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HIGHER-ORDER FINITE VOLUME METHODS WITH MOVING LEAST SQUARES APPROXIMATIONS

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Outline

- Introduction
- The FV-MLS method
- Multiscale properties of MLS: MLS-based shock detection
- A formulation for all-speed flows
- A MLS-based sliding mesh technique
- Application to Navier-Stokes-Korteweg equations
- Conclusions

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A Coruña...OK. But... where is it?

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Introduction

► Origin of this research:

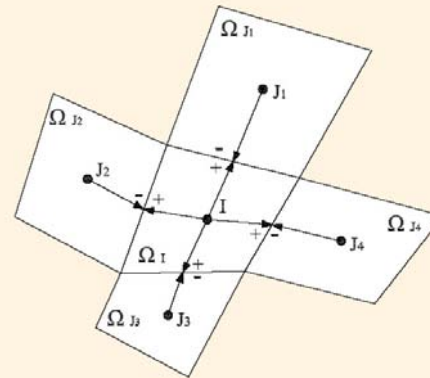
- Development of more accurate numerical methods for turbomachinery.
- Standard industrial codes: 2^{nd} order.
- We need high-resolution schemes for unstructured grids.
- Turbomachinery \Rightarrow Relative motion rotor/stator.





Introduction

- ▶ It is not straightforward to obtain finite volume methods with order higher than two on **unstructured grids**.
- ▶ One of the main difficulties is the **computation of high-order derivatives**.





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The MLS method in a nutshell

- ▶ MLS is an approximation method very used by the meshless community.
- ▶ MLS performs a reconstruction of $u(\mathbf{x})$ at a point \mathbf{x} by using a **weighted LS approximation** in the vicinity of \mathbf{x} .
- ▶ The approximation is written in terms of MLS shape functions.

$$\hat{u}(\mathbf{x}) = \sum_{j=1}^{n_x} N_j(\mathbf{x}) u_j$$

- ▶ The approximation basically depends on a kernel and a basis function.

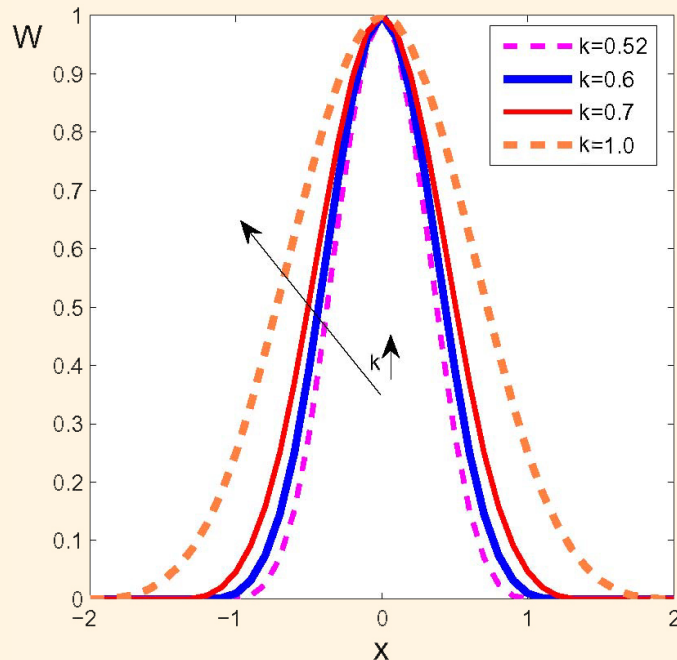




Kernel functions

- ▶ Many functions used as kernels: splines, gaussians
- ▶ An example, the cubic spline:

$$W_j(\mathbf{x}) = W(\mathbf{x} - \mathbf{x}_j, h) = \frac{\alpha}{h^\nu} \begin{cases} 1 - \frac{3}{2}s^2 + \frac{3}{4}s^3 & s \leq 1 \\ \frac{1}{4}(2-s)^3 & 1 < s \leq 2 \\ 0 & s > 2 \end{cases}$$



$$s = \frac{\|\mathbf{x} - \mathbf{x}_j\|}{h}$$

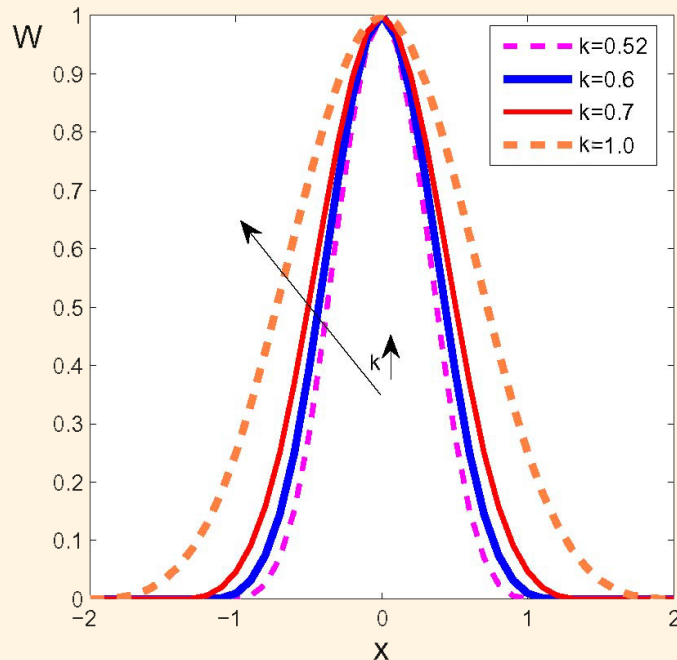
$$h = k \max(\|\mathbf{x} - \mathbf{x}_j\|)$$



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$$s = \frac{\|\mathbf{x} - \mathbf{x}_j\|}{h}$$

$$h = \mathbf{k} \max(\|\mathbf{x} - \mathbf{x}_j\|)$$

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Kernel functions

- ▶ Another example: Exponential Kernel.

$$W(x, x^*, \kappa) = \frac{e^{-\left(\frac{s}{c}\right)^2} - e^{-\left(\frac{d_m}{c}\right)^2}}{1 - e^{-\left(\frac{d_m}{c}\right)^2}}$$

$$s = |x - x^*|, d_m = 2 \max(|x_j - x^*|), c = \frac{d_m}{2\kappa}$$

- ▶ A 2D kernel is obtained by multiplying two 1D kernels:

$$W_j(\mathbf{x}, \mathbf{x}^*, \kappa_x, \kappa_y) = W_j(x, x^*, \kappa_x)W_j(y, y^*, \kappa_y)$$





Kernel functions

- ▶ Another example: Exponential Kernel.

$$W(x, x^*, \kappa) = \frac{e^{-\left(\frac{s}{c}\right)^2} - e^{-\left(\frac{d_m}{c}\right)^2}}{1 - e^{-\left(\frac{d_m}{c}\right)^2}}$$

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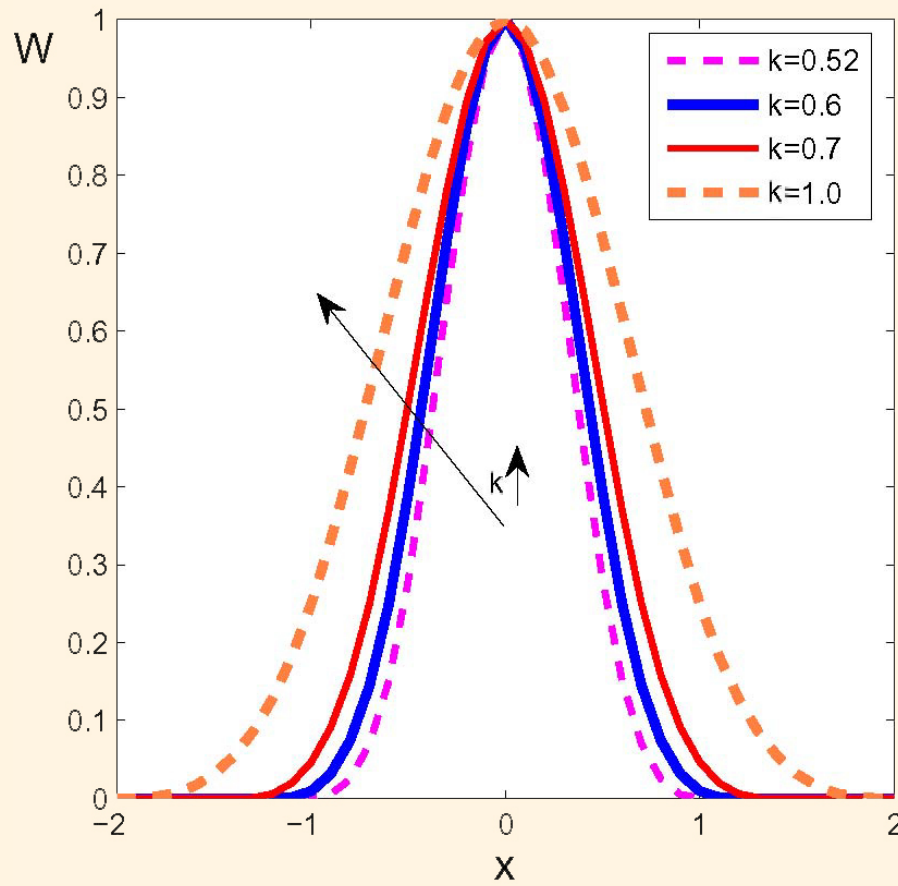
$$W_j(\mathbf{x}, \mathbf{x}^*, \kappa_x, \kappa_y) = W_j(x, x^*, \kappa_x)W_j(y, y^*, \kappa_y)$$



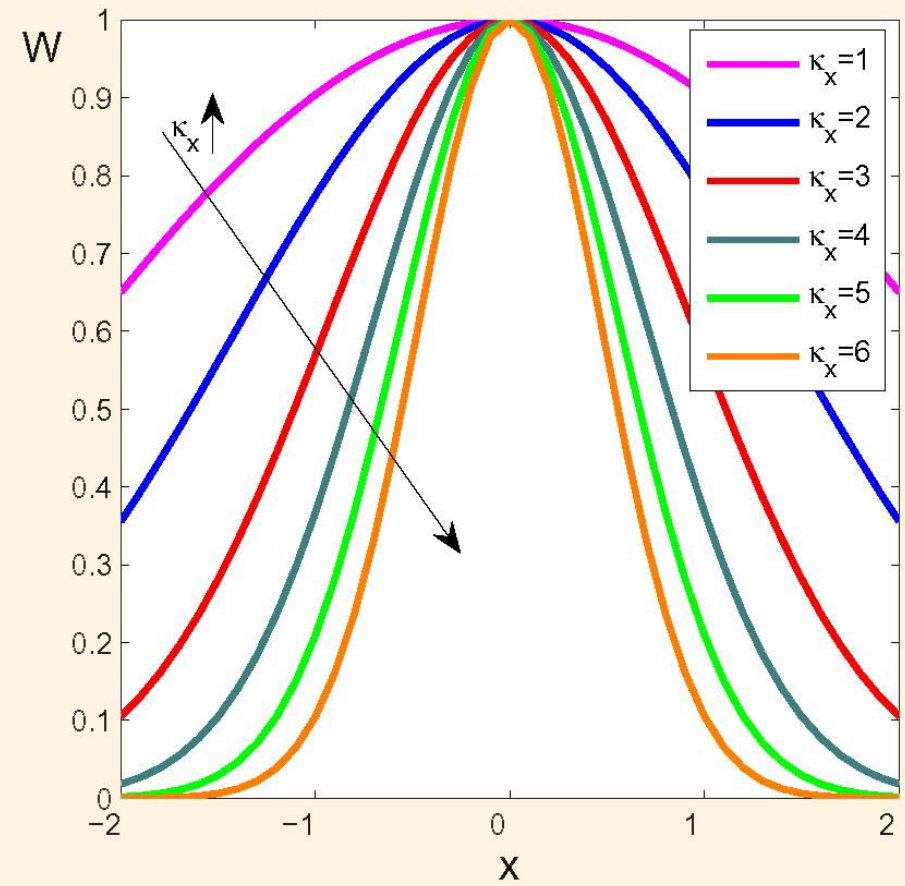


Kernel functions

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CUBIC SPLINE



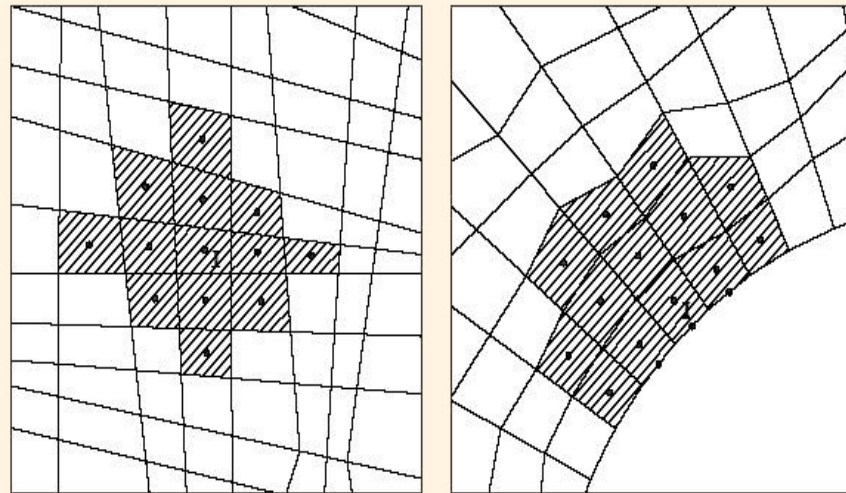
EXPONENTIAL KERNEL





A practical note

- ▶ Vertices and/or centroids of the control cells are the “particles” to perform the MLS approximation.
- ▶ We need to define **stencils** to “mark” the neighbor particles that define the cloud of points.



- ▶ We use a polynomial **cubic basis** in all the computations.

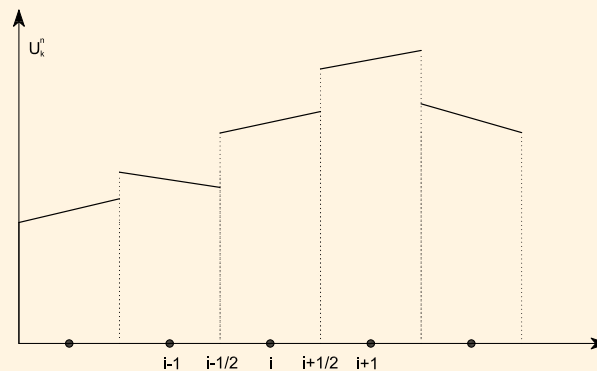


The FV-MLS method

► In order to develop high-order finite volume schemes:

- Compute fluxes more accurately.
- Improve function reconstruction at an integration point \mathbf{x} placed at the interface between elements.

$$U(x) = U_I + \nabla U_I \cdot (\mathbf{x} - \mathbf{x}_I) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_I)^T \mathbf{H}_I (\mathbf{x} - \mathbf{x}_I) + \dots$$



Piece-wise linear reconstruction of a function.



The FV-MLS method

- ▶ Computation of high-order derivatives:
 - Easy on structured grids.
 - Unstructured grids ⇒ **PROBLEM**.
- ▶ We propose:
 - The use of **Moving Least Squares (MLS)** to obtain an **accurate** and **multidimensional** approximation of derivatives on unstructured grids.





The FV-MLS method

- ▶ This scheme acknowledges the **different nature** of convective and diffusive terms.
- ▶ We start from a high-order, **continuous** MLS approximation of the solution:
- ▶ **Convective** terms discretization:
 - **Breaks** the continuous representation of the MLS approximation.
 - Obtains a continuous representation of the variables **inside each cell**.
- ▶ **Diffusive** terms discretization is:
 - Centered.
 - Continuous.
 - Highly accurate.





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MLS-based shock detection



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Mach cone. (Source: www.airliners.net)





MLS-based shock detection

► Slope limiters are used to design TVD schemes.

- A slope limiter limits the Taylor reconstruction of a high-order finite volume scheme as follows:

$$U(\mathbf{x}) = U_I + \chi_I \nabla U_I \cdot (\mathbf{x} - \mathbf{x}_I)$$

- ▷ $\chi_I = 0 \Rightarrow$ First-order scheme
- ▷ $\chi_I = 1 \Rightarrow$ No limitation
- Slope limiters present some drawbacks.
 - ▷ They avoid the convergence of the numerical method.
 - ▷ They may be active in **cells where the flow is smooth**.
 - ▷ Straightforward application to higher-order schemes is not obvious.





MLS-based filtering (I)

- We propose to use the **MLS multiresolution properties** to detect shock waves¹. (Generalization of the work of Sjögren and Yee ² for unstructured grids)
- The use of the Reproducing Kernel Particle Method as a **filter** for turbulence problems was proposed in 2000 by Wagner and Liu.
- MLS approximation of a variable can be seen as a **low-pass filtering**.

$$\overline{\Phi}_I = \sum_{j=1}^n N_j(\mathbf{x}) \Phi_j$$

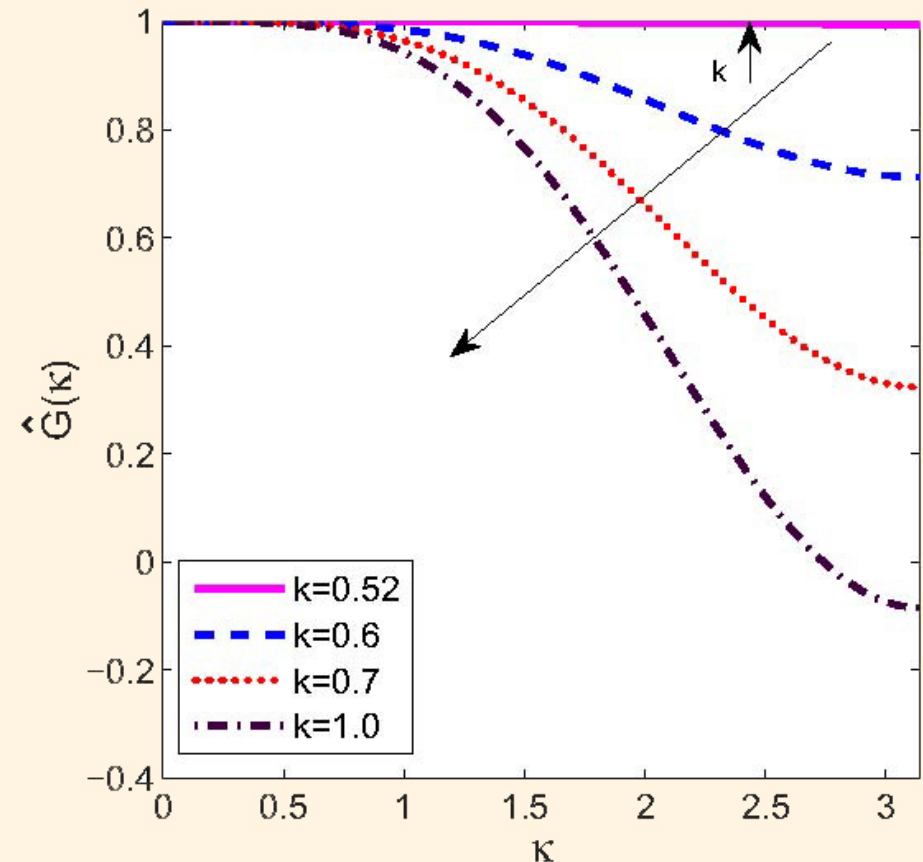
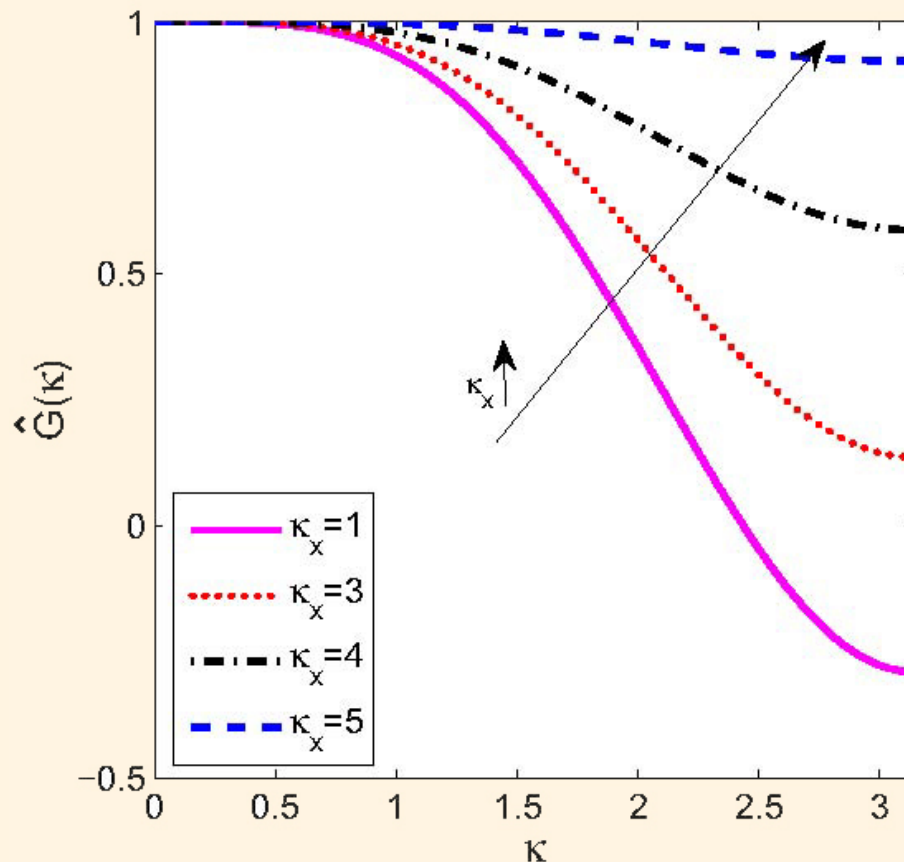
¹X. Nogueira, L. Cueto-Felgueroso, I. Colominas, F. Navarrina, M. Casteleiro, *A new shock-capturing technique based on moving least squares for higher-order numerical schemes on unstructured grids*, CMAME, 2010

²Sjögren, B., Yee, H. C., *Multiresolution wavelet based adaptive numerical dissipation control for high order methods*, Journal of Scientific Computing, 20:211-255, 2004.



MLS-based filtering (II)

- ▶ The filter properties are analyzed by the study of its transfer function



Transfer function for the exponential (left) and for the cubic (right) kernels.

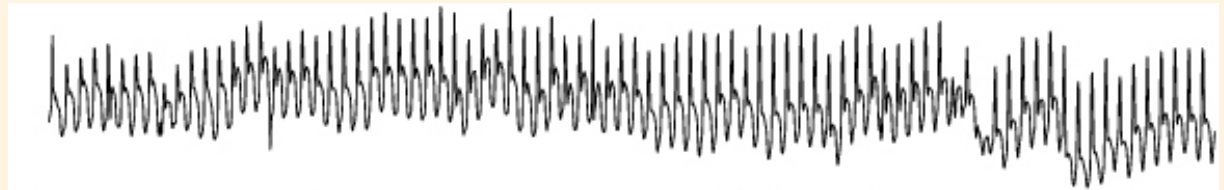


MLS-based shock detection (II)

- ▶ We can decompose a given data series in:

$$u = \hat{u} + u'$$

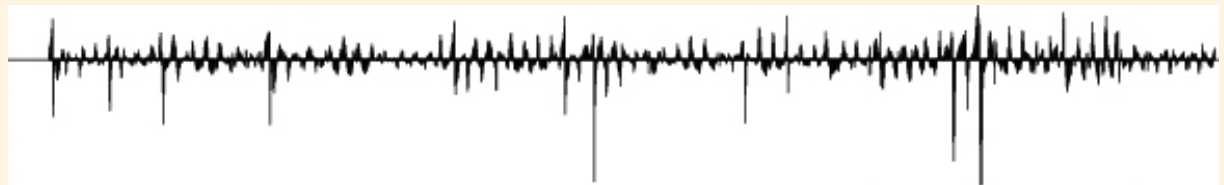
Raw Data (u)



Low frequencies (\hat{u})



High frequencies (u')



- ▶ The **cut frequency** of the filter varies according to its transfer function.



MLS-based shock detection

► Wavelets connection.

- We define two sets of MLS shape functions, $\mathbf{N}^h(\mathbf{x})$ y $\mathbf{N}^{2h}(\mathbf{x})$, computed with h and $2h$ (Two different cut frequencies).
- Set of wavelet functions:

$$\Phi^{2h}(\mathbf{x}) = \mathbf{N}^h(\mathbf{x}) - \mathbf{N}^{2h}(\mathbf{x})$$

- ▷ h (smoothing length) is the **scale parameter** of the wavelet function.
- ▷ We can do the same procedure with κ_x and exponential kernels.
- h -scale solution is the sum of the low-scale part and its complementary high-scale part:

$$u_h(\mathbf{x}) = u_{2h}(\mathbf{x}) + \Psi(\mathbf{x})$$

$$\Psi(\mathbf{x}) = \sum_{j=1}^n \mathbf{u}_j \Phi_j^{2h}(\mathbf{x}) = \sum_{j=1}^n \mathbf{u}_j (\mathbf{N}^h(\mathbf{x}) - \mathbf{N}^{2h}(\mathbf{x}))$$





MLS-based shock detection

► MLS-based selective limiting:

- $\Psi \Rightarrow$ indicates the smoothness of the solution.
- We use Ψ to **decide** if a slope limiter algorithm is activated or not.
- We select the **density** as the reference variable.
- We need to define a threshold value for the function $\Psi_\rho(\mathbf{x})$.
 - ▷ We propose a **possible choice**, that depend on a parameter C_{lc} :
 - T_v defined from the **gradient** of the reference variable in cell I .

$$T_v = \frac{C_{lc} |\nabla \rho|_I A_I^{\frac{1}{d}}}{M}$$

A_I is the size (area in 2D) of the control volume I , d is the number of spatial dimensions and M is the Mach number



MLS-based shock detection

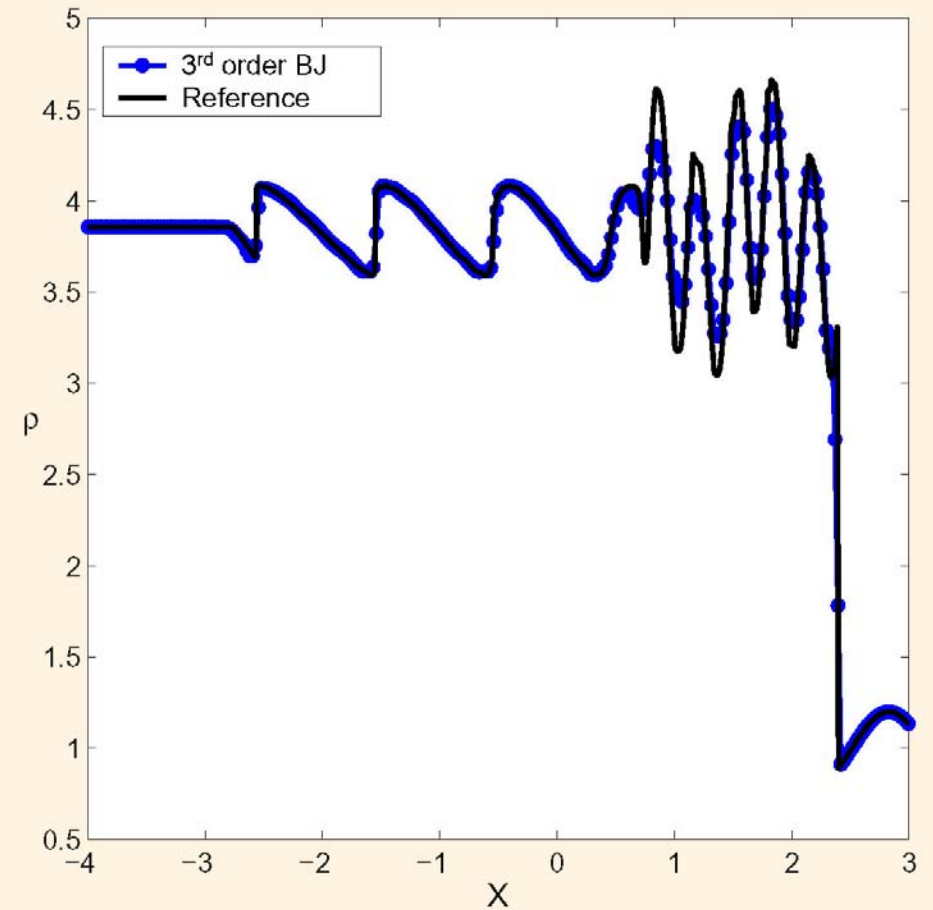
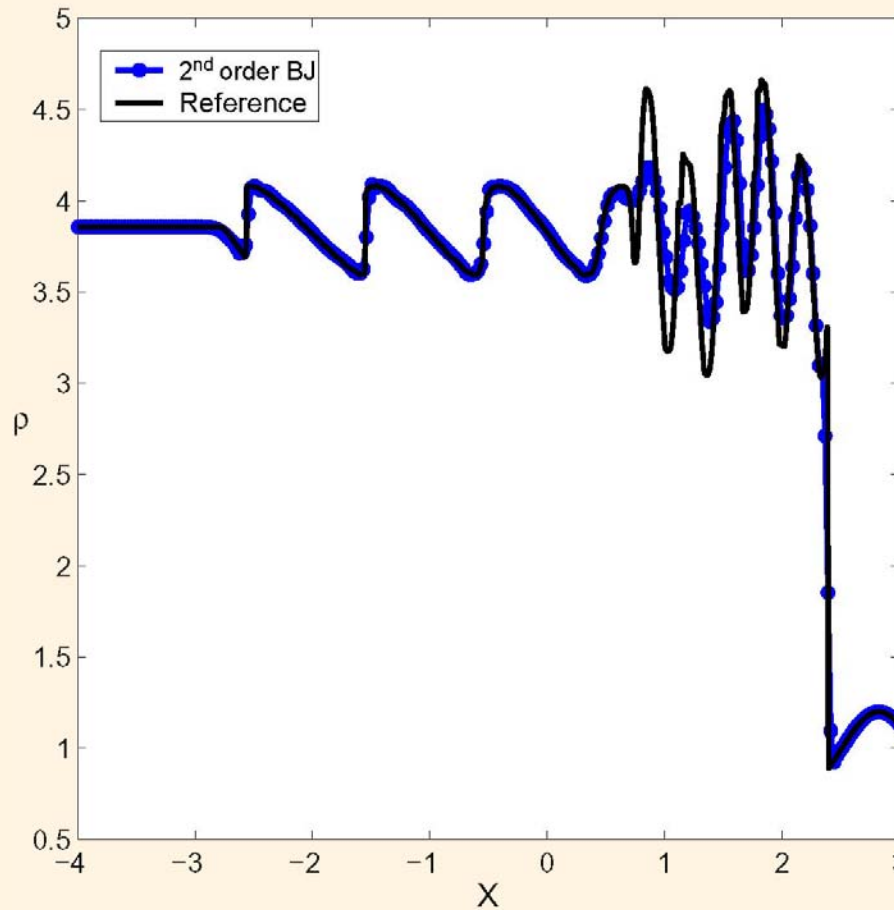
- ▶ The slope limiter is active when:

$$|\Psi_\rho| = \left| \sum_{j=1}^{n_I} \rho_j (\mathbf{N}^h(\mathbf{x}) - \mathbf{N}^{2h}(\mathbf{x})) \right| > T_v$$

- ▶ MLS-based detection method can be applied to **structured and unstructured** grids.
- ▶ This **selective limiting** allows the extension of slope limiters to higher-order schemes.
- ▶ It avoids the limitation of **smooth extrema**.
- ▶ It **improves the convergence** of the numerical method.



MLS-based shock detection. A first 1D test (I)



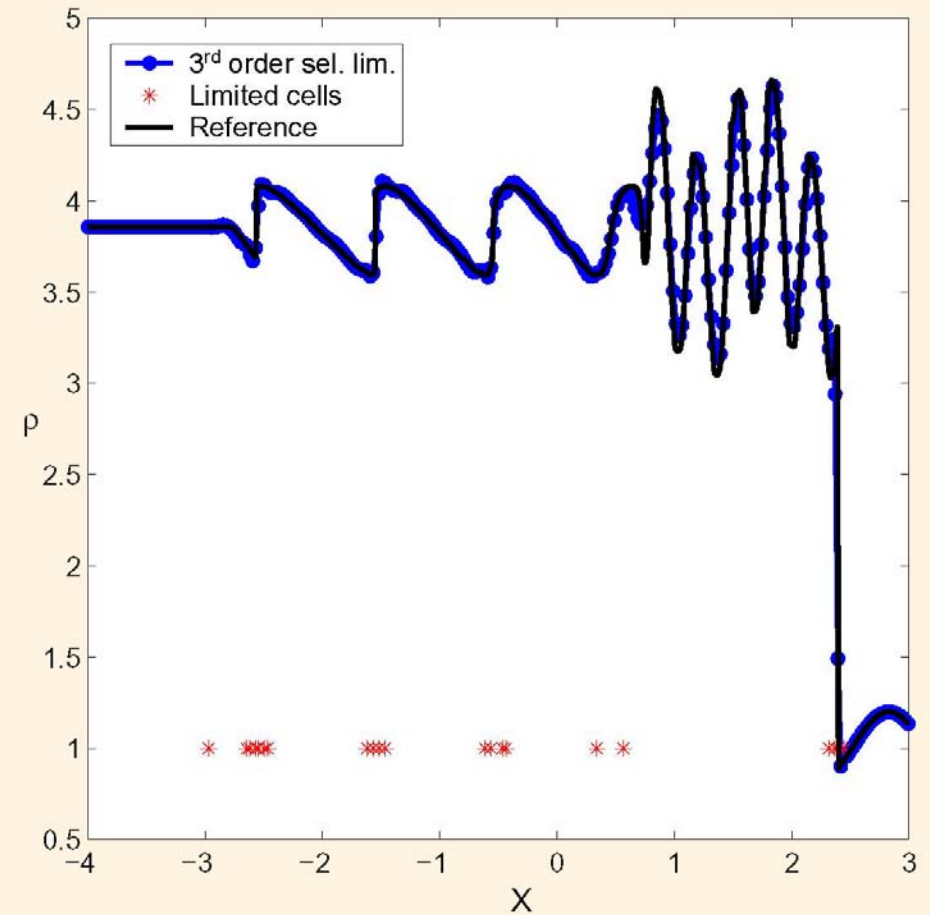
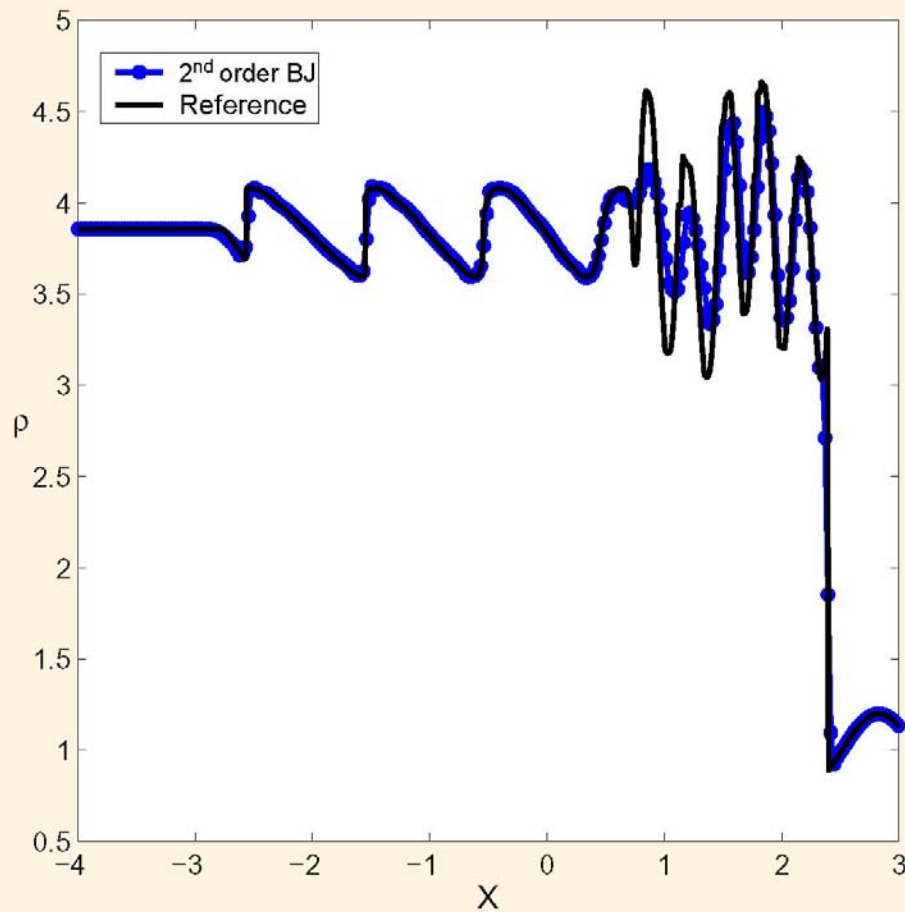
Linear reconstruction (left) and quadratic reconstruction (right) with the BJ limiter for the 1D Shu-Osher problem.





