu = \nu \omega \rightarrow \) linear range, tuning needed
Mathematical model

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Mathematical model

- From the total force (added mass coefficients $f_i = \sum_j -A_{ij}\ddot{x}_j - B_{ij}\dot{x}_j$), the resonance frequency can be estimated.
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Added mass coefficient w.r.t. frequency, *undamped* simulation
Damping of a forced system

A multi-story building can be simplified to a single degree of freedom (SDF) structure for the first natural frequency:
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A multi-story building can be simplified to a single degree of freedom (SDF) structure for the first natural frequency:

\[ x \quad y \]

\[ K_s \quad C_s \quad M_s \]

\[ F_x \]

\[ \hat{H}(\omega) / \hat{H}_0 \]

\[ \nu = 0.05 \quad \nu = 0.1 \quad \nu = 0.5 \quad \cdots \text{Undamped} \]
The free surface for the first natural frequency
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3. $P$-convergence $T$ and $q$
4. Numerical results:
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   - DCVFEM comparable to DGFEM
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$$\phi_V(x) = \begin{cases} 
1 & \text{if } x \in V \\
0 & \text{otherwise}
\end{cases}$$
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Modified wavenumber: diffusion

![Graph showing modified wavenumber over wave number](image_url)
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DCVFEM: $P$-convergence
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Sketch of a 2D Tuned Liquid Damper
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The weighted schemes
- attain high-order by a convex combination of lower-order stencils
- non-linear weights $\omega_{0,1,2}$ associated to "smoothness"
Weighted schemes WCS and WENO: foundation

Candidate stencils for the approximation of the numerical flux $\hat{F}$.

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Why WCS + WENO → MWCS?

\[ \hat{F}_{j-1/2}^{(MWCS)} = \alpha_j \hat{F}_{j-1/2}^{(WCS)} + (1 - \alpha_j) \hat{F}_{j-1/2}^{(WENO)} \quad (2) \]

**Figure:** Fourier analysis of the 1st order derivative. The WCS in multidimensional applications is unstable (in TVD sense).
Why $\text{WCS+WENO} \rightarrow \text{MWCS}$?

\begin{equation}
F_{j-1/2}^{(\text{MWCS})} = \alpha_j F_{j-1/2}^{(\text{WCS})} + (1 - \alpha_j) F_{j-1/2}^{(\text{WENO})}
\end{equation}

Figure: Fourier analysis of the 1$^{st}$ order derivative. The WCS in multidimensional applications is \textit{unstable} (in TVD sense).
The mixing function

The blending factor $\alpha = \alpha(\lambda)$ in (2) is based on a shock-detector:

$$\lambda_i = \frac{1}{2} \left[ 1 - \tanh \left( 2.5 + 40 \frac{\Delta_i}{C_i} \nabla \cdot u_i \right) \right]$$

(3)

where

- $0 \leq \lambda_i \leq 1$
- $\Delta$ is the magnitude of grid size
- $C$ is the speed of sound
- $\mathbf{u}$ is the velocity vector
- $2 \frac{\Delta_i}{C_i}$ is the time scale of the highest frequency acoustic wave

$$\alpha_i = 0.75 \left( 1.0 - \bar{\lambda}_i \right) \rightarrow \text{Stability 2D}$$

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The mixing function

The blending factor $\alpha = \alpha(\lambda)$ in (2) is based on a shock-detector:

$$\lambda_i = \frac{1}{2} \left[ 1 - \tanh \left( 2.5 + 40 \frac{\Delta_i}{C_i} \nabla \cdot u_i \right) \right]$$  \hspace{1cm} (3)

where

- $0 \leq \lambda_i \leq 1$
- $\Delta$ is the magnitude of grid size
- $C$ is the speed of sound
- $u$ is the velocity vector
- $2 \frac{\Delta_i}{C_i}$ is the time scale of the highest frequency acoustic wave

$$\alpha_i = 0.75 \left( 1.0 - \bar{\lambda}_i \right) \rightarrow \text{Stability 2D}$$  \hspace{1cm} (4)
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Outline

1. Why high-order in CFD?

2. On a discontinuous hybrid CV & FE algorithm
   - The idea: motivations and features
   - Governing equations
   - Fourier analysis
   - Numerical results
   - Conclusions I

3. Finite-difference high-order MWCS (WCS+WENO)
   - Weighted schemes: insight
   - Motivations and objectives
   - Numerical results
   - Conclusions II

4. General concluding remarks
Numerical results
Compressible Euler equations

The Euler equations are solved:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + \rho \mathbf{l}) = 0
\]  \hspace{1cm} (5)

