GPU Accelerated High-Order Hybrid Methods for Shock Problems

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w/
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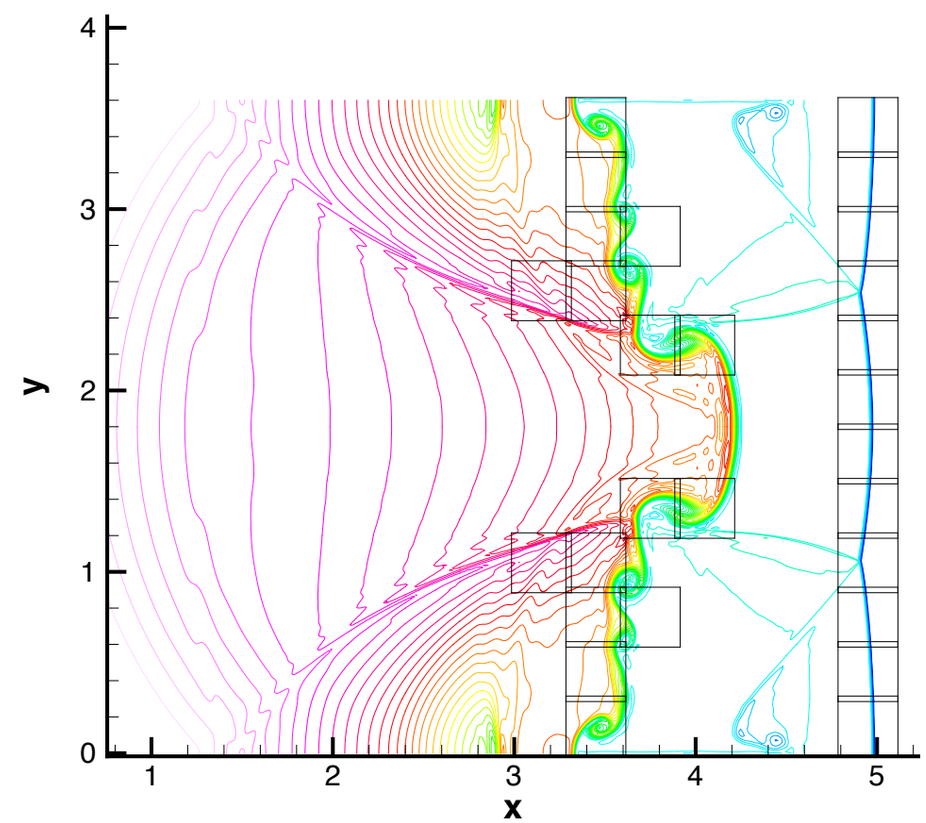

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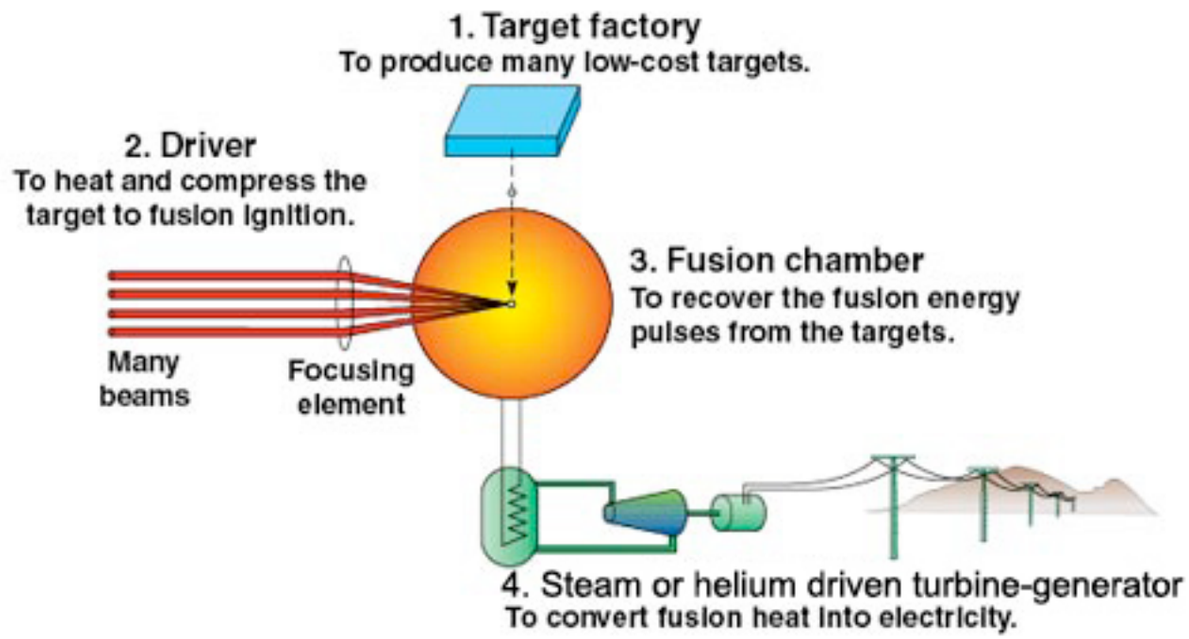
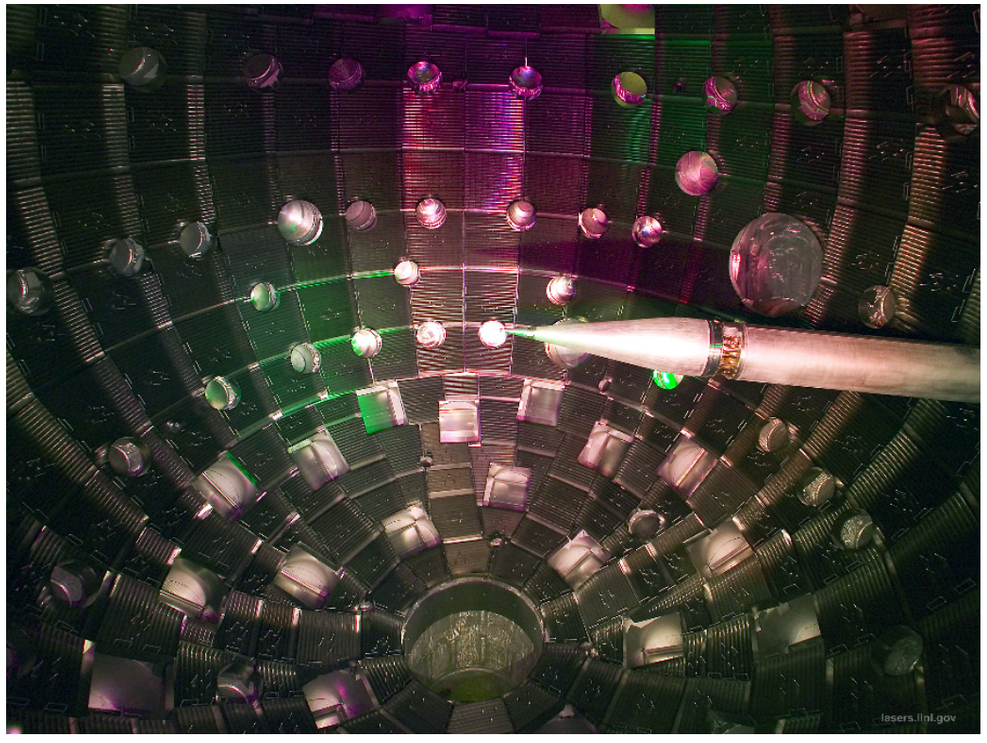
A bit of motivation

Laser induced fusion

NIF - National Ignition Facility

192 Lasers, delivering 4MJ in a few pico seconds



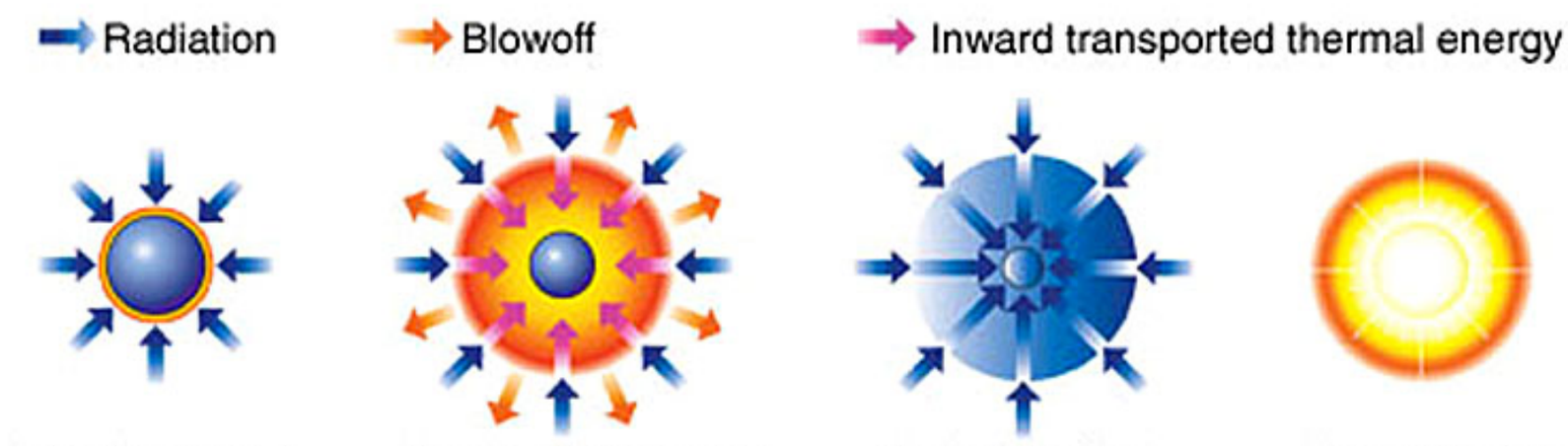


50 l of water ~ 200,000 kwh

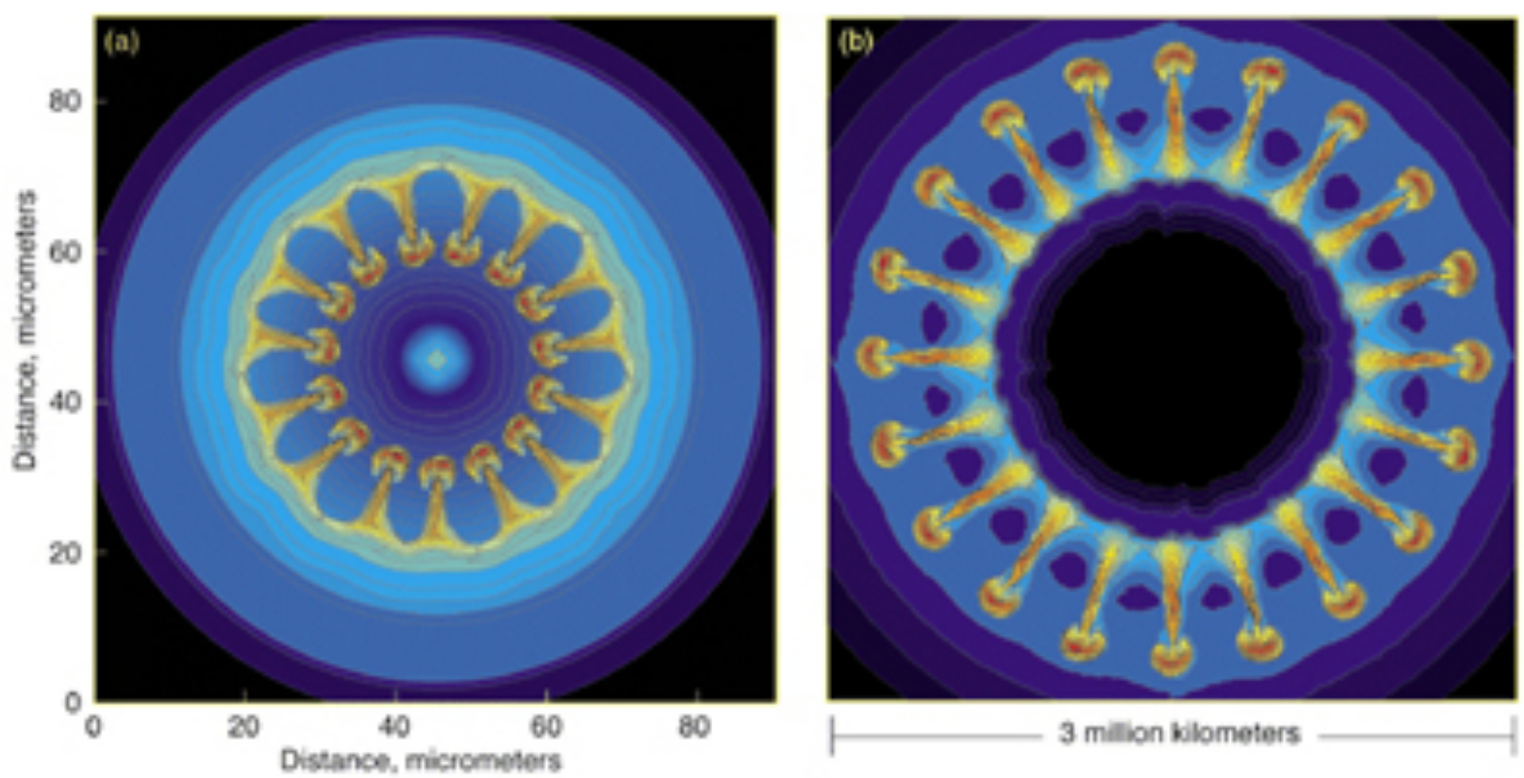
Energy ad libitum

A bit of motivation

How does it work ?