MLS-based shock detection. A first 1D test (II)

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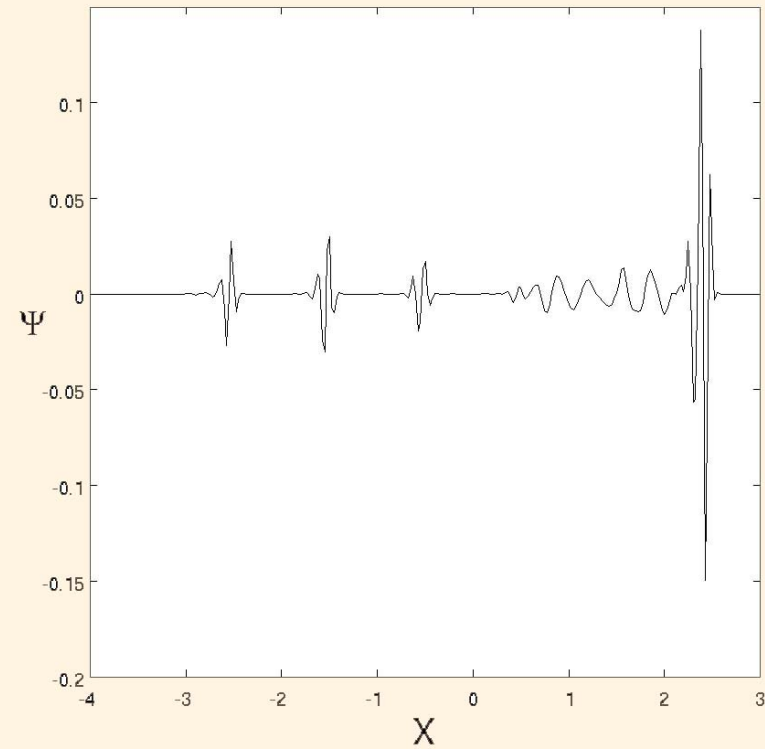
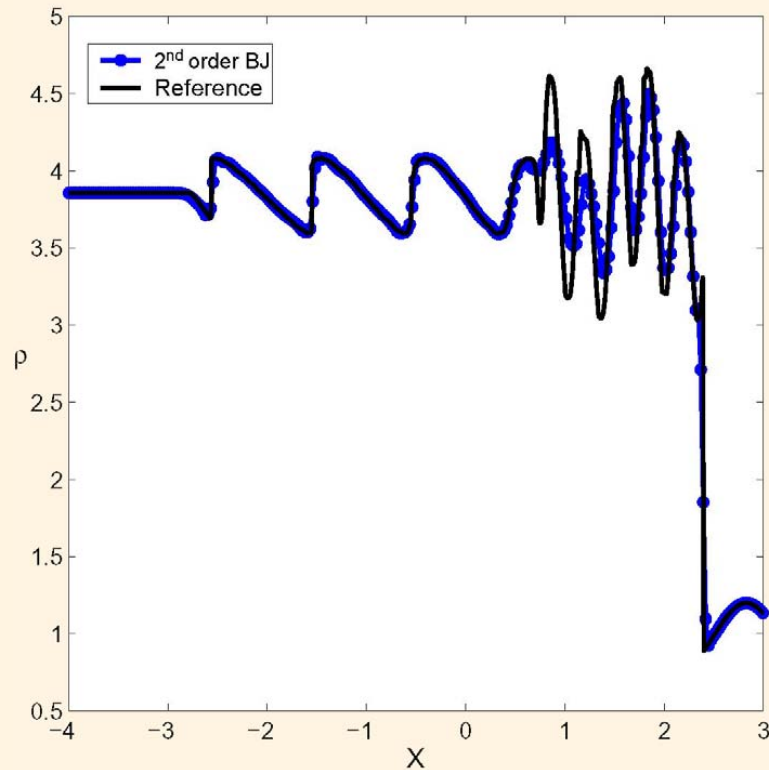
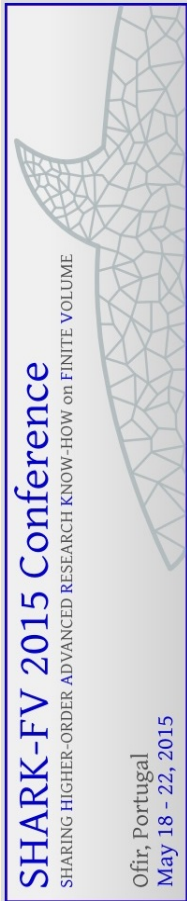
Quadratic reconstruction without detector (left) and with detector (right) for the 1D Shu-Osher problem.





MLS-based shock detection. A first 1D test (III)

► $\Psi \Rightarrow$ indicates the smoothness of the solution.



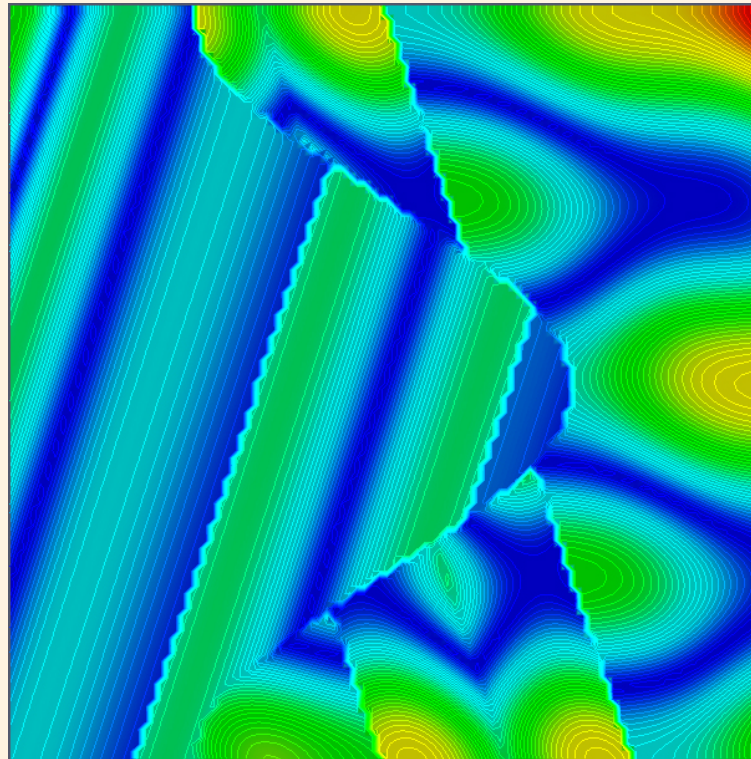
Shape of Ψ for the 1D Shu-Osher problem.





Multiple dimensions detection test

- ▶ We test the ability of the proposed method to detect shock waves in a multidimensional data distribution.



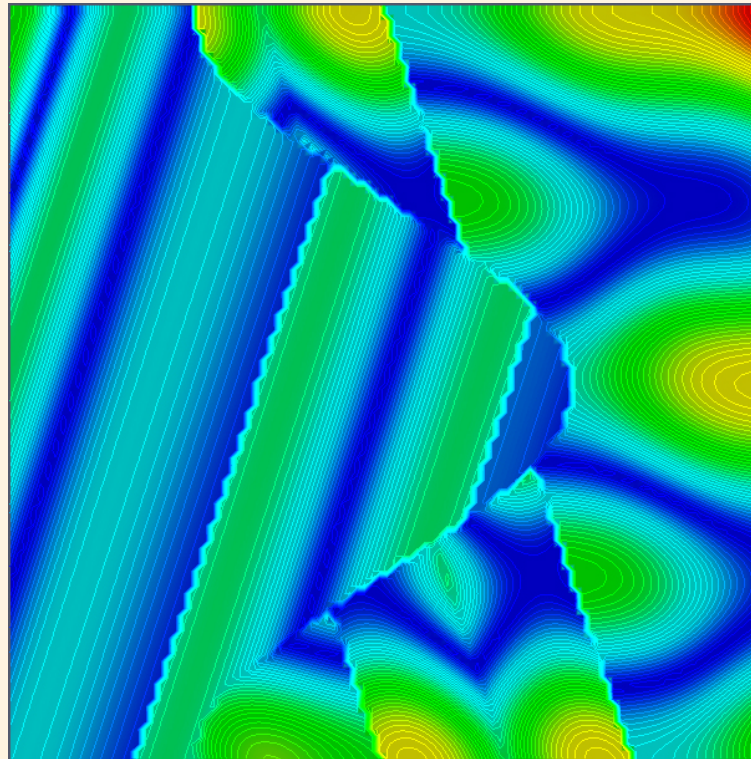
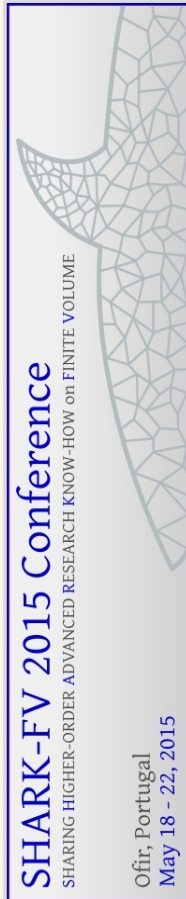
Abgrall function for the multidimensional detection test.





Multiple dimensions detection test

- ▶ We test the ability of the proposed method to detect shock waves in a multidimensional data distribution.



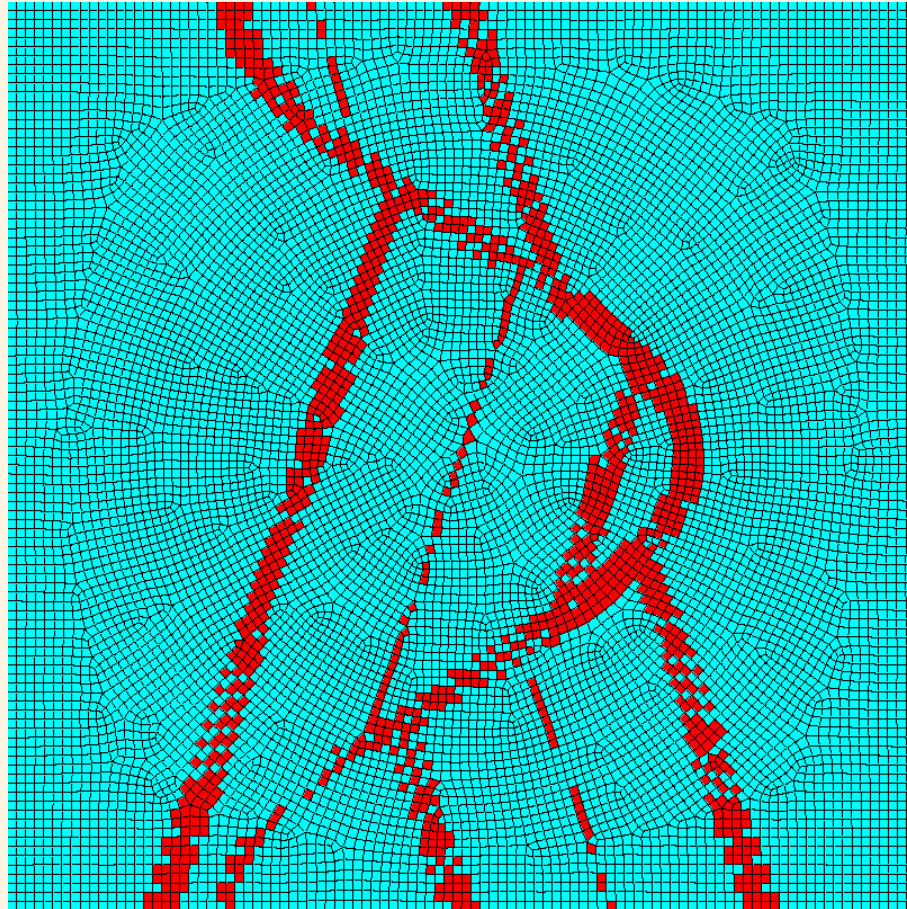
Abgrall function for the multidimensional detection test.



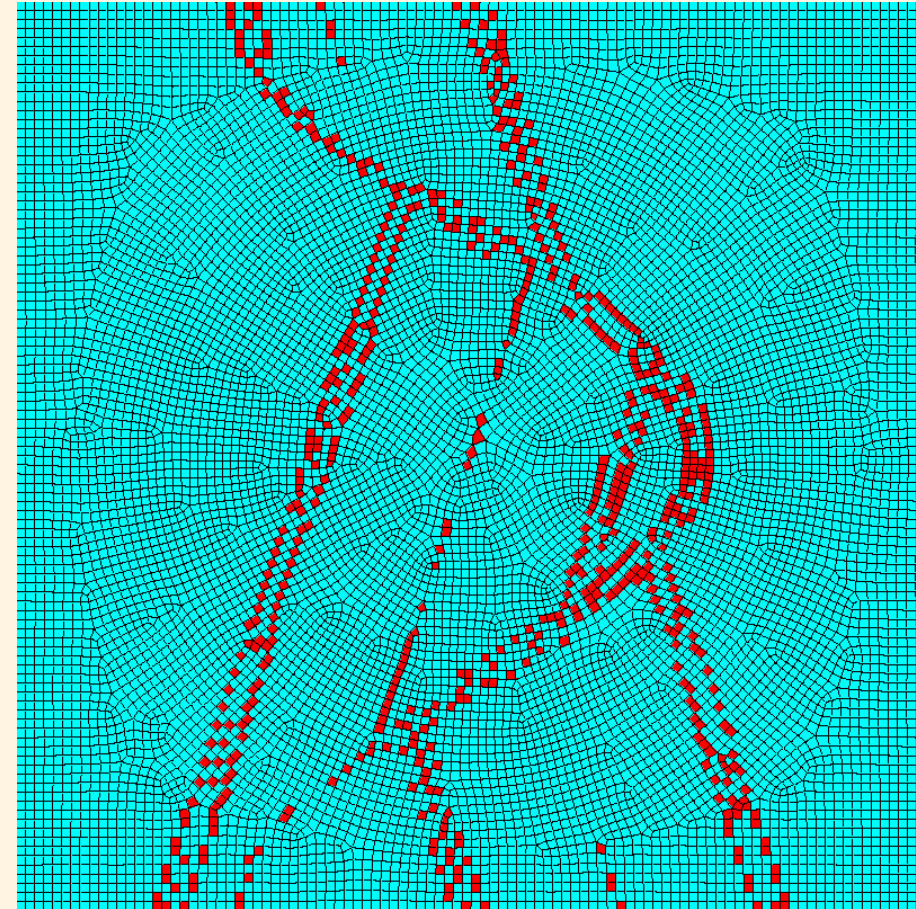


Multiple dimensions detection test.

$$C_{lc} = 0.2$$



$$C_{lc} = 0.4$$





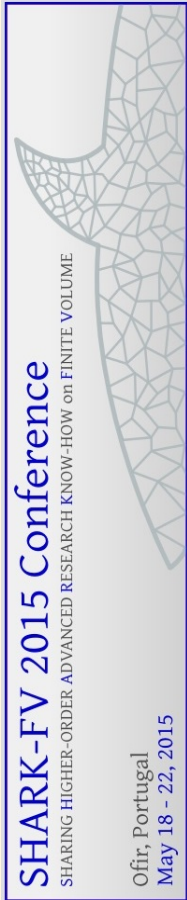
Multiple dimensions detection test.

- ▶ General grids \Rightarrow this approach may become **unstable**.
- ▶ **Solution**: If the slope limiter is activated in a cell it is activated in the **whole stencil** of that cell.
- ▶ We choose a **less restrictive parameter** for the detection $\Rightarrow C_{lc2} = 0.32$.





Multiple dimensions detection test. Unstructured grid



$$C_{lc2} = 0.32$$



Detection results for the Abgrall function with the methodology for general grids.





2D Examples. A subsonic case

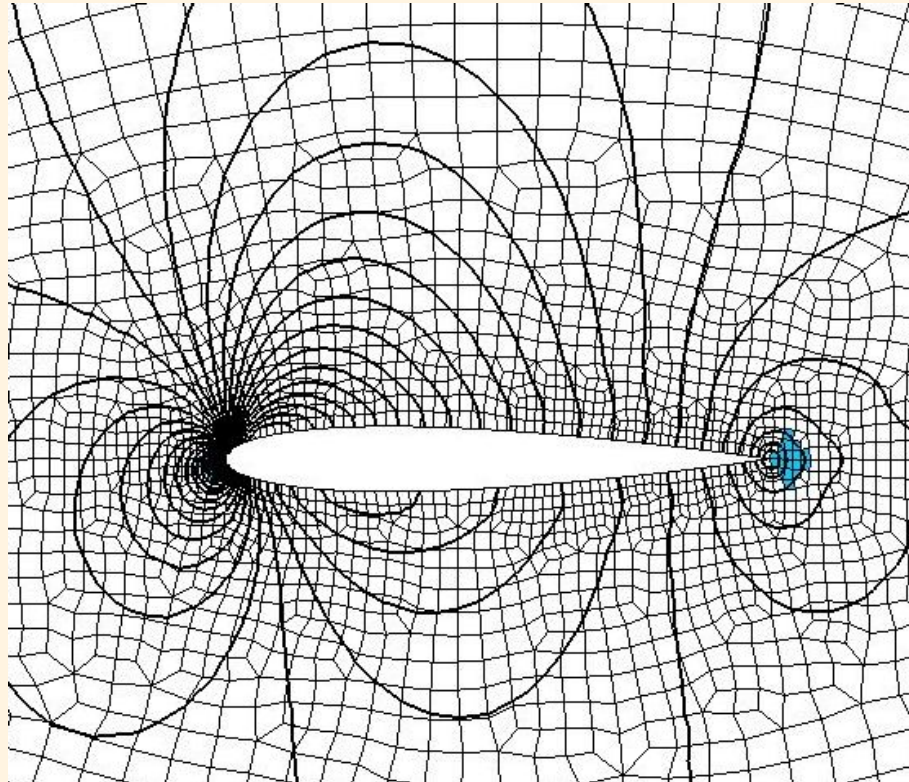
- ▶ Slope limiters may limit even for **smooth flows**
- ▶ Slope limiters may difficult to achieve **convergence**
- ▶ MLS-based selective limiting **alleviate** these problems.
- ▶ We check these effects by solving the **subsonic flow** past a NACA 0012 profile
 - Mach number=0.63, Angle of attack=2°



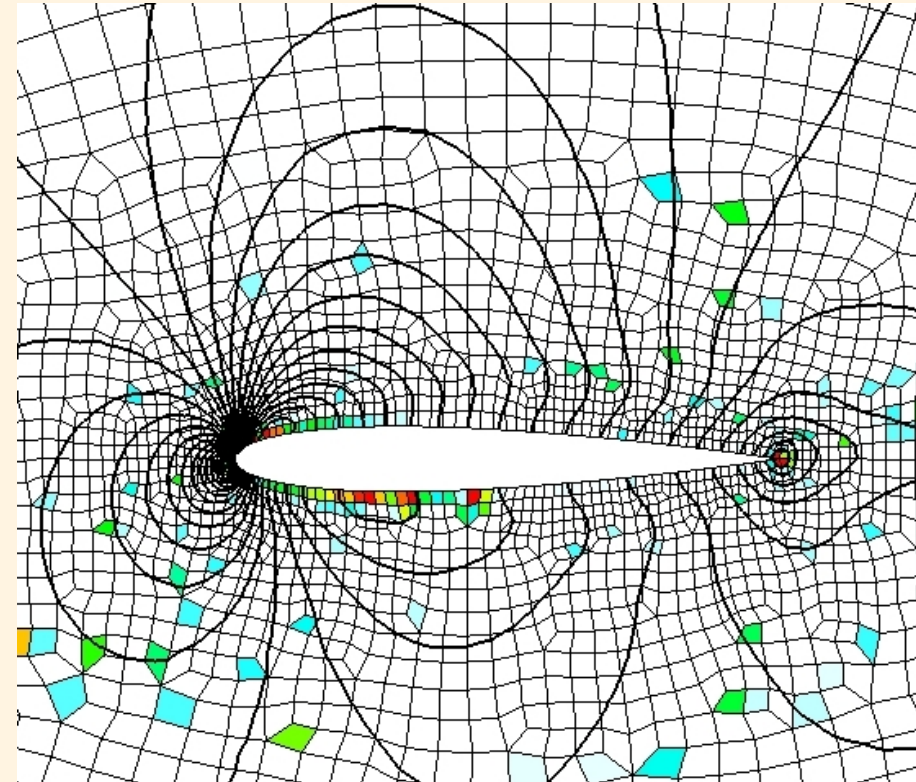


2D Examples. A subsonic case

Selective limiting



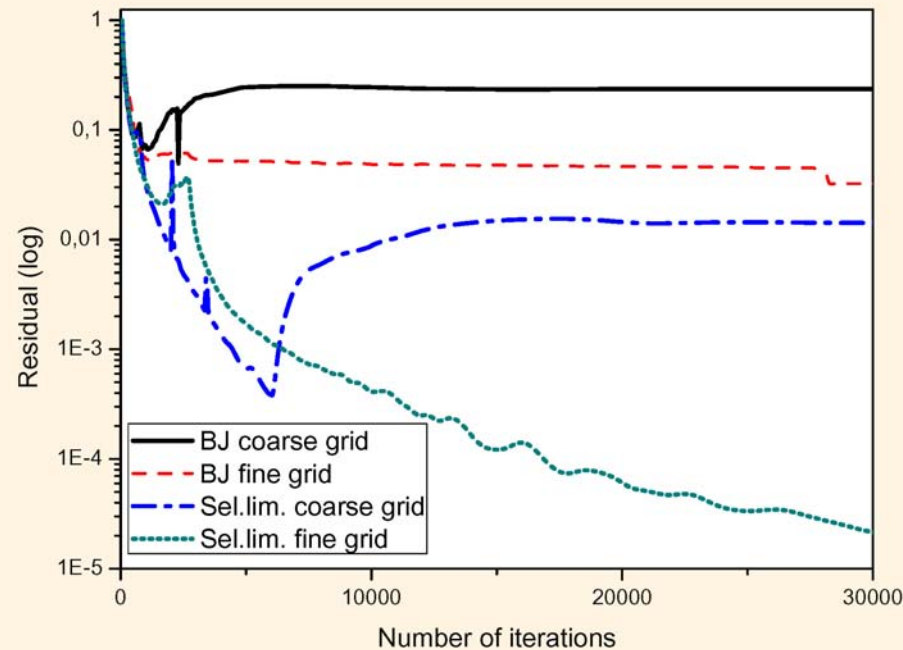
BJ limiter





2D Examples. A subsonic case

Numerical Scheme	C_L	C_D
Hodography method	0.335	0
FV-MLS 3 rd order + BJ	0.318	5.29E-03
FV-MLS 3 rd order BJ + selective limiting	0.328	1.24E-03

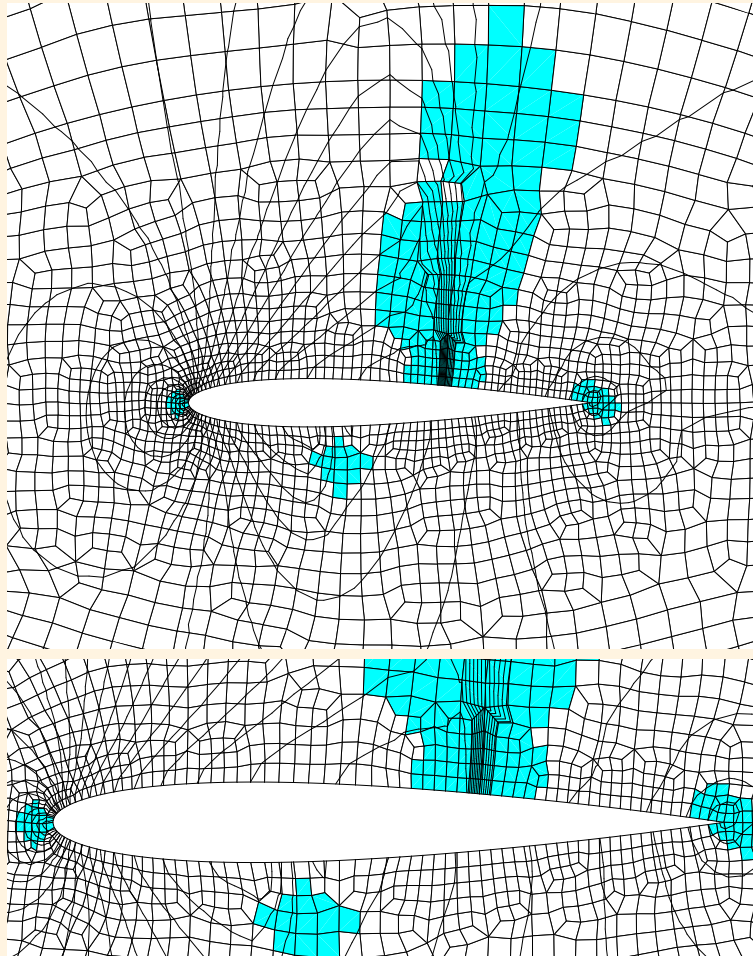




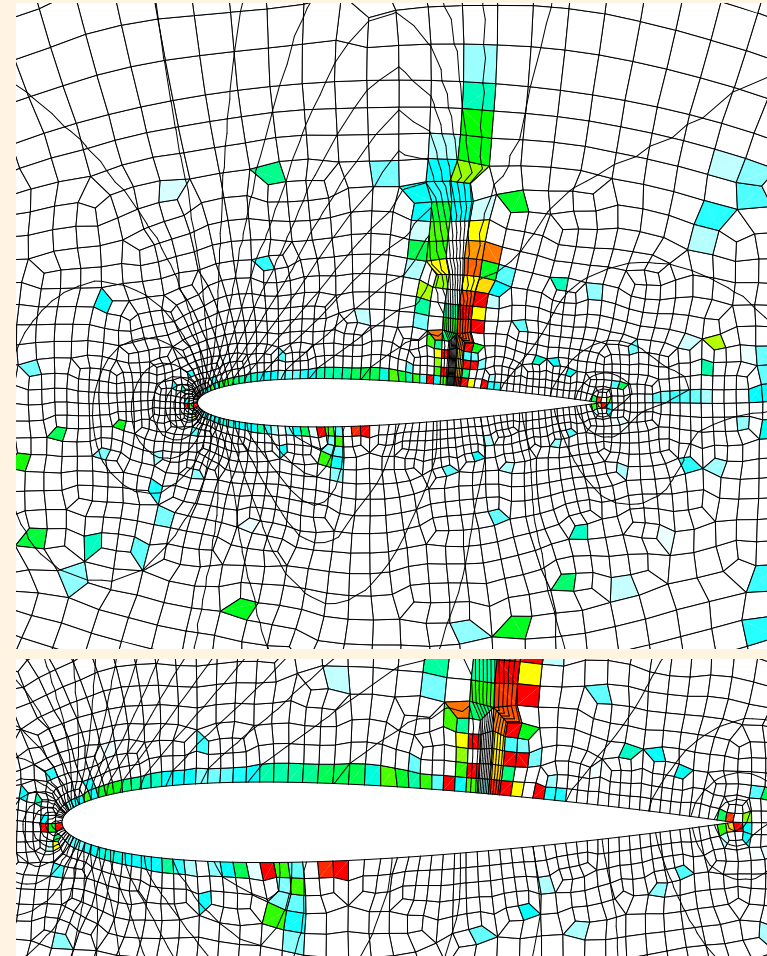
2D Examples. Transonic flow past a NACA 0012

Mach number=0.8, Angle of attack=1.25°

Selective limiting



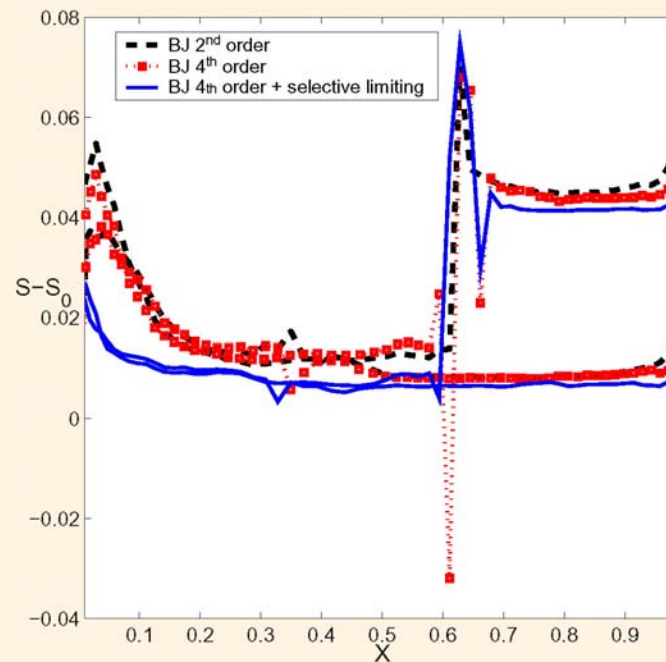
BJ limiter





2D Examples. Transonic flow past a NACA 0012

Numerical Scheme	C_L	C_D
FV-MLS 2 nd order + BJ	0.341	2.465E-02
FV-MLS 4 th order + BJ	0.342	2.486E-02
FV-MLS 4 th order BJ + selective limiting	0.343	2.317E-02
AGARD Reference	0.347	2.221E-02



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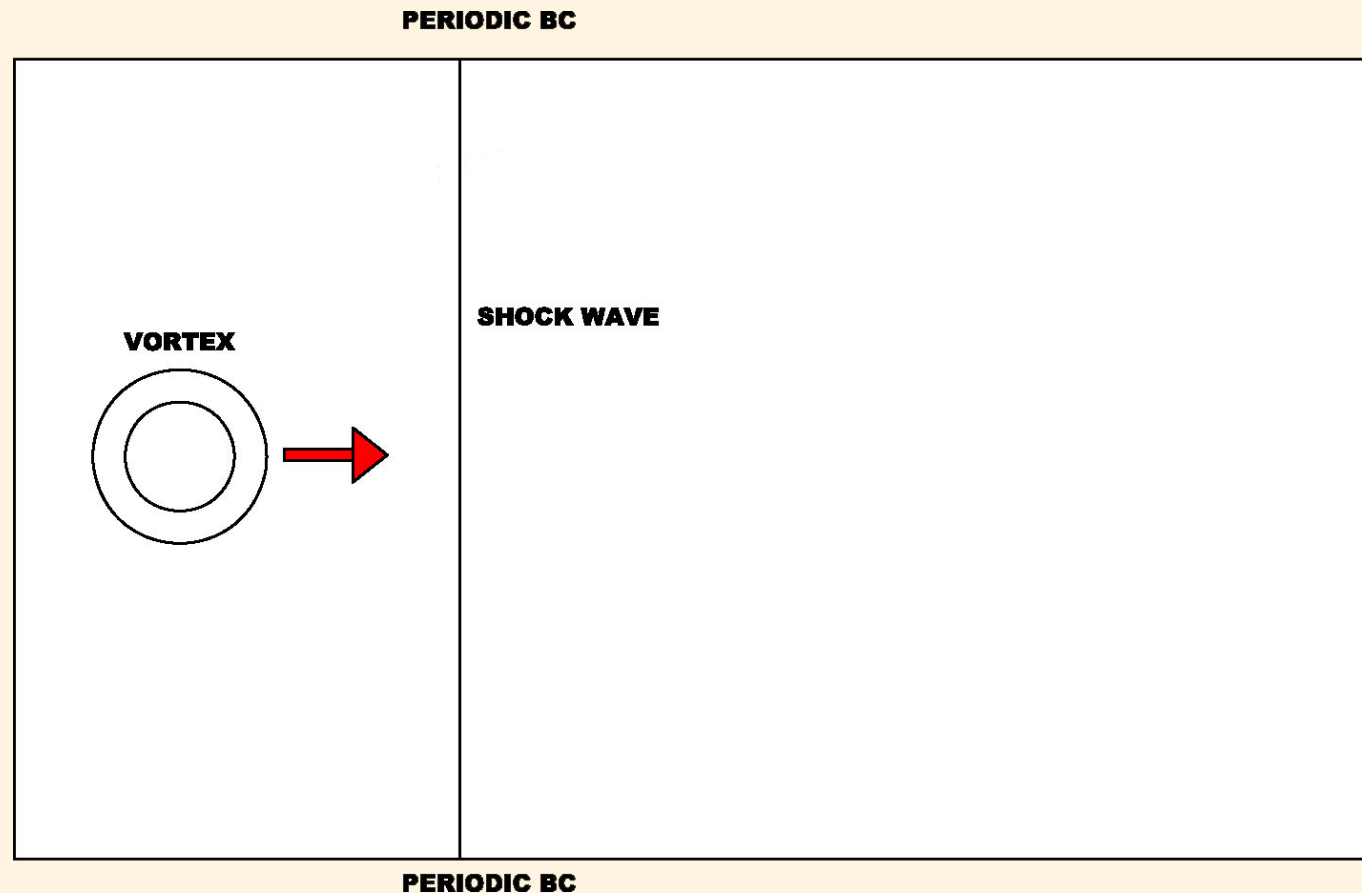


2D Examples. Shock-wave-vortex Interaction

Shock-wave-vortex Interaction.