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot ((\rho E + p) \mathbf{u}) = 0
\]

coupled with suitable initial conditions
Shu-Osher interaction problem

\[(\rho, u, p) = \begin{cases} (3.857143, 2.629369, 10.33333) & t = 0, x < -4 \\ (1 + 0.2 \sin(5x), 0, 1) & t = 0, x \geq -4 \end{cases}\]
Shu-Osher problem

(c) WENO

(d) Enlargement
The shock-sensor (Shu-Osher problem)

(e) MWCS

(f) Shock-sensor
Shock reflection over an inviscid wall

- Shock angle 35.24°
- Mach 2

Sketch of the oblique shock reflection.
Shock reflection over an inviscid wall

Exact solution of the pressure contour.
Shock reflection over an inviscid wall

MWCS, pressure, 12 equally spaced contours. Mesh 33 × 33.
Shock reflection over an inviscid wall

WENO, pressure, 12 equally spaced contours. Mesh 33 $\times$ 33.
Shock reflection over an inviscid wall

(a) Pressure at $y = 0.34$

(b) Enlargement
Shock reflection over an inviscid wall: animation
The shock-sensor (shock reflection over an inviscid wall)
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Conclusions II

1. MWCS: linear combination WENO & WCS
2. New mixing function based on shock-detector
3. Better resolution and shock-capturing w.r.t. WENO
4. Numerical stability (TVD) and non-oscillatory property in multidimensions
5. The shock-sensor formula accurately detects the shock location
6. No adjustable parameters are introduced
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\[ \hat{F}_{j-1/2}^{(MWCS)} = \alpha_j \hat{F}_{j-1/2}^{(WCS)} + (1 - \alpha_j) \hat{F}_{j-1/2}^{(WENO)} \]
Conclusions II

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\[ \lambda_i \sim \tanh(\nabla \cdot u_i) \]
Conclusions II

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Location of oblique shock
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General concluding remarks

1. Two high-order methods:
   - DCVFEM $\rightarrow$ Diffusion
   - MWCS $\rightarrow$ Hyperbolic

2. DCVFEM: arbitrary triangulation, interpolation nodes

3. MWCS: regular geometry, efficiency 2-3D

4. Accuracy:
   - MWCS: 6\textsuperscript{th} order
   - DCVFEM: any order
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DCVFEM (○) and DGFEM (●): the Hemker problem
Two high-order methods:
- DCVFEM $\rightarrow$ Diffusion
- MWCS $\rightarrow$ Hyperbolic

DCVFEM: arbitrary triangulation, interpolation nodes

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- MWCS: $6^{th}$ order
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MWCS: Shu-Osher problem

\( \rho \)

\( x \)
General concluding remarks

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DCVFEM: element in the transformed space
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MWCS: oblique shock reflection
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Future work and difficulties

1. DCVFEM:
   - 3D extension for hexahedrons
   - 3D extension for triangles/tetrahedrons
   - Bottleneck: computational cost

2. MWCS:
   - Improvement in resolution and stability (mixing function)
Future work and difficulties

DCVFEM:
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Hexahedral element, arbitrary order
Future work and difficulties

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Tetrahedral element, arbitrary order
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   - 3D extension for triangles/tetrahedrons
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2. **MWCS:**
   - Improvement in resolution and stability (mixing function)

![Graph showing oblique shock reflection, pressure vs. x](image-url)
Thank you
Weighted schemes: foundation

Consider the conservation equation in 1D:

\[
\frac{\partial q}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad (6)
\]

and its semi-discrete form:

\[
\frac{\partial q_j}{\partial t} = - \frac{\hat{F}_{j+1/2} - \hat{F}_{j-1/2}}{h_j} \quad (7)
\]

where \( \hat{F} \) is the numerical flux at cell interfaces

\[
F_j = F(q(x_j, t)) \equiv \int_{x_{j-1/2}}^{x_{j+1/2}} \hat{F}(\xi) d\xi \quad (8)
\]

With definition (8), Eq. (7) is an exact expression, i.e. 
\[
F'_j = \frac{\hat{F}_{j+1/2} - \hat{F}_{j-1/2}}{h_j} \quad (bcam)
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Consider the conservation equation in 1D:

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Total variation diminishing

In systems described by partial differential equations, such as the following hyperbolic advection equation,

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

the total variation (TV) is given by

$$TV = \int \left| \frac{\partial u}{\partial x} \right| \, dx$$

and the total variation for the discrete case is,

$$TV = \sum_{j} |u_{j+1} - u_{j}|$$

A numerical method is said to be total variation diminishing (TVD) if,

$$TV \left( u^{n+1} \right) \leq TV \left( u^{n} \right)$$
Weak formulation: formal derivation I