Problems ? -- the real world is not ideal

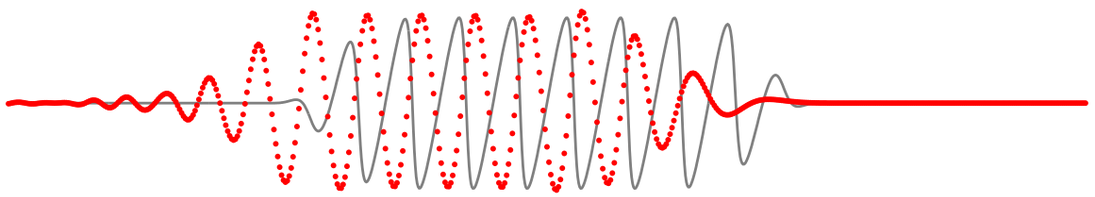


Why is this a hard problem ?

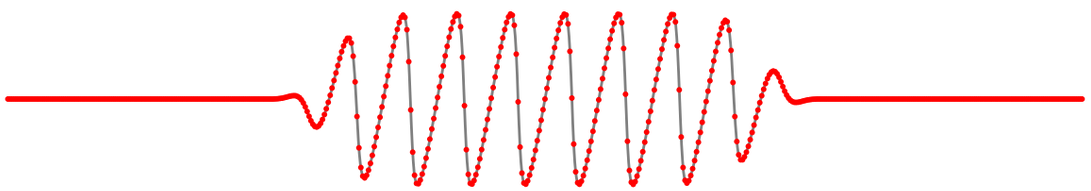
- ✓ Strong shocks are present
- ✓ Considerable mixing after shock
- ✓ Very long time evolution
- ✓ Complex physics - multi physics, multi scale

This suggests that high-order accurate methods are suitable and likely required

Spectral methods perform very well for smooth problems



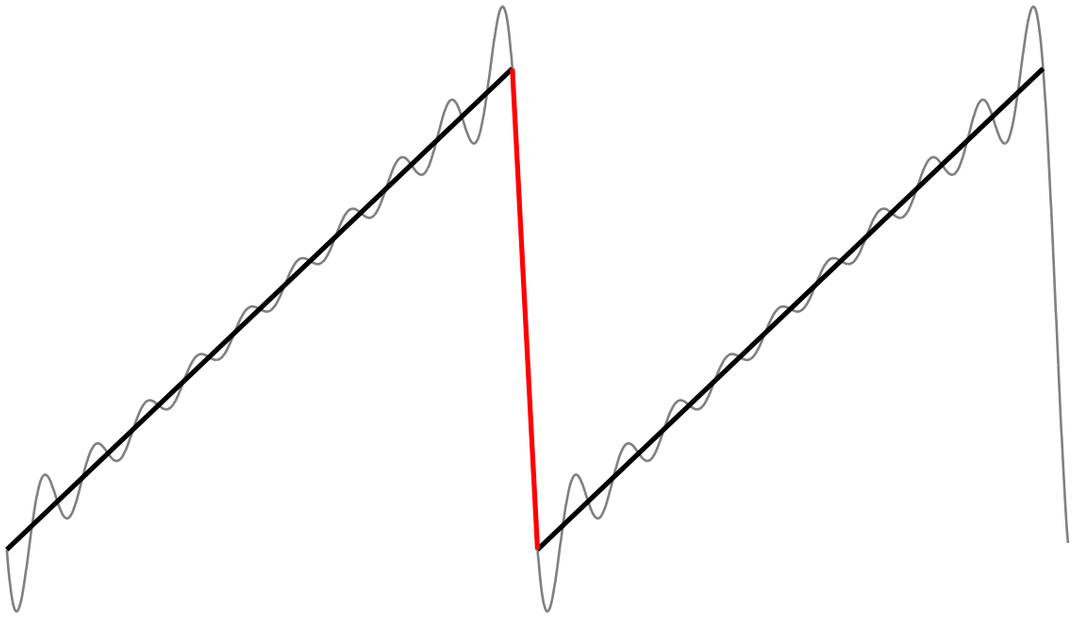
2nd-order FD



Fourier Spectral

Problems !

.. but has problems
for shocks



What we need is a high-order method that can deal with shocks without introducing oscillations

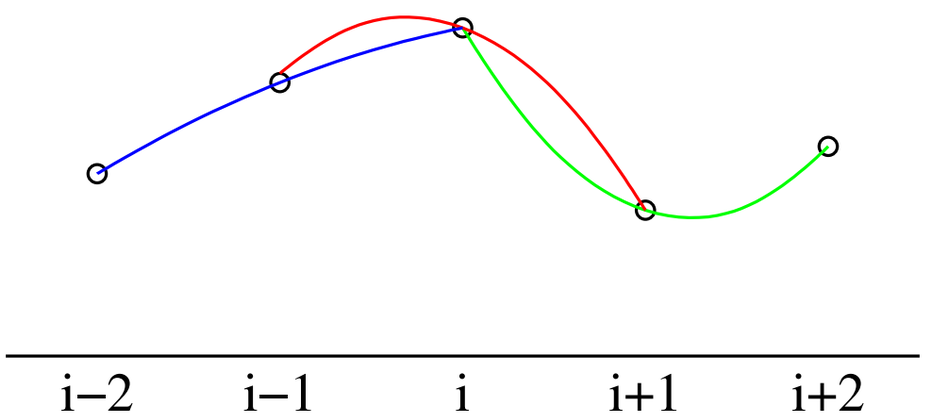
Problem - such a scheme <u>must</u> be nonlinear, i.e., costly

WENO methods

The most popular and powerful way is through weighted essentially non-oscillatory methods (WENO)

Basic idea - never evaluate across a shock

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}(f_{i+1/2}^n - f_{i-1/2}^n).$$



To update cell, there are 3 options

$$f_{i+1/2} = f_i^k$$

$$\begin{aligned} f_i^{-2} &= \frac{1}{3}f_{i-2} - \frac{7}{6}f_{i-1} + \frac{11}{6}f_i \\ f_i^{-1} &= -\frac{1}{6}f_{i-1} + \frac{5}{6}f_i + \frac{1}{3}f_{i+1} \\ f_i^{0} &= \frac{1}{3}f_i + \frac{5}{6}f_{i+1} - \frac{1}{6}f_{i+2} \end{aligned}$$

Which one is preferred depends on smoothness

WENO methods

Observation -

✓ ENO scheme with 2p points is order p

✓ Central scheme with 2p points is order 2p-1

This leads to the Weighted ENO schemes (Jiang/Shu'94)

$$f_{i+1/2} = \omega_{-2} f^{-2}_{i+1/2} + \omega_{-1} f^{-1}_{i+1/2} + \omega_0 f^{0}_{i+1/2}$$

$$\begin{aligned}
IS_{-2} &= 13/12(f_{i-2} - 2f_{i-1} + f_i)^2 + 1/4(f_{i-2} - 4f_{i-1} + 3f_i)^2 \\
IS_{-1} &= 13/12(f_{i-1} - 2f_i + f_{i+1})^2 + 1/4(f_{i-1} - f_{i+1})^2 \\
IS_0 &= 13/12(f_i - 2f_{i+1} + f_{i+2})^2 + 1/4(3f_i - 4f_{i+1} + f_{i+2})^2
\end{aligned}$$

$$\alpha_k = \frac{C_k}{(\epsilon + IS_k)^2}, \quad \omega_k = \frac{\alpha_k}{\alpha_{-2} + \alpha_{-1} + \alpha_0}$$

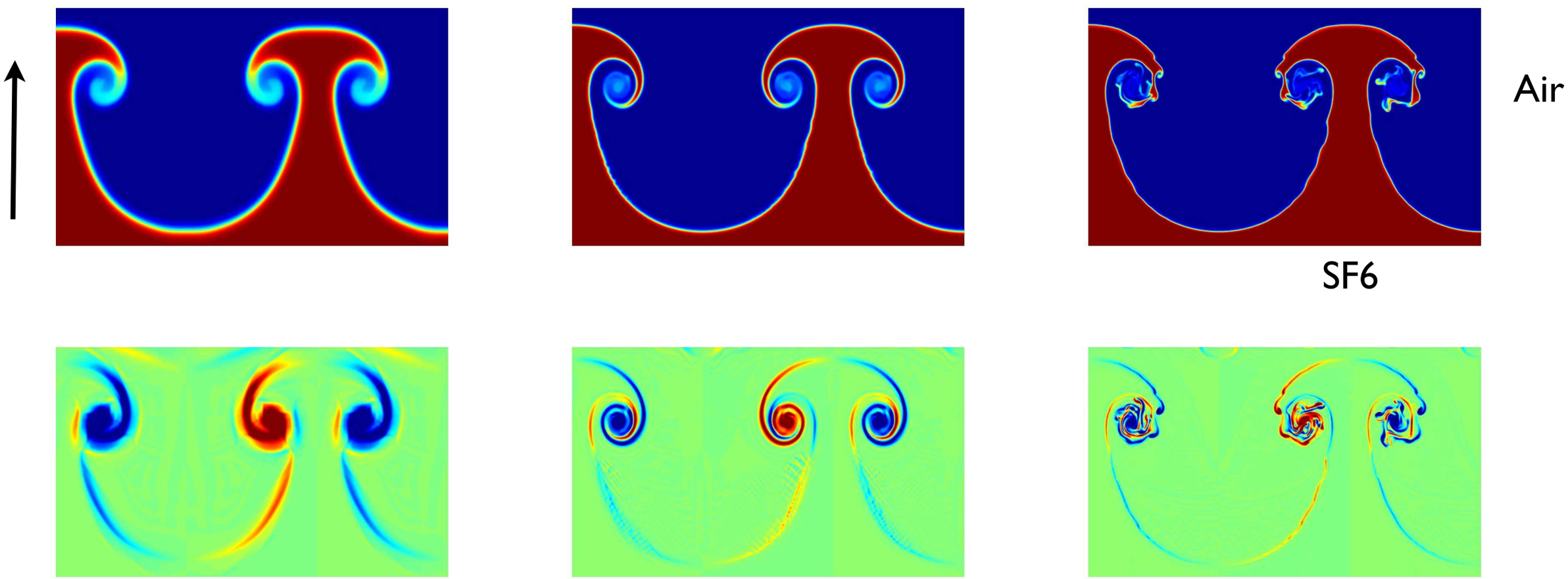
WENO methods

To test the value of such methods consider

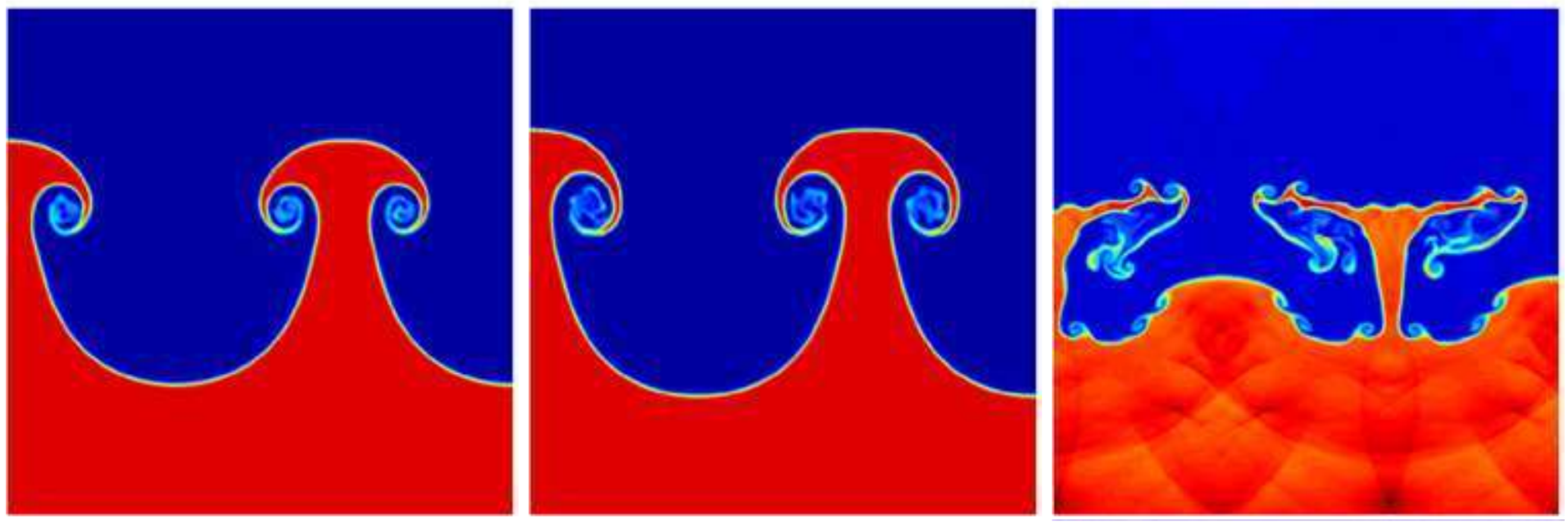
- ✓ 2D compressible Euler equations
- ✓ Mix of SF6 and air
- ✓ Mach 1.21 shock