$M_v = 0.4$, $M_s = 1.2$, 200×200 grid

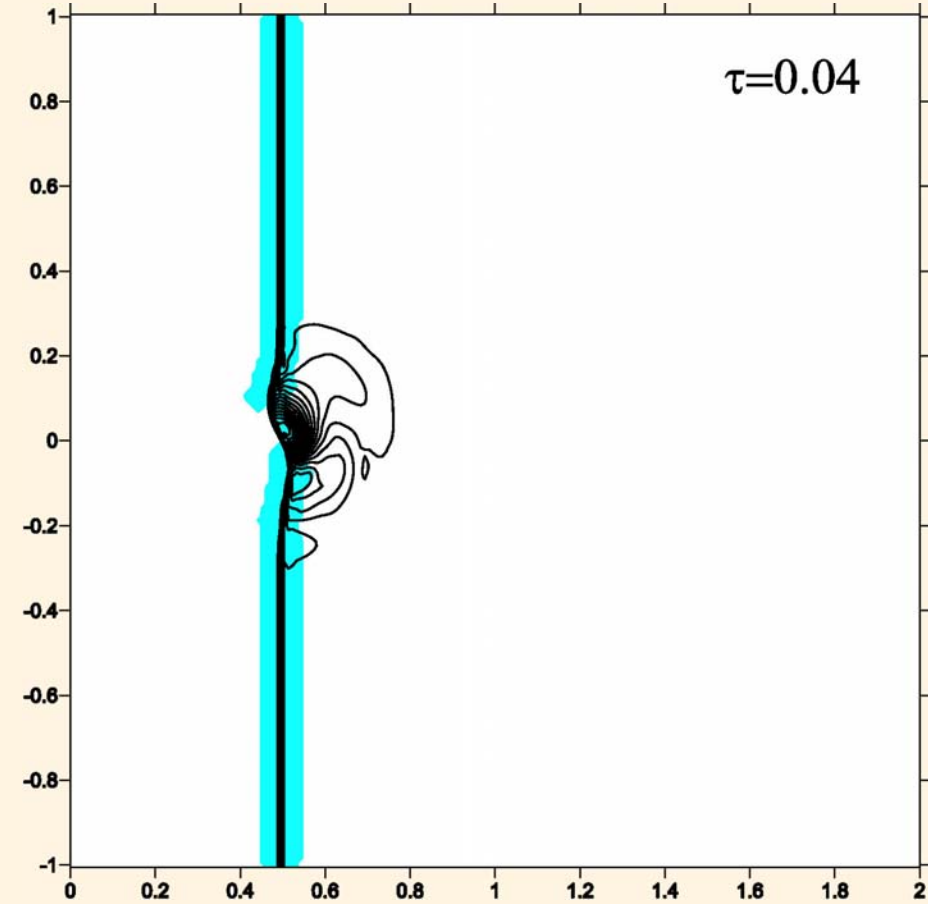
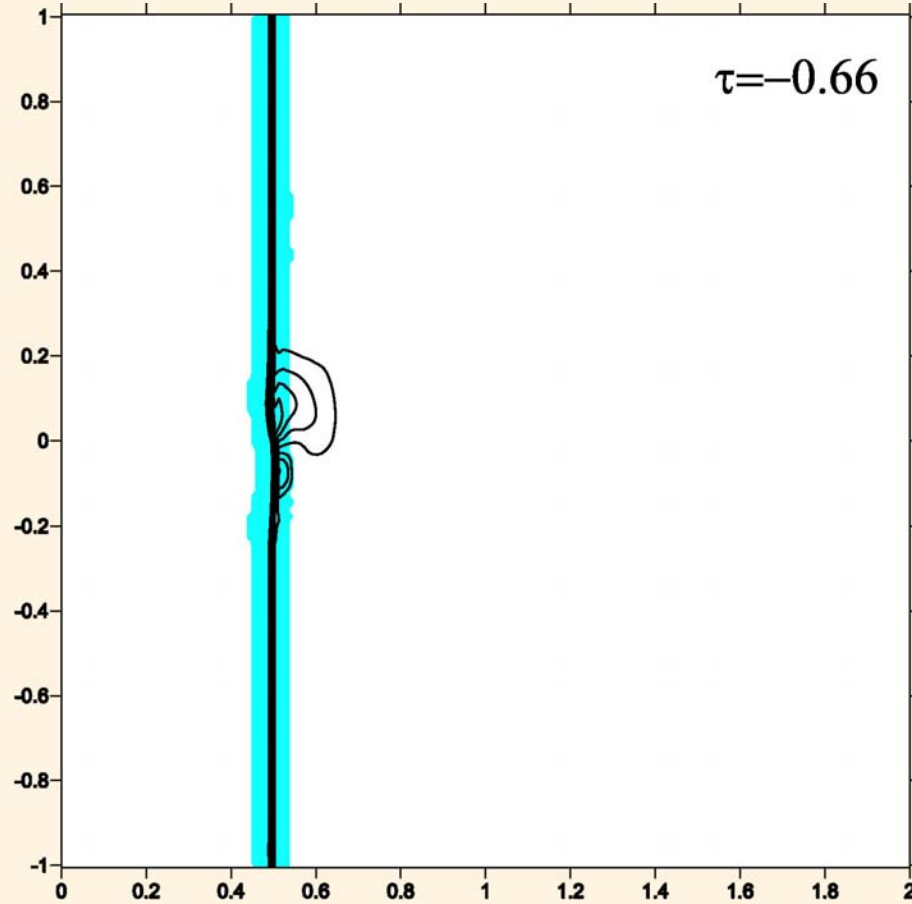
Third-order FV-MLS scheme, Barth-Jespersen limiter





2D Examples. Shock-wave-vortex Interaction

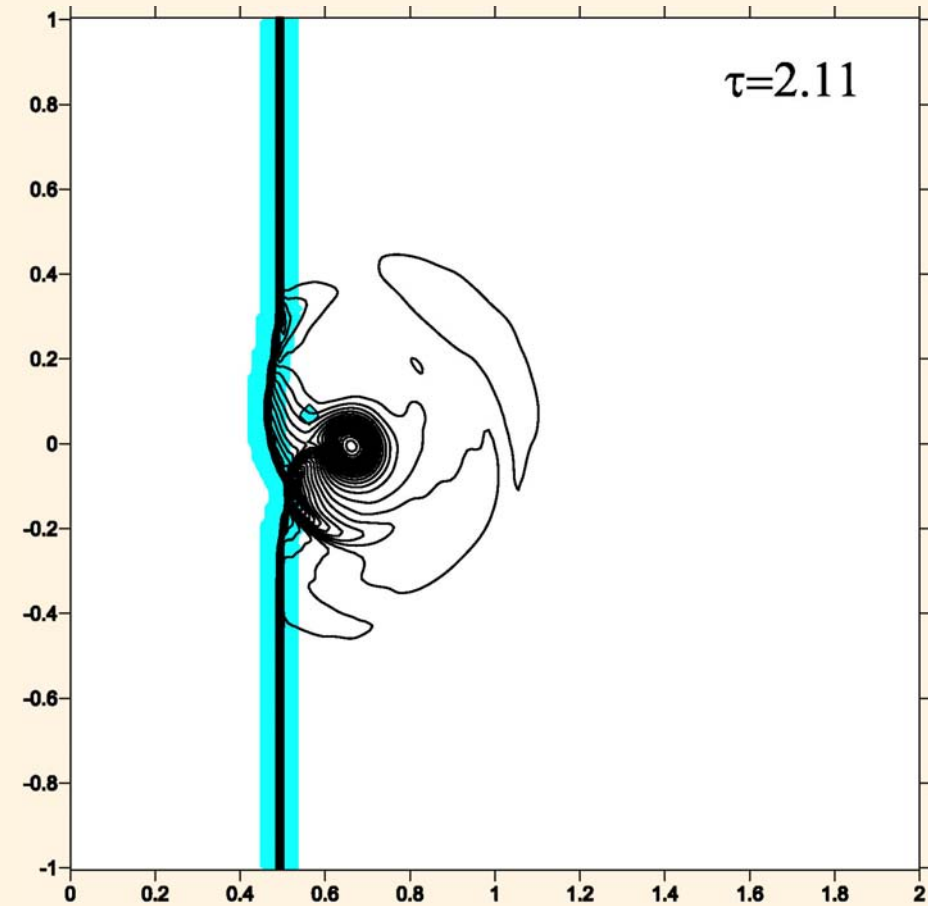
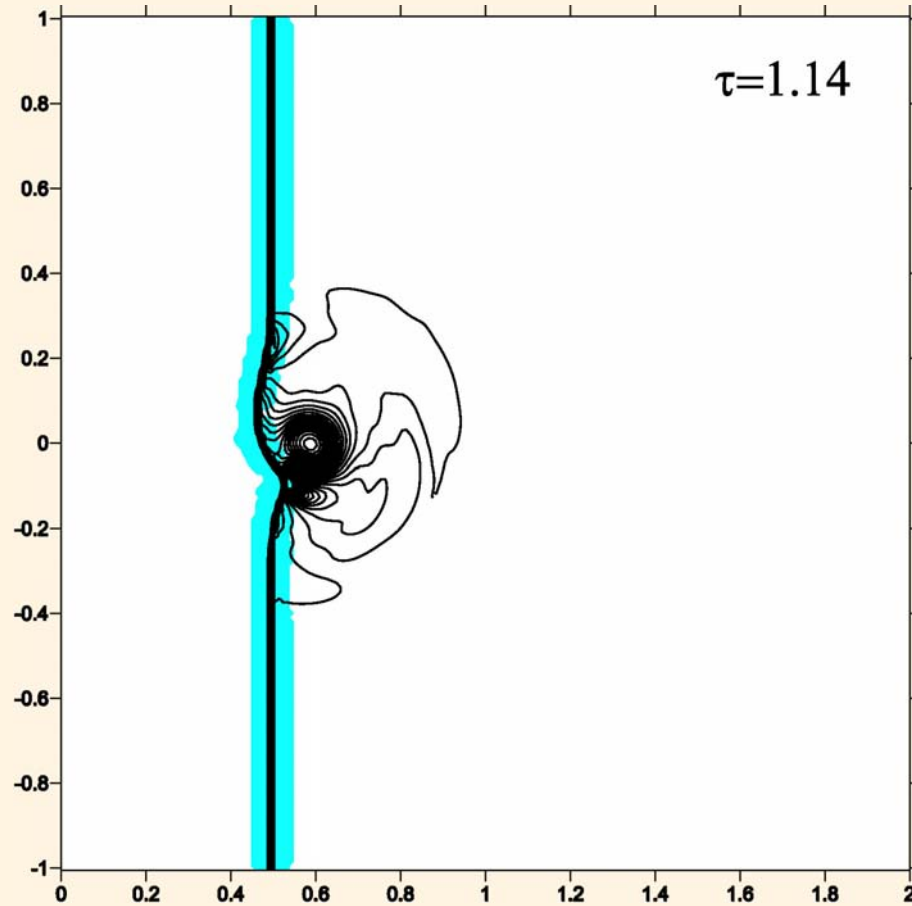
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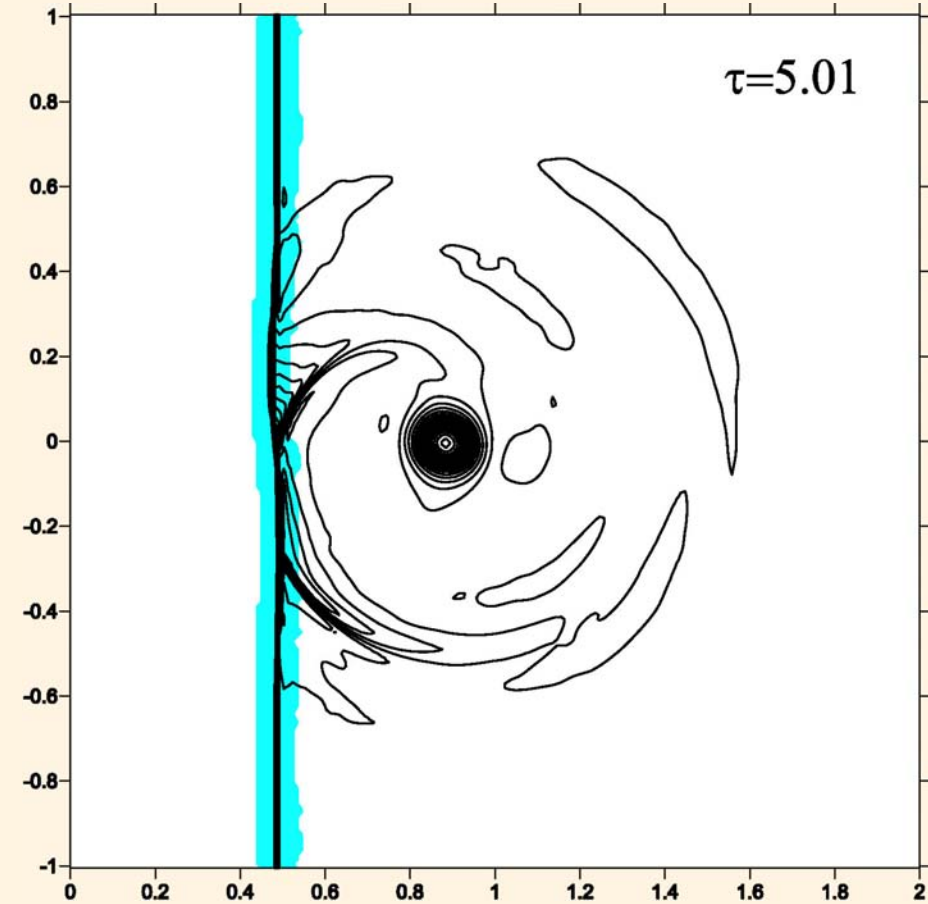
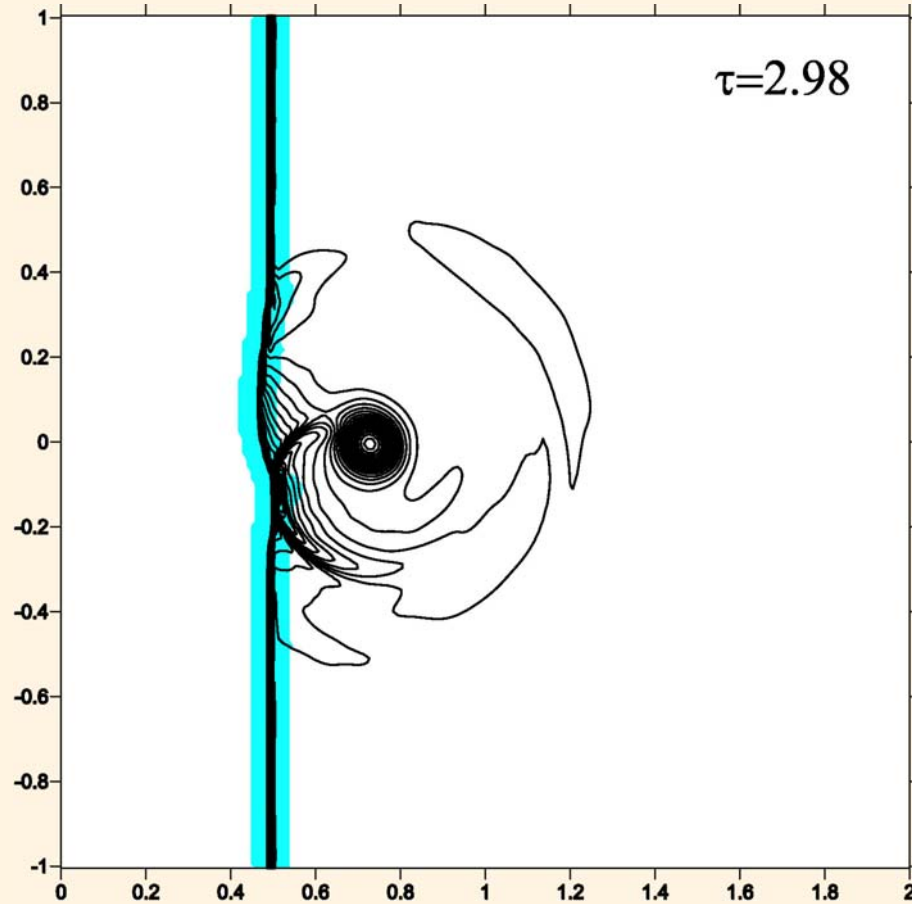


2D Examples. Shock-wave-vortex Interaction

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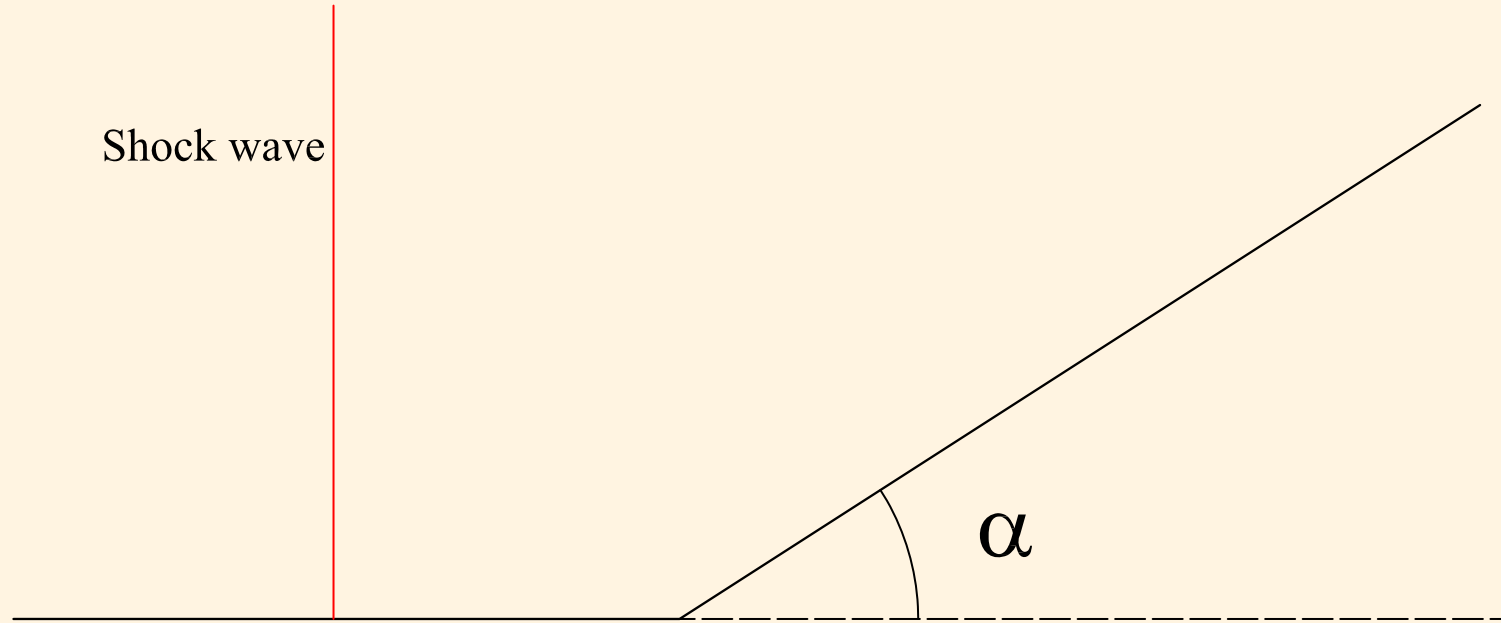
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2D Examples. Double Mach Reflection

Shock wave

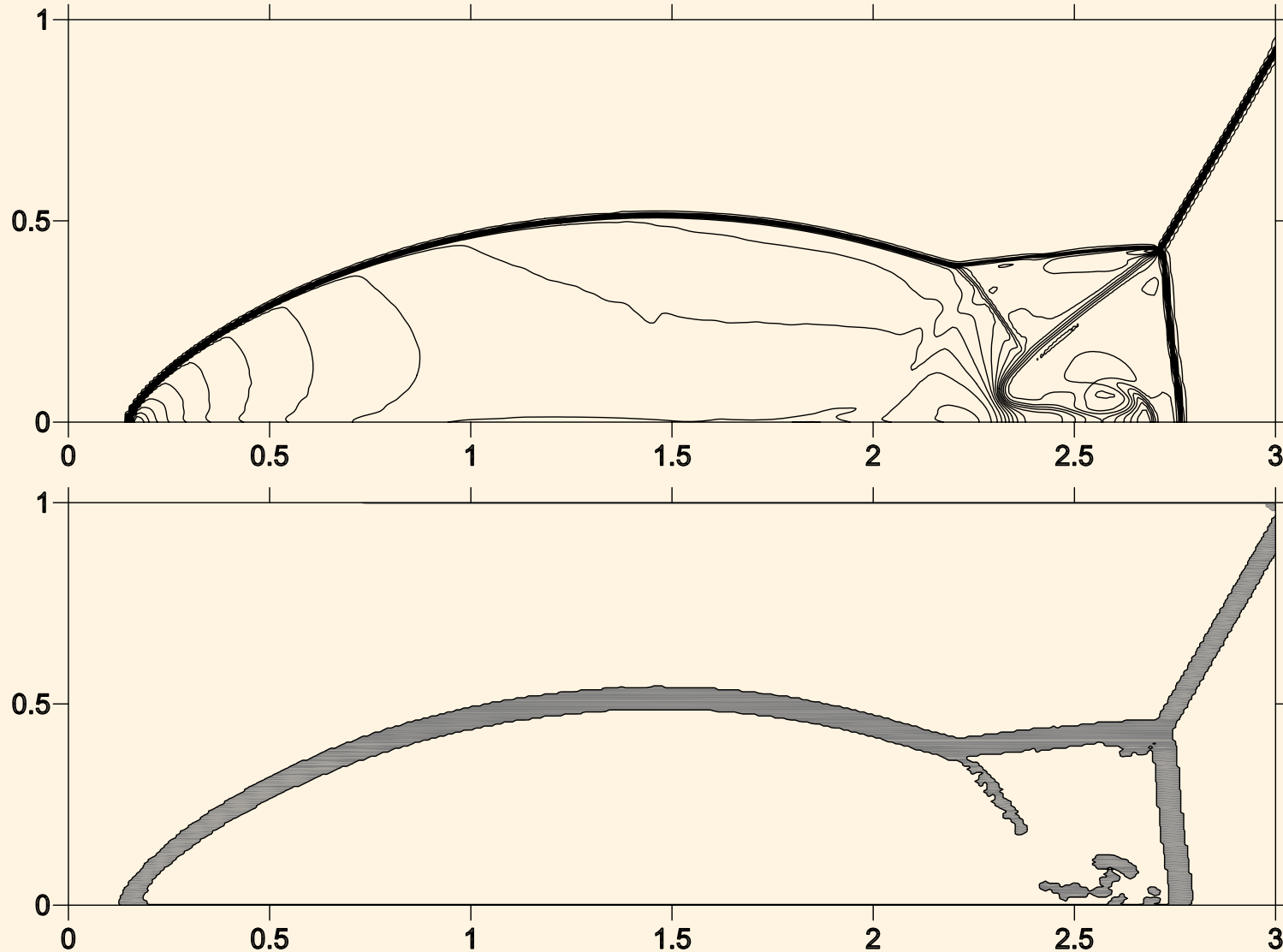


Schematic representation of the Double Mach reflection problem.

- ▶ The size of the elements is $\Delta x = \Delta y = \frac{1}{200}$
- ▶ Mach 10 right-moving shock
- ▶ $\alpha = 60$ degrees
- ▶ Third-order **FV-MLS** scheme, Van Albada limiter



2D Examples. Double Mach Reflection



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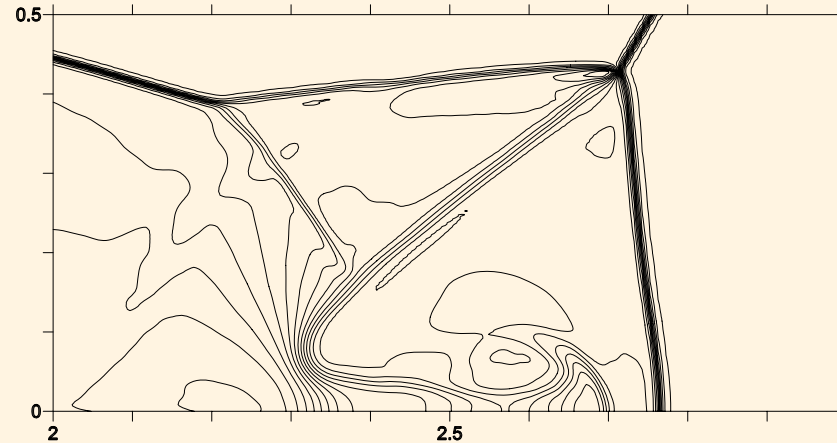




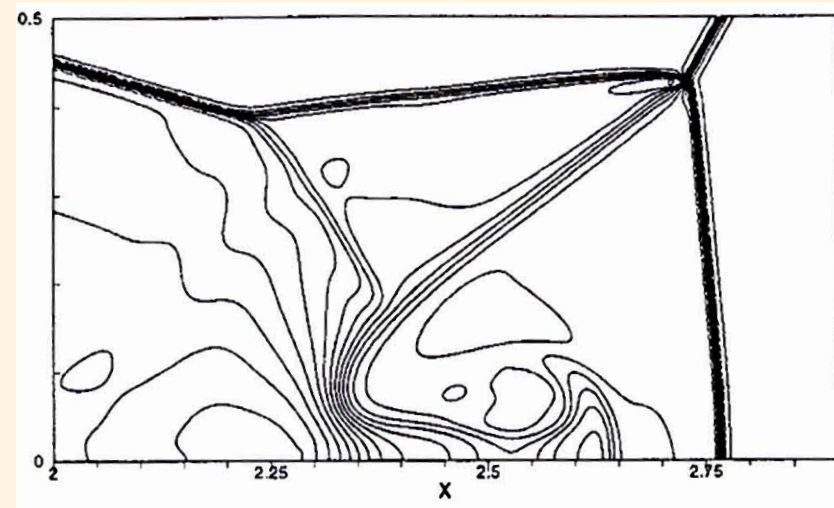
Double Mach Reflection. Detail of the Mach stems region

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Present Approach

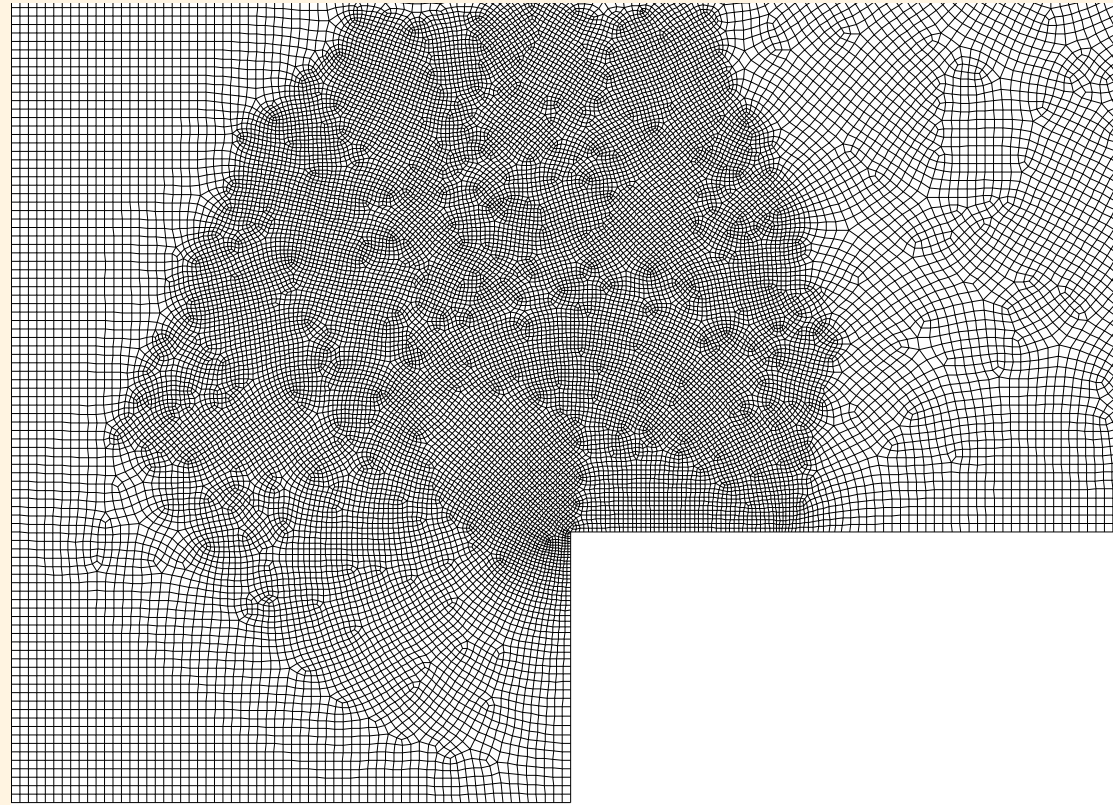


WENO (Shu, JCP,150 (1999))





2D Examples. Mach 3 Forward step

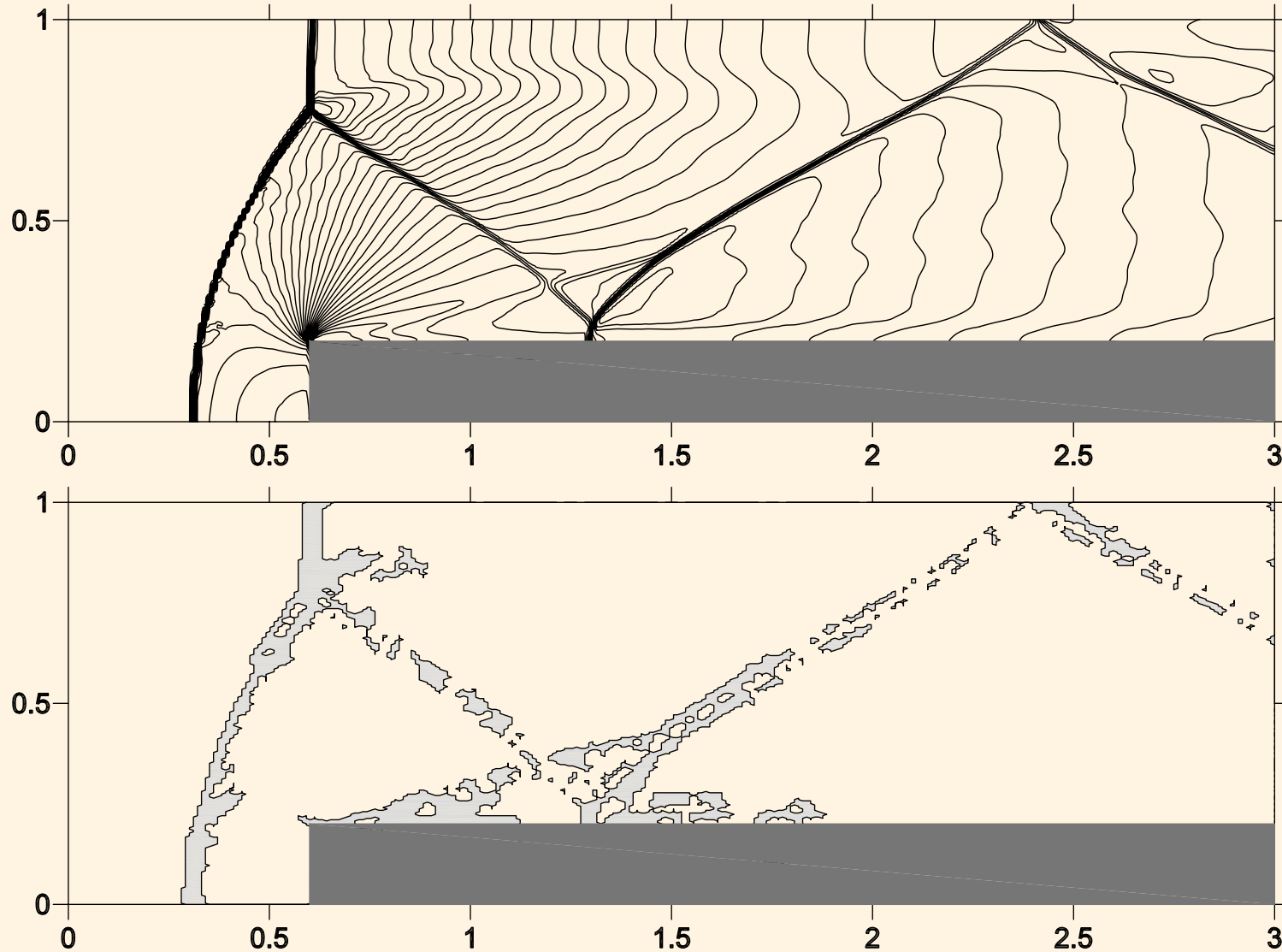


Detail of the mesh in the corner region.

- ▶ The size of the elements away from the corner is ($\Delta x = \Delta y = \frac{1}{160}$). Size of elements near the corner is **one-half** that.
- ▶ Third-order **FV-MLS** scheme, Jawahar limiter



2D Examples. Mach 3 Forward step



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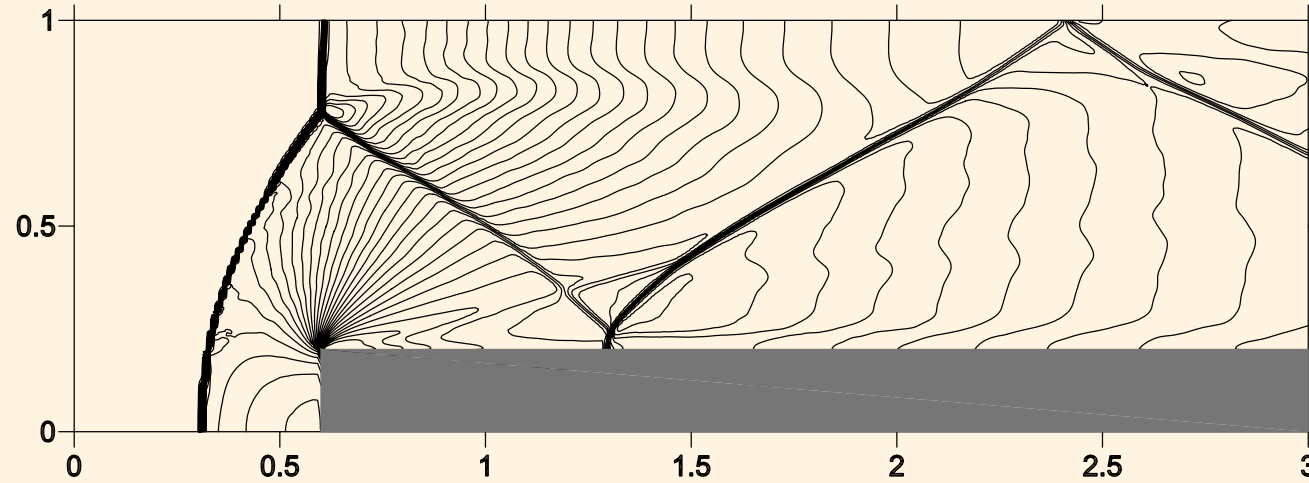




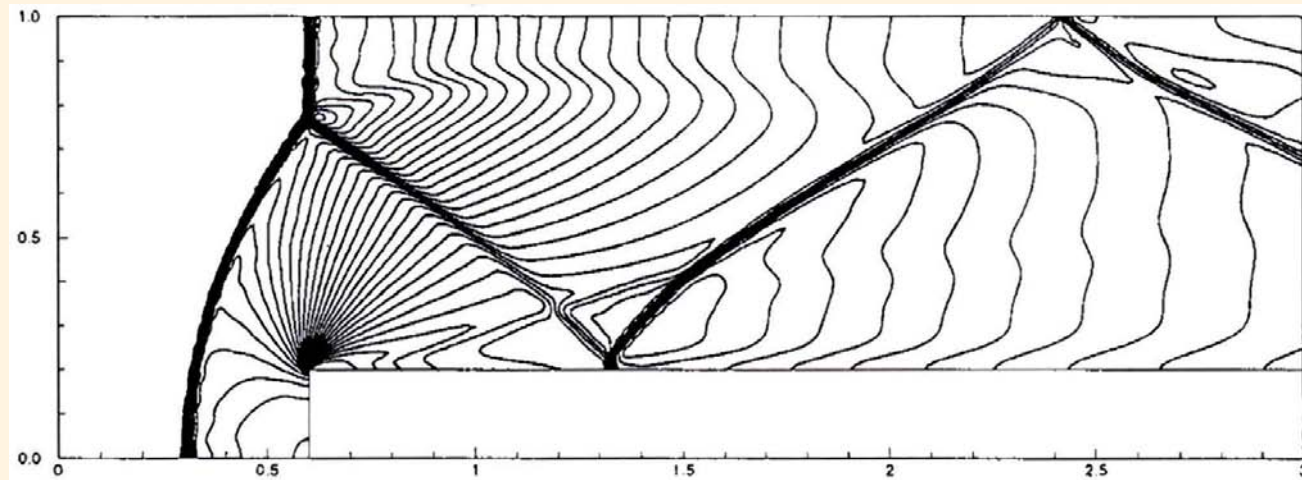
2D Examples. Mach 3 Forward step

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Present Approach



WENO (Shu, JCP,150 (1999))





A high-order formulation for all-speed flows

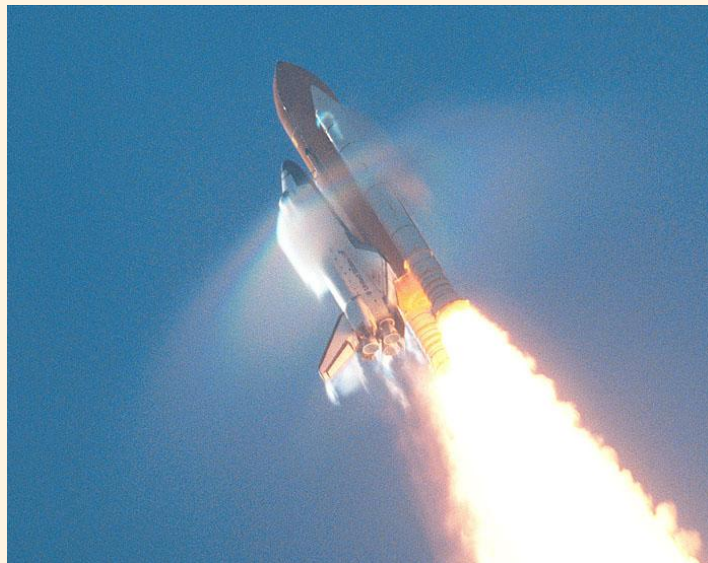
- Introduction
- The FV-MLS method
- A high-order formulation for all-speed flows
- High-order Sliding Mesh techniques
- Phase-transition phenomena
- Conclusions





A high-order formulation for all-speed flows

- ▶ Two families of FV schemes:
 - Density-based solvers \Rightarrow Compressible flows
 - Pressure-based solvers \Rightarrow Incompressible flows
- ▶ The difference is in the computation of pressure field, and in the density.



Compressible Flow



Incompressible Flow



A high-order formulation for all-speed flows

► Density-based solvers:

- Density \Rightarrow computed from the continuity equation
- Pressure \Rightarrow obtained via an **EQUATION OF STATE**

► Fails to compute low Mach number flows:

- Discretized equations do not verify the right scaling of the pressure fluctuations with M^2





A high-order formulation for all-speed flows

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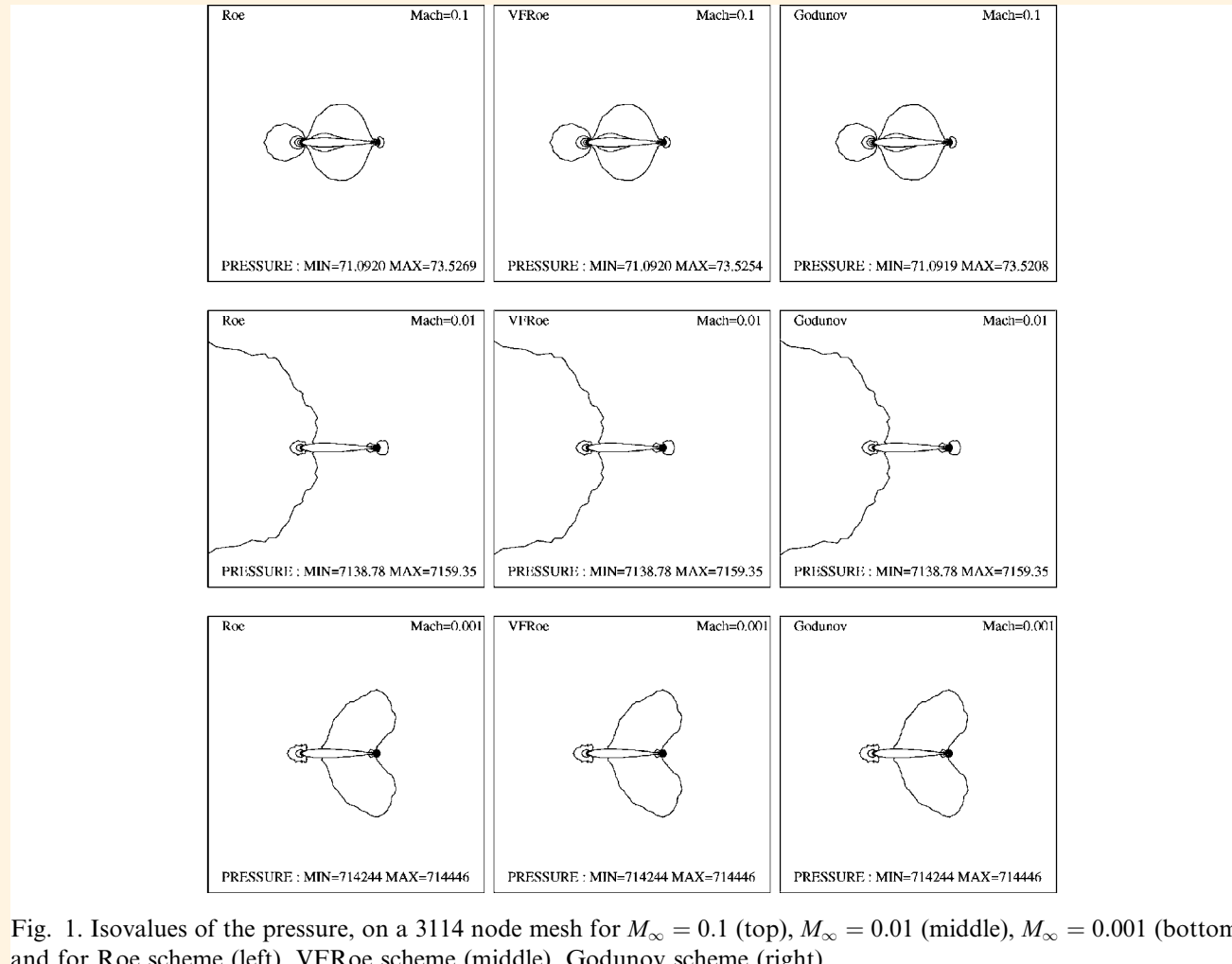


Fig. 1. Isovalues of the pressure, on a 3114 node mesh for $M_\infty = 0.1$ (top), $M_\infty = 0.01$ (middle), $M_\infty = 0.001$ (bottom) and for Roe scheme (left), VFRoe scheme (middle), Godunov scheme (right).