Consider the volume indicator function

\[
\phi_V(x) = \begin{cases} 
1 & \text{if } x \in V \\
0 & \text{otherwise}
\end{cases}
\] (9)

And take the constitutive equation \( q_d + D \nabla T = 0 \). After

1. multiplication with (9)
2. integration over the whole domain \( \Omega \)
3. application of the divergence theorem

we have

\[
\int_V D^{-1} q_d \, dx + \int_{\partial V} T^- n \, ds = 0
\] (10)

where \( T^- \) denotes the trace on \( \partial V \) of the restriction of the function \( T \) to the control volume \( V \).
Weak formulation: formal derivation I

Consider the volume indicator function

\[ \phi_V(x) = \begin{cases} 
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Consider the volume indicator function

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And take the *constitutive* equation \( \mathbf{q}_d + D \nabla T = 0 \). After

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$$

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where $T^-$ denotes the trace on $\partial V$ of the restriction of the function $T$ to the control volume $V$. 
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Consider the volume indicator function

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Weak formulation: formal derivation II

Regularity conditions:

\( T \in H^1 \left( \mathbb{V}; \mathbb{R}^2 \right) \rightarrow \) theory of the \textit{mollifiers} [Salsa, 2007].

A family of mollifiers \( \rho_\epsilon \in C_0^\infty (\mathbb{R}^2), \epsilon > 0 \) is defined as follows

\[
\rho_\epsilon (x) = \begin{cases} 
\frac{1}{\epsilon^2} \exp \left( - \frac{1}{1 - \frac{|x|}{\epsilon}} \right) & \text{for } |x| < 1 \\
0 & \text{for } |x| \geq 1
\end{cases}
\] (11)

A sequence of smooth functions \( T_\epsilon \) is defined using the \textit{convolution}

\[
T_\epsilon (x) = \int_{\mathbb{R}^2} \rho_\epsilon (x - y) E \left( T(y) \right) \, dy
\]

where \( E (\cdot) \) is a linear \textit{extension} operator

\[
E : H^1 (\mathbb{V}) \longrightarrow H^1 (\mathbb{R}^2)
\]
Weak formulation: formal derivation II

Regularity conditions:

\[ T \in H^1(V; \mathbb{R}^2) \rightarrow \text{theory of the mollifiers [Salsa, 2007].} \]

A family of mollifiers \( \rho_\epsilon \in C^\infty_0(\mathbb{R}^2), \epsilon > 0 \) is defined as follows

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\end{cases}
\]  

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A sequence of smooth functions \( T_\epsilon \) is defined using the convolution

\[
T_\epsilon(x) = \int_{\mathbb{R}^2} \rho_\epsilon(x - y) E(T(y)) \, dy
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E : H^1(V) \rightarrow H^1(\mathbb{R}^2)
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Weak formulation: formal derivation II

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\]
Weak formulation: formal derivation III

It can be proven that $T_{\epsilon}$ converges to $T$

$$\lim_{\epsilon \to 0} \| T - T_{\epsilon} \|_{H^1(V)} = 0 \quad (12)$$

The second integral in the constitutive equation can be rearranged as:

$$\int_{\Omega} \nabla T \cdot \Phi_x \, dx = \int_V \frac{\partial T}{\partial x} \, dx = \lim_{\epsilon \to 0} \int_V \frac{\partial T_{\epsilon}}{\partial x} \, dx =$$

$$\lim_{\epsilon \to 0} \int_{\partial V} T_{\epsilon} n_x \, ds = \int_{\partial V} T n_x \, ds \quad (13)$$

Analogously for the conservation equation. Choosing $T, q \in H^1(V)$ guarantees the existence of the integrals on the control volume $V$. 
Weak formulation: formal derivation III

It can be proven that $T_\epsilon$ converges to $T$

$$\lim_{\epsilon \to 0} \| T - T_\epsilon \|_{H^1(V)} = 0 \quad (12)$$

The second integral in the constitutive equation can be rearranged as:

$$\int_{\Omega} \nabla T \cdot \Phi_x \, dx = \int_V \frac{\partial T}{\partial x} \, dx = \lim_{\epsilon \to 0} \int_V \frac{\partial T_\epsilon}{\partial x} \, dx = \lim_{\epsilon \to 0} \int_{\partial V} T_\epsilon n_x \, ds = \int_{\partial V} T^- n_x \, ds \quad (13)$$

Analogously for the conservation equation. Choosing $T, q \in H^1(V)$ guarantees the existence of the integrals on the control volume $V$. 
Weak formulation: formal derivation III

It can be proven that $T_\epsilon$ converges to $T$

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Analogously for the conservation equation. Choosing $T, \, q \in H^1(V)$ guarantees the existence of the integrals on the control volume $V$. 