Density
6ms

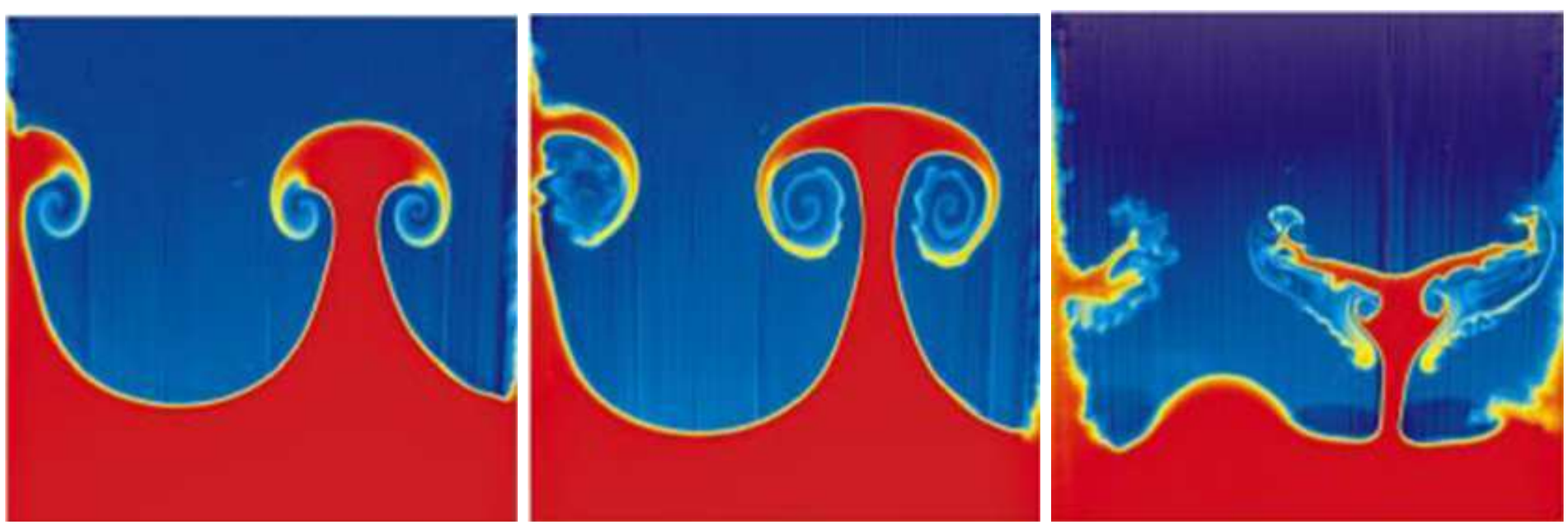
WENO3 WENO5 WENO9



WENO methods



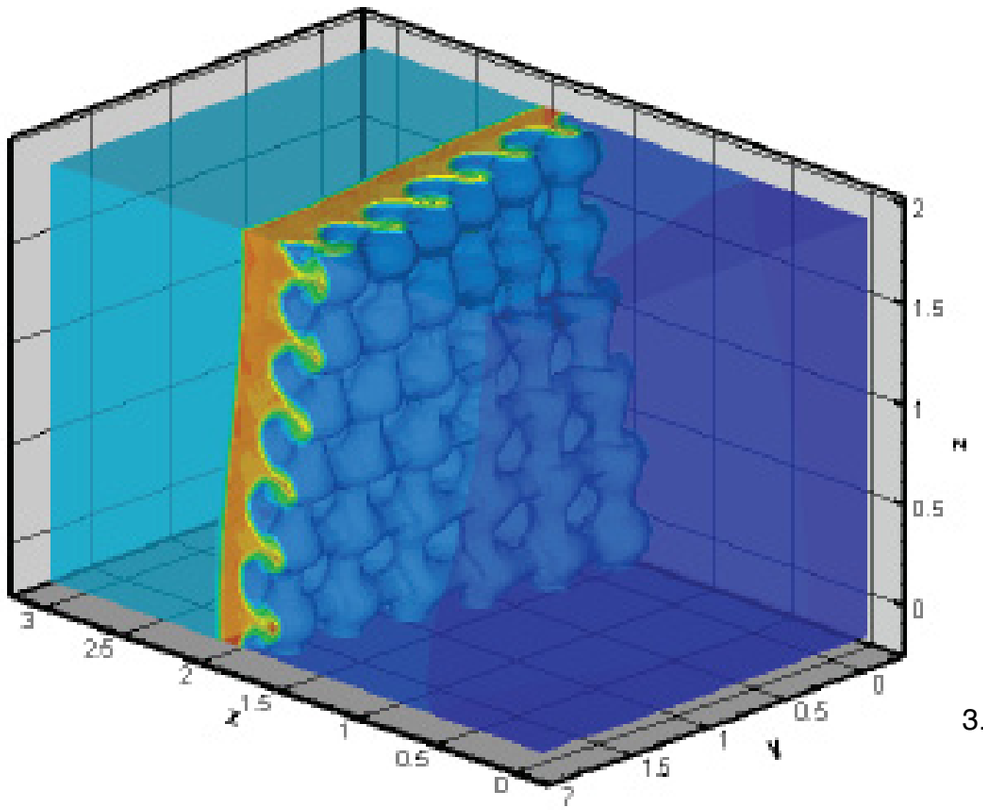
WENO9



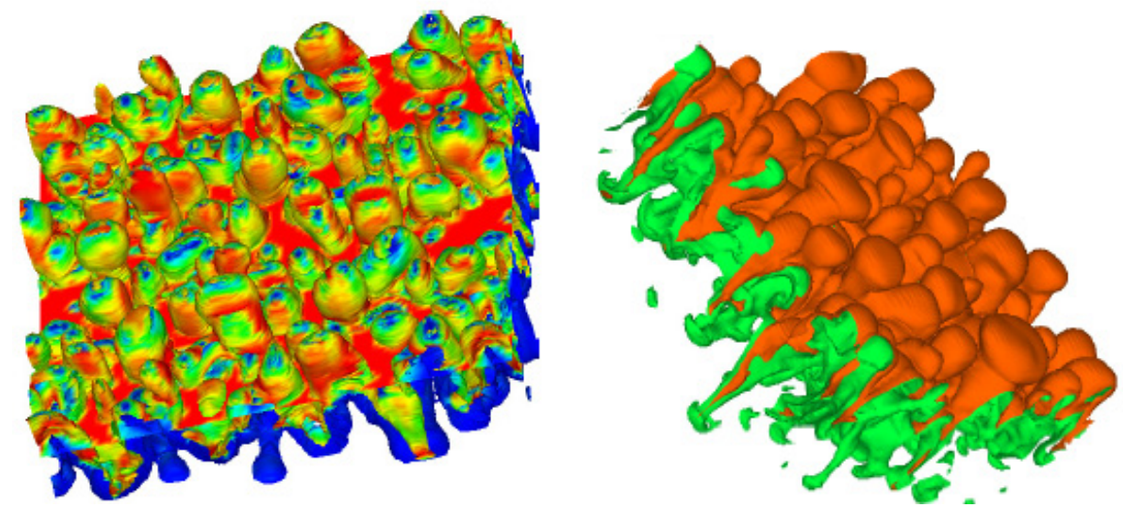
Experiment Collins/Jacobs, 2002

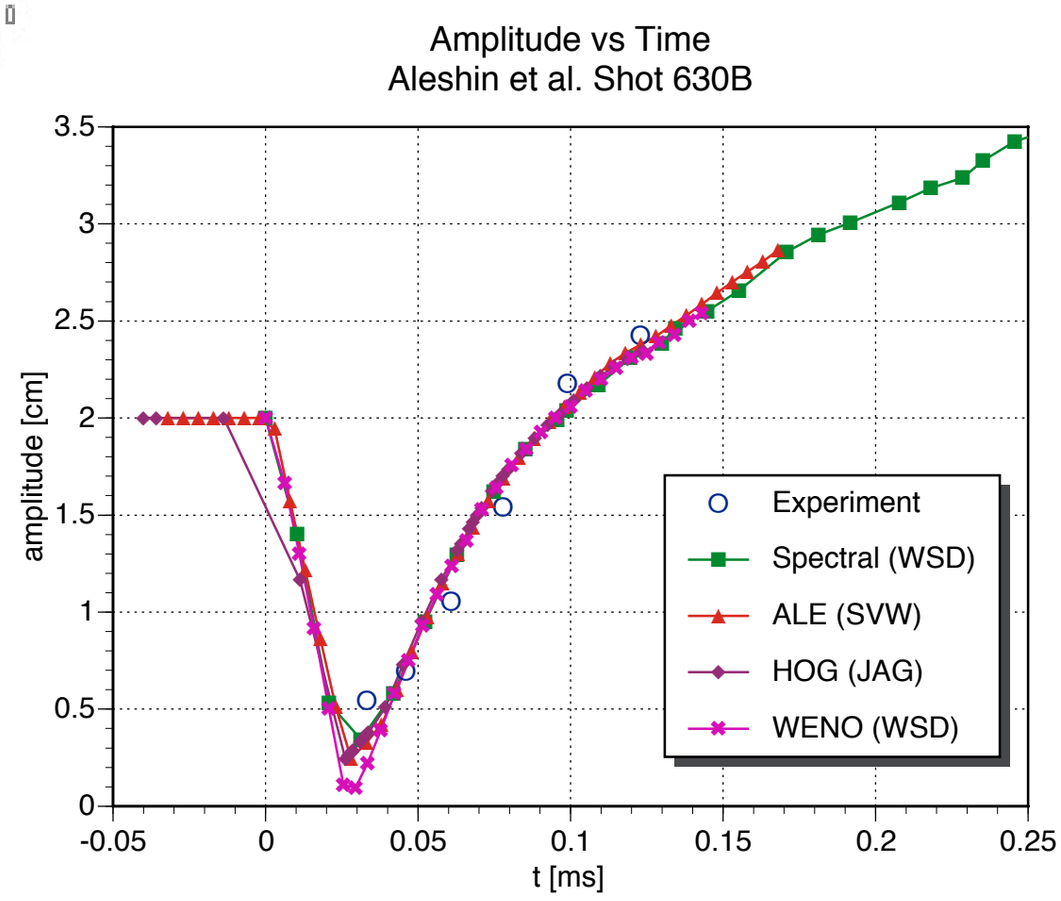
5ms 6ms 6.88ms

3D and Validation



Navier-Stokes extension





A hybrid method

Problems

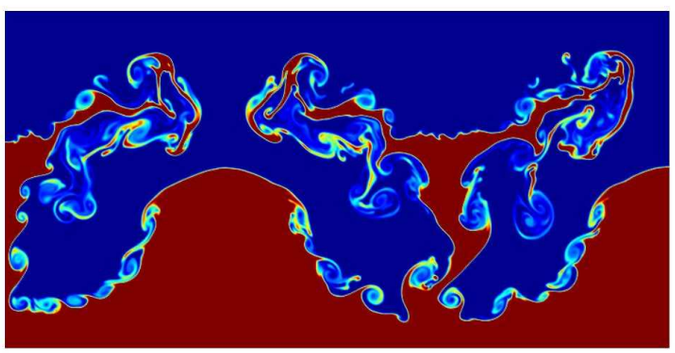
- ✓ Computational expense (nonlinearity, characteristics etc)
- ✓ Limited order of accuracy in smooth regions

What we seek is a method that

- ✓ Uses WENO in regions with shocks and steep gradients
- ✓ Uses spectral methods in regions with smooth solutions

A few problems to address to enable this

- ✓ What do we do in the smooth regions ?
- ✓ How do we decide ?
- ✓ How do we connect ?