H. Guillard and A.Murrone, Computers & Fluids, 2004





A high-order formulation for all-speed flows

- ▶ Pressure-based solvers:
 - Continuity and momentum equations \Rightarrow Poisson equation
 - Pressure \Rightarrow Solve Poisson equation
- ▶ Not well-suited to compute high Mach flows





A high-order formulation for all-speed flows

We want to develop solvers for

ALL THE REGIMES OF A FLOW





A high-order formulation for all-speed flows

► Conservation laws

$$\frac{\partial U}{\partial t} + \nabla \cdot (\mathcal{F}^{\mathcal{H}} - \mathcal{F}^{\mathcal{V}}) = S \quad \text{in } \Omega_T$$

► Numerical discretization:

$$\Omega_I \frac{\partial U_I}{\partial t} + \sum_{j=1}^{N_f} \sum_{ig=1}^{N_G} [\mathcal{H}(U_j^+, U_j^-, \hat{\mathbf{n}}_j) - \mathcal{F}^{\mathcal{V}}_j \cdot \hat{\mathbf{n}}_j]_{ig} \mathcal{W}_{ig} = \int_{\Omega_I} S d\Omega$$

- Time integration \rightarrow 3rd order Runge-Kutta of Shu and Osher
- $\mathcal{H}(U_j^+, U_j^-, \hat{\mathbf{n}}_j) \rightarrow$ Numerical flux



A high-order formulation for all-speed flows

► Approximate Riemann solvers

- Roe numerical flux

$$\mathcal{H}_j = \frac{1}{2}(\mathcal{F}^{\mathcal{H}}(U_j^+) + \mathcal{F}^{\mathcal{H}}(U_j^-)) \cdot \hat{\mathbf{n}} - \frac{1}{2} \sum_{k=1}^4 \tilde{\alpha}_k |\tilde{\lambda}_k| \tilde{\mathbf{r}}_k$$

▷ $\tilde{\lambda}$ → eigenvalues

▷ $\tilde{\mathbf{r}}$ → eigenvectors

$$\tilde{\alpha}_1 = \frac{1}{2\tilde{c}^2} [\Delta(p) - \tilde{\rho}\tilde{c} (\Delta(u)n_x + \Delta(v)n_y)]$$

$$\tilde{\alpha}_2 = \frac{\tilde{\rho}}{\tilde{c}} [\Delta(v)n_x - \Delta(u)n_y]$$

$$\tilde{\alpha}_3 = \frac{1}{\tilde{c}^2} [\Delta(p) - \tilde{c}^2 \Delta(\rho)]$$

$$\tilde{\alpha}_4 = \frac{1}{2\tilde{c}^2} [\Delta(p) + \tilde{\rho}\tilde{c} (\Delta(u)n_x + \Delta(v)n_y)]$$

- Rusanov numerical flux

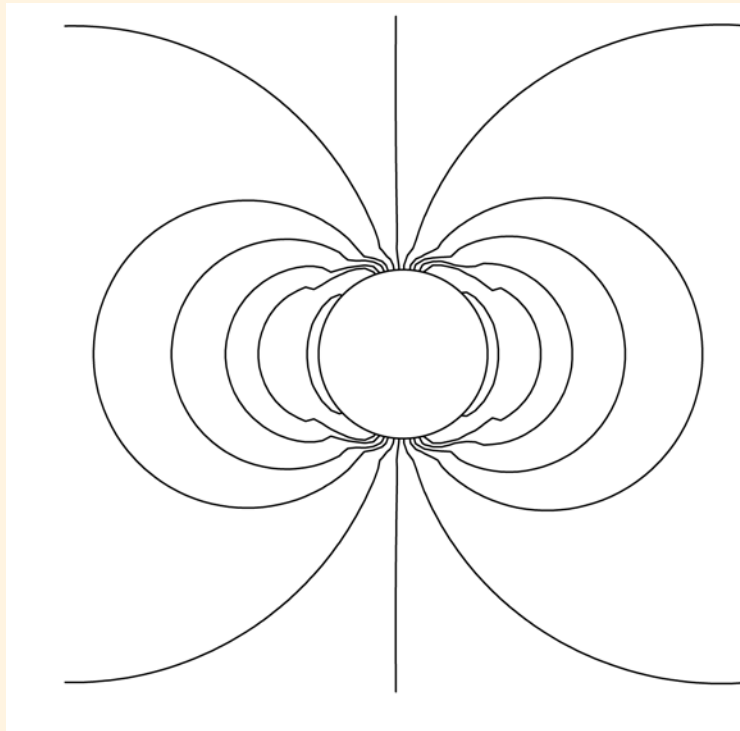
$$\mathcal{H}_j = \frac{1}{2}(\mathcal{F}^{\mathcal{H}}(U_j^+) + \mathcal{F}^{\mathcal{H}}(U_j^-)) \cdot \hat{\mathbf{n}} - \frac{1}{2} S^+ \Delta(\mathbf{U})$$

▷ $S^+ = \max(|\mathbf{v}^+| + c^+, |\mathbf{v}^-| + c^-)$

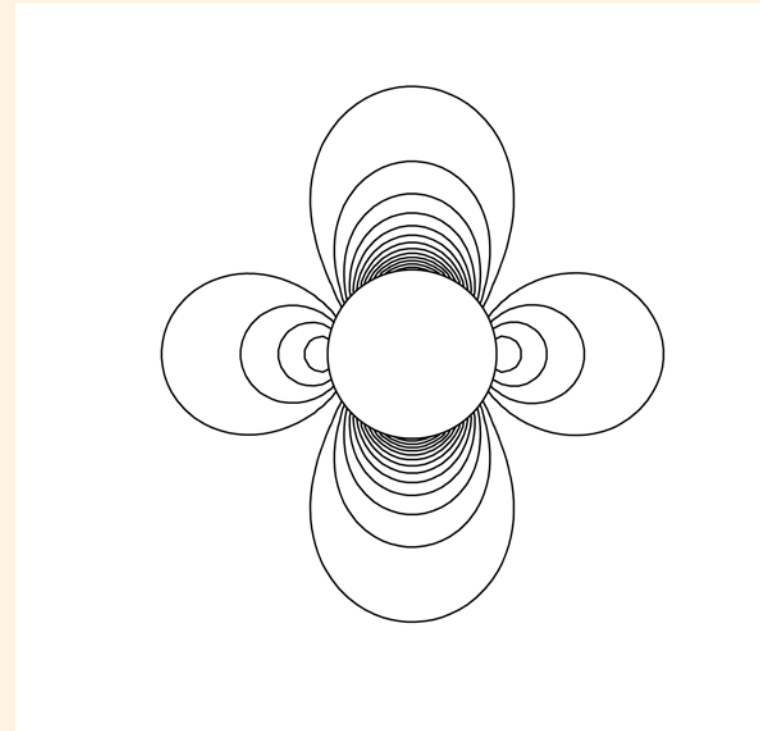


A high-order formulation for all-speed flows

- ▶ Inviscid Flow past a cylinder. $M_\infty = 10^{-3}$



First-order FV



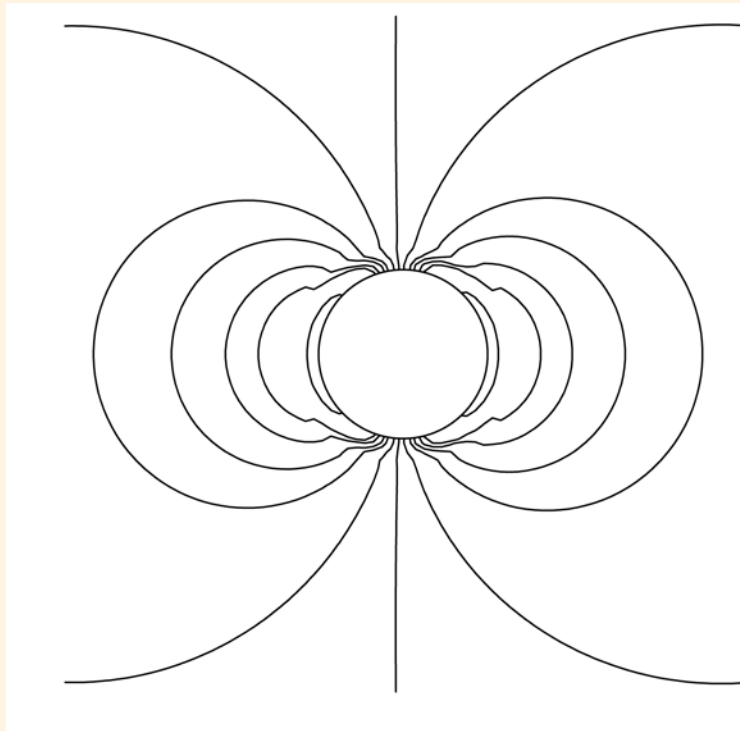
Fourth-order FV-MLS



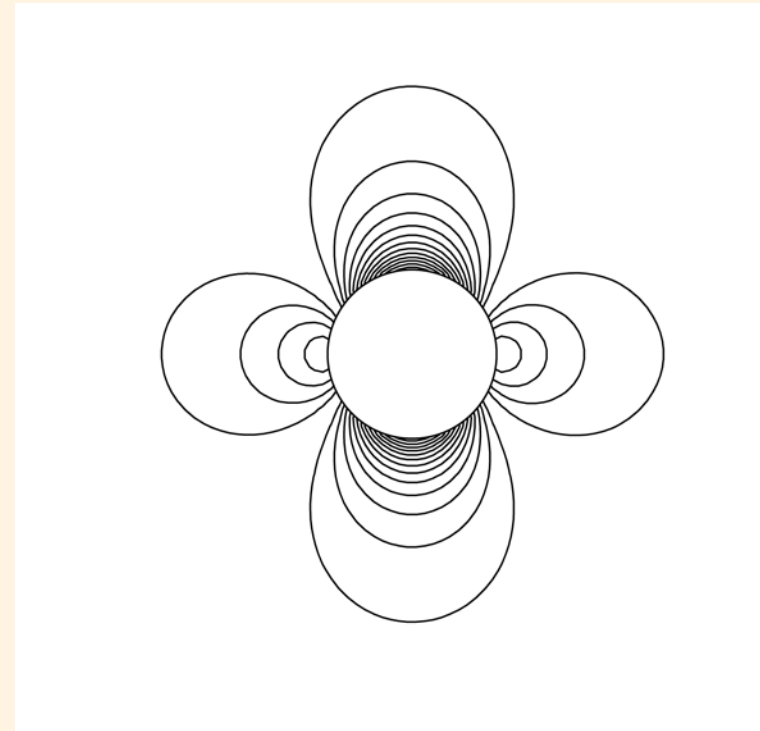


A high-order formulation for all-speed flows

- ▶ Inviscid Flow past a cylinder. $M_\infty = 10^{-3}$



First-order FV



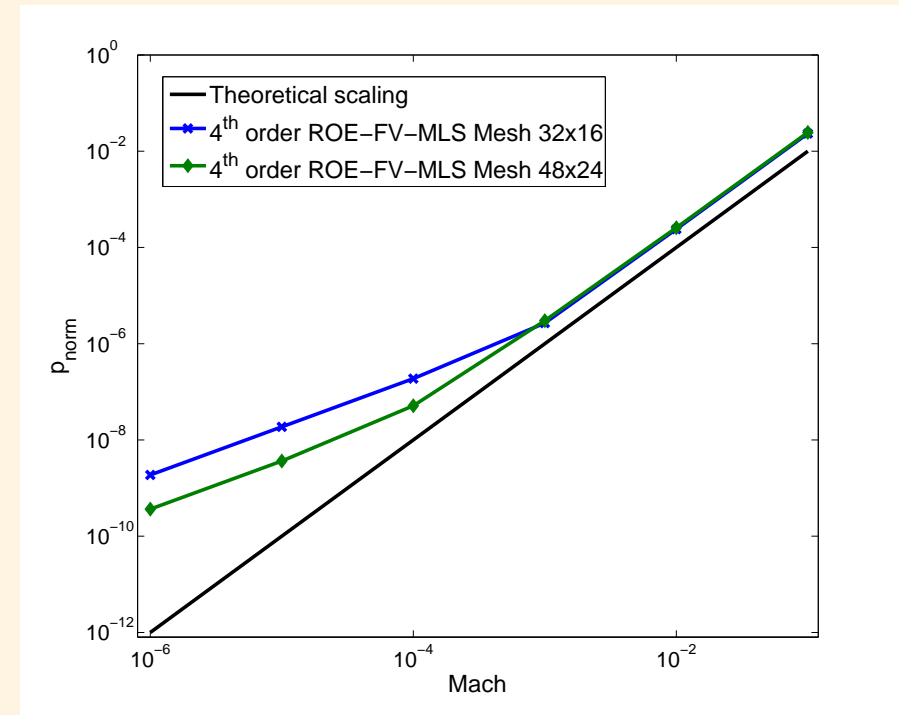
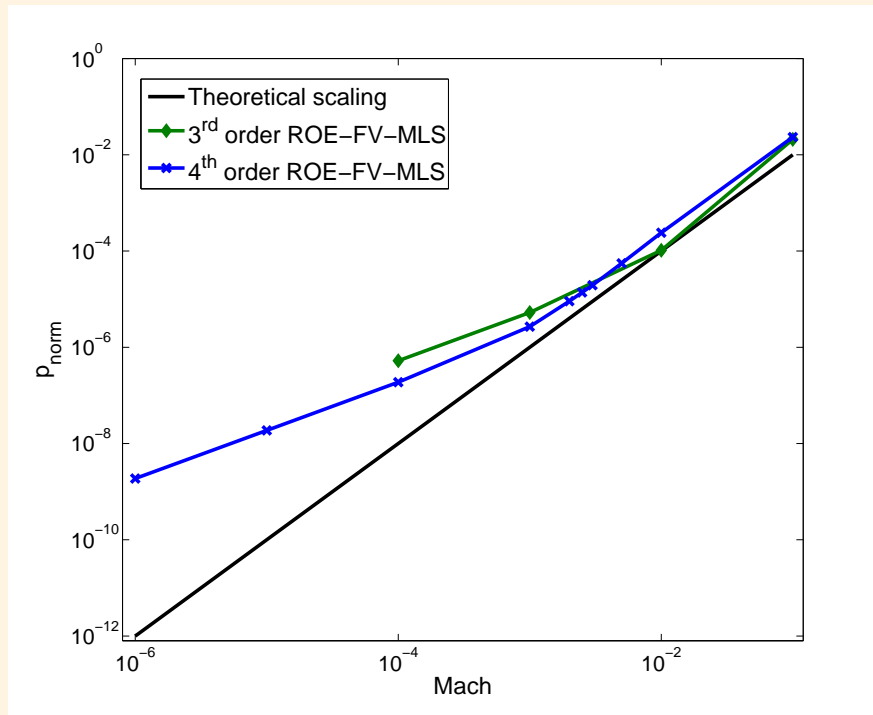
Fourth-order FV-MLS

Unphysical solution!



Formulation

► Physical solution → Mach, mesh and order dependency



$$p_{norm} = \frac{p_{max} - p_{min}}{p_{max}}$$

$$p_{norm} \sim \mathcal{O}(M_\infty^2)$$

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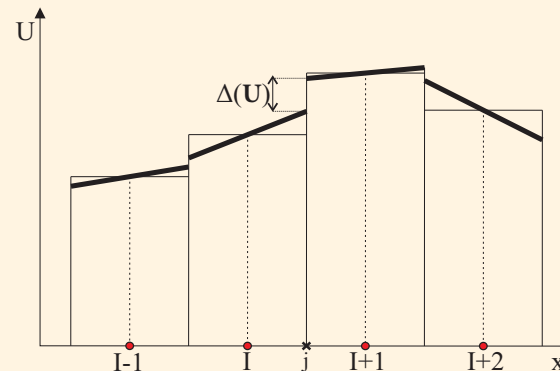


Formulation

- The numerical dissipation of the continuity and momentum equations can always be expressed as:

$$c_u \Delta \mathbf{u} + c_p \Delta p$$

- ▷ c_u and c_p are the coefficients of the velocity difference and pressure difference terms
- ▷ The accuracy problem is only attributable to $c_u = O(c)$ of the momentum equation
- ▷ Checkerboard problems are attributable to the order of c_p especially for the continuity equation. A reasonable interval is $c_p \in [c_p^{-1}, c_p^0]^1$



¹X. -s. Li, C. -w. Gu *Mechanism of Roe-type schemes for all-speed flows and its application*, C&F, 2013



A high-order formulation for all-speed flows

► Rieper's fix for the Roe flux

$$\mathcal{H}_j = \frac{1}{2}(\mathcal{F}^{\mathcal{H}}(U_j^+) + \mathcal{F}^{\mathcal{H}}(U_j^-)) \cdot \hat{\mathbf{n}} - \frac{1}{2} \sum_{k=1}^4 \tilde{\alpha}_k |\tilde{\lambda}_k| \tilde{\mathbf{r}}_k$$

$$\tilde{\alpha}_1 = \frac{1}{2\tilde{c}^2} [\Delta(p) - \tilde{\rho}\tilde{c}f(M_l) (\Delta(u)n_x + \Delta(v)n_y)]$$

$$\tilde{\alpha}_2 = \frac{\tilde{\rho}}{\tilde{c}} [\Delta(v)n_x - \Delta(u)n_y]$$

$$\tilde{\alpha}_3 = \frac{1}{\tilde{c}^2} [\Delta(p) - \tilde{c}^2 \Delta(\rho)]$$

$$\tilde{\alpha}_4 = \frac{1}{2\tilde{c}^2} [\Delta(p) + \tilde{\rho}\tilde{c}f(M_l) (\Delta(u)n_x + \Delta(v)n_y)]$$

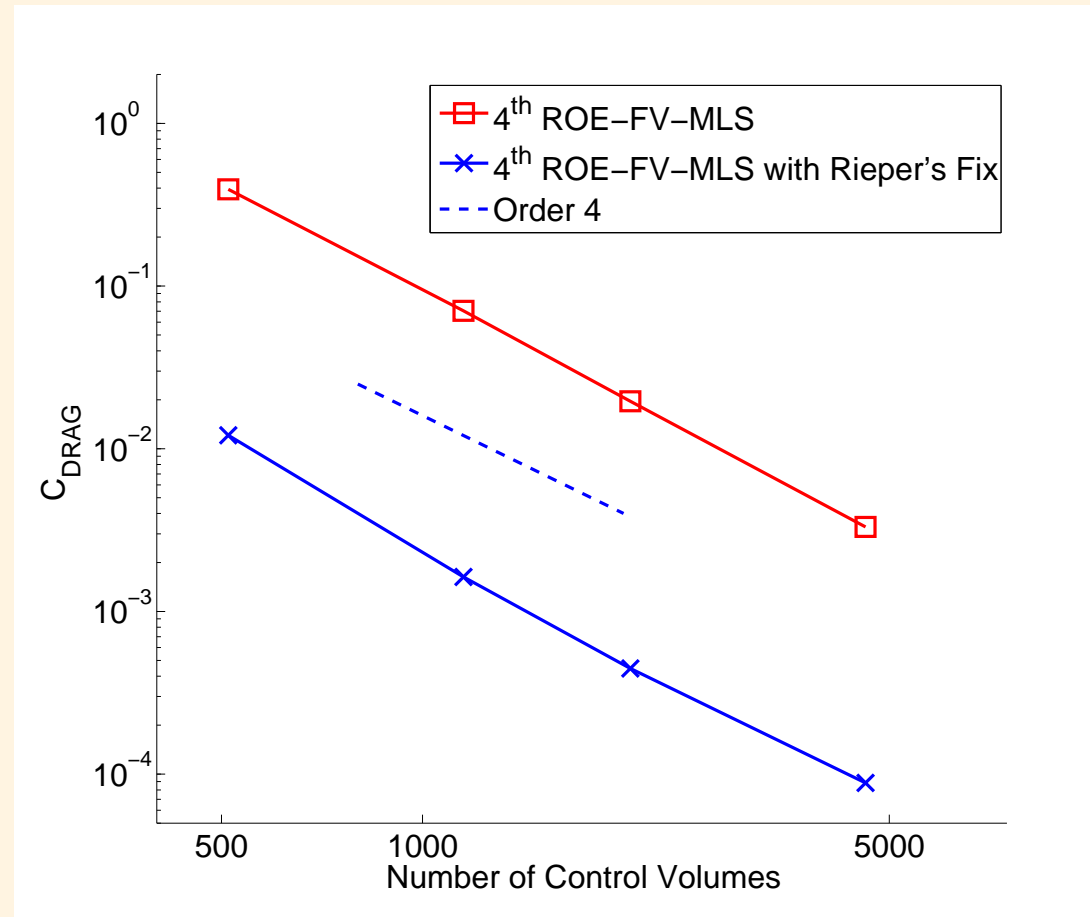
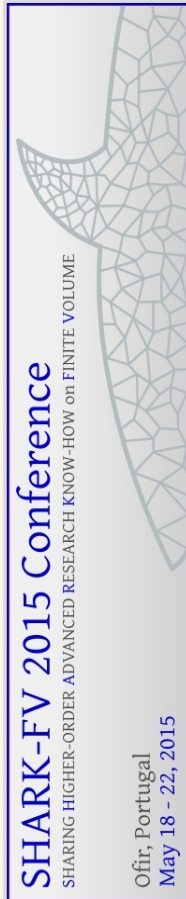
$$f(M_l) = \min(M_l, 1) \quad M_l = \frac{|\tilde{u}|_I + |\tilde{v}|_I}{\tilde{c}_I}$$





A high-order formulation for all-speed flows

- Inviscid Flow past a cylinder. $M_\infty = 10^{-2}$



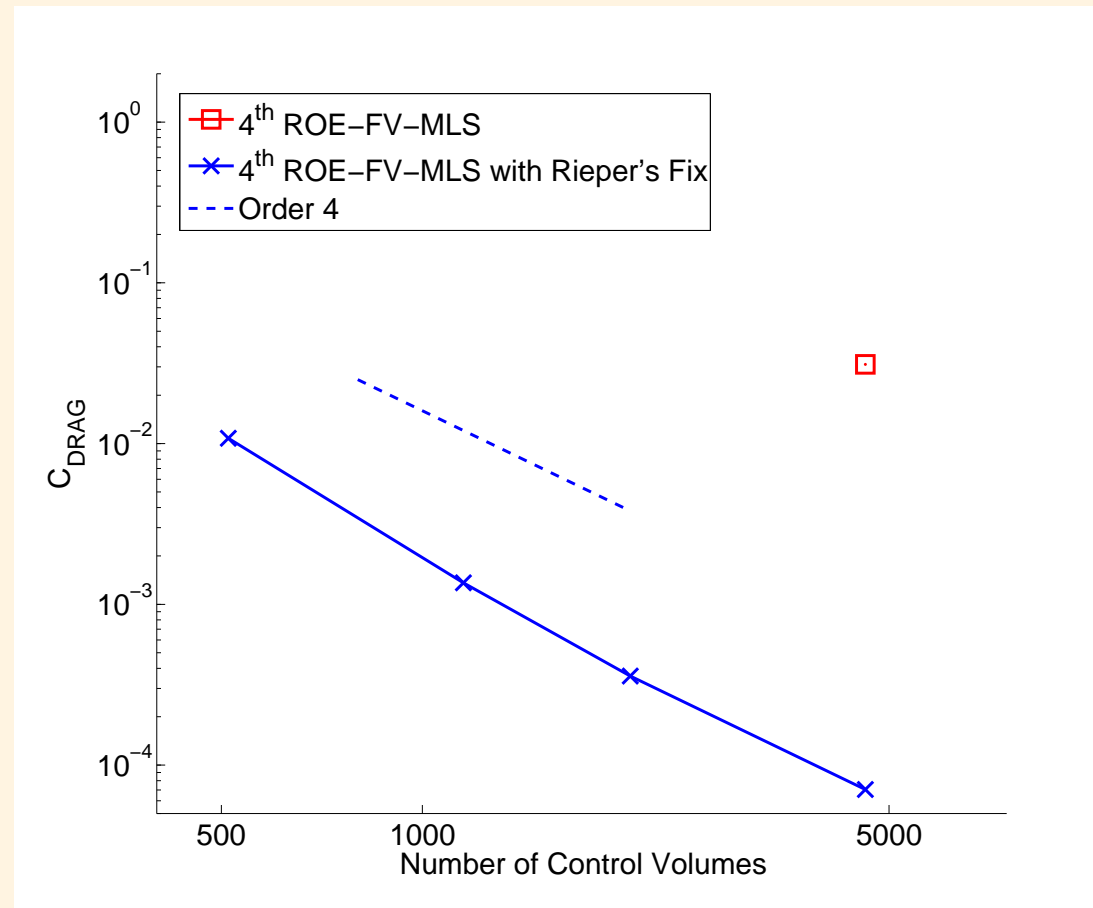
- The formal order of accuracy is recovered





Formulation

- ▶ Inviscid Flow past a cylinder. $M_\infty = 10^{-3}$



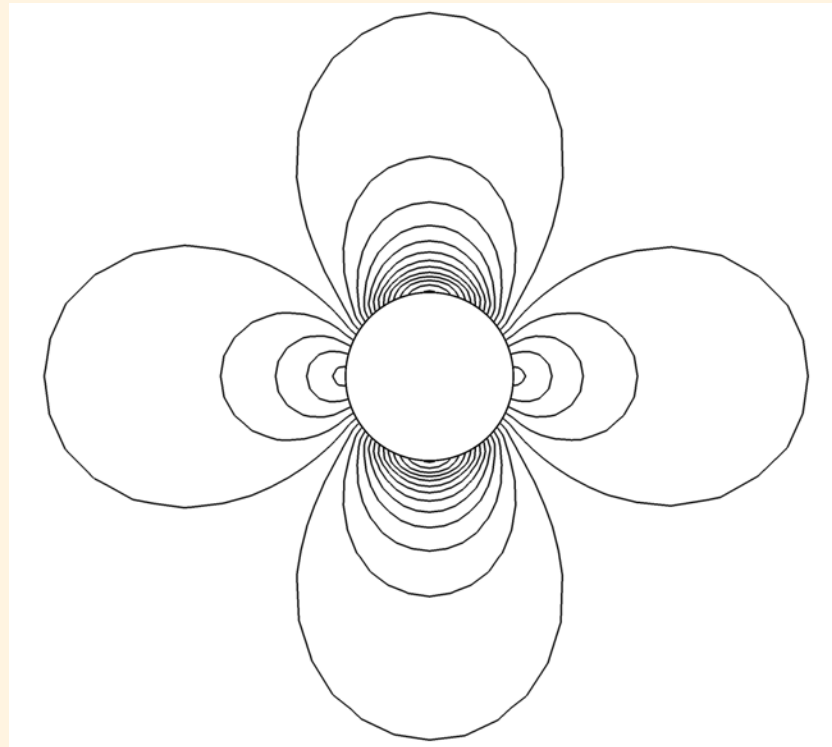
- The formal order of accuracy is recovered with the fix





A high-order formulation for all-speed flows

- ▶ Inviscid Flow past a cylinder. $M_\infty = 10^{-6}$.
- 4th ROE-FV-MLS with Rieper's fix
- 32×16 grid



Pressure contours



A high-order formulation for all-speed flows

- ▶ Li and Gu's fix for the Rusanov flux

$$\mathcal{H}_j = \frac{1}{2}(\mathcal{F}^{\mathcal{H}}(U_j^+) + \mathcal{F}^{\mathcal{H}}(U_j^-)) \cdot \hat{\mathbf{n}} - \frac{1}{2}S^+ \Delta(\mathbf{U})$$

$$S^+ = \max(|\mathbf{v}^+| + c^+, |\mathbf{v}^-| + c^-)$$

$$\Delta(\mathbf{U}) = \left\{ \begin{array}{l} \Delta(\rho) \\ f(M_l) \Delta(\rho u) \\ f(M_l) \Delta(\rho v) \\ \Delta(\rho E) \end{array} \right\}$$

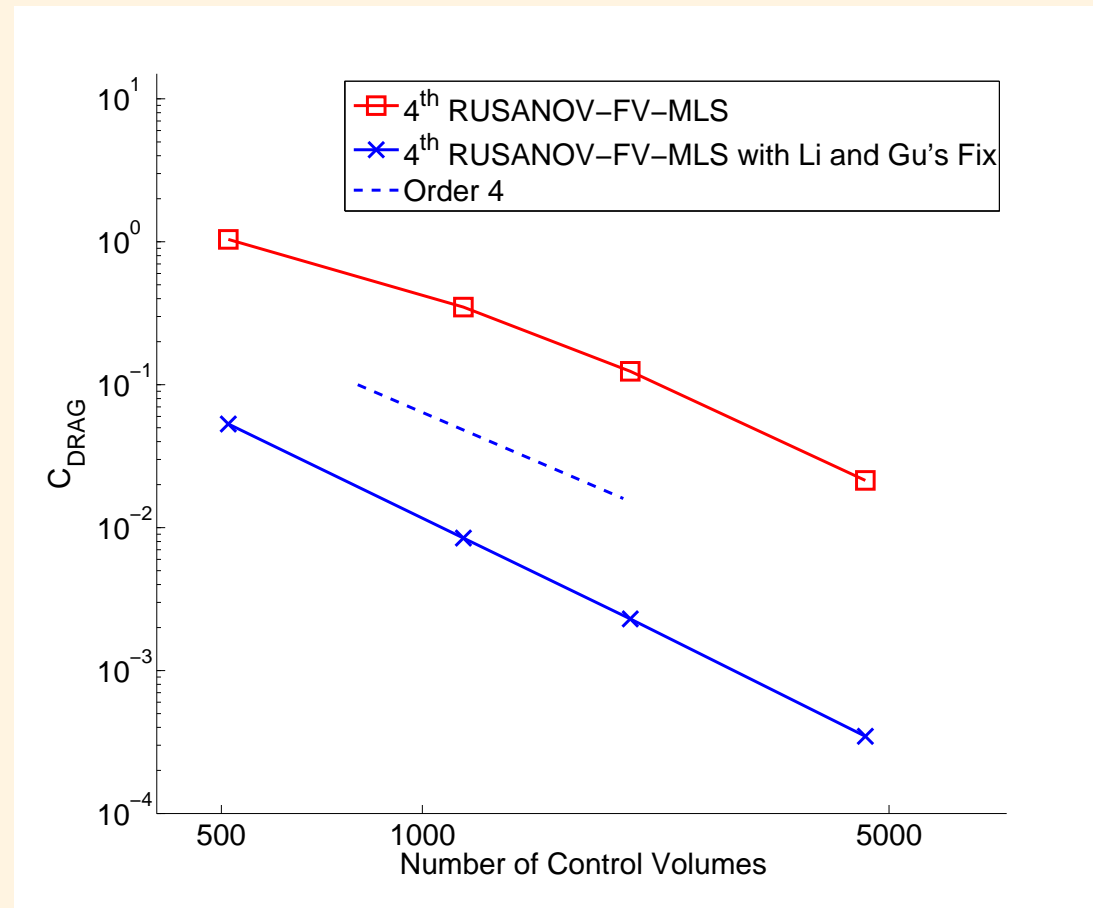
$$f(M_l) = \min(M_l, 1) \quad M_l = \frac{|u|_I + |v|_I}{c_I}$$





Formulation

- ▶ Inviscid Flow past a cylinder. $M_\infty = 10^{-2}$



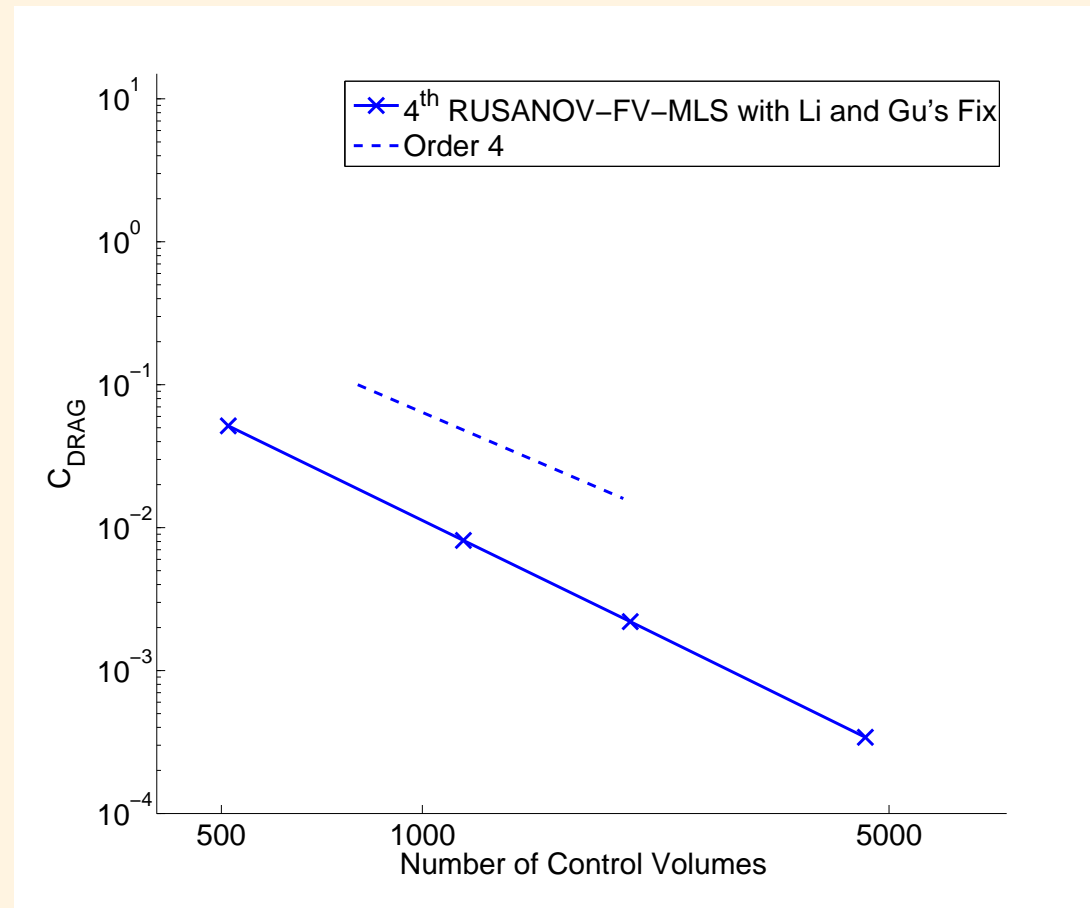
- The formal order of accuracy is recovered





Formulation

- ▶ Inviscid Flow past a cylinder. $M_\infty = 10^{-3}$



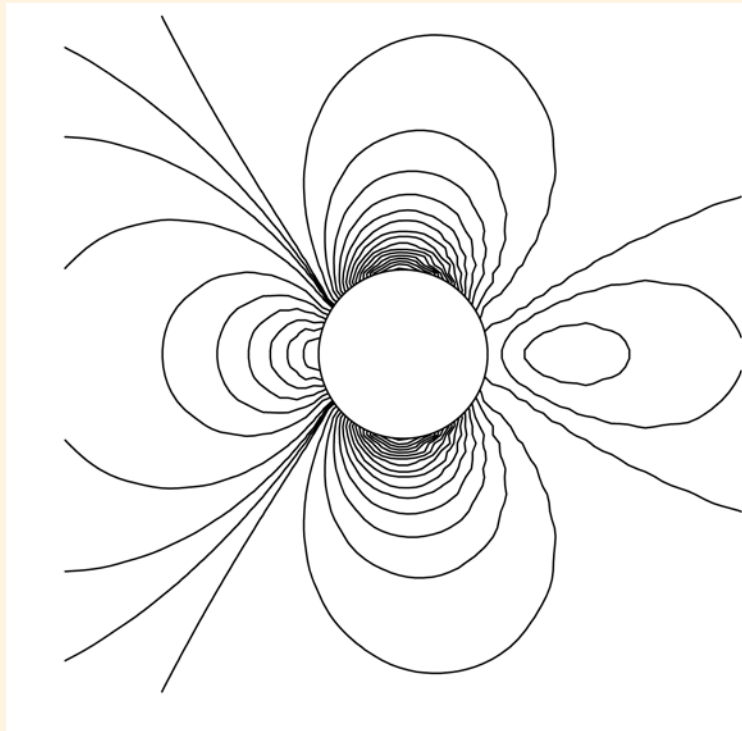
- The formal order of accuracy is recovered with the fix



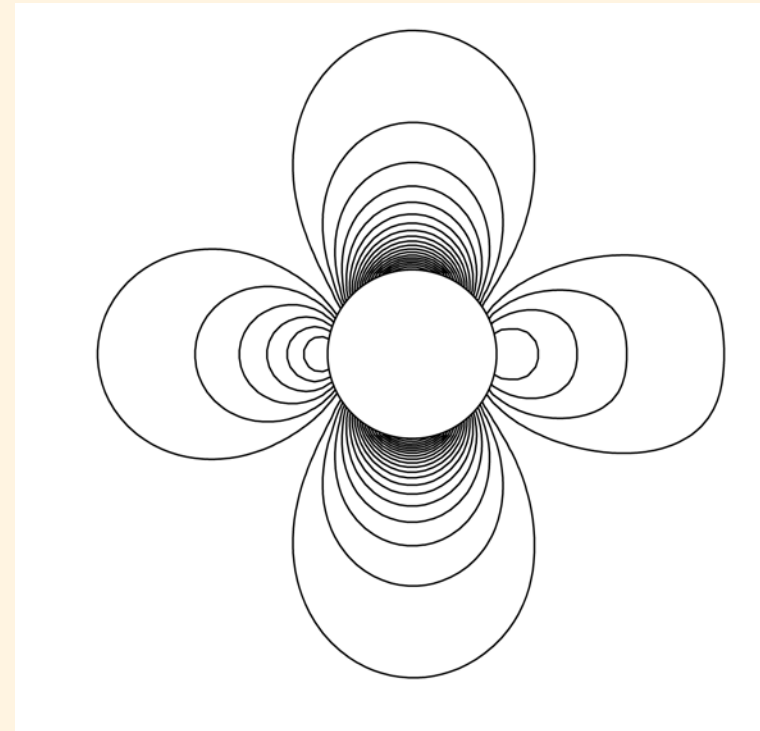


A high-order formulation for all-speed flows

- ▶ Inviscid Flow past a cylinder. $M_\infty = 10^{-2}$.
 - RUSANOV-FV-MLS with Li and Gu's fix
 - 96×48 grid



1st order

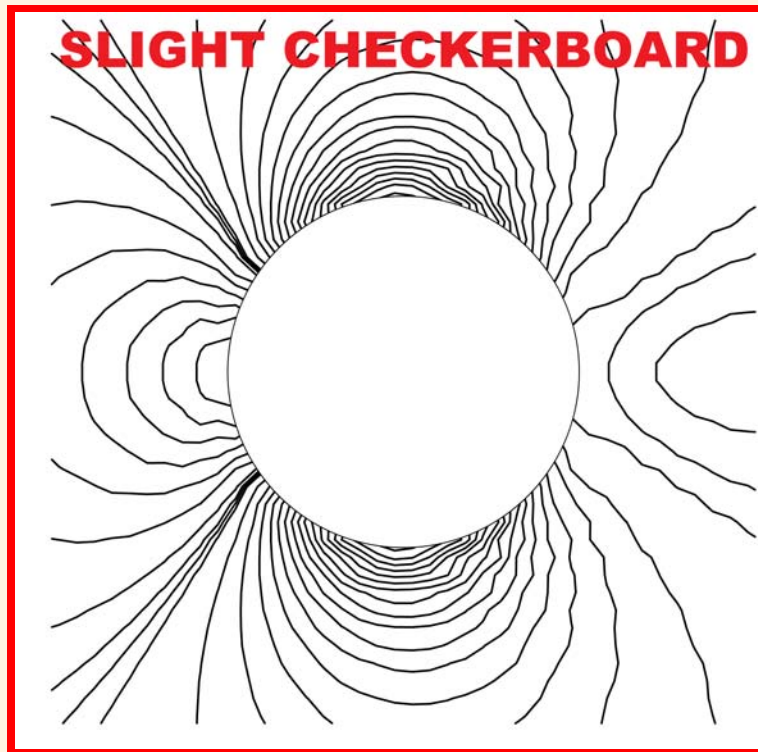


4th order

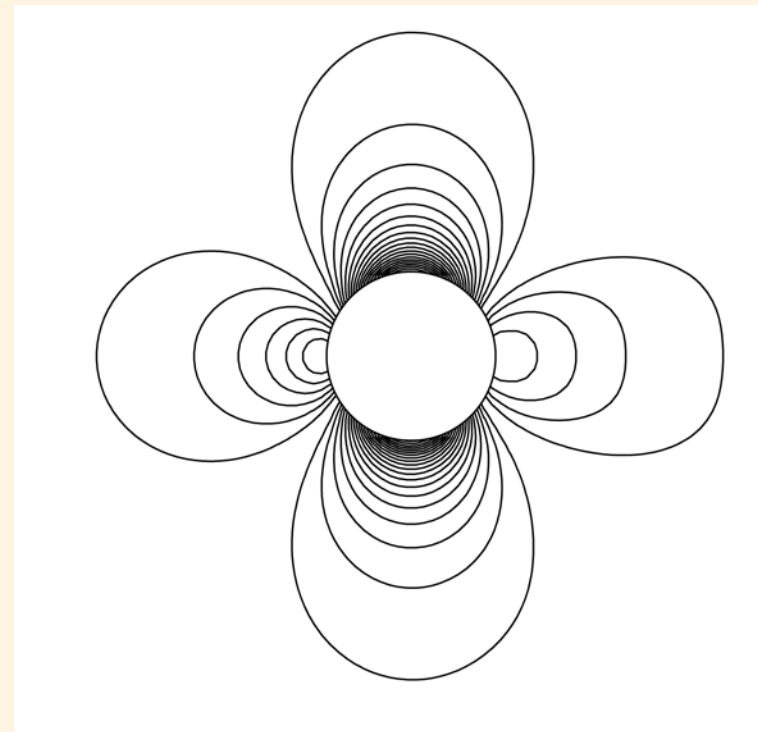


A high-order formulation for all-speed flows

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1st order

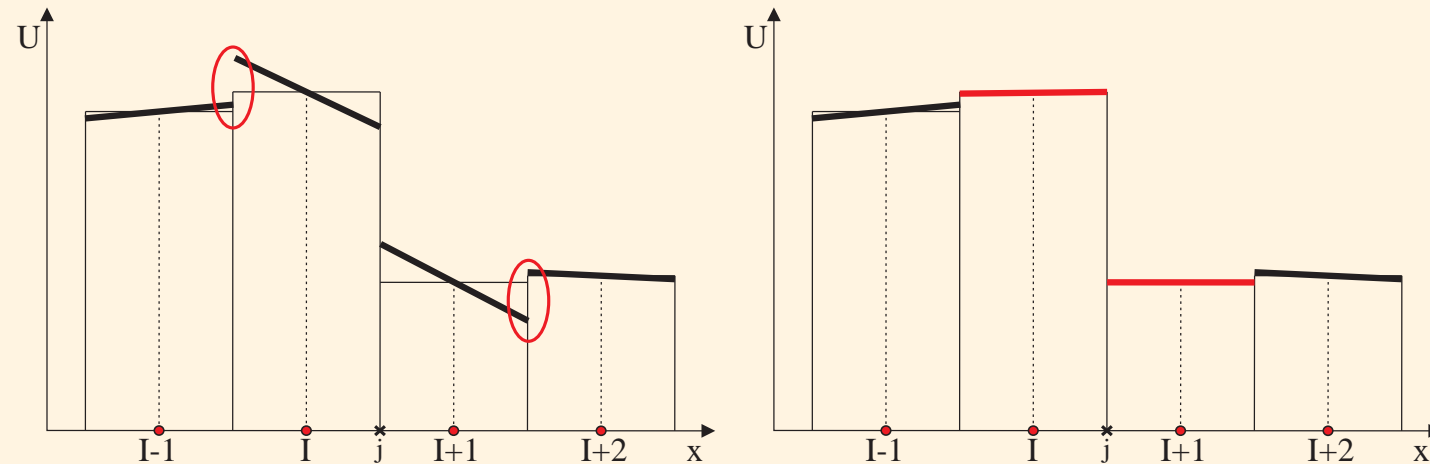


4th order



Slope limiters

- ▶ Slope limiters are used to design TVD schemes.



- A slope limiter limits the Taylor reconstruction of a high-order finite volume scheme as follows:

$$U(\mathbf{x}) = U_I + \chi_I \nabla U_I \cdot (\mathbf{x} - \mathbf{x}_I)$$

- ▷ $\chi_I = 0 \Rightarrow$ First-order scheme
- ▷ $\chi_I = 1 \Rightarrow$ No limitation



Slope limiters

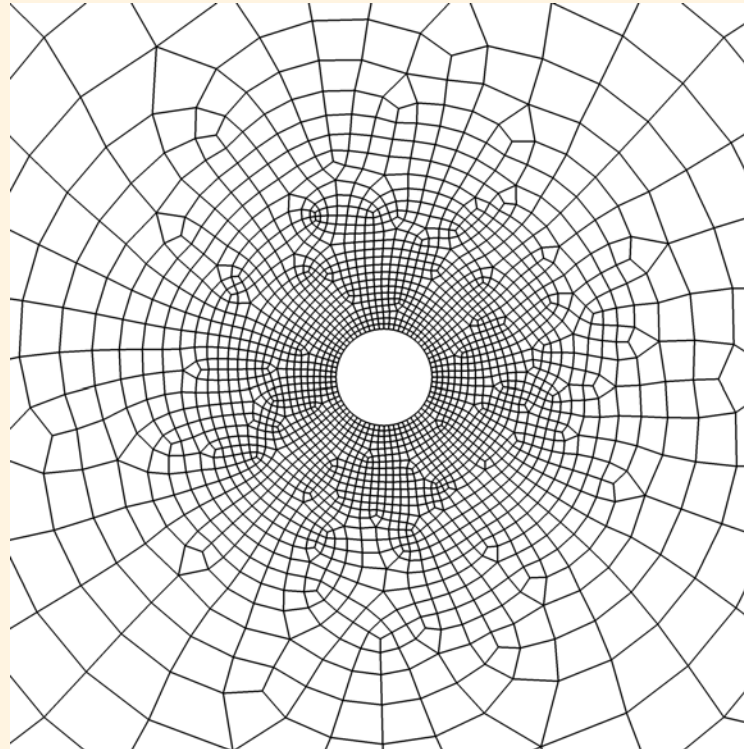
► Slope limiters:

- Barth and Jespersen slope limiter
 - ▷ Non-differential limiter
- Venkatakrishnan slope limiter
 - ▷ Differentiable limiter
 - ▷ Near strong shocks may introduce deviations from the monotone solution
- Van-Albada limiter
 - ▷ Non-differential limiter



Slope limiters

- ▶ Inviscid Flow past a cylinder. $M_\infty = 10^{-3}$.
 - 4th FV-MLS
 - Unstructured grid of 2320 elements.





Slope limiters

- Inviscid Flow past a cylinder. $M_\infty = 10^{-3}$.

Method	Barth-Jespersen	Van Albada	Venkatakrishnan
4^{th} ROE+ Rieper's fix			
4^{th} RUSANOV+Li and Gu's fix			

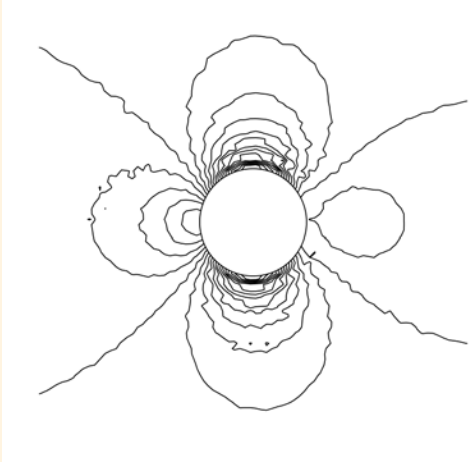
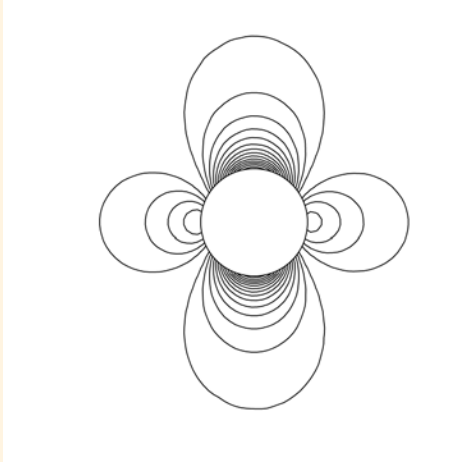
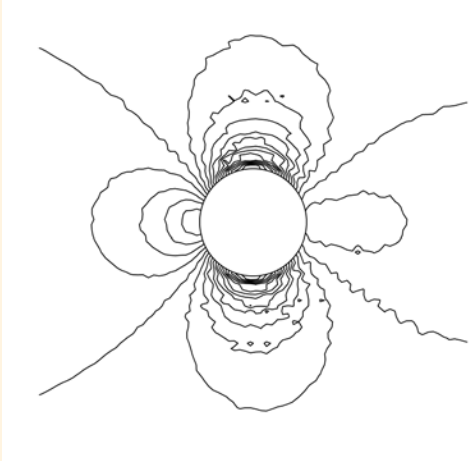
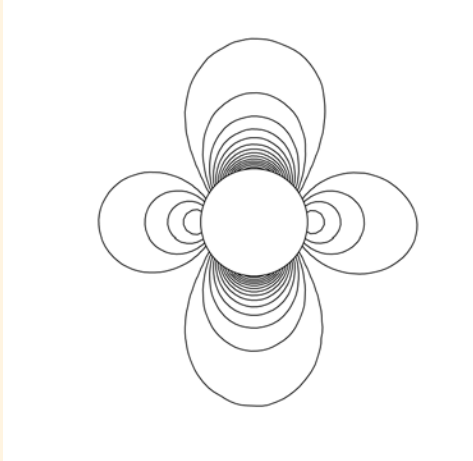
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Slope limiters

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Method	Van Albada	Van Albada + MLS-based sensor
4^{th} ROE+ Rieper's fix		
4^{th} RUSANOV+Li and Gu's fix		





Numerical Examples

► 3D decay of compressible isotropic turbulence

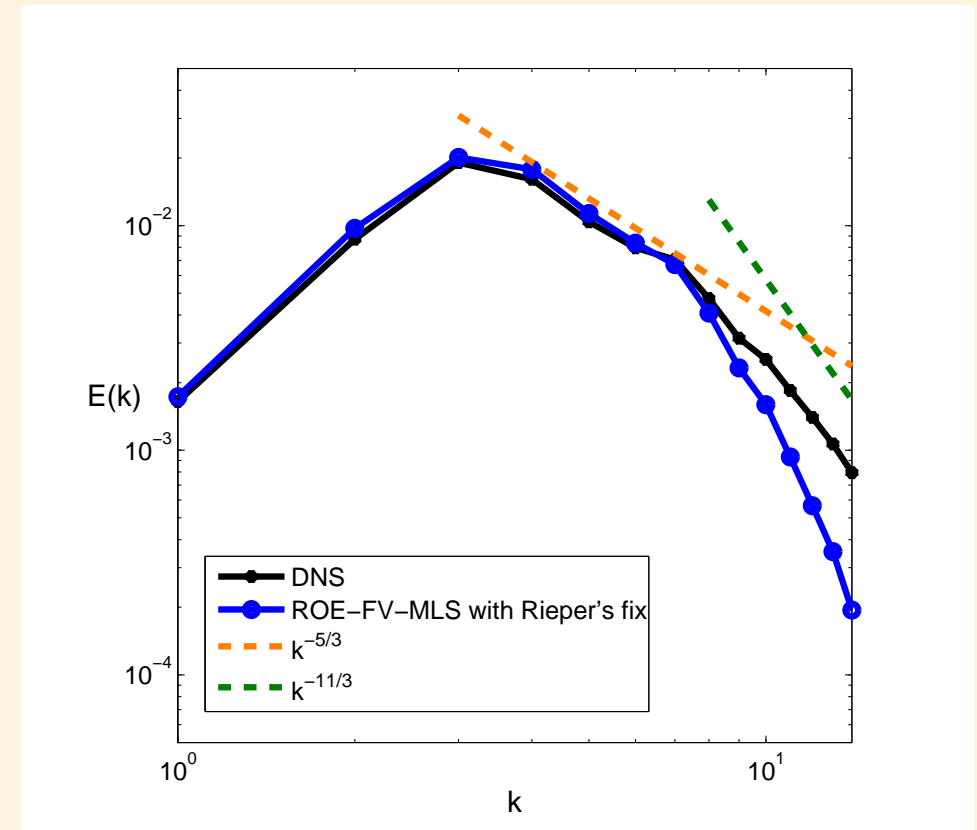
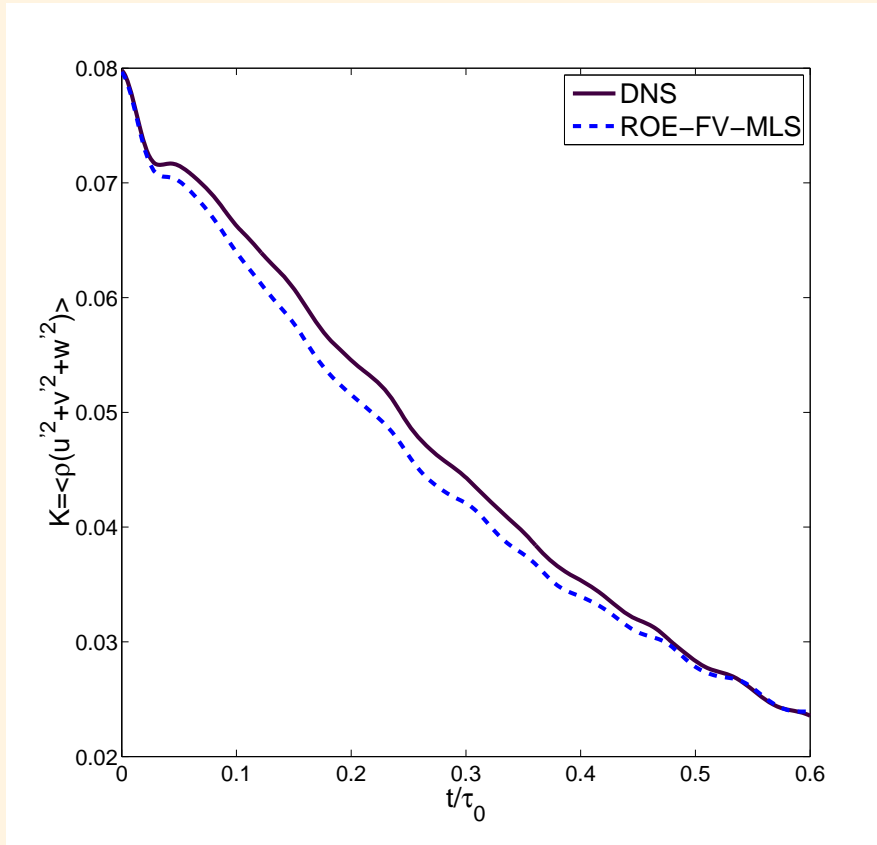
- Domain: $\Omega_T = [-\pi, \pi]^3 \rightarrow 32^3$ elements.
- Periodic boundary conditions.
- 3^{rd} order ROE-FV-MLS with Rieper's fix.
- Van Albada limiter with the MLS-based sensor.
- Reference solution: 6^{th} order FD + LES.





Numerical Examples

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$$t/\tau_0 = 0.3$$

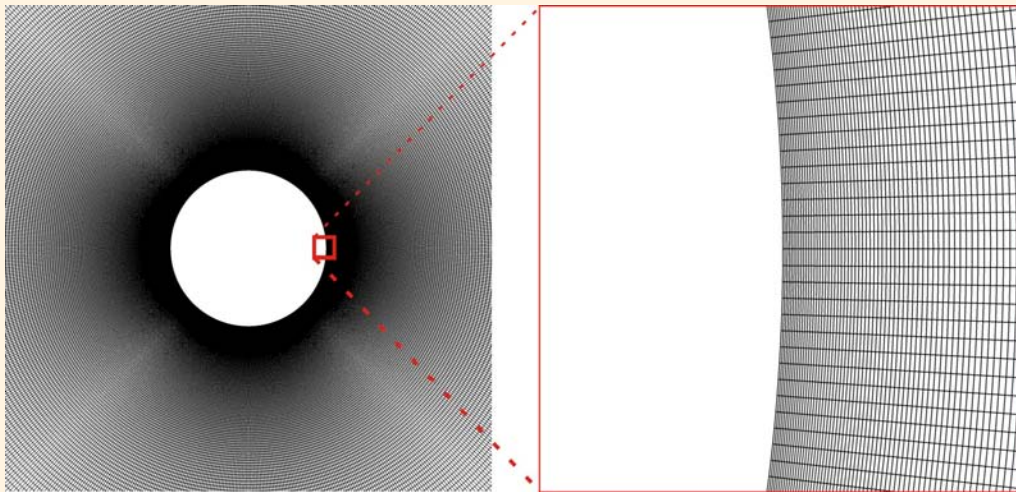




Numerical Examples

► Unsteady transonic viscous flow over a circular cylinder

- $M_\infty = 0.80$. $Re = 166.000$.
- 3rd ROE-FV-MLS with Rieper's Fix.

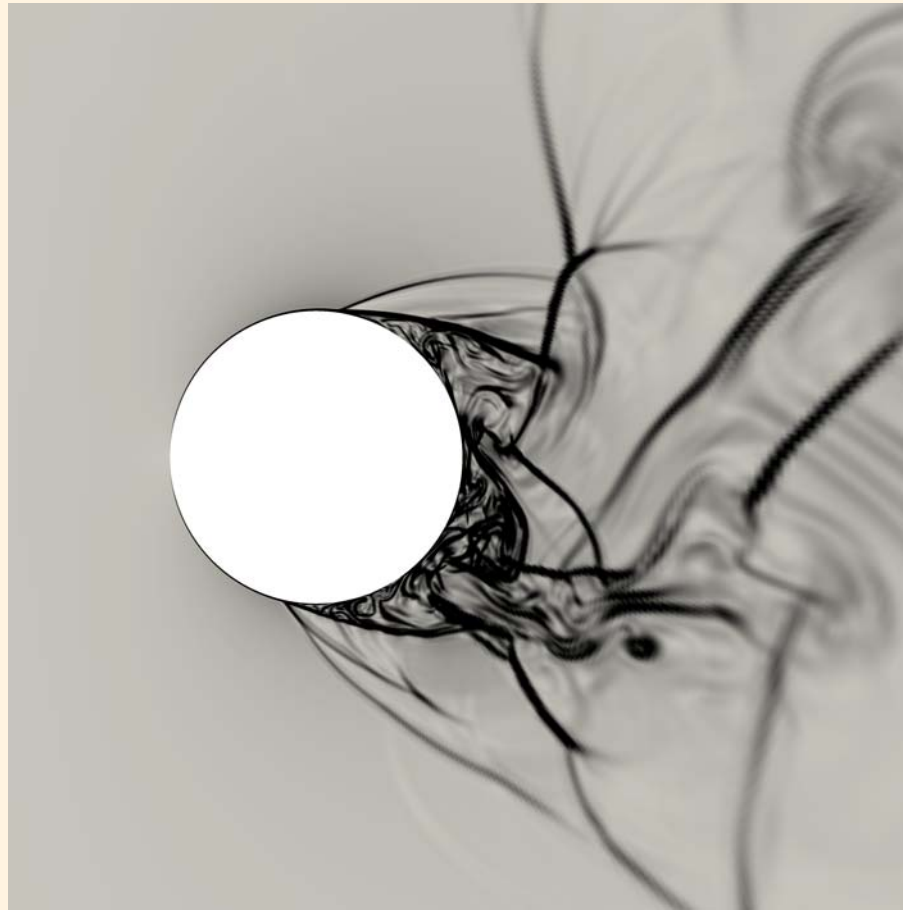


- 720 CV around the cylinder.
- $y_n = 2.85 \times 10^{-4} D$
- Total: 206.150 CV.



Numerical Examples

- ▶ Unsteady transonic viscous flow over a circular cylinder

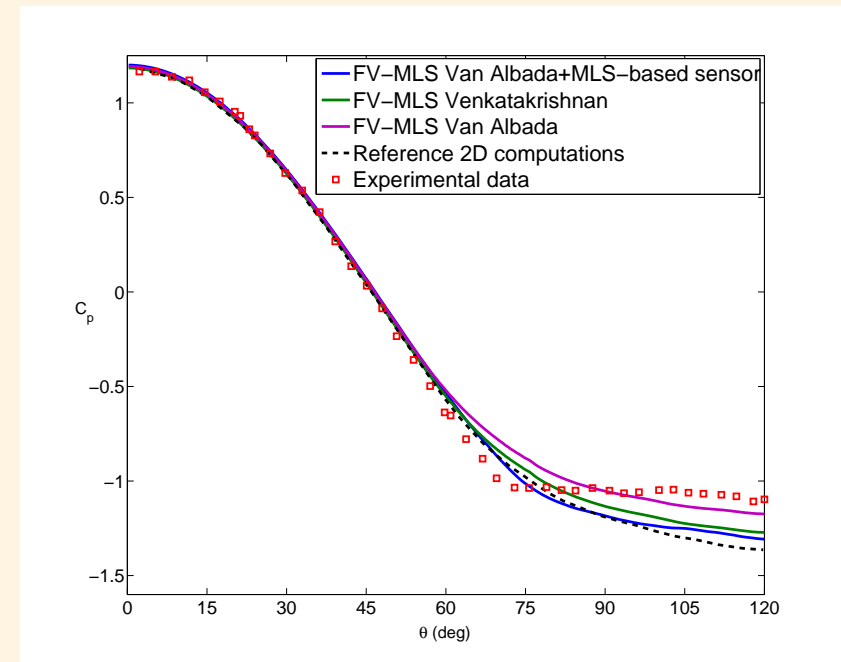




Numerical Examples

► Unsteady transonic viscous flow over a circular cylinder

Method	C_{DRAG}
Reference 2D computations	1.86
FV-MLS Van Albada	1.82
FV-MLS Venkatakrisnan	1.84
FV-MLS Van Albada+MLS-based sensor	1.81
Experimental	1.50



Experimental reference: Murthy, V.S., Rose, W.C., *Detailed Measurements on a Circular Cylinder in Cross Flow*, AIAA Journal, 57, 549–550, 1978.

2D reference: Garcia, R., Bobenrieth, R.F., *Detached Eddy simulation of the transonic flow over a circular cylinder*, Proceedings of COBEM, 2005.



A MLS-based sliding mesh technique

- Introduction
- The FV-MLS method
- Multiscale properties of MLS: MLS-based shock detection
- A formulation for all-speed flows
- **A MLS-based sliding mesh technique**
- Application to Navier-Stokes-Korteweg equations
- Conclusions





A MLS based sliding-mesh technique

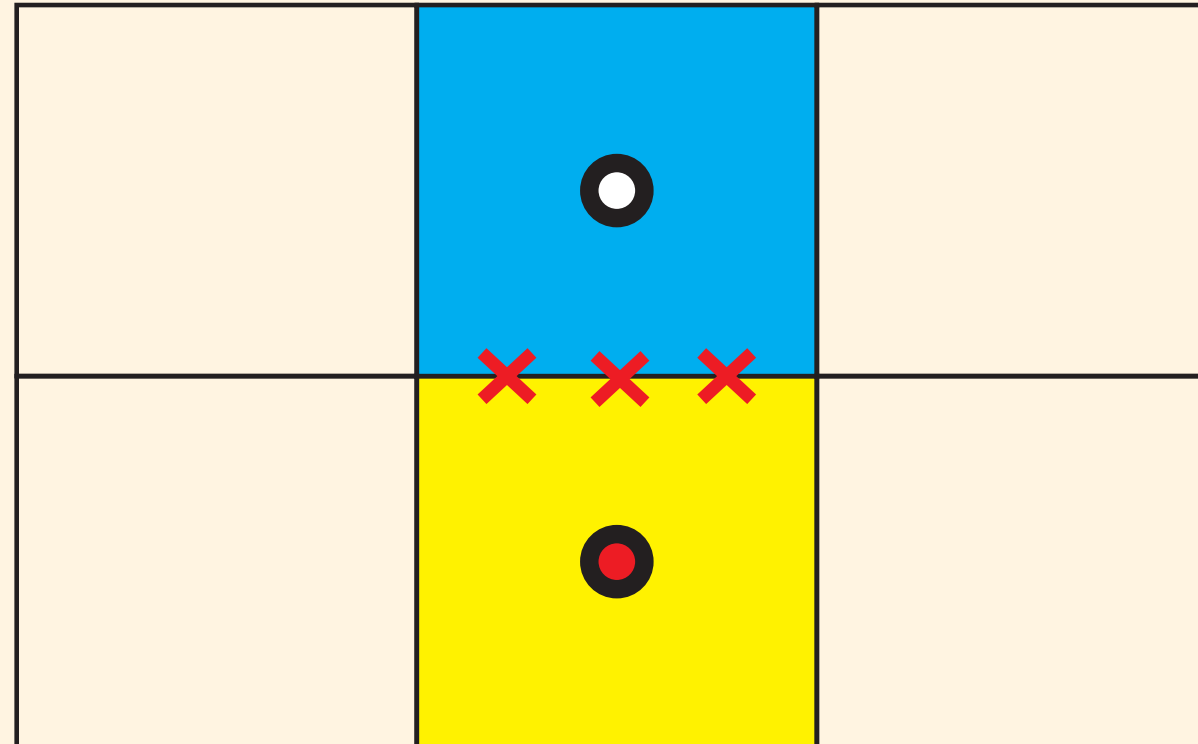
▶ Two different approaches

- 1. MLS-based sliding mesh with intersections.
- 2. Interface halo-cell sliding mesh.



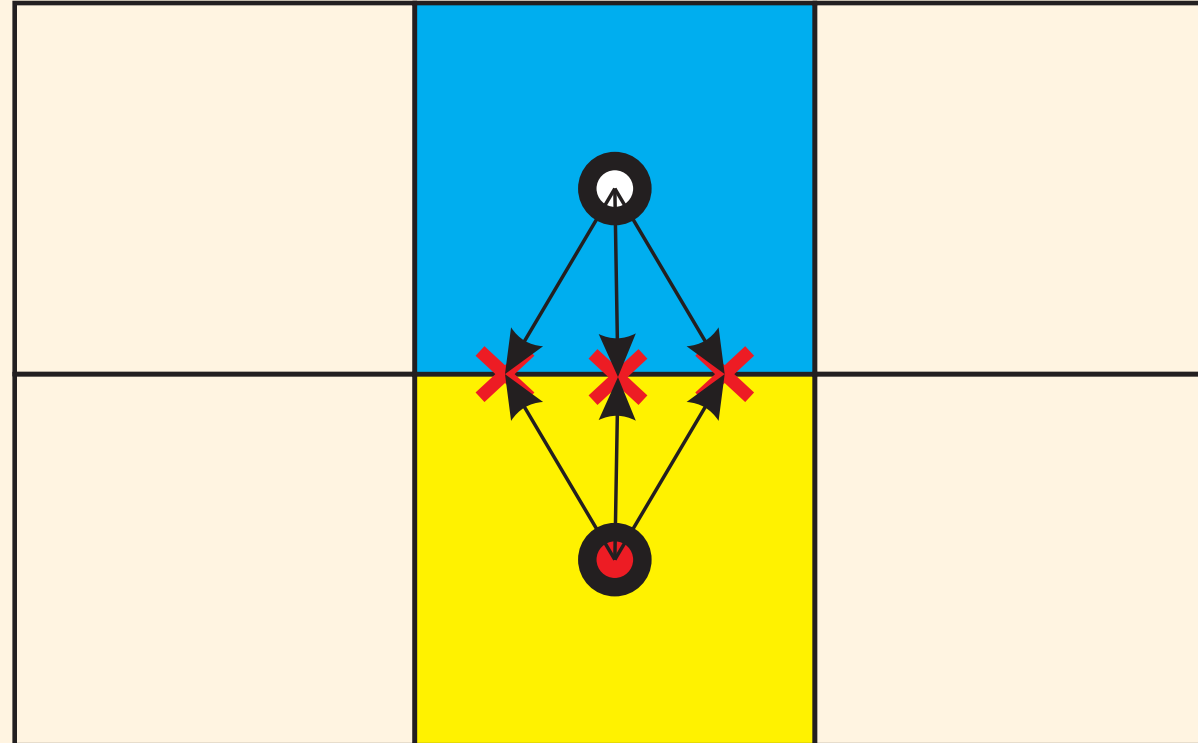


MLS-based sliding mesh with intersections





MLS-based sliding mesh with intersections

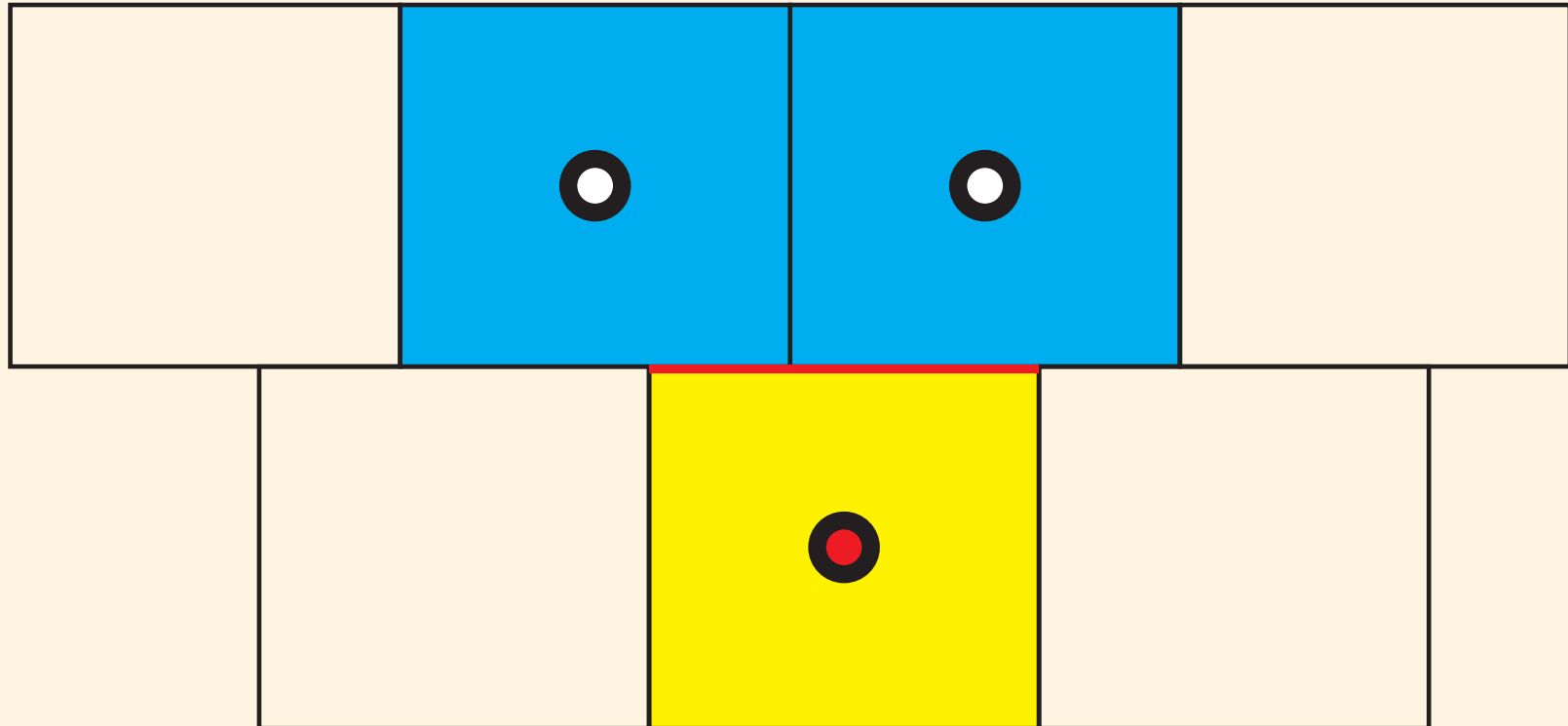


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MLS-based sliding mesh with intersections



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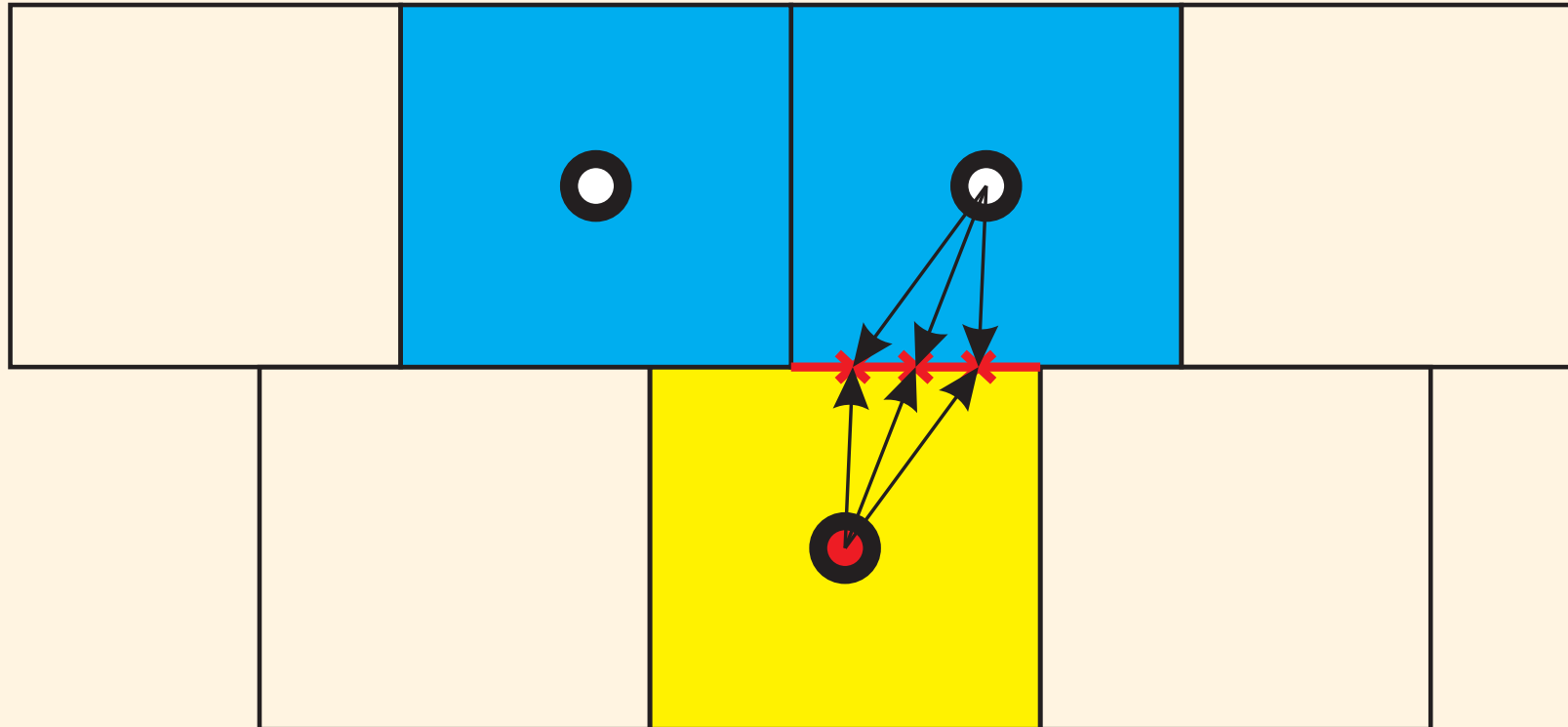
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MLS-based sliding mesh with intersections