Element based hybrid

The foundation of the algorithm

- ✓ Split computational domain into elements
- ✓ In each element use WENO or spectral method
- ✓ Dynamically change WENO/Spectral approach based on smoothness
- ✓ Connection elements through overlaps

We use spectral methods in the smooth domains

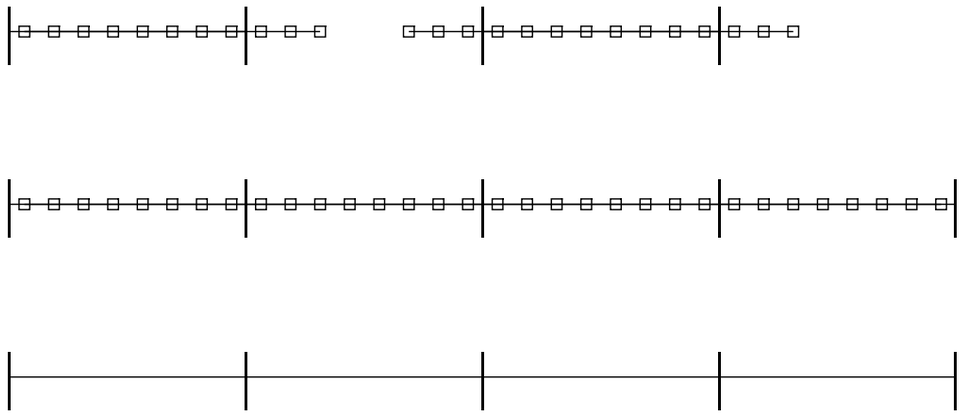
$$I_N f(x) = \sum_{j=0}^{N} f(x_j) g_j(x), \qquad x_j = -\cos\frac{\pi i}{N}$$

This is well known and well understood for smooth problems

A hybrid method

The devil is always in the details

✓ Connecting the regions - through overlaps



✓ Imposing boundary conditions - through penalty terms

$$U_h(t,x) = u_h(t,x) + (g_D(t) - u_h(t,x_0))\mathcal{L}_0(x)$$

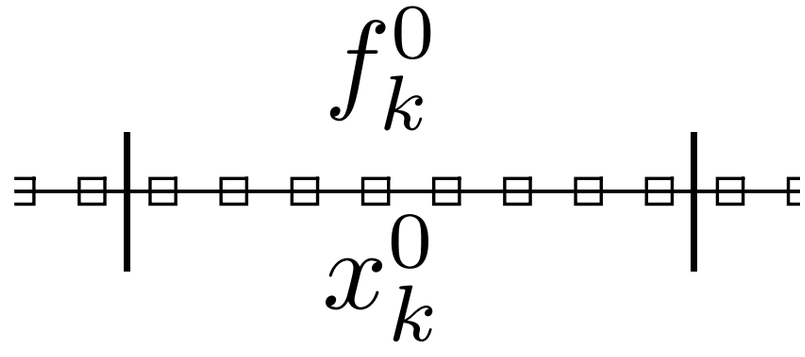
$$\frac{\partial U_h(t,x)}{\partial x} = \frac{\partial u_h(t,x)}{\partial x} + (g_D(t) - u_h(t,x_0))\frac{\partial \mathcal{L}_0(x)}{\partial x}$$

$$\mathcal{L}_0(xe_0) = 1$$

$$\mathcal{L}_0(xe_k) = 0 \qquad k = 1, \cdots, N-1.$$

A hybrid method

Detecting shocks through multi-resolution -



Define

$$f_k^1 = \frac{f_{2k}^0 + f_{2k+1}^0}{2} \qquad \forall k = 1, \cdots, N.$$

Compute

$$d_k = f_k^0 - p_s(x_k^0)$$

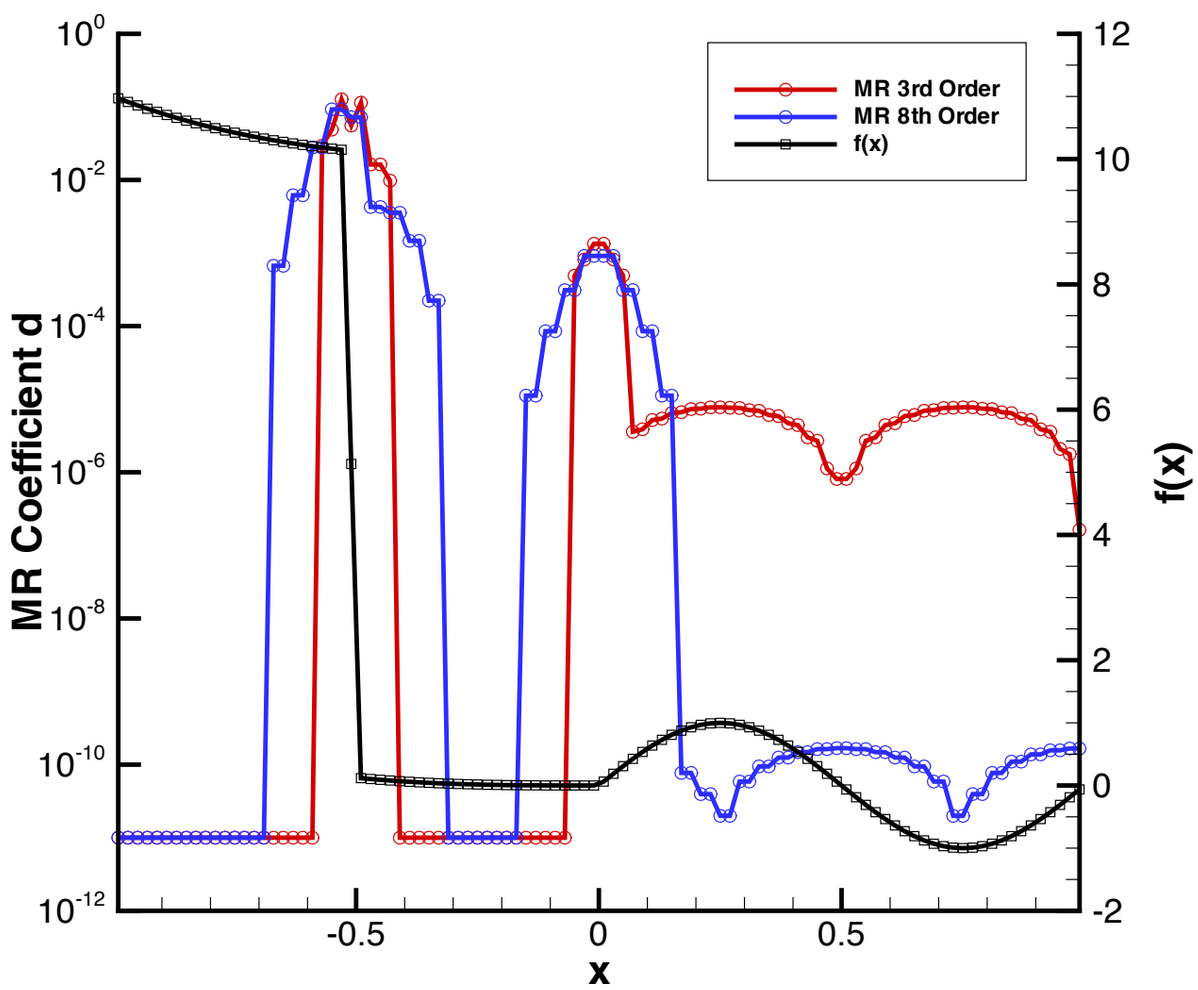
One can show (Harten'94)

$$d_k = \begin{cases} \Delta x^r [\frac{d^r f_k}{dx^r}] & s \geq r, \\ \Delta x^s \frac{d^s f_k}{dx^s} & s < r, \end{cases}$$

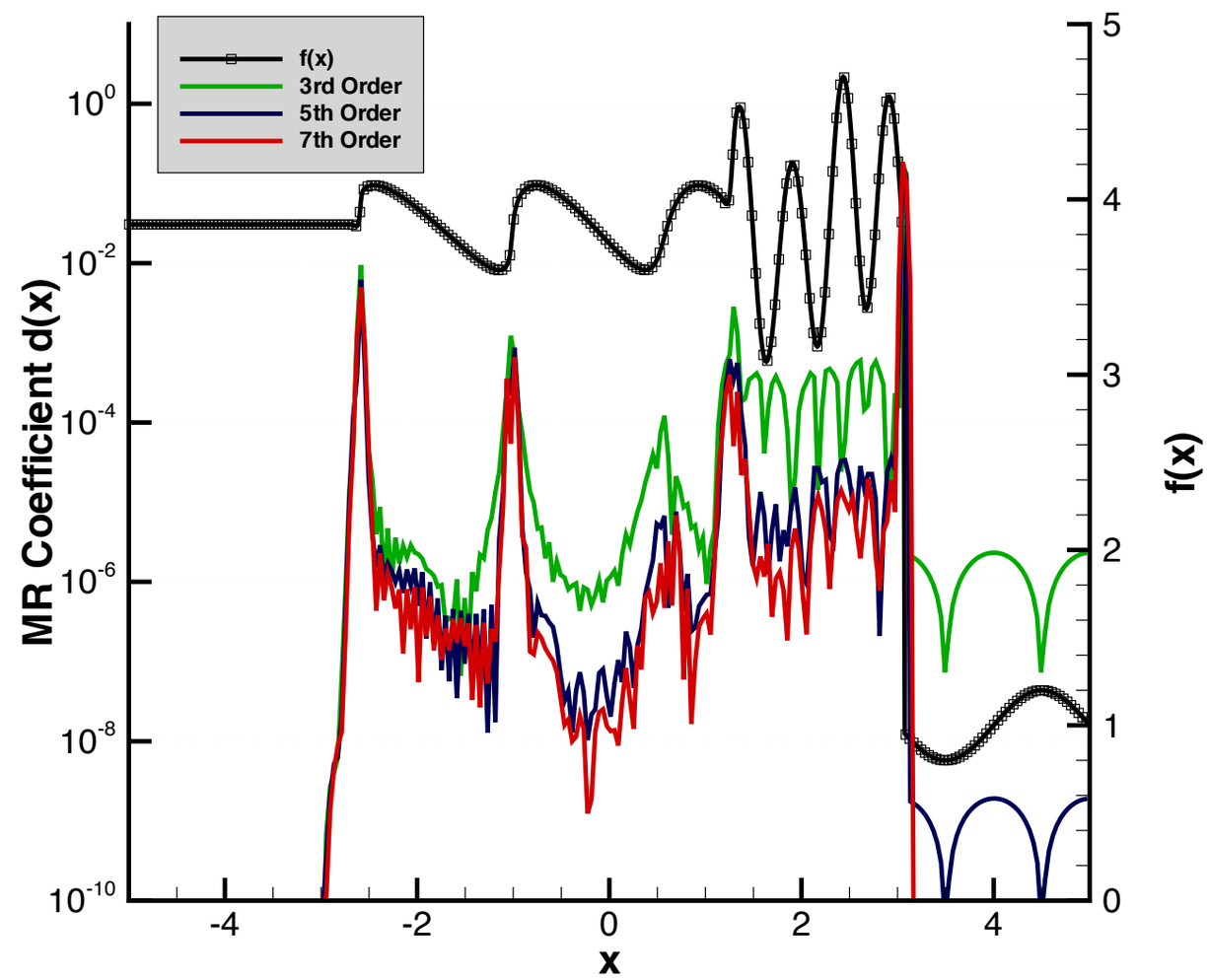
Small 'd' - smooth

A hybrid method

$$f(x) = \begin{cases} 10 + x^3 & -1 \le x < -0.5 \\ x^3 & -0.5 \le x < 0 \\ \sin(2\pi x) & 0 \le x \le 1 \end{cases}$$