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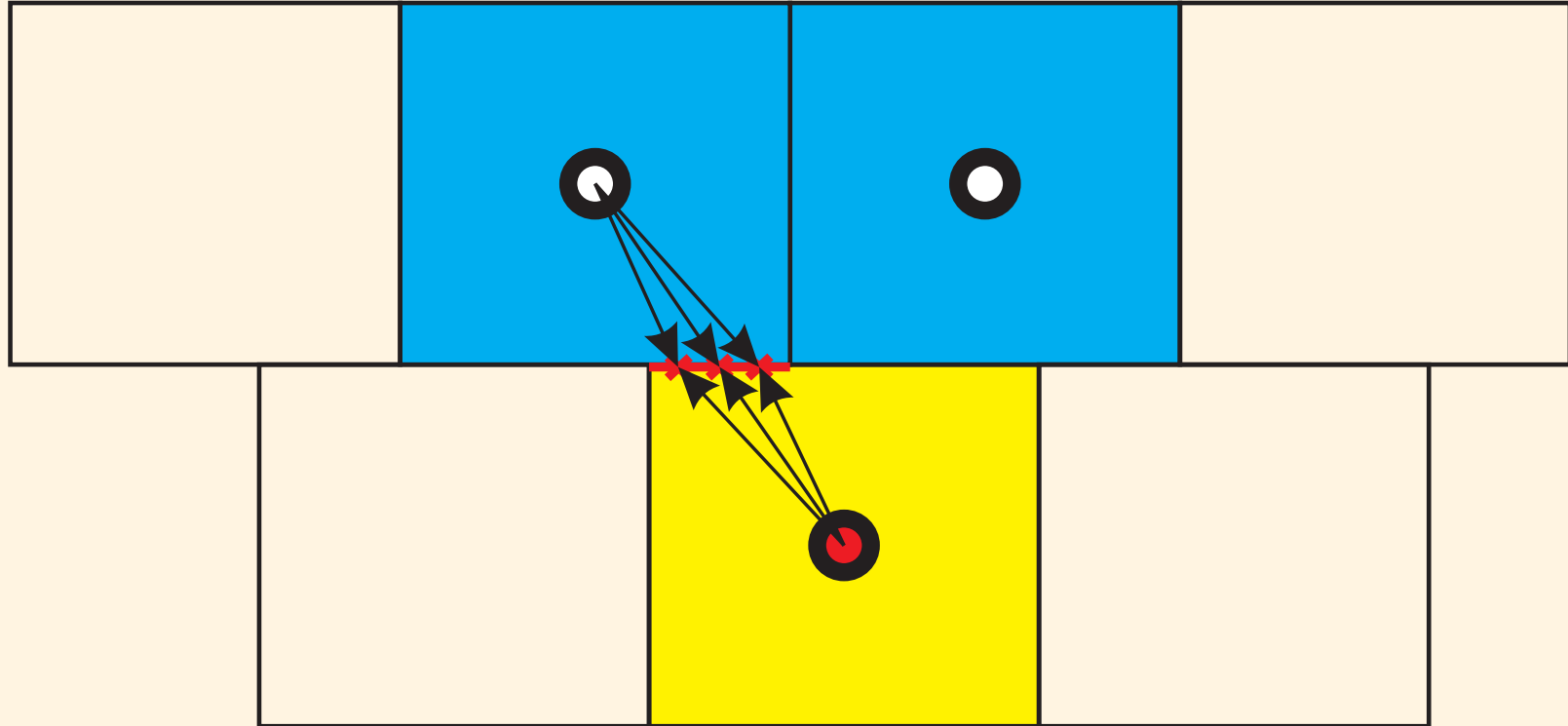
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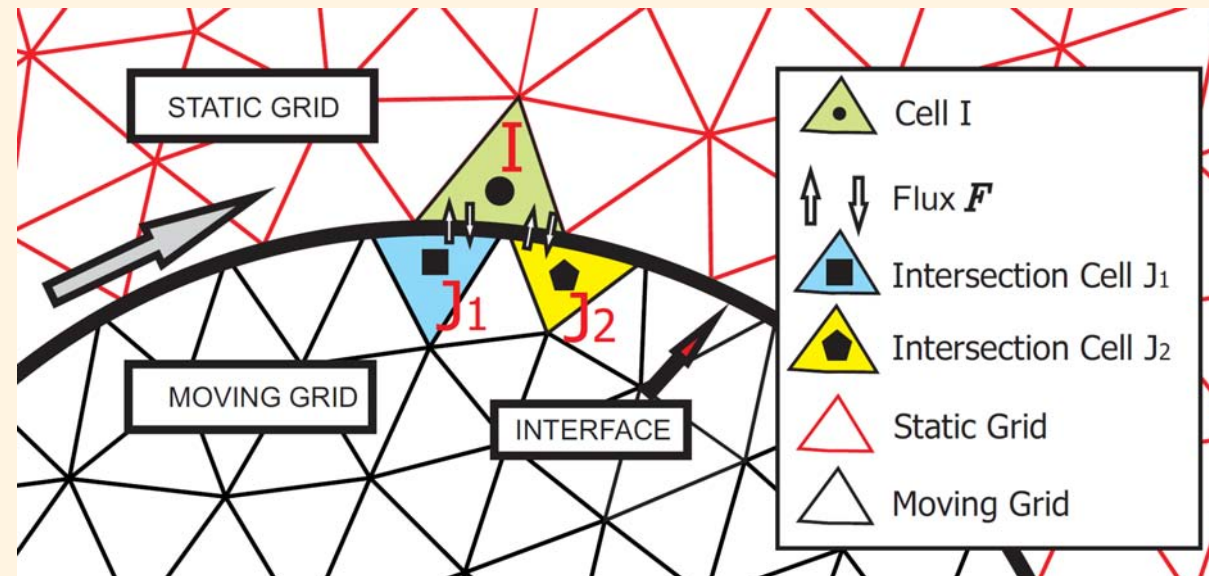
MLS-based sliding mesh with intersections





A MLS-based sliding mesh technique

- ▶ MLS-based sliding mesh with intersections.
 - Recursive searching of intersection nodes.
 - Computation of the numerical flux at interface.

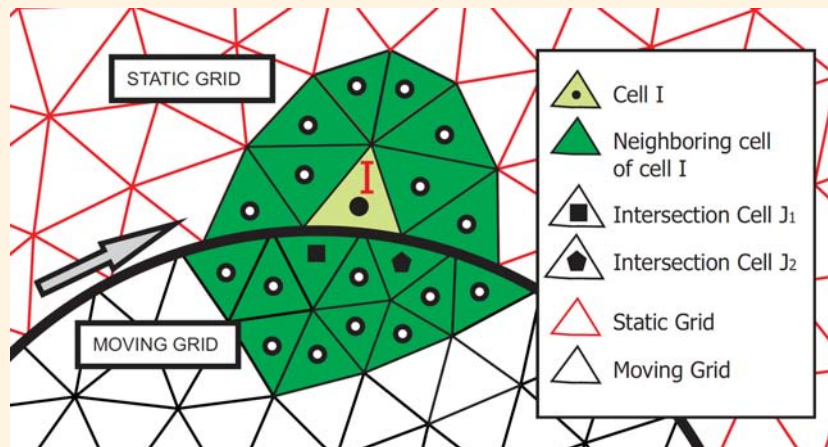




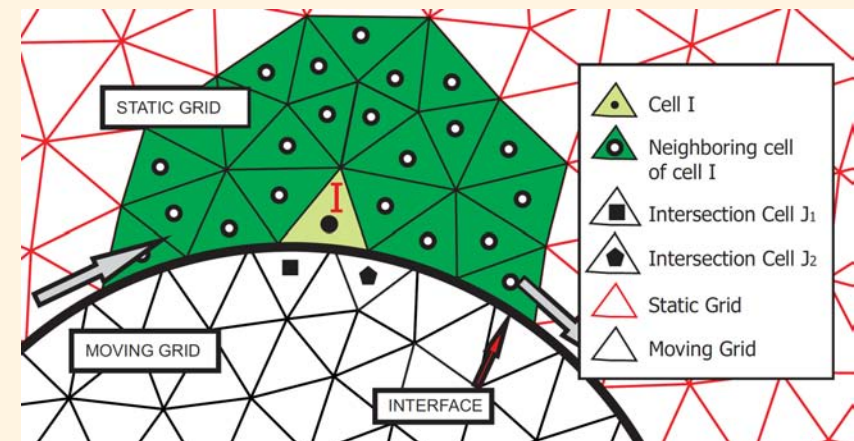
A MLS-based sliding mesh technique

► MLS-based sliding mesh with intersections.

- The stencil can be defined as:



Full Stencil



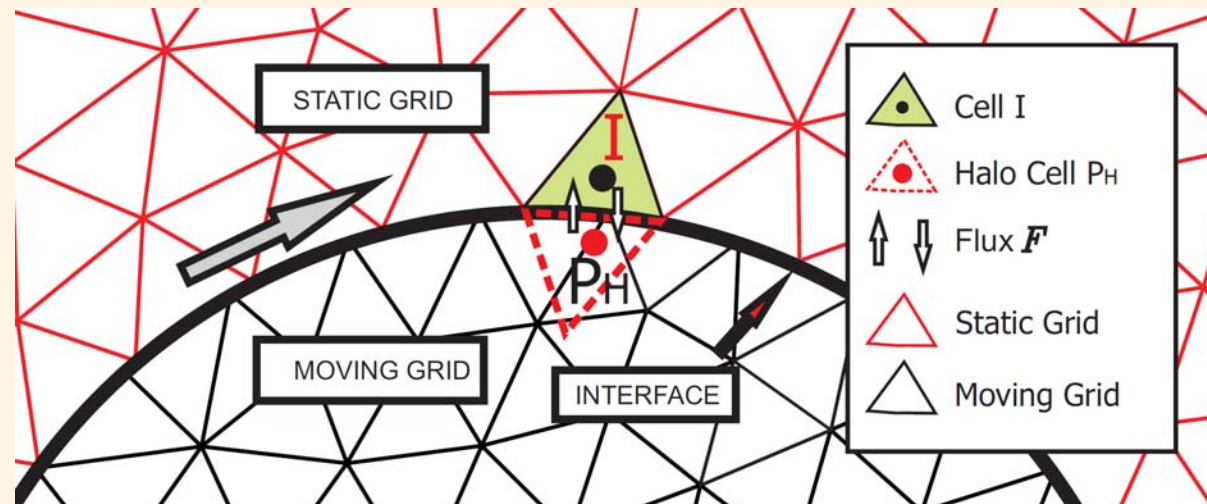
Half Stencil



A MLS-based sliding mesh technique

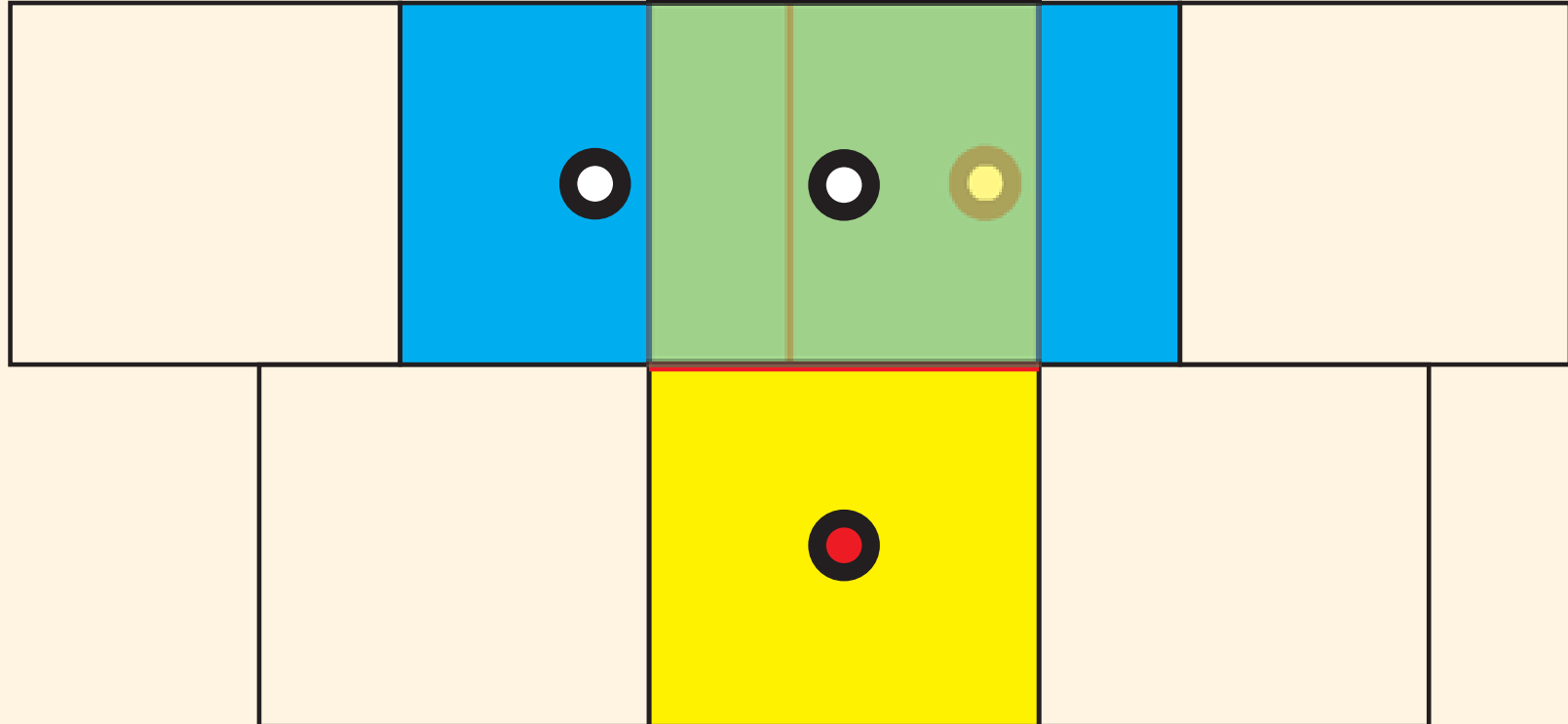
► Interface halo cell sliding mesh.

- Create a **halo** cell.
- Computation of the numerical flux at interface.






A MLS-based sliding mesh technique

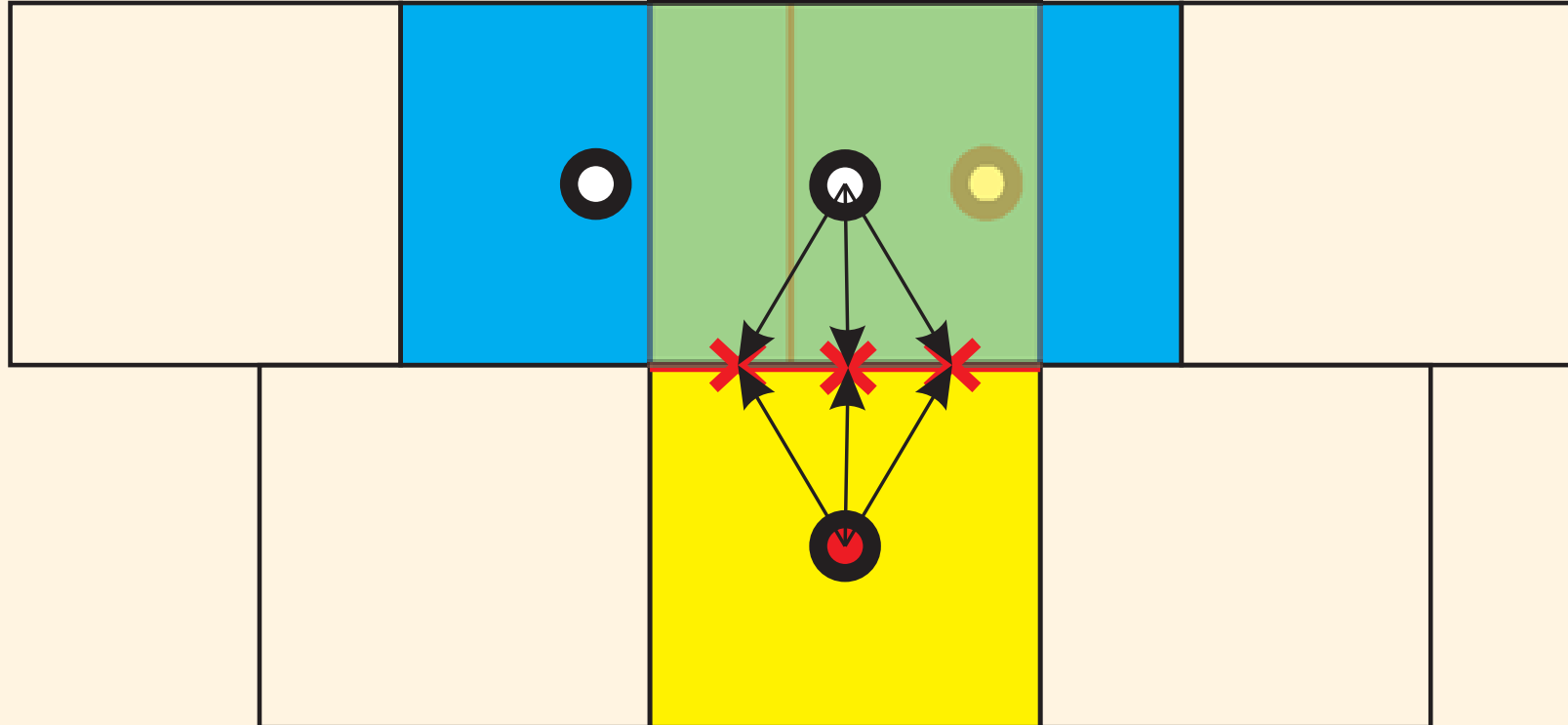


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A MLS-based sliding mesh technique



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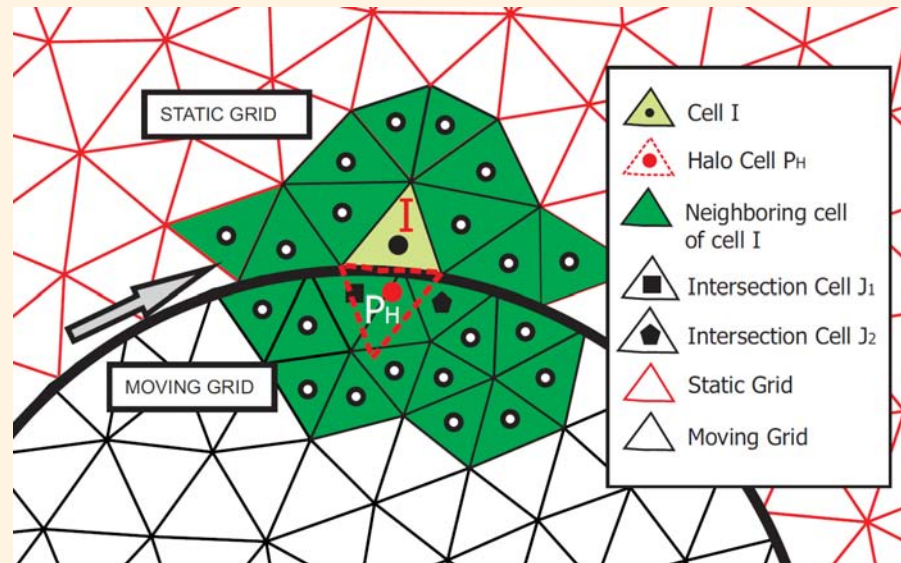




A MLS-based sliding mesh technique

- U_{P_H} is defined as

$$U_{P_H} = \frac{1}{A_{P_H}} \int U dA = \frac{1}{A_{P_H}} \int \sum_{j=1}^{n_x} N_j(\mathbf{x}_{P_H}) U_j dA$$



- It avoids the computation of intersection points!



Numerical Examples

► 1D Steady Shock

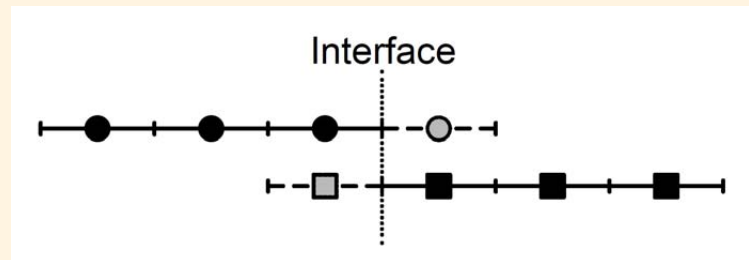
- Initial Conditions

$$\rho_L = 1, \quad \rho_R = 1.8621$$

$$u_L = 1.5, \quad u_R = 0.8055$$

$$p_L = 0.71429, \quad p_R = 1.7559$$

- Computational domain $0 \leq x \leq 10$ discretized in two regions of 25 elements
- The Interface is located at $x = 5.0$



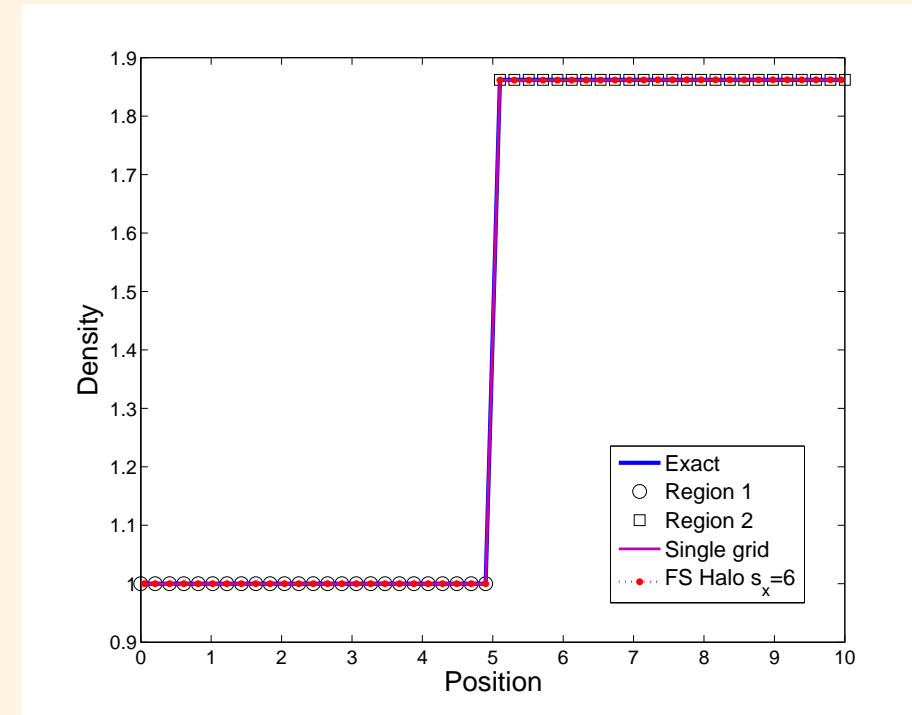
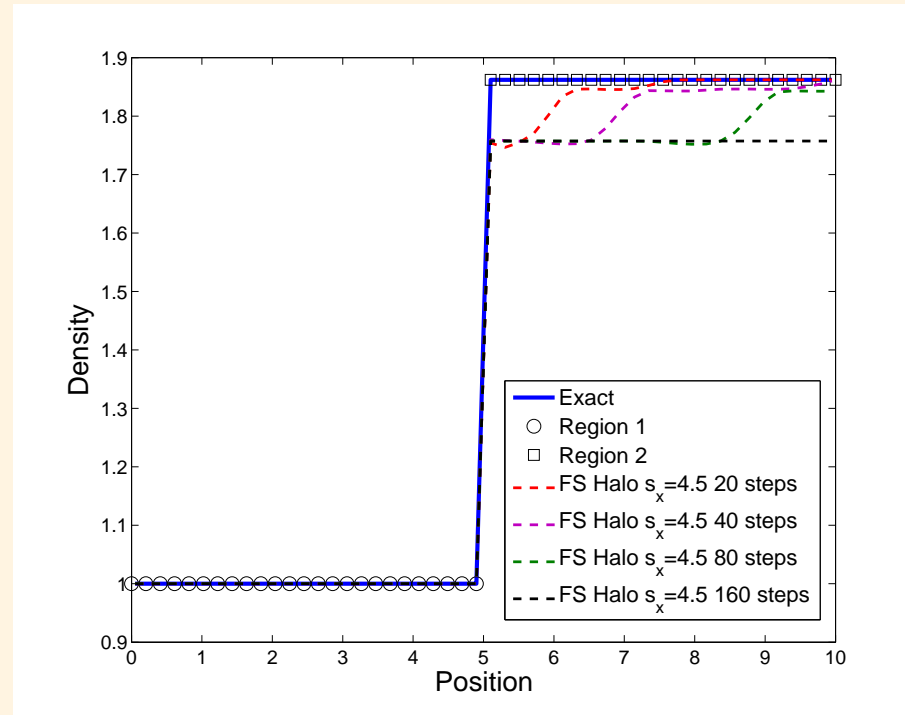
Z.J.Wang et al.. Recent development on the conservation property of chimera. IJCFD, 15,265-278,2001.



Numerical Examples

► 1D Steady Shock

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Numerical Examples

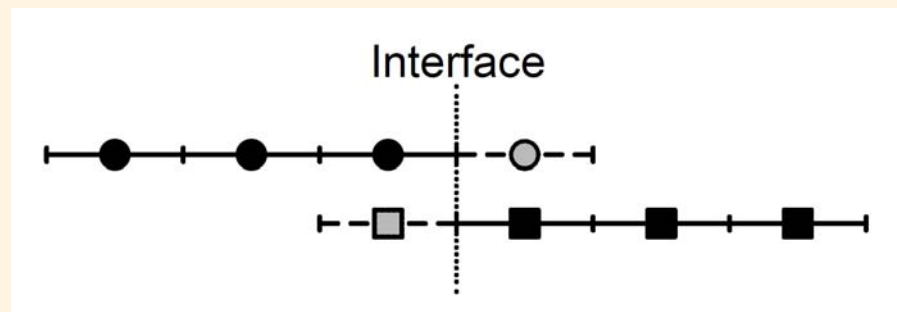
► 1D Unsteady Shock

- First test case of: *Riemann solvers and numerical methods for fluid dynamics. A practical introduction. Springer, 1999.*

- Initial Conditions

$$\begin{aligned}\rho_L &= 1.0, & \rho_R &= 0.125 \\ u_L &= 0.75, & u_R &= 0.0 \\ p_L &= 1.0, & p_R &= 0.1\end{aligned}$$

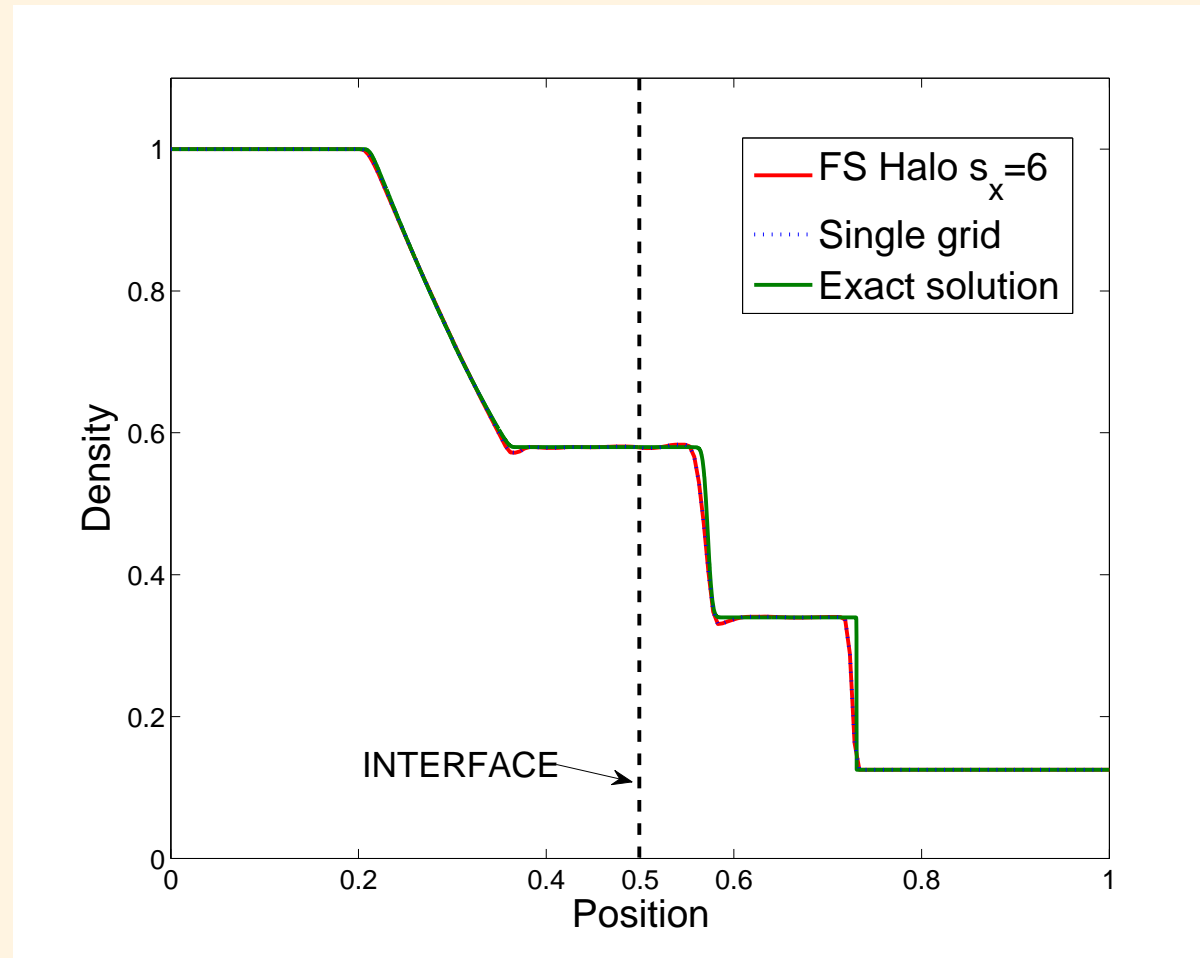
- Computational domain $0 \leq x \leq 1$ discretized in two regions of 150 elements
- The Interface is located at $x = 0.5$





Numerical Examples

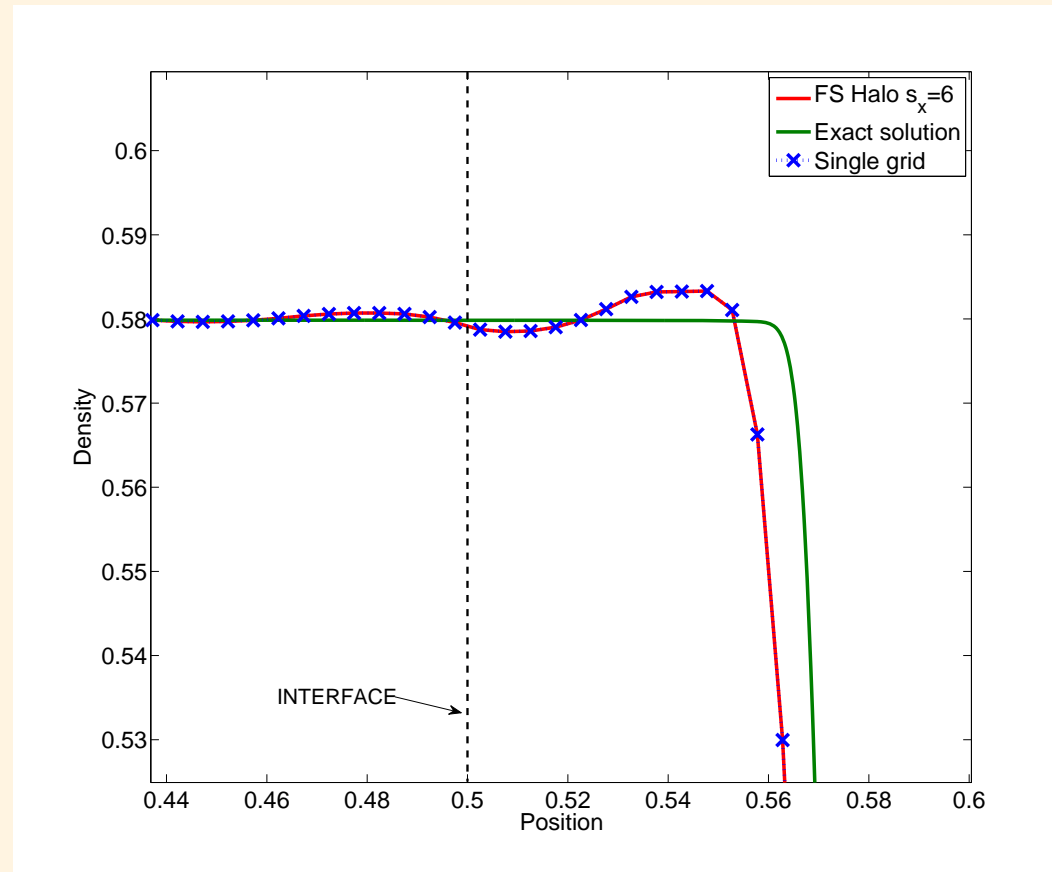
► 1D Unsteady Shock





Numerical Examples

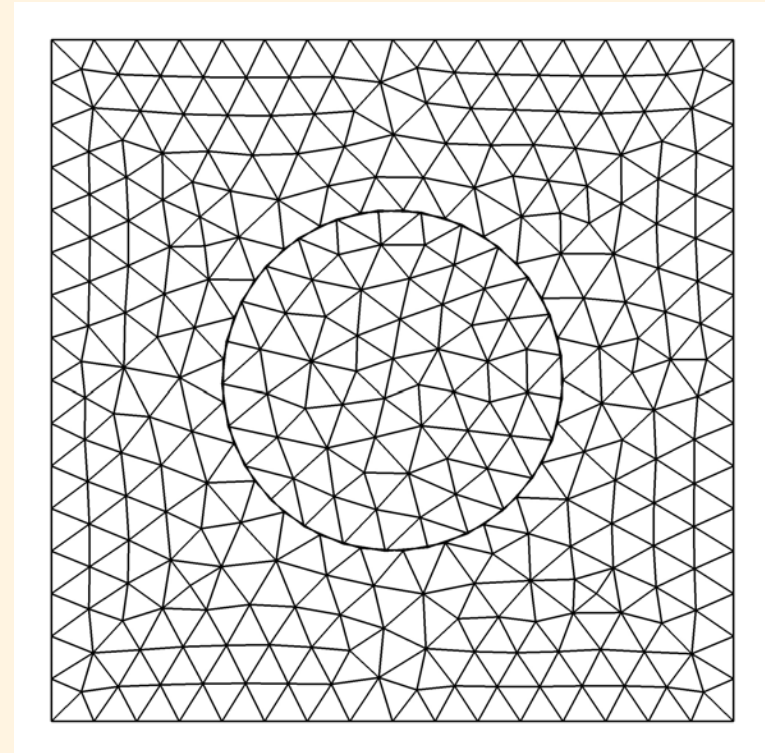
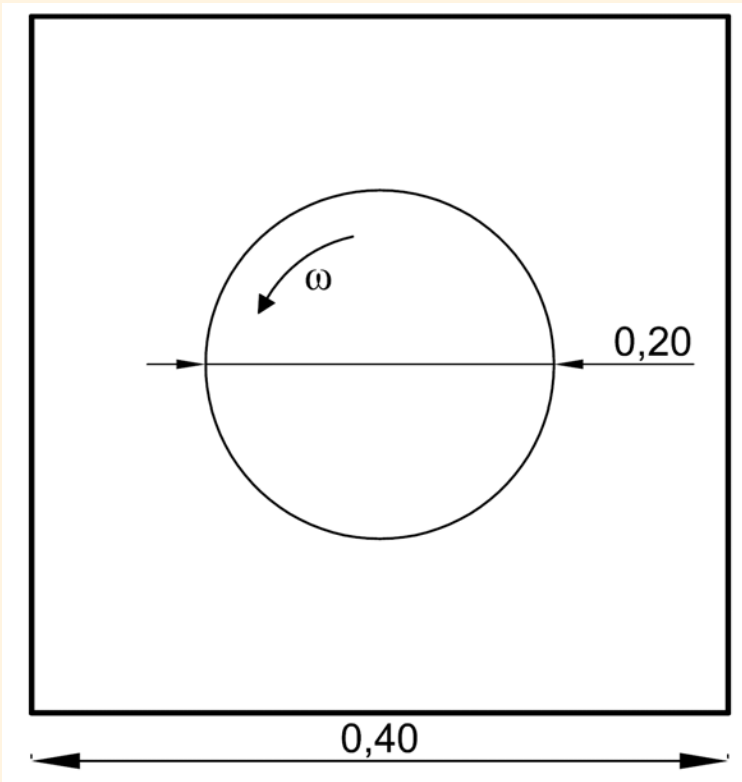
► 1D Unsteady Shock