Mach 3 density for Shock-Density problem



Euler's equations

Closer to reality

$$\mathbf{f}(\mathbf{u}) = [\rho v, \rho v^2 + p, (\rho E + p)v]$$

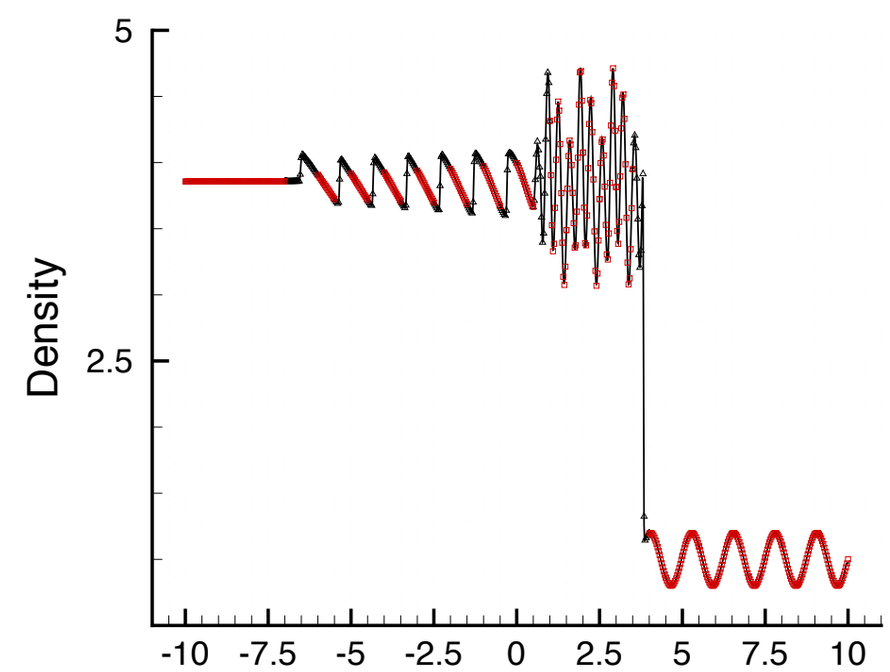
$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0,$$

$$\mathbf{u} = [\rho, \rho v, \rho E]$$

Osher-Shu shock entropy problem

$$(\rho, v, p)(0, x) = \begin{cases} (3.857143, 2.629369, 10.33333) & x \leq -9.5, \\ (1.0, 0.0, 1.0) & -9.5 \leq x \leq -8.85, \\ (\exp(-0.01 \sin(13(x - 8.85))), 0, 1.0) & x > -8.85, \end{cases}$$

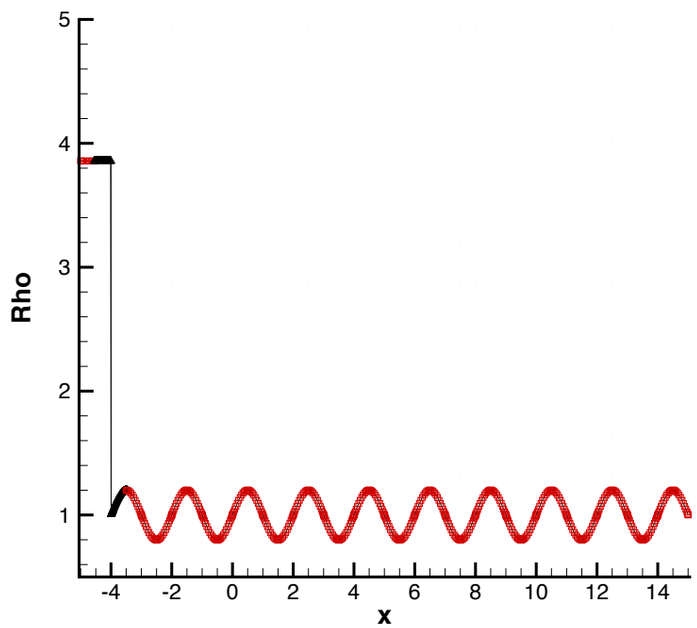
Classic test case that combined shocks with mixing



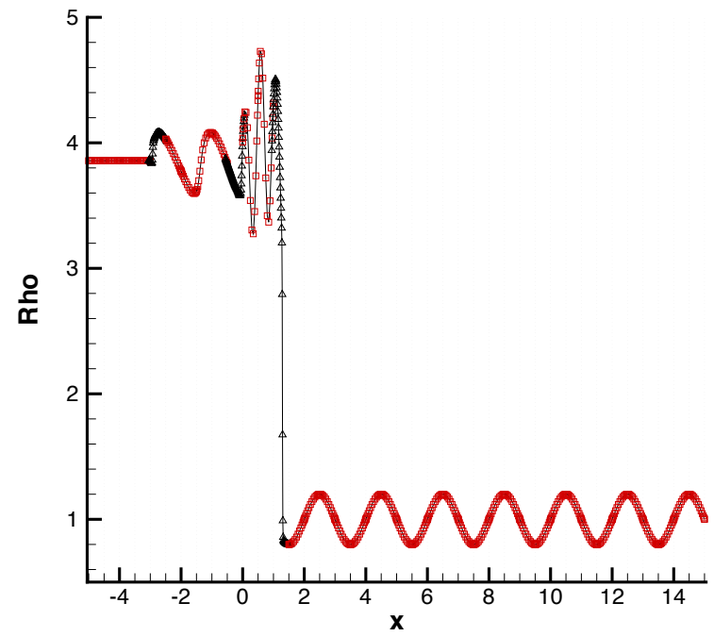
(d)