Numerical Examples

► Ringleb flow test case

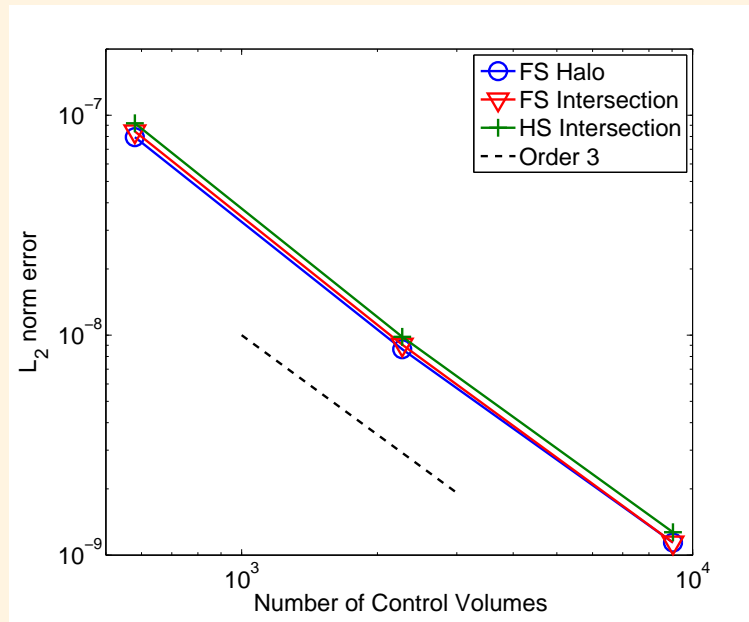




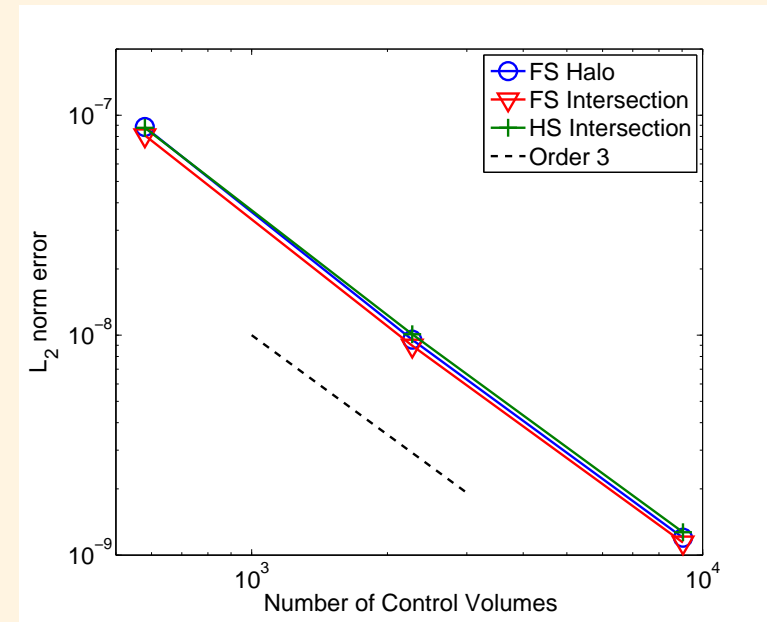
Numerical Examples

► Ringleb flow test case

- Third order FV-MLS



$$\omega = 0 \text{ rad/s}$$



$$\omega = 0.01 \text{ rad/s}$$

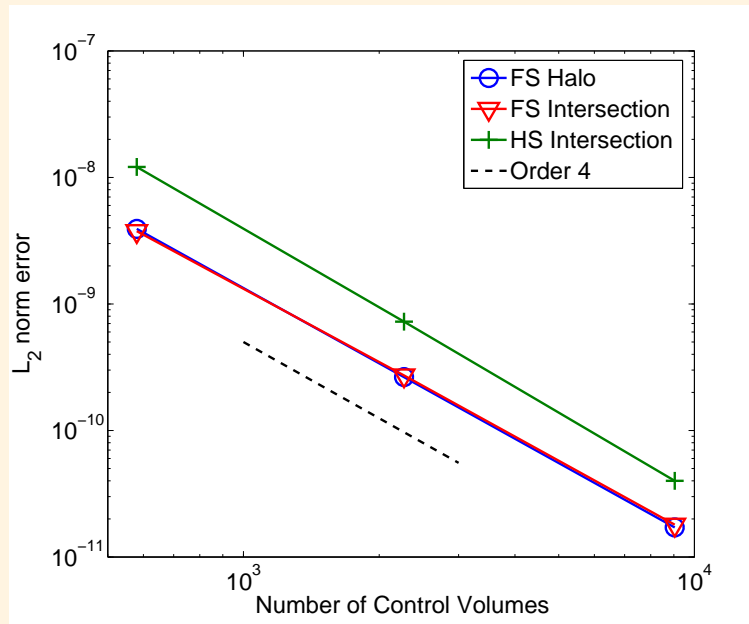




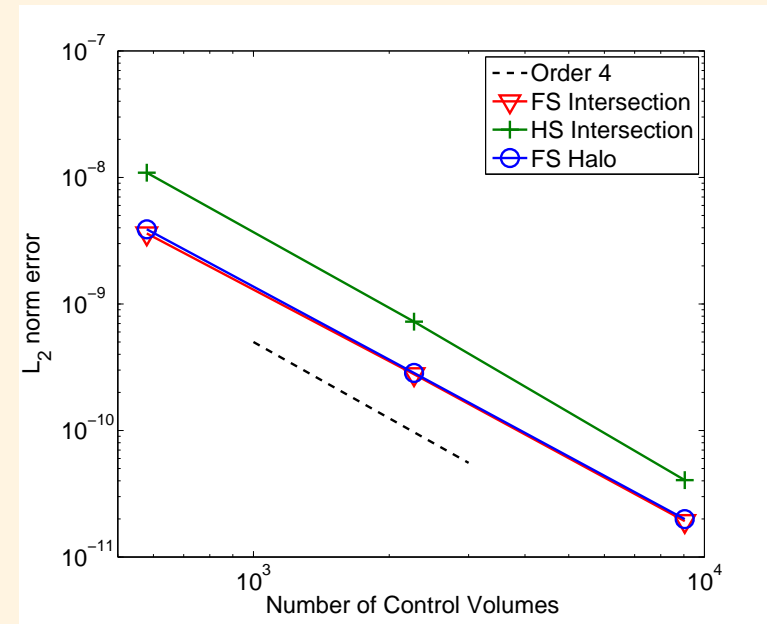
Numerical Examples

► Ringleb flow test case

- Fourth order FV-MLS



$$\omega = 0 \text{ rad/s}$$



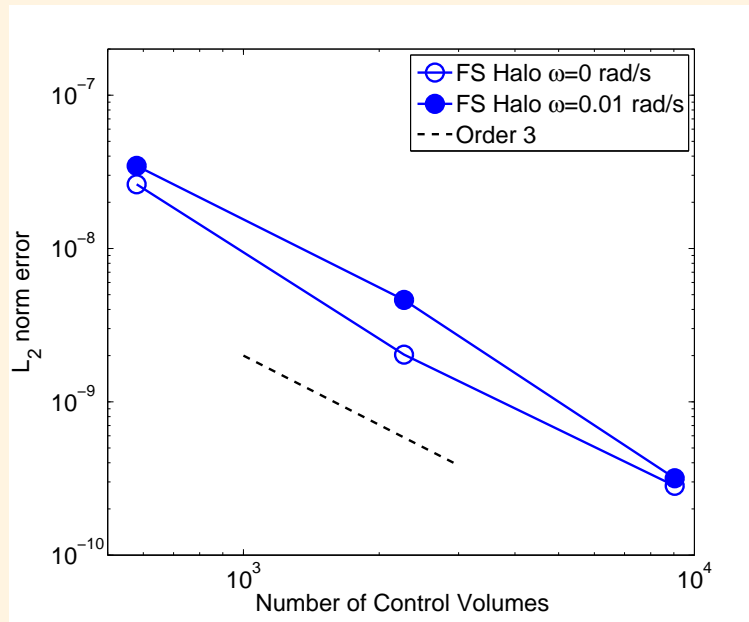
$$\omega = 0.01 \text{ rad/s}$$



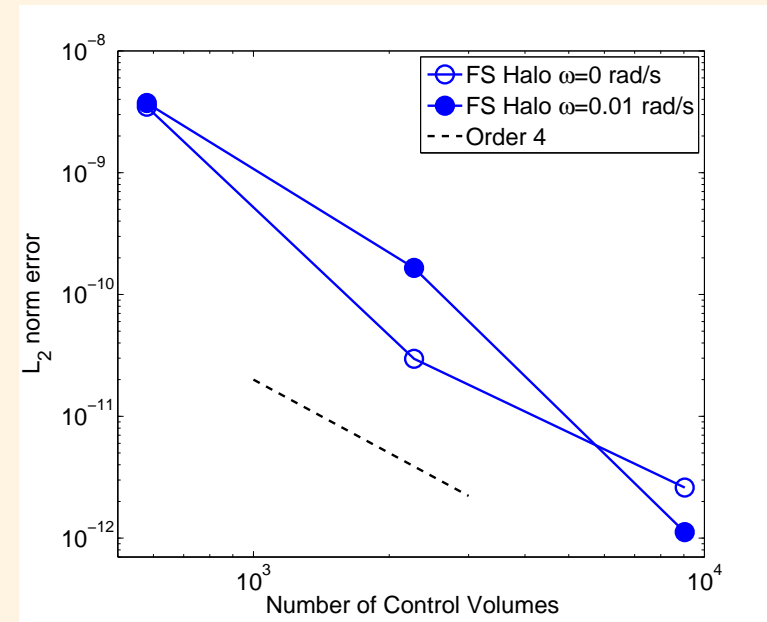
Numerical Examples

► Ringleb flow test case

- Conservation Error



Third order

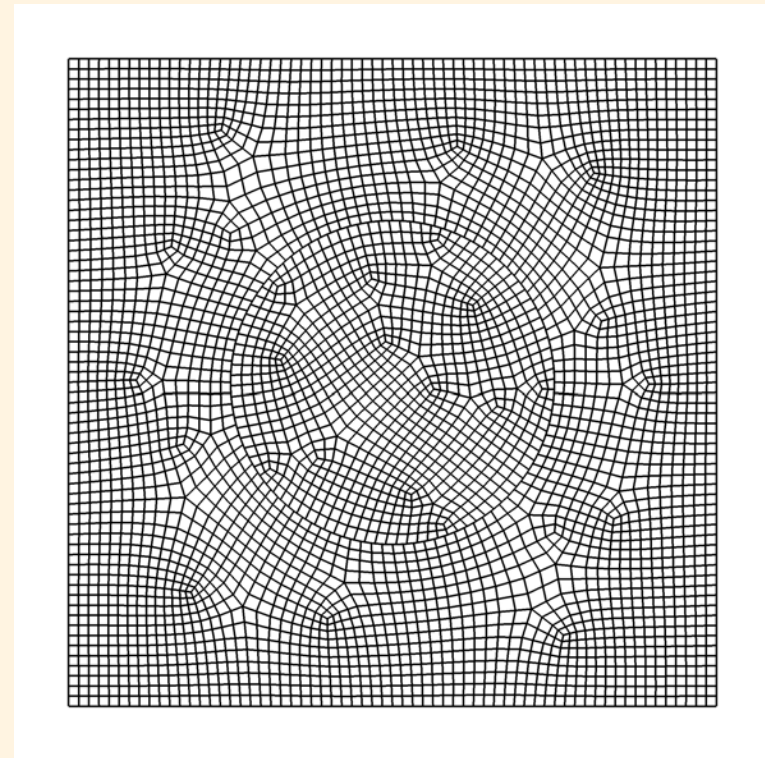
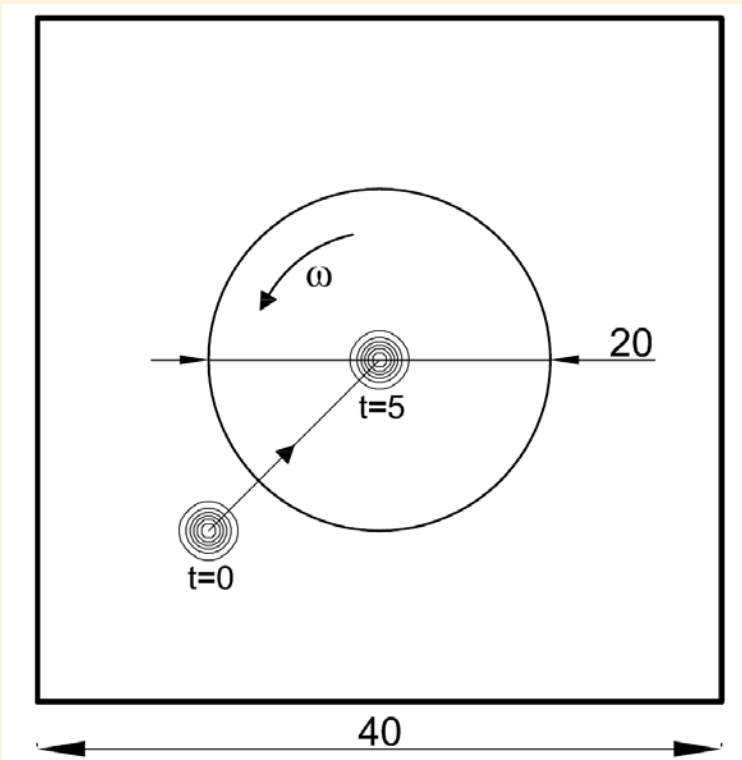


Fourth order



Numerical Examples

► 2D Vortex Convection

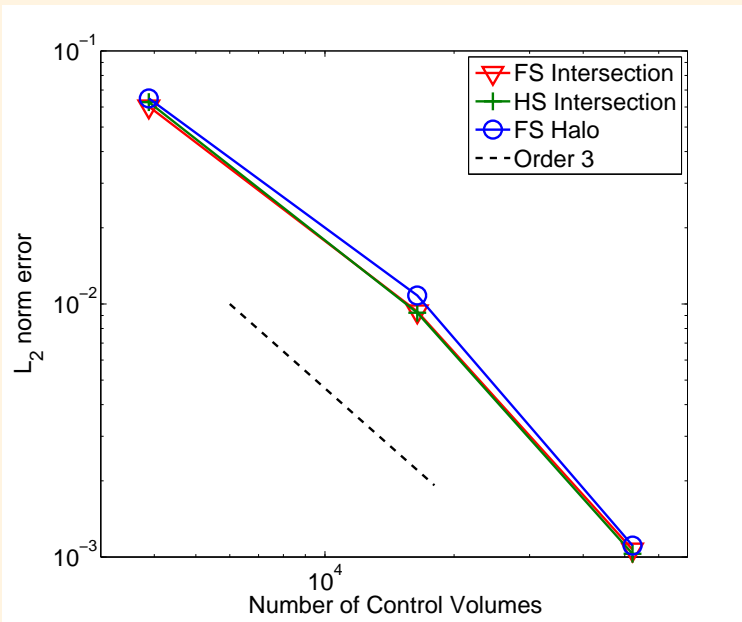




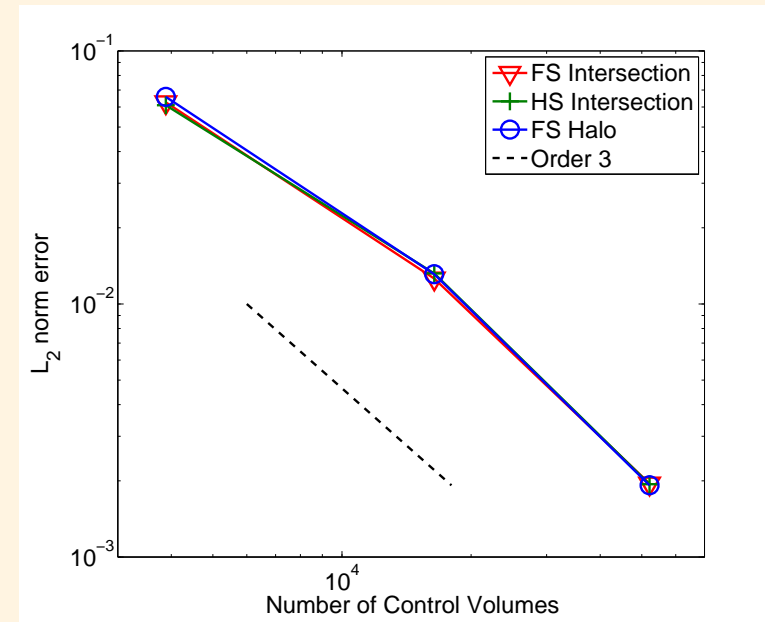
Numerical Examples

► 2D Vortex Convection

- Third order FV-MLS



$$\omega = 0 \text{ rad/s}$$



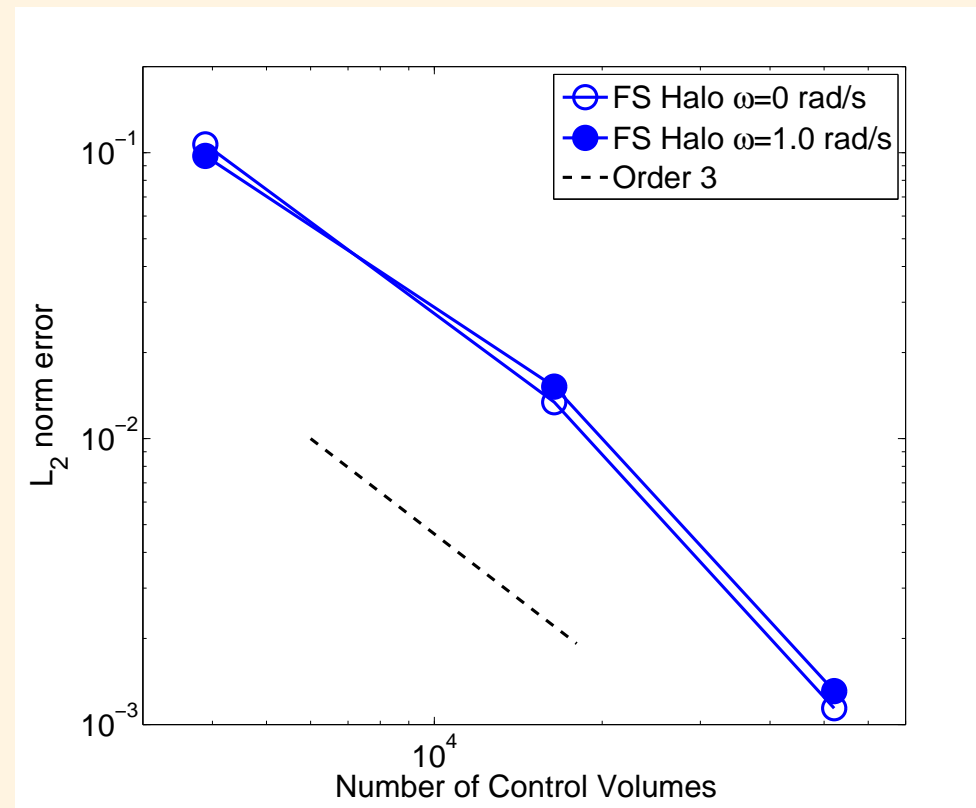
$$\omega = 1.00 \text{ rad/s}$$



Numerical Examples

► 2D Vortex Convection

- Conservation Error



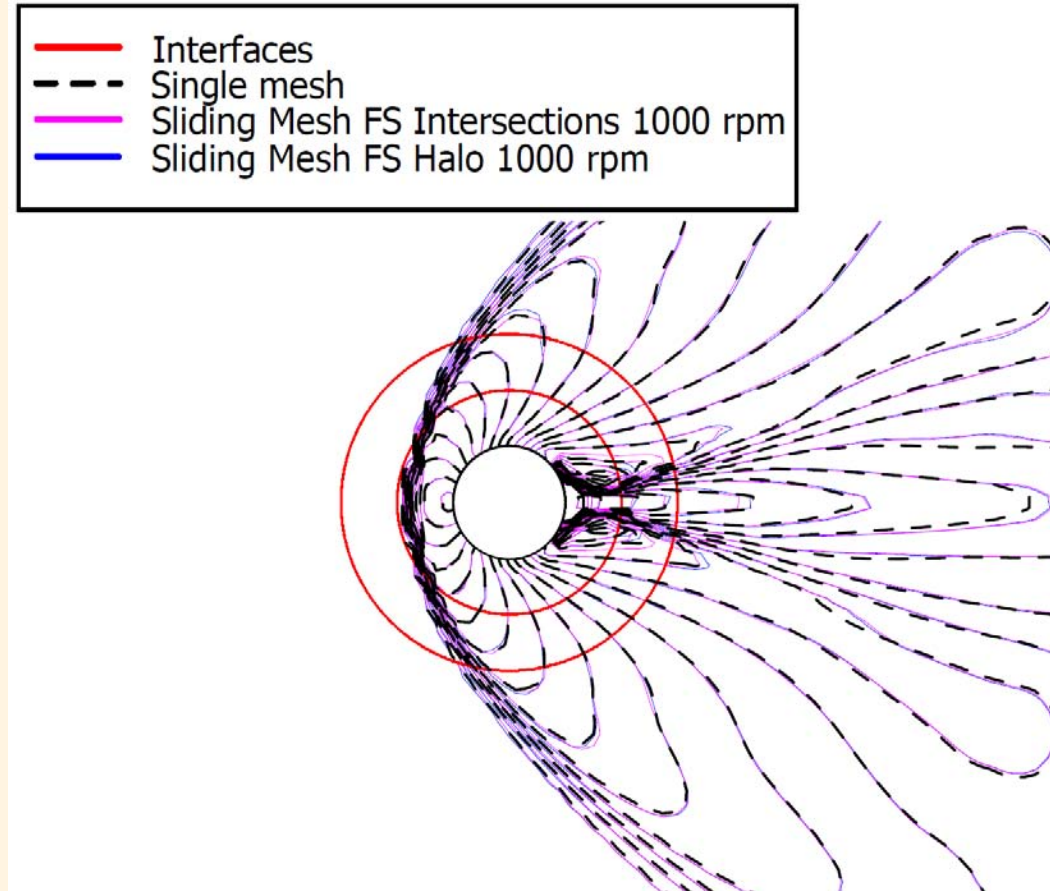
Third order





Numerical Examples

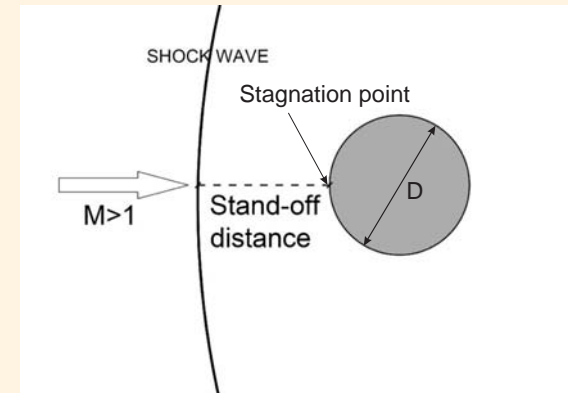
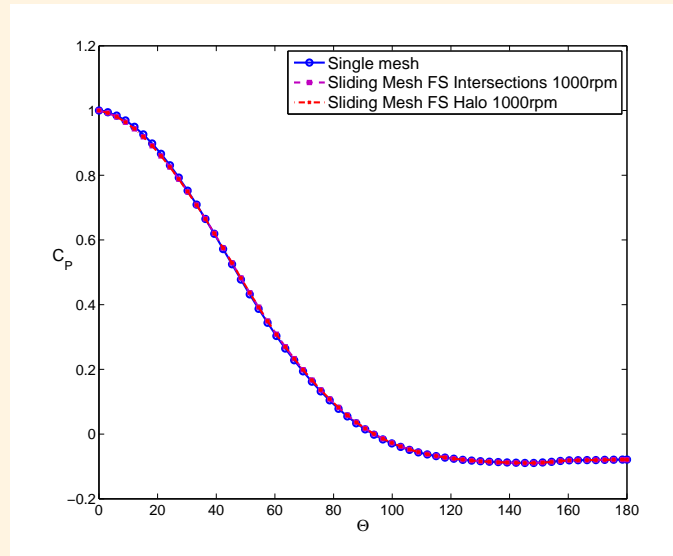
► Supersonic inviscid Flow over a cylinder. Mach 3





Numerical Examples

► Supersonic Flow over a cylinder. Mach 3

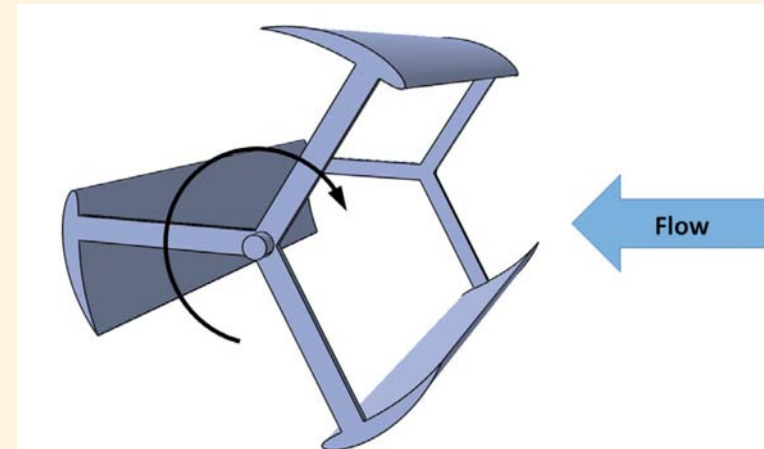
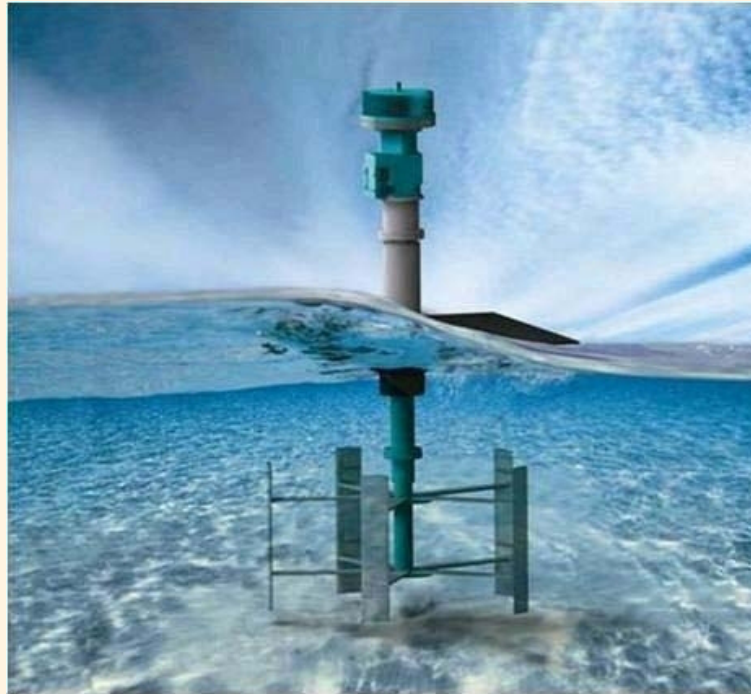


Method	$p_0/(p)_\infty$	Stand-off distance/D
Single mesh	0.327	0.405
Sliding Mesh FS Halo 0 rpm	0.324	0.407
Sliding Mesh FS Halo 1000 rpm	0.324	0.408
Sliding Mesh FS Intersections 1000 rpm	0.324	0.408
Reference solution	0.328	—



Numerical Examples

- ▶ Incompressible flow around a cross-flow turbine.



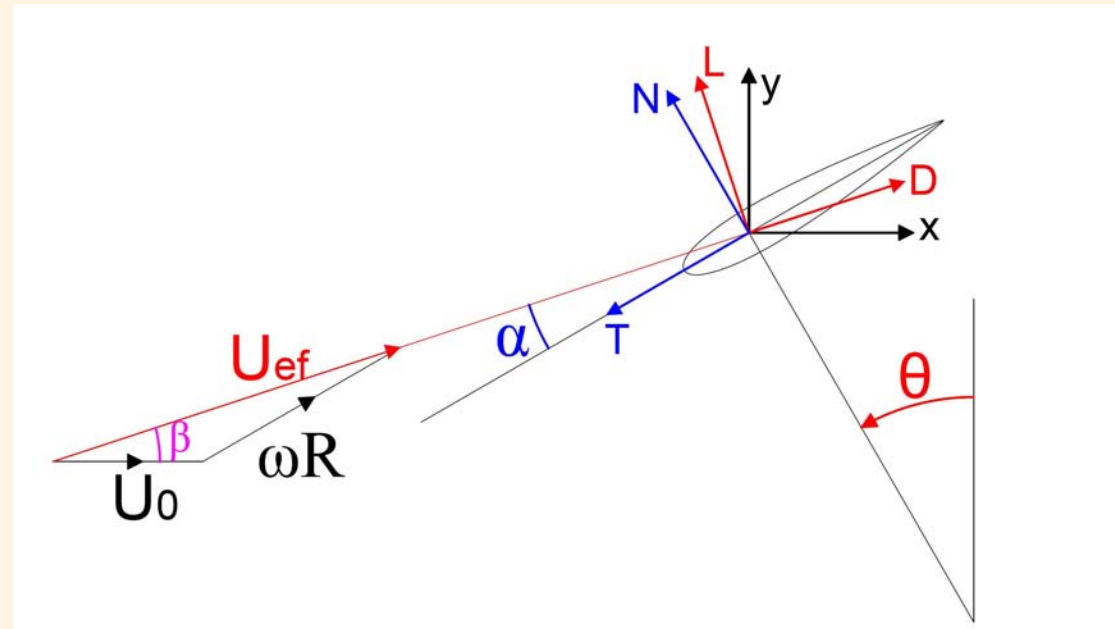
- Two test cases:
 - ▷ Single-bladed cross-flow turbine
 - ▷ Three-bladed cross-flow turbine

Problems Setup: E. Ferrer et al. A high order discontinuous galerkin fourier incompressible 3D Navier-Stokes solver with rotating sliding meshes. JCP, 231:7037-7056, 2012.



Numerical Examples

- Incompressible flow around a cross-flow turbine.



$$\vec{f} = \begin{Bmatrix} f_x \\ f_y \end{Bmatrix} = \oint (p\vec{n} - \nu(\nabla\vec{U} \cdot \vec{n}))d\Gamma$$

$$f_N = f_y \cos\theta - f_x \sin\theta \quad f_T = -f_x \cos\theta - f_y \sin\theta$$

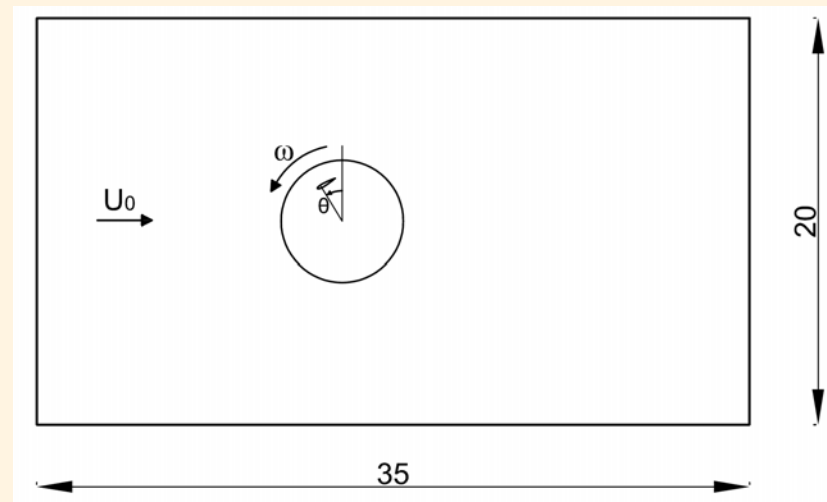


Numerical Examples

► Single-bladed cross-flow turbine

- Problem setup:

Free-stream velocity U_0	Rotational Speed ω	Tip Speed Ratio $\lambda = \omega R / U_0$
0.2	0.5	5
0.5	0.5	2
1.0	0.5	1

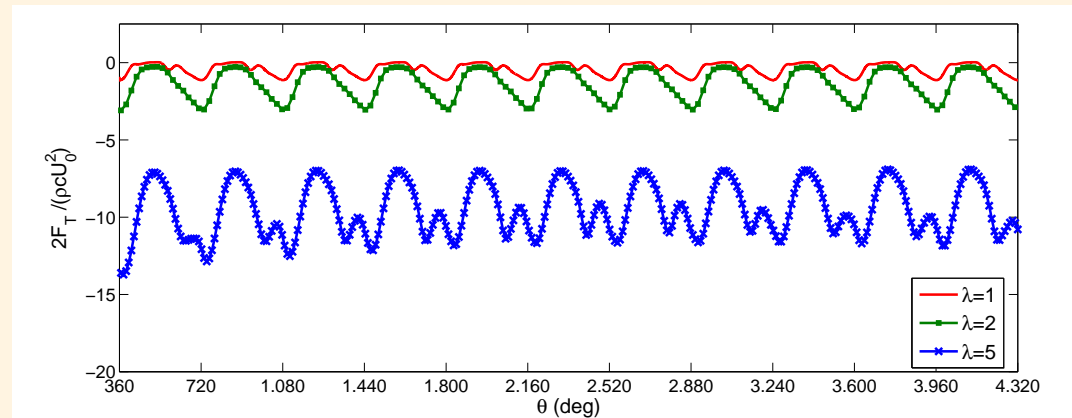
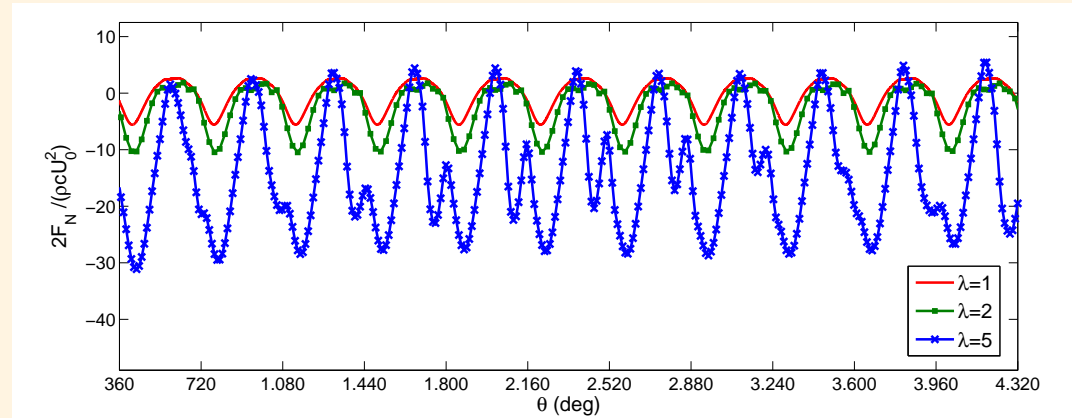
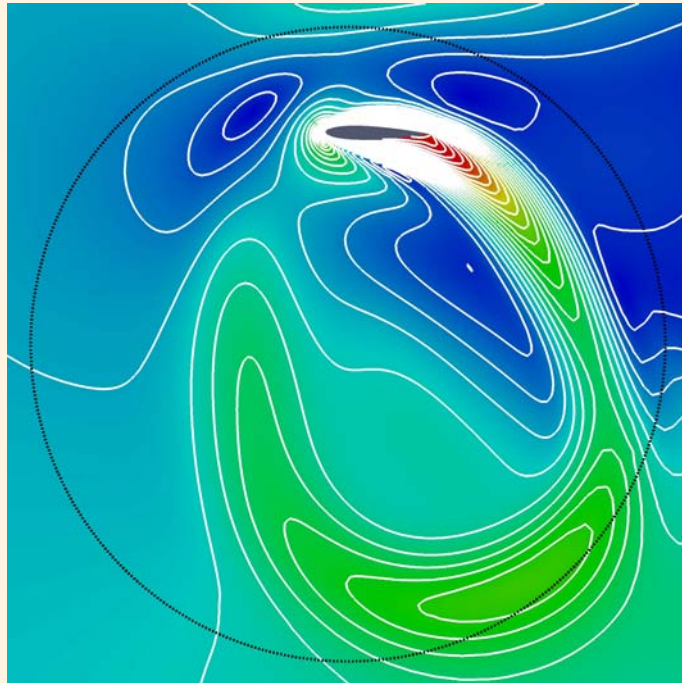




Numerical Examples

► Single-bladed cross-flow turbine

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Numerical Examples

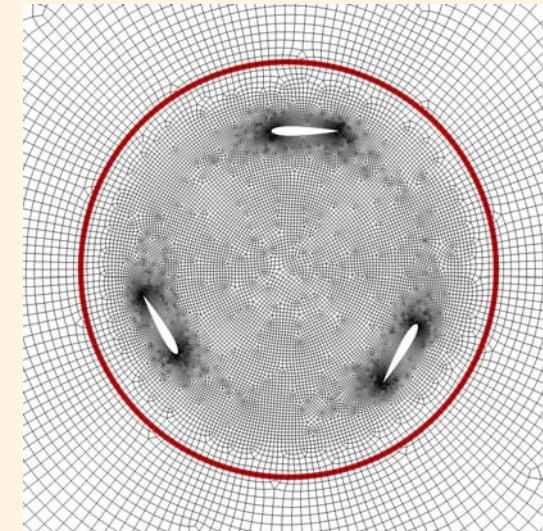
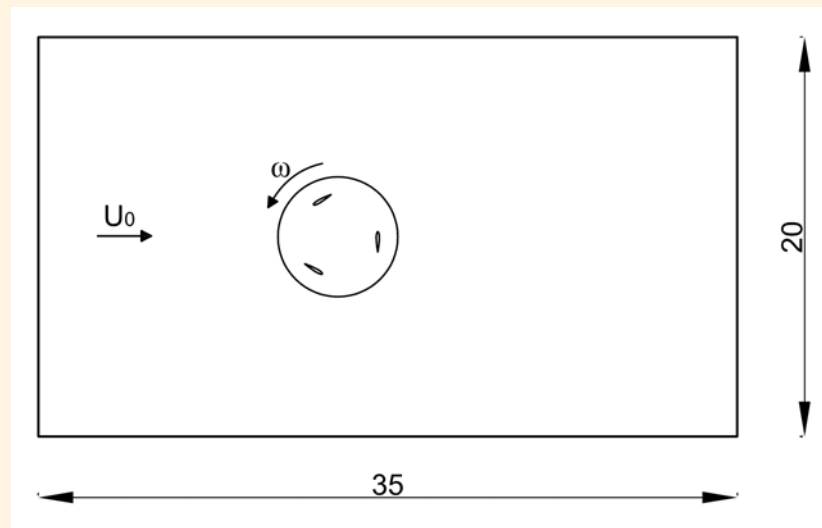
▶ Three bladed cross-flow turbine