Euler equations

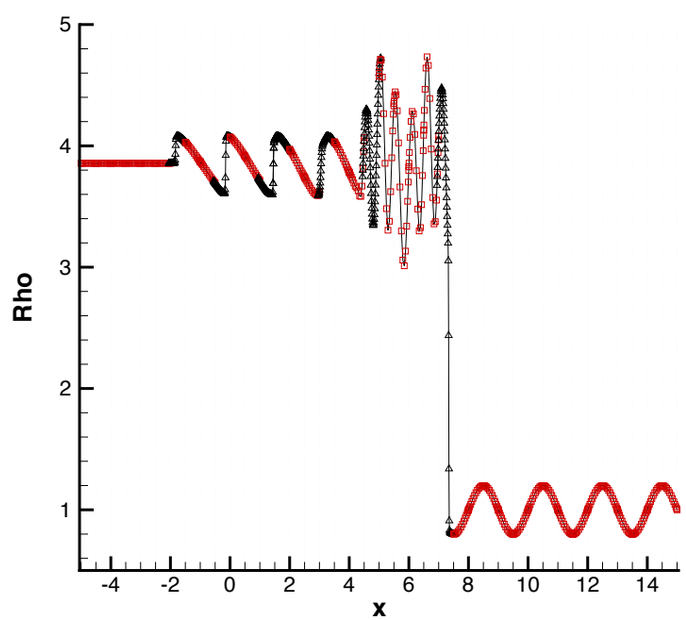
T=0.0



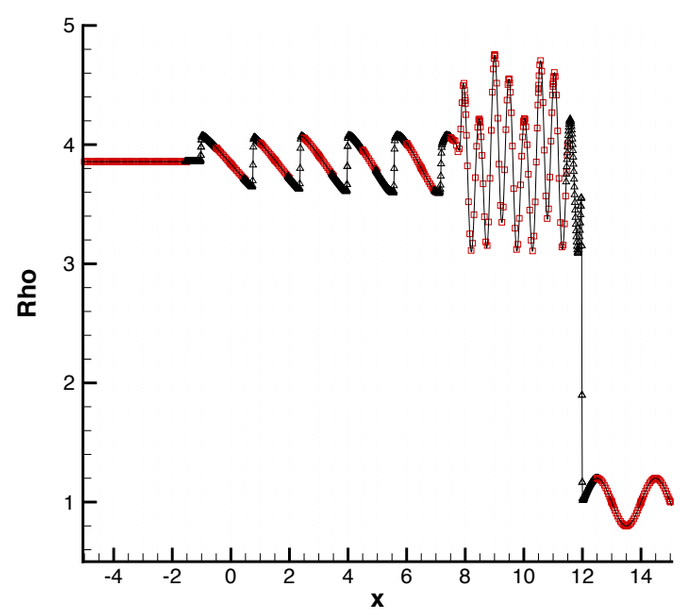
T=1.5



K=40
N=16
M=50



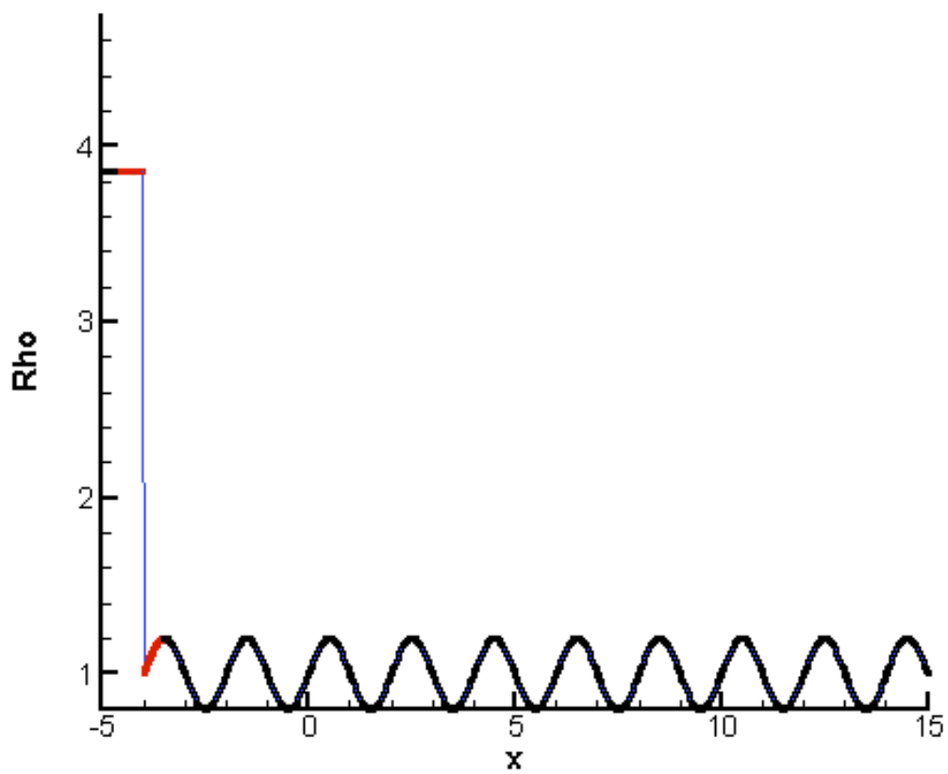
T=3.2



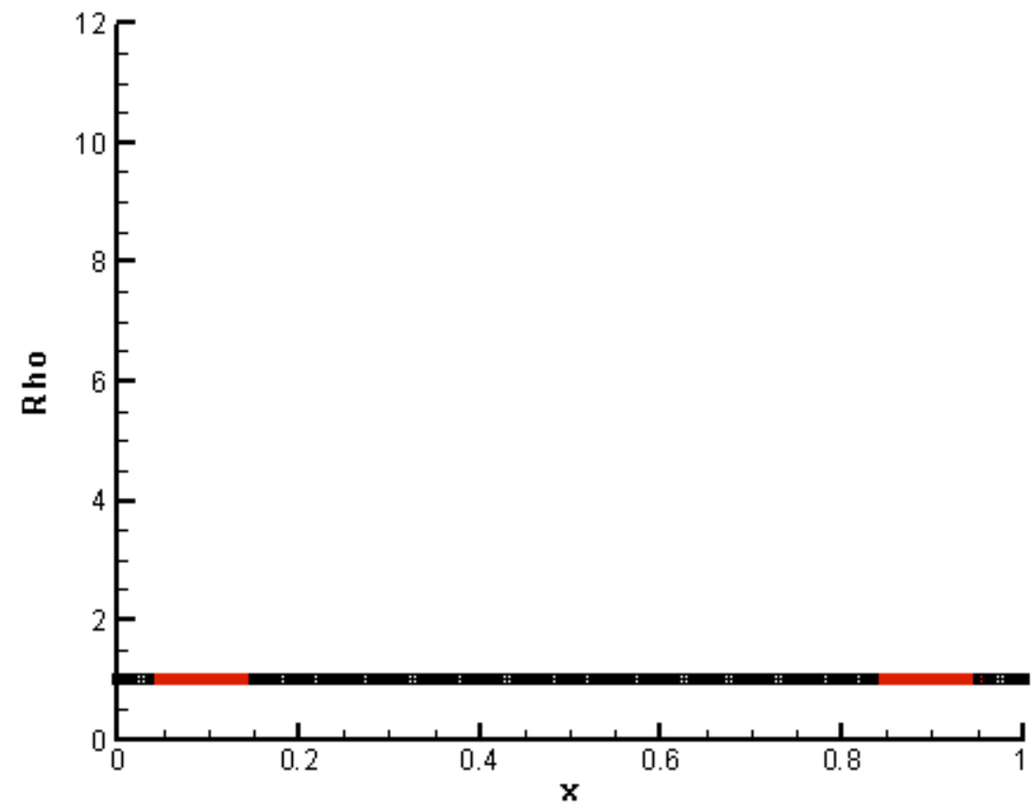
T=4.5

Euler equations

Shock-Wave Problem

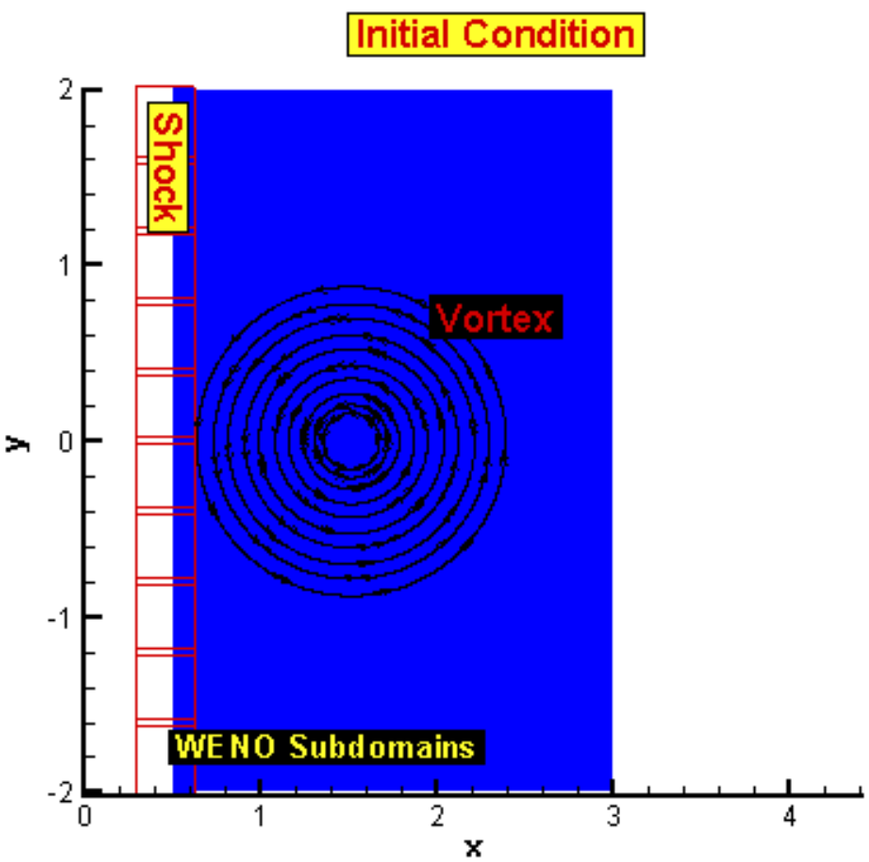


Blast Wave Problem

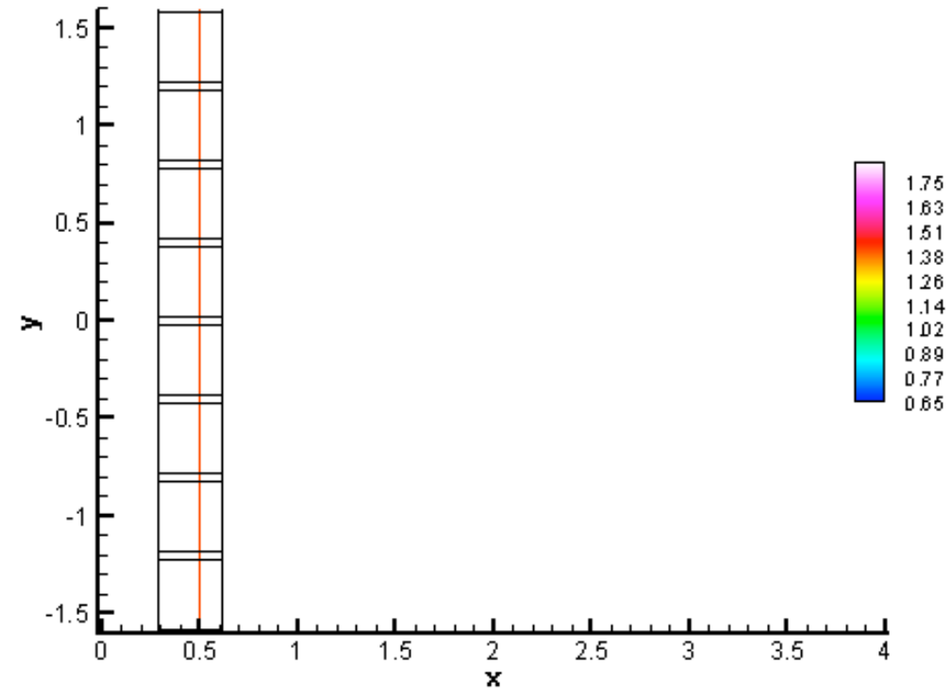


Extension to 2D ? -- fairly straightforward

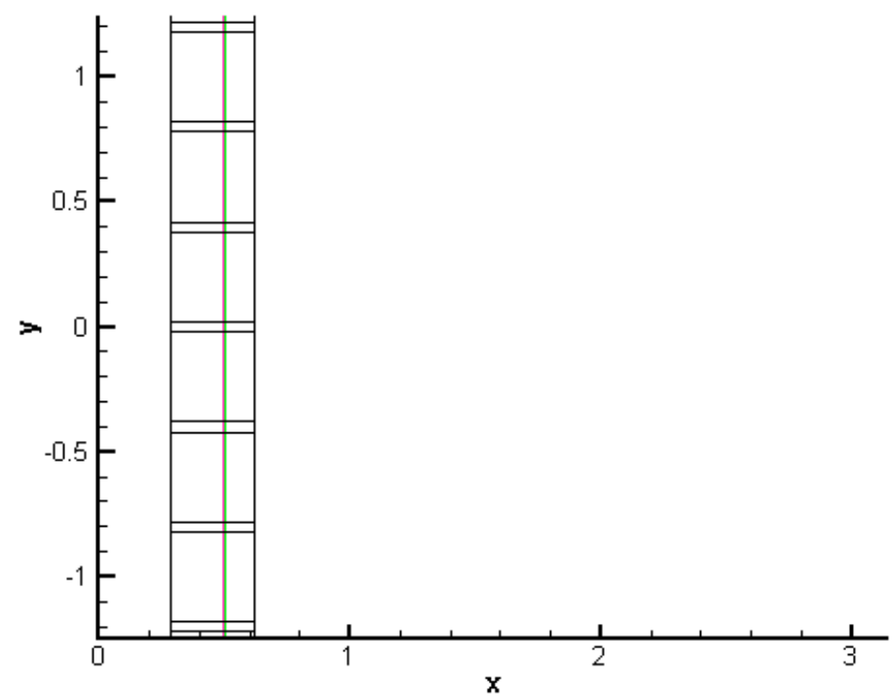
2D RMI tests



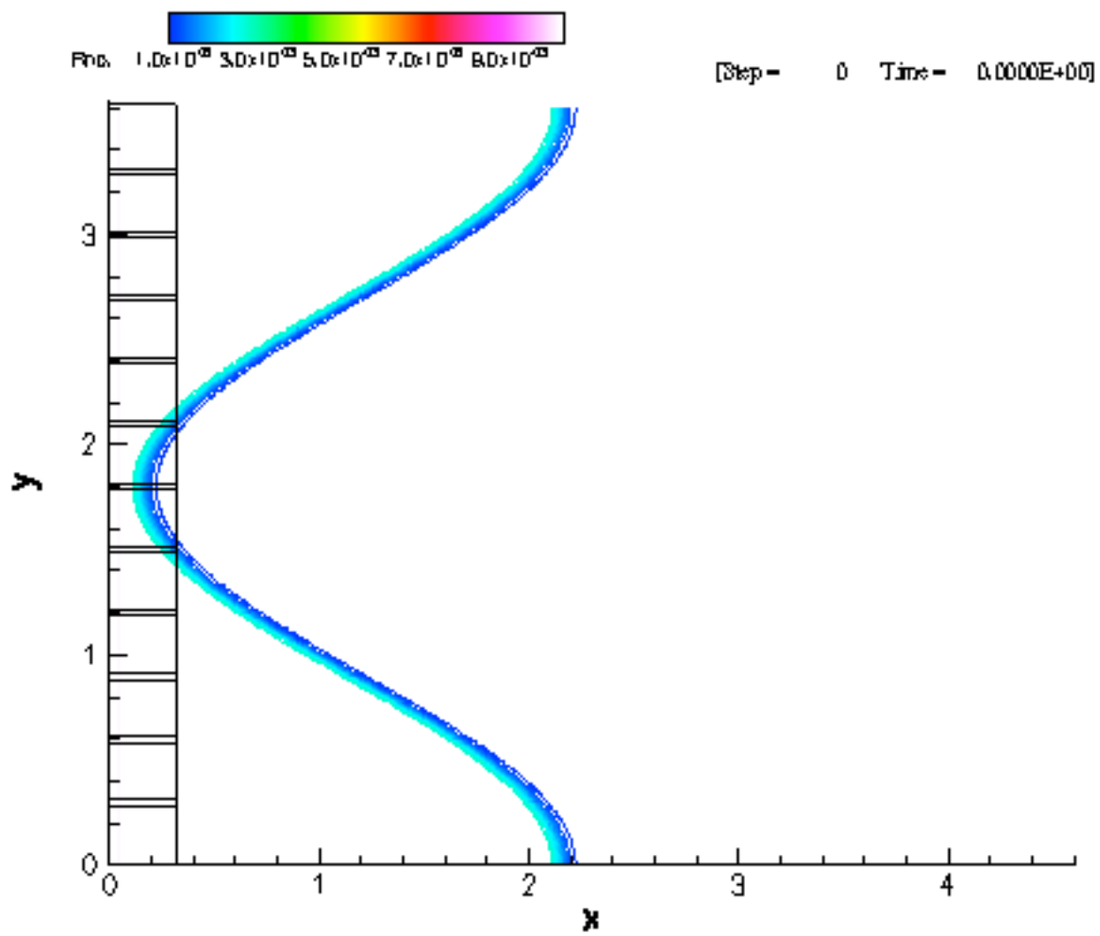
Ma = 1.25



Ma = 3.00



Main goal was acceleration



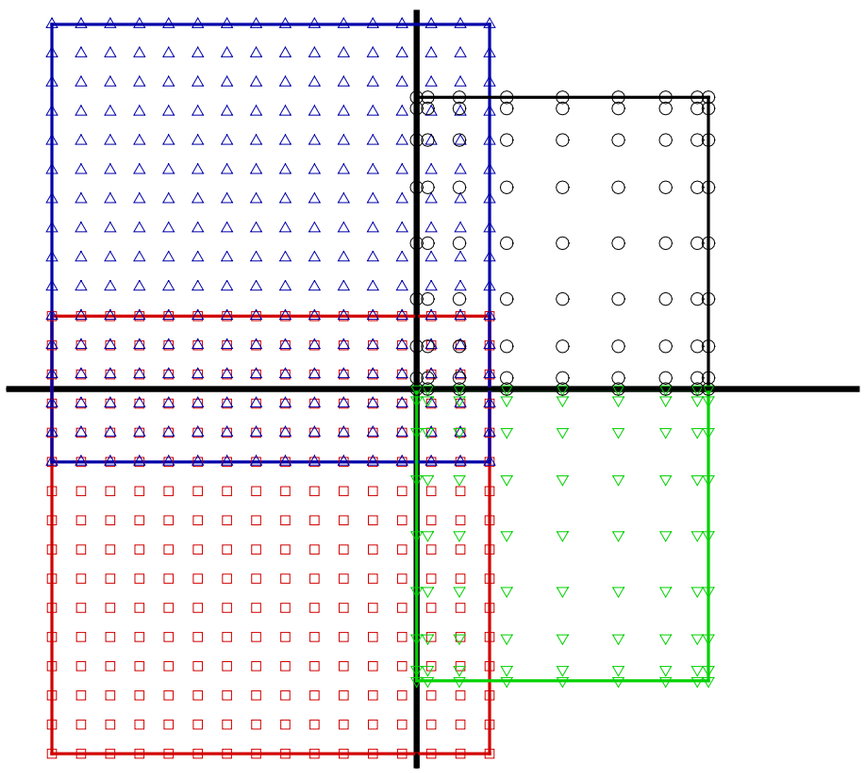
Ma = 4.46

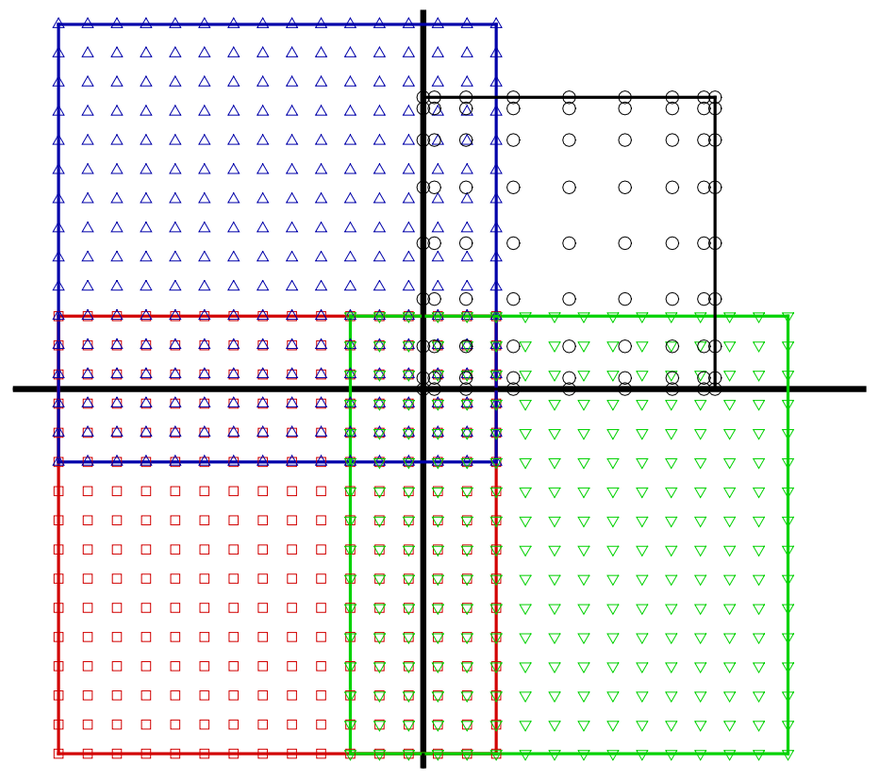
Number of subdomains	Grid size	Hybrid S12W20	WENO5	Speedup
10x10	200x200	265	282	1.06
20x20	400x400	2009	2762	1.37
40x40	800x800	14410	26090	1.81
80x80	1600x1600	112900	253996	2.24

Main goal was acceleration

Two main reasons -

Different block meshes





Time-step in spectral elements scale as

$$\Delta t \propto \frac{h}{N^2}$$

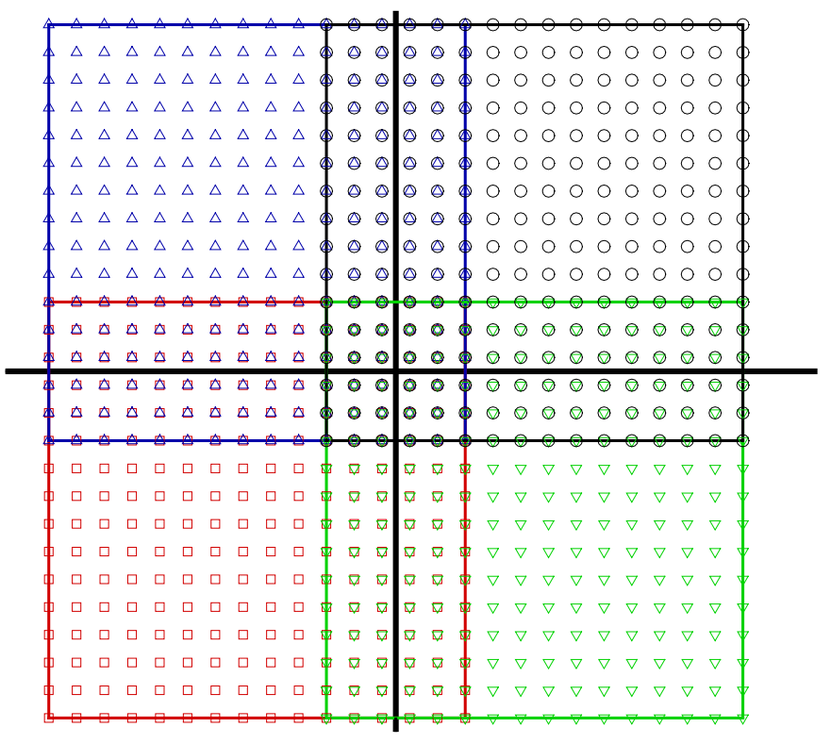
vs

$$\Delta t \propto \frac{h}{N}$$

A Fourier based hybrid method

If we can use a Fourier spectral method in the 'smooth domains' we obtained two things