- Problem setup:

- ▷ $U_0 = 0.5$ m/s

- ▷ $Re = 50$

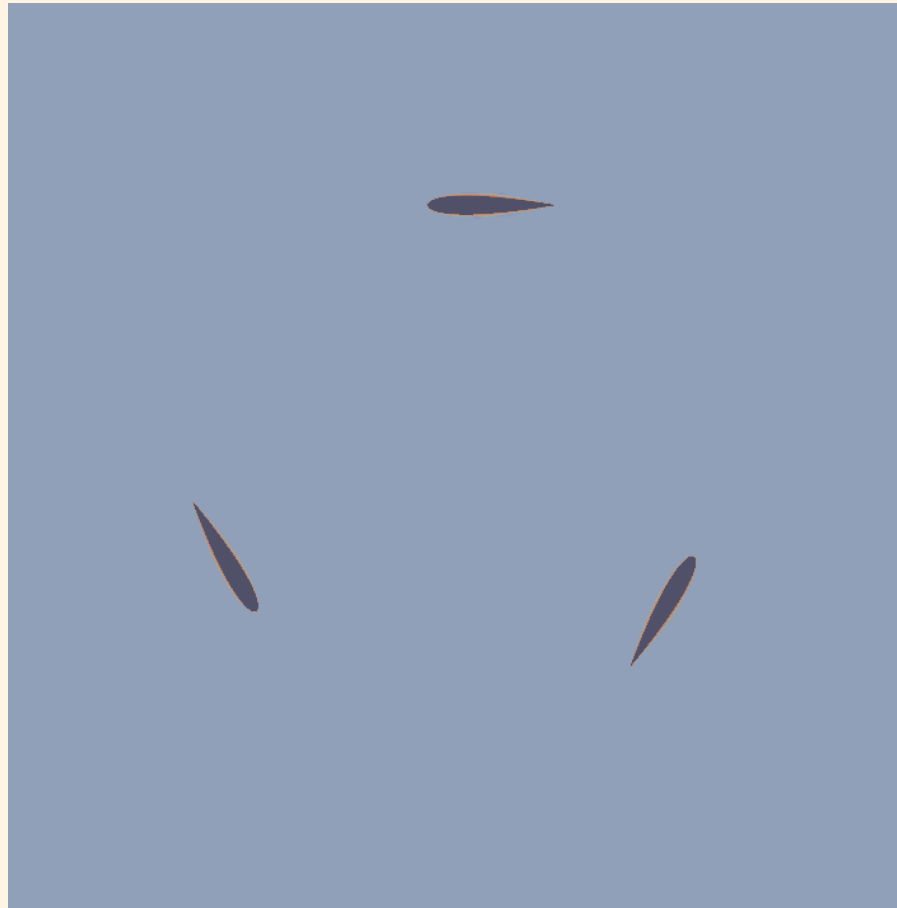
- ▷ $\omega = 0.5$ rad/s \rightarrow Tip-Speed Ratio (TSR) = $\frac{\omega R}{U_0} = 2$





Numerical Examples

▶ Three bladed cross-flow turbine

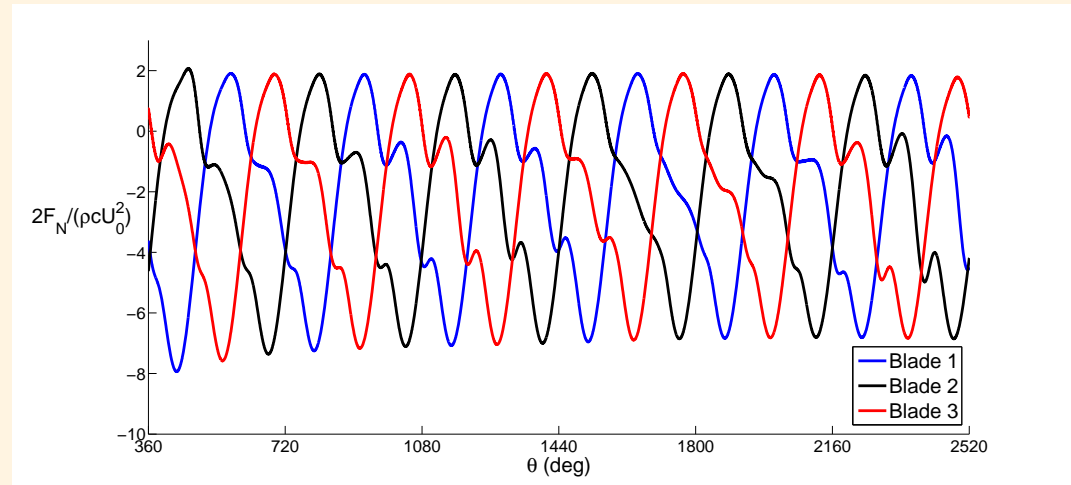




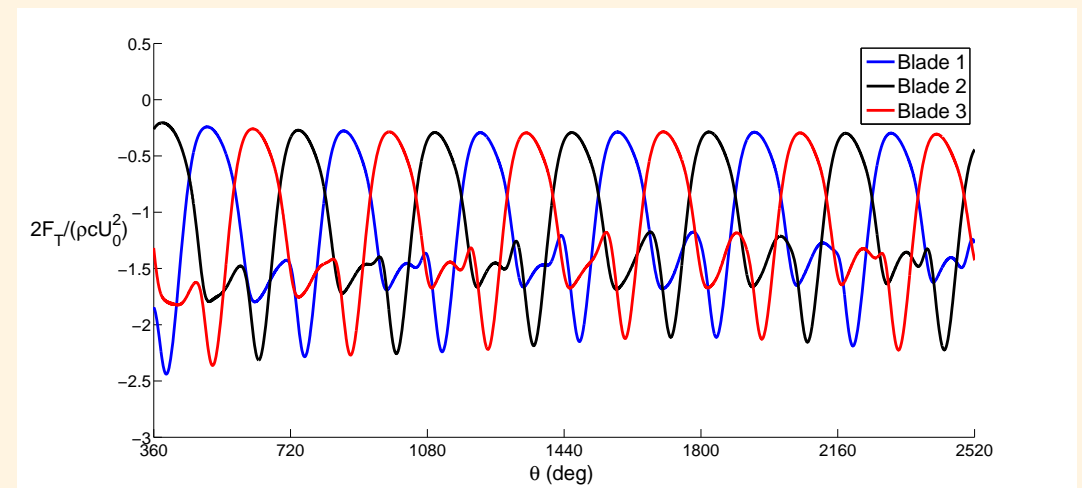
Numerical Examples

► Three bladed cross-flow turbine

Normalized Normal Force



Normalized Tangential Force





Application to Navier-Stokes-Korteweg equations

- Introduction
- The FV-MLS method
- Multiscale properties of MLS: MLS-based shock detection
- A formulation for all-speed flows
- A MLS-based sliding mesh technique
- Application to Navier-Stokes-Korteweg equations
- Conclusions





Application to Navier-Stokes-Korteweg equations

- ▶ Navier-Stokes-Korteweg equations:
 - Density is the phase-field parameter
 - Simplest model for vaporization is the isothermal version
 - Spatial derivatives of order three
 - Very few numerical solutions (see D. Diehl, PhD. Thesis)

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Application to Navier-Stokes-Korteweg equations

► Phase-field modeling:

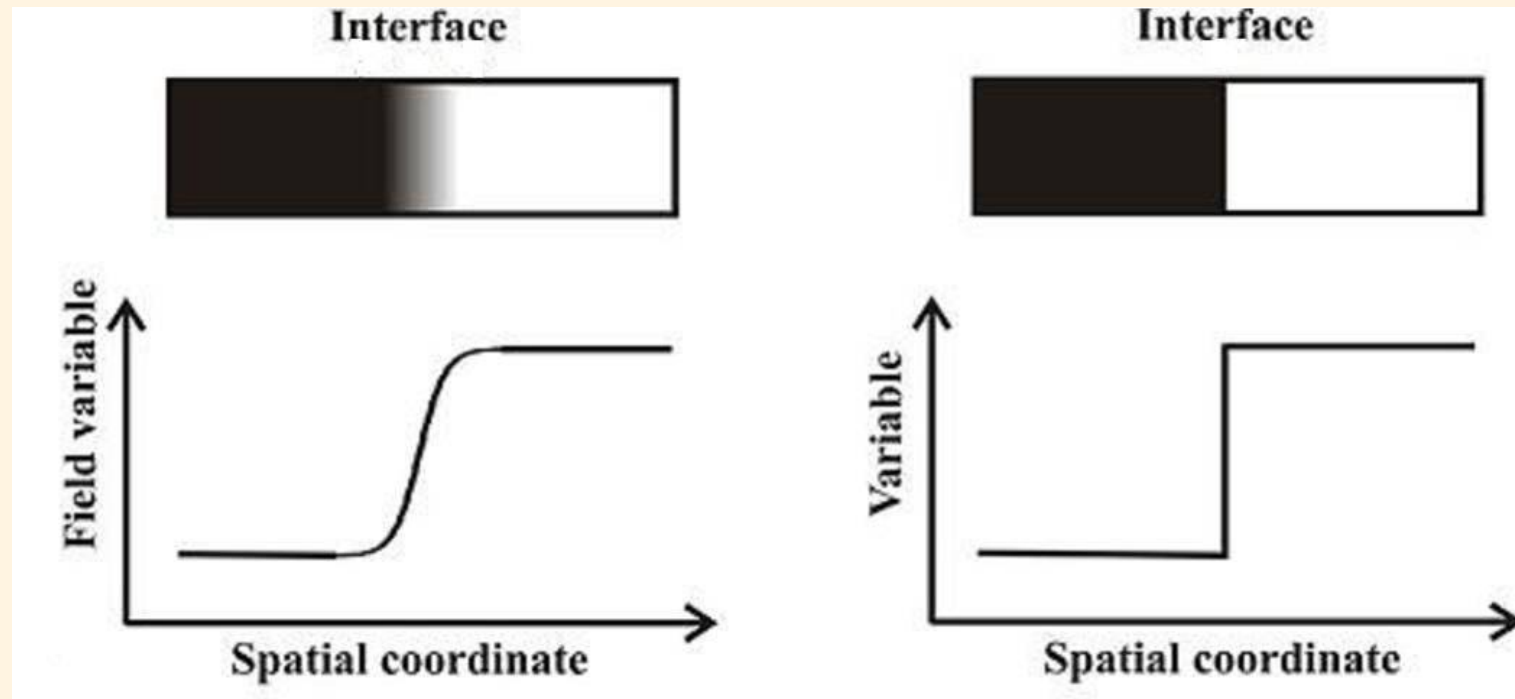
- Initiated for phase evolution/transition problems
 - ▷ Phase separation of immiscible fluids
 - ▷ Vaporization and condensation
 - ▷ Solidification
- Sound mathematics and thermodynamics
- Successfully applied to other phenomena
 - ▷ Crack propagation
 - ▷ Thin liquid films
 - ▷ Porous media flow
 - ▷ Cancer growth





Application to Navier-Stokes-Korteweg equations

► Phase-field modeling





Application to Navier-Stokes-Korteweg equations

▶ Sharp-interface models

- Partial differential equations of the individual phases are coupled through interface boundary conditions
- Very difficult numerically

▶ Phase-field models

- Sharp interfaces approximated by thin layers described by higher-order differential operators
- All variables are continuous across the interface
- Examples:
 - ▷ Cahn-Hilliard equation
 - ▷ Navier-Stokes-Korteweg equations





Application to Navier-Stokes-Korteweg equations

► Navier-Stokes-Korteweg equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) + \nabla p - \nabla \cdot \tau - \nabla \cdot \varsigma = S_b$$

where

$$\tau = \bar{\mu}(\nabla u + \nabla u^T) + \bar{\lambda} \nabla \cdot u \mathbf{I}$$

$$\varsigma = \lambda(\rho \nabla \rho + \frac{1}{2} |\nabla \rho|^2) \mathbf{I} - \lambda \nabla \rho \otimes \nabla \rho$$

The capillarity term may be written in non conservative form:

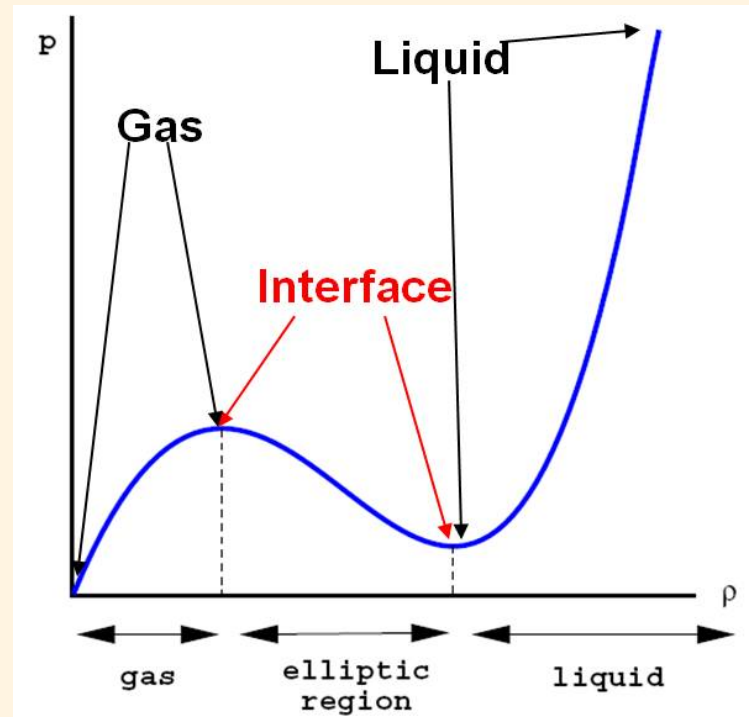
$$\nabla \cdot \varsigma = \lambda \rho \nabla(\Delta \rho)$$





Application to Navier-Stokes-Korteweg equations

- Model based on van der Waals equations



$$p(\rho) = Rb \frac{\rho\theta}{b - \rho} - a\rho^2$$

θ is the temperature, a , b are the van der Waals constants and R is the universal gas constant



Application to Navier-Stokes-Korteweg equations

- ▶ Convective term: Rusanov flux with Li and Gu's fix
- ▶ Korteweg term: Direct computation at Gauss points using MLS
- ▶ Interface upscaling
 - There is a very limited number of numerical solutions to the Navier–Stokes–Korteweg equations in the literature.
 - One of the main reasons is that NSK equations are only a realistic model if the thickness of the interfaces is extremely small.
 - The interfaces must be resolved by the computational mesh, which imposes severe restrictions on any numerical method.
 - We use a scaling according to which the thickness of the interfaces is adapted to the computational mesh¹.

¹H. Gomez, T.J.R. Hughes, X. Nogueira, V. Calo *Isogeometric analysis of the isothermal Navier–Stokes–Korteweg equations*, CMAME, 199, 2010



Application to Navier-Stokes-Korteweg equations

► Refinement methodology

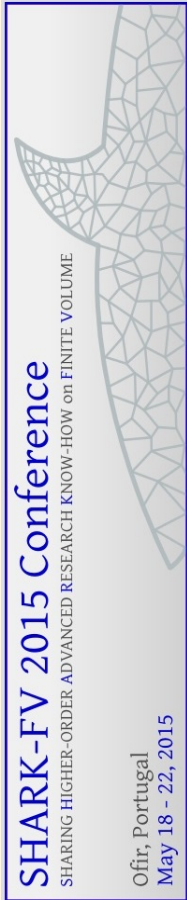
- Ca expresses the ratio between a characteristic length scale of the NSK equations and the arbitrary length scale L_0
- Ca scales as the thickness of the interfaces.
- We propose to scale the capillarity number as:

$$Ca = \frac{h}{L_0}$$

- From dimensional analysis the product of Re and Ca must be a constant.

$$Re = \alpha \frac{L_0}{h}$$

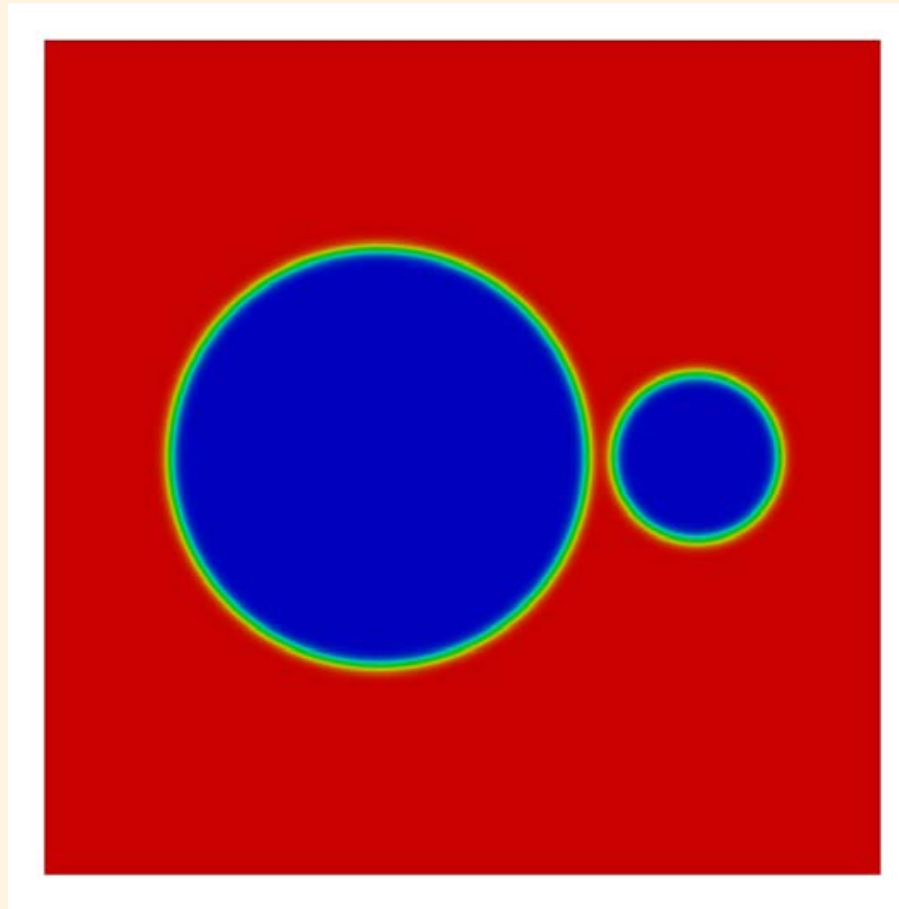
$$L = 1, \alpha = 2, h = \max(V_i)^{1/d}$$





Application to Navier-Stokes-Korteweg equations

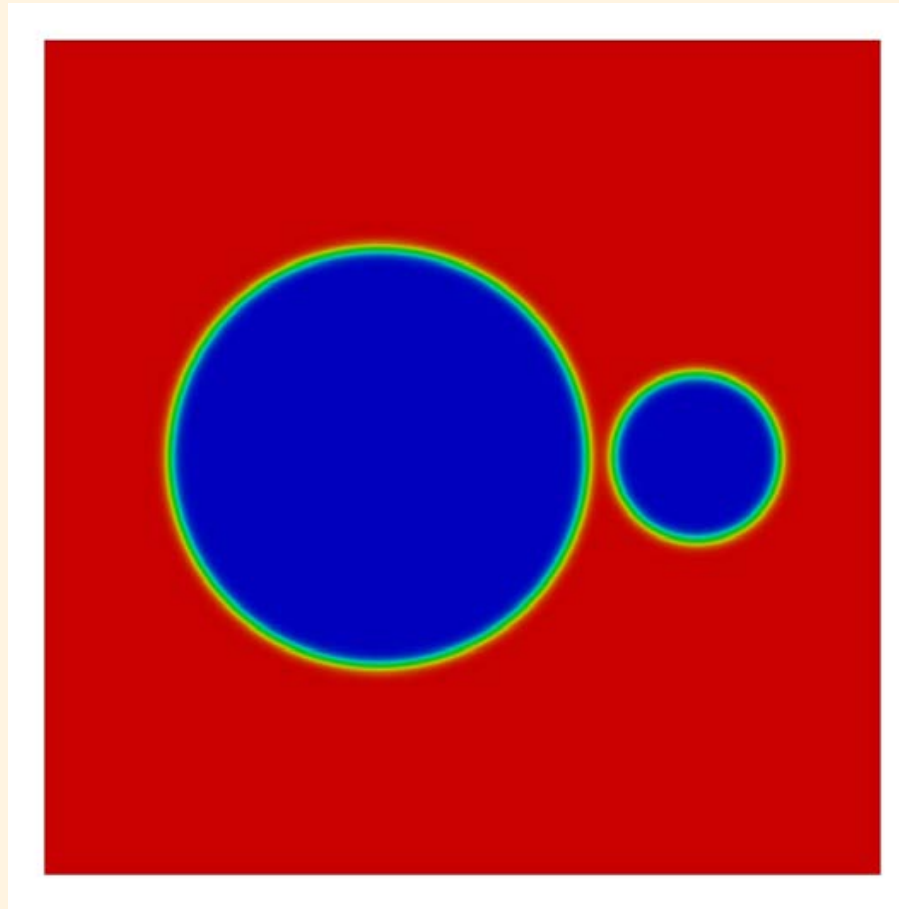
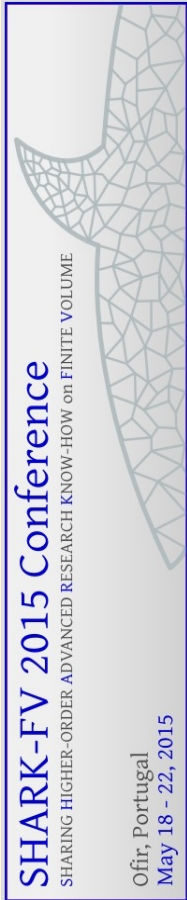
- ▶ Two bubbles coalescence: 256^2 grid





Application to Navier-Stokes-Korteweg equations

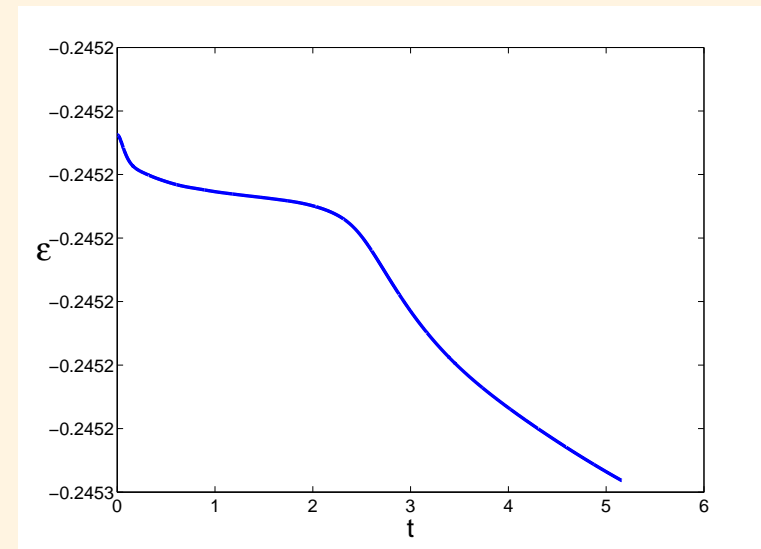
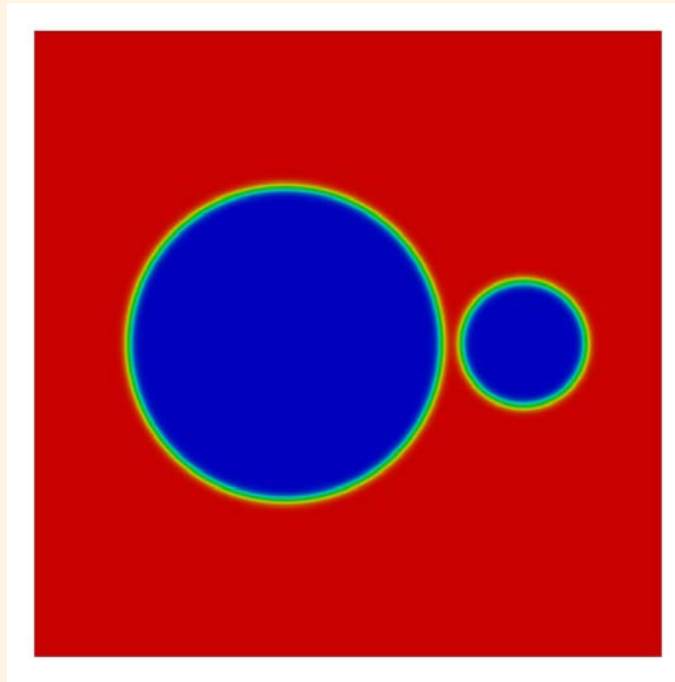
- ▶ Two bubbles coalescence: 256^2 grid





Application to Navier-Stokes-Korteweg equations

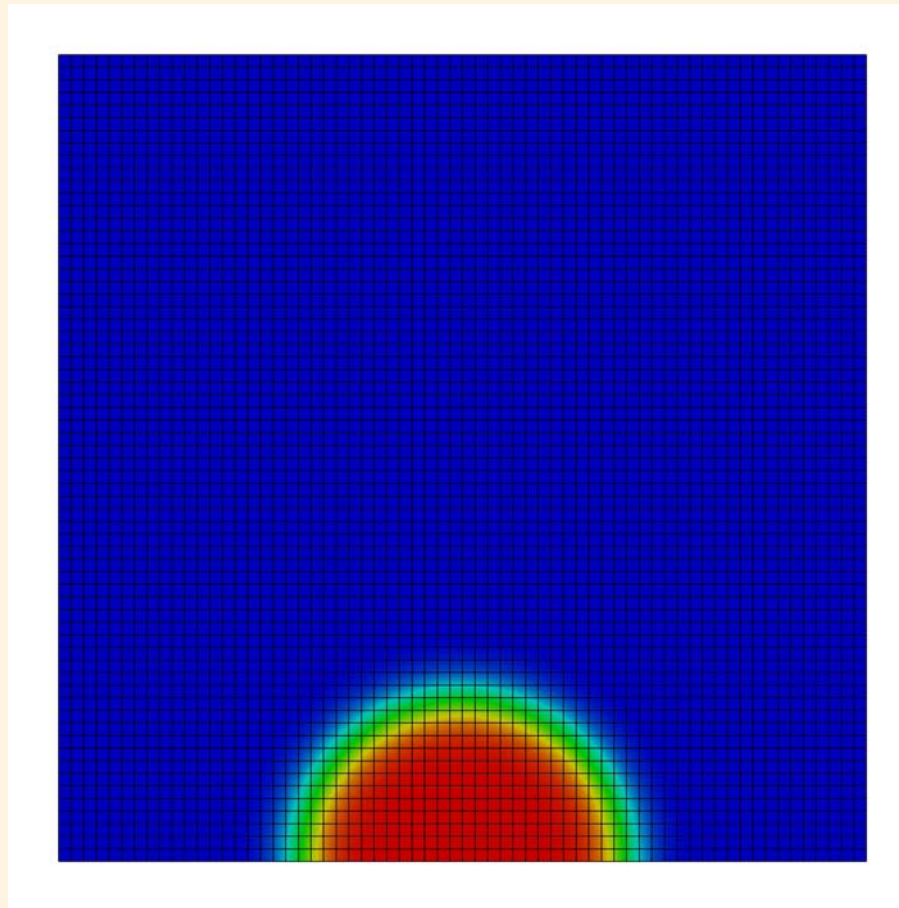
- ▶ Two bubbles coalescence: 256^2 grid





Application to Navier-Stokes-Korteweg equations

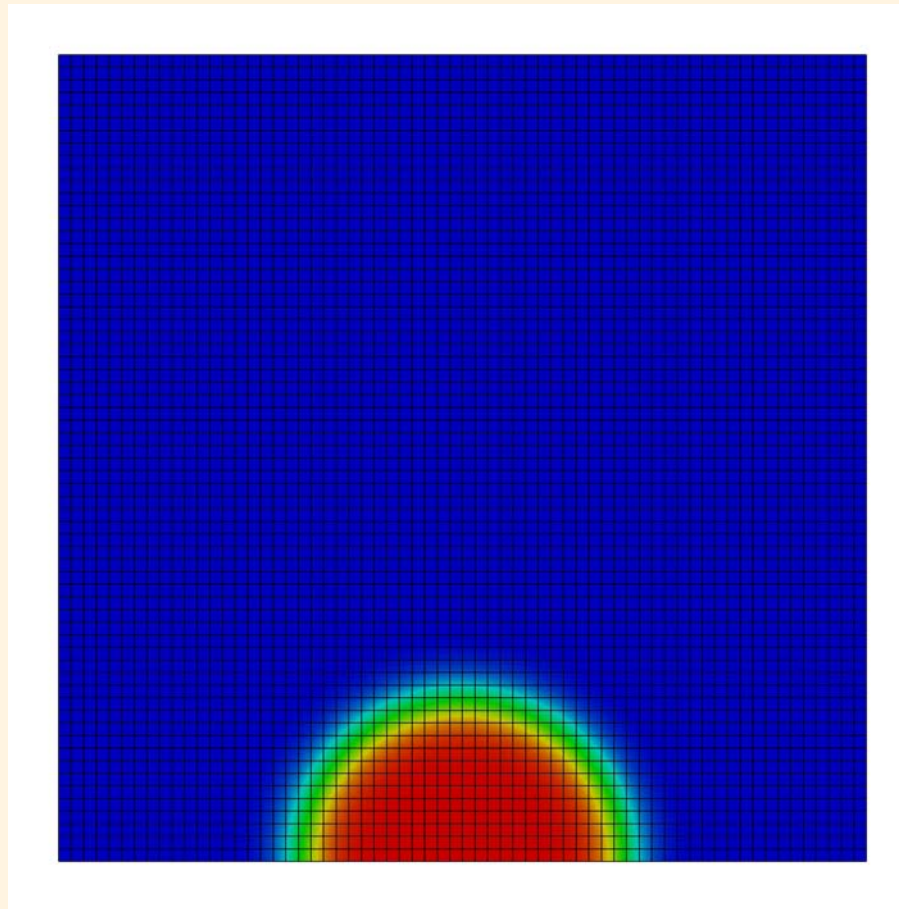
- ▶ Wet-wall boundary condition: 64^2 grid





Application to Navier-Stokes-Korteweg equations

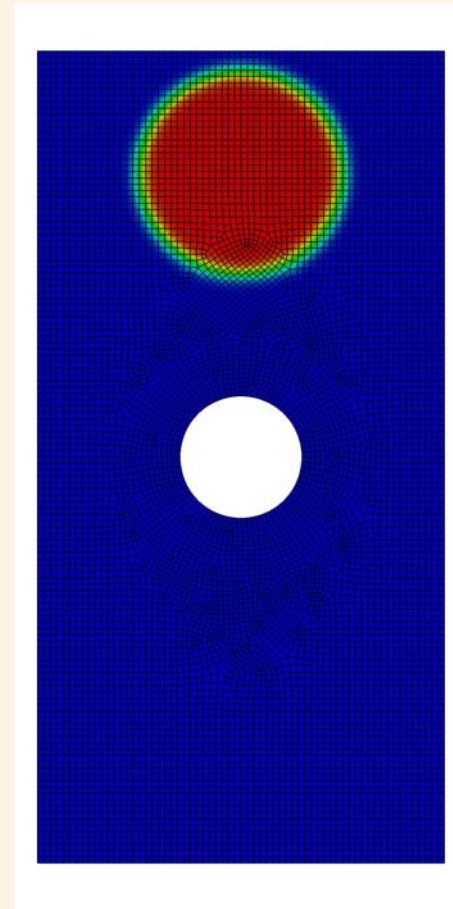
- ▶ Wet-wall boundary condition (intense gravity): 64^2 grid





Application to Navier-Stokes-Korteweg equations

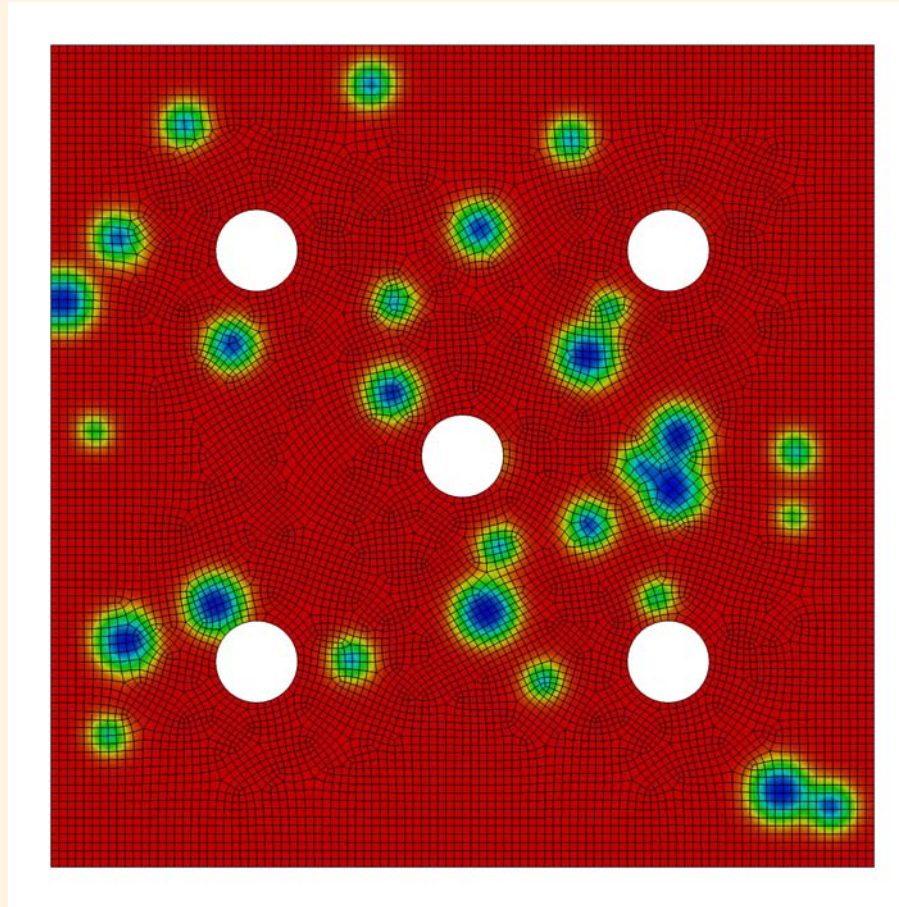
- ▶ Droplet falling interacting with an obstacle: 64^2 grid





Application to Navier-Stokes-Korteweg equations

- ▶ Two-phase spinodal decomposition with obstacles:
 64^2 grid





Outline

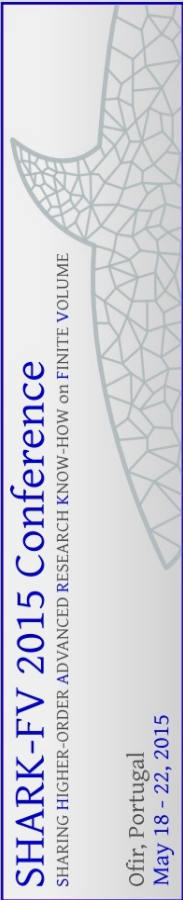
- Introduction
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- **Conclusions**





Conclusions

- ▶ Many numerical applications using MLS with FV schemes have been presented.
- ▶ The accuracy and robustness of the new methodologies have been shown with different numerical test cases.
- ▶ MLS allows increasing the accuracy and capabilities of current FV codes.
- ▶ FV-MLS is a good method for phase field models.





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HIGHER-ORDER FINITE VOLUME METHODS WITH MOVING LEAST SQUARES APPROXIMATIONS

Xesús Nogueira

email: xnogueira@udc.es

Thank you

—





Acknowledgments

► This work has been partially supported by:

- The *Ministerio de Educación y Ciencia* of the Spanish Government,
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- the *Universidade da Coruña (UDC)*, and
- the *Group of Numerical Methods in Engineering - GMNI*





Some FV-MLS references

- L. Cueto-Felgueroso, I. Colominas, X. Nogueira, F. Navarrina, and M. Casteleiro, *Finite-volume solvers and moving least-squares approximations for the compressible Navier-Stokes equations on unstructured grids*, CMAME, 2007
- X. Nogueira, I. Colominas, L. Cueto-Felgueroso, and S. Khelladi, *On the simulation of wave propagation with a higher-order finite volume scheme based on reproducing kernel methods*, CMAME, 2010
- X. Nogueira, L. Cueto-Felgueroso, I. Colominas, F. Navarrina, and M. Casteleiro, *A new shock-capturing technique based on moving least squares for higher-order numerical schemes on unstructured grids*, CMAME, 2010
- X. Nogueira, L. Cueto-Felgueroso, I. Colominas, H. Gómez, *Implicit Large Eddy Simulation of non-wall-bounded turbulent flows based on the multiscale properties of a high-order finite volume method*, CMAME, 2010
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