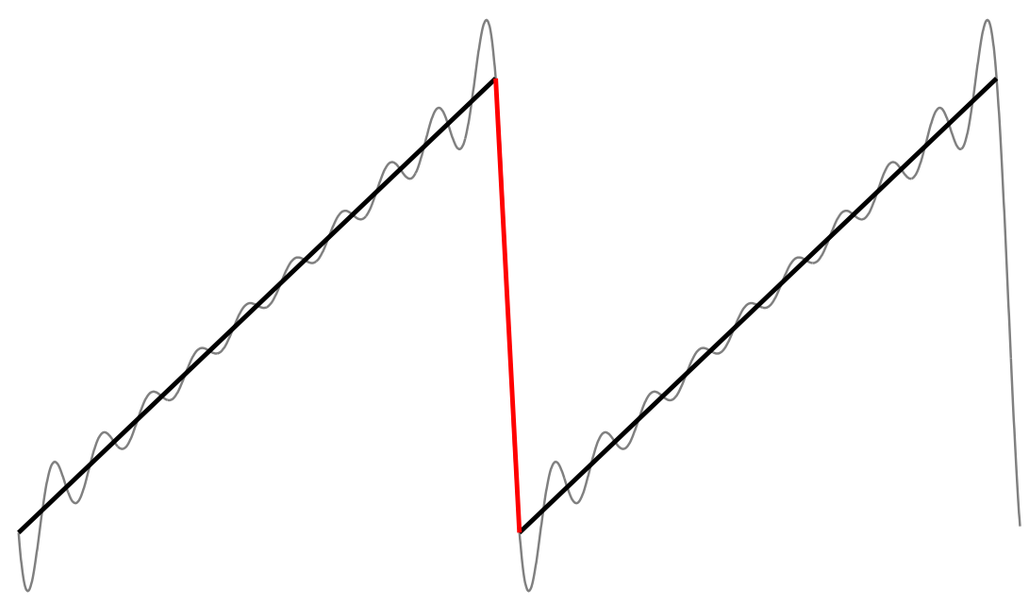
Simpler connection between elements



Comparable timestep

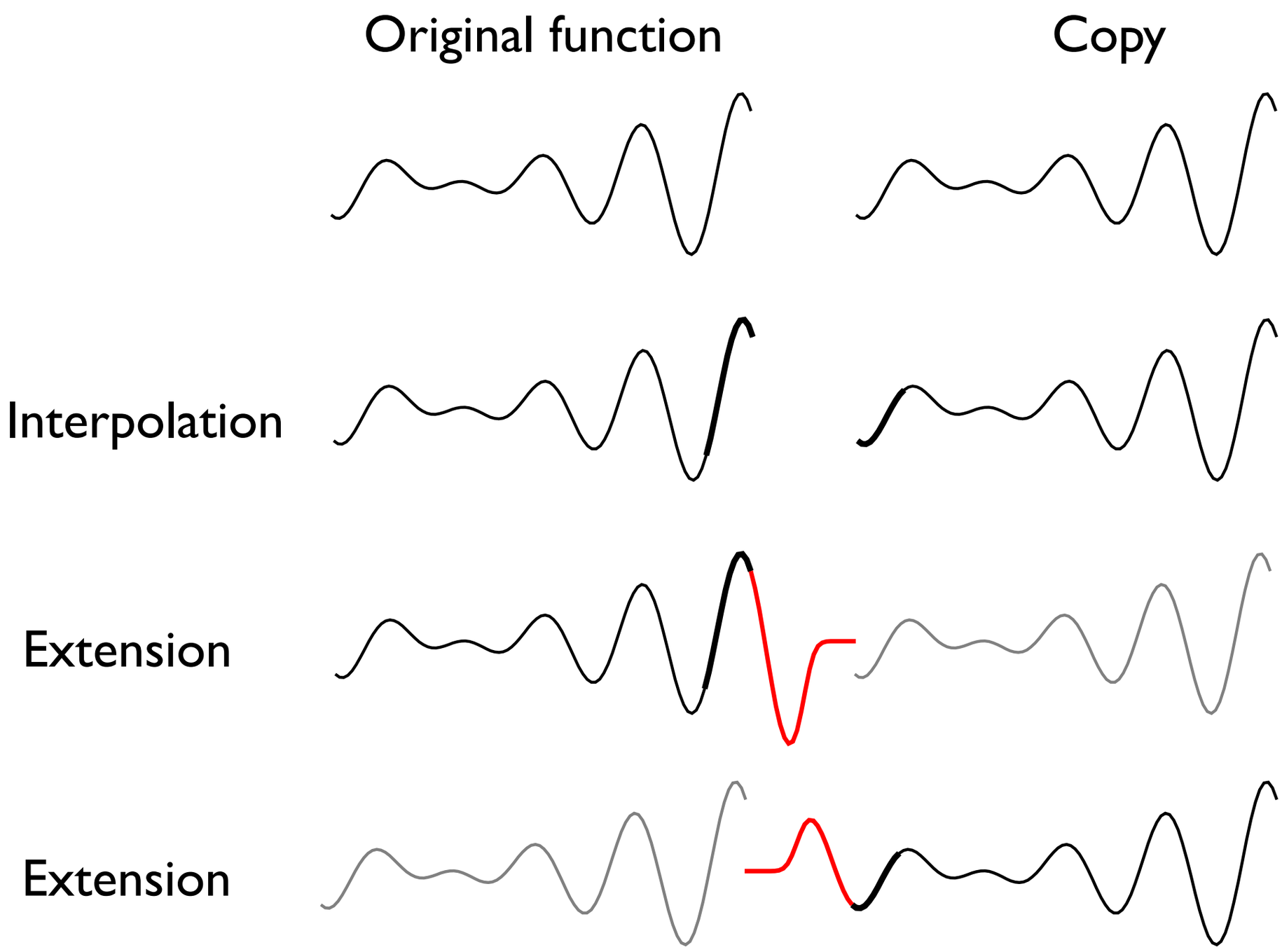
$$\Delta t \propto \frac{h}{N}$$

Problem - periodicity



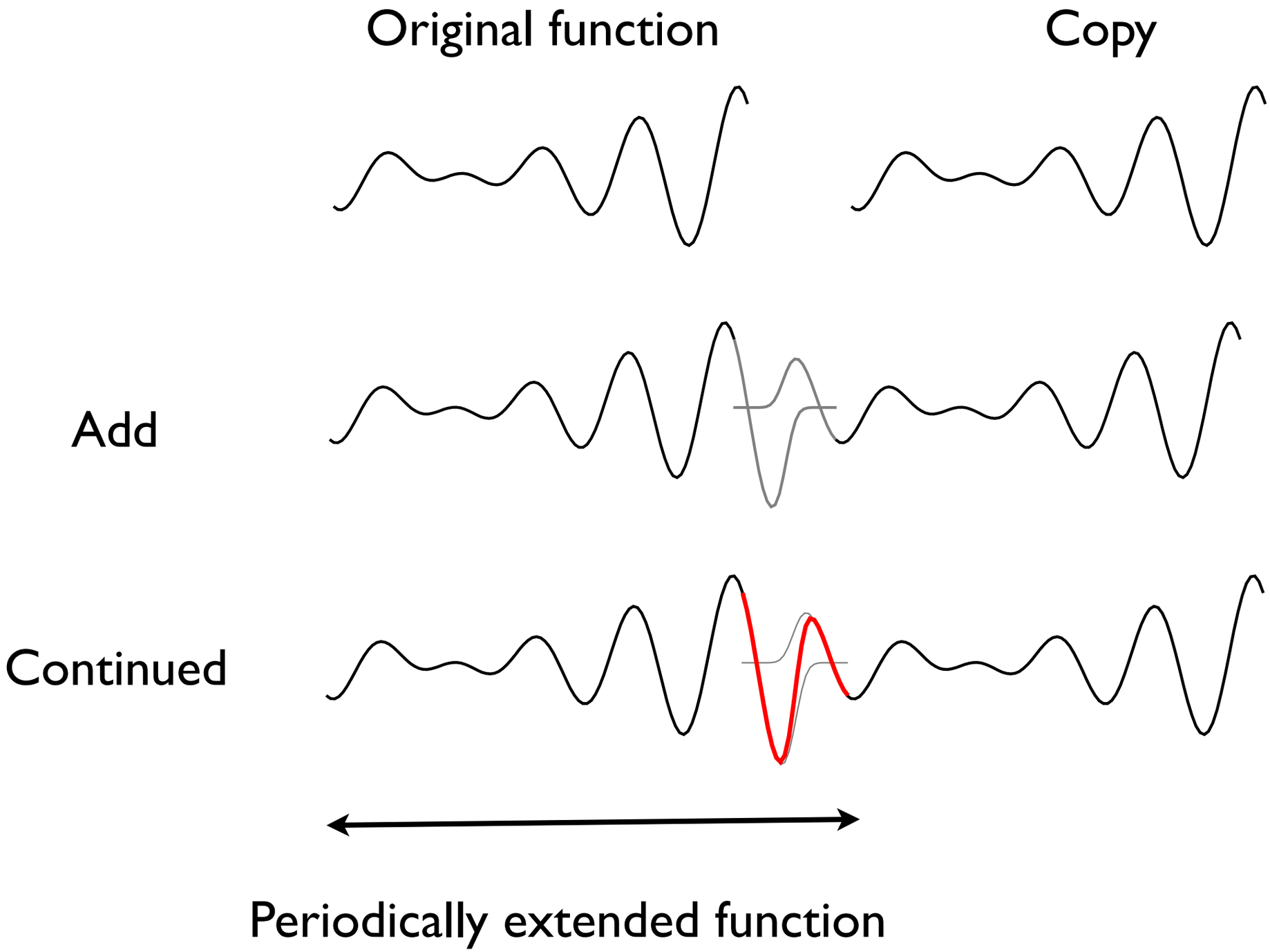
A Fourier Continuation Method

Based on smooth polynomial continuation



A Fourier Continuation Method

Based on smooth polynomial continuation



Euler's equations

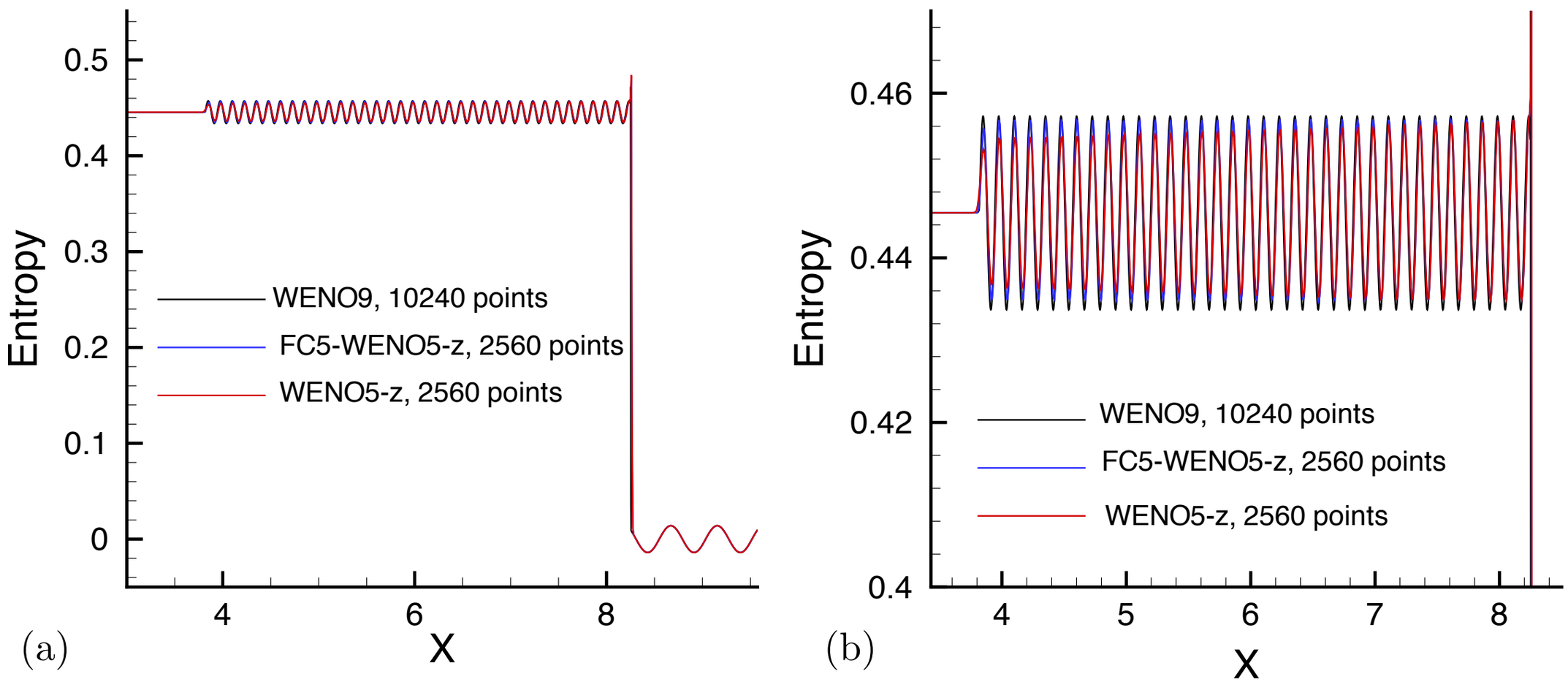


Table 1: Error in entropy amplification, Mach $= 3.0$, $T = 5.0$, $ND = 80, NP = 32$, $\Delta t = 4.4 \times 10^{-4}$

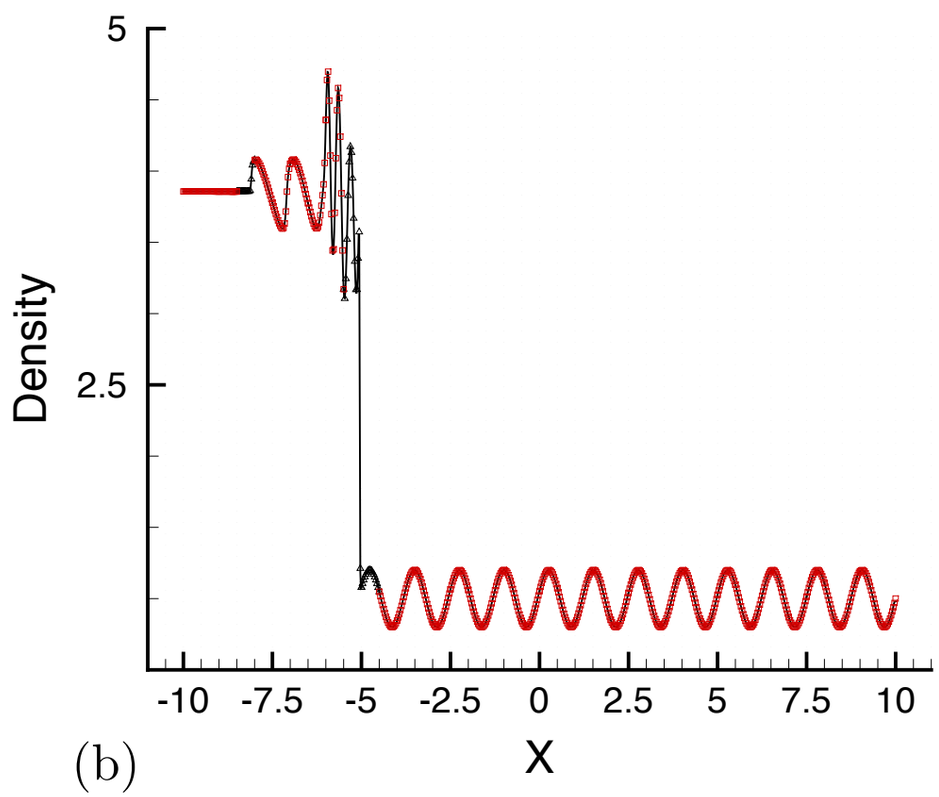
Method	Error near shock	Error far from shock	CPU time(s)
WENO5	22.1%	56.2%	99.0
WENO5-z	10.5%	22.6%	99.0
FC5-WENO5-z	10.4%	10.2%	32.0
WENO9	4.4%	4.0%	188.0
FC5-WENO9	4.4%	4.1%	35.0

Euler's equations

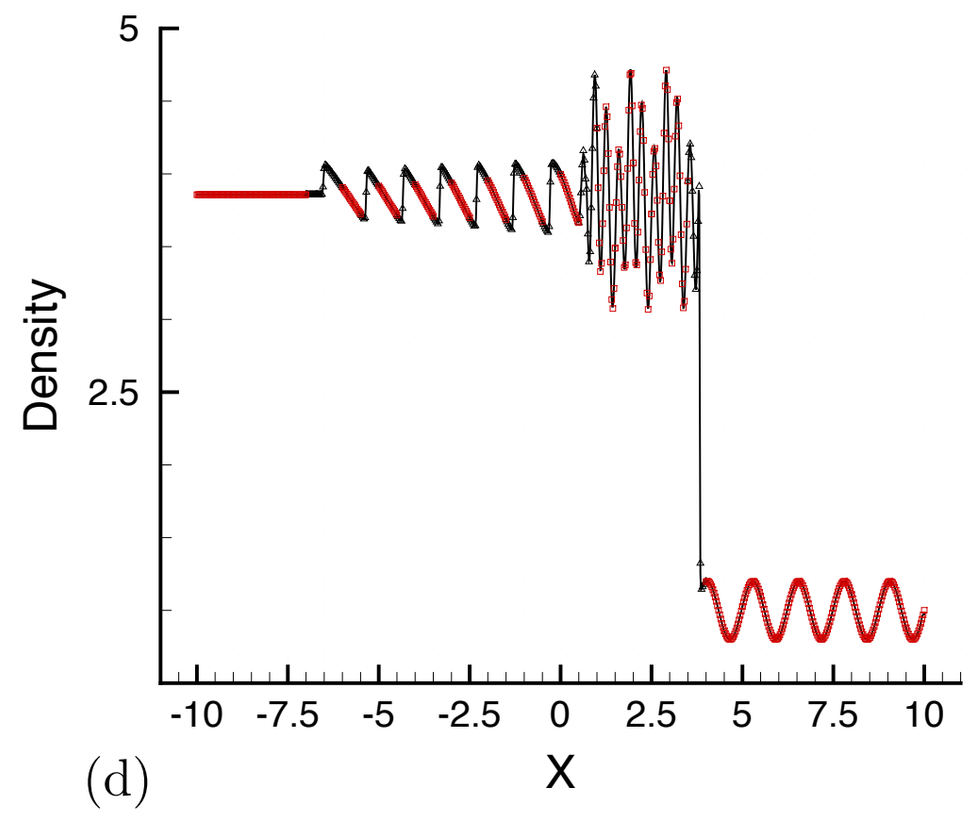
Table 3: Error in entropy amplification, Mach $= 6.0$, $T = 2.5$, $ND = 160, NP = 32$, $\Delta t = 1.1 \times 10^{-4}$

Method	Error near shock	Error far from shock	CPU time(s)
WENO5-z	6.5%	7.7%	325.0
FC5-WENO5-z	7.3%	7.2%	98.0
WENO9	1.8%	1.7%	618.0
FC5-WENO9	1.8%	1.8%	106.0

About 6 times faster - 1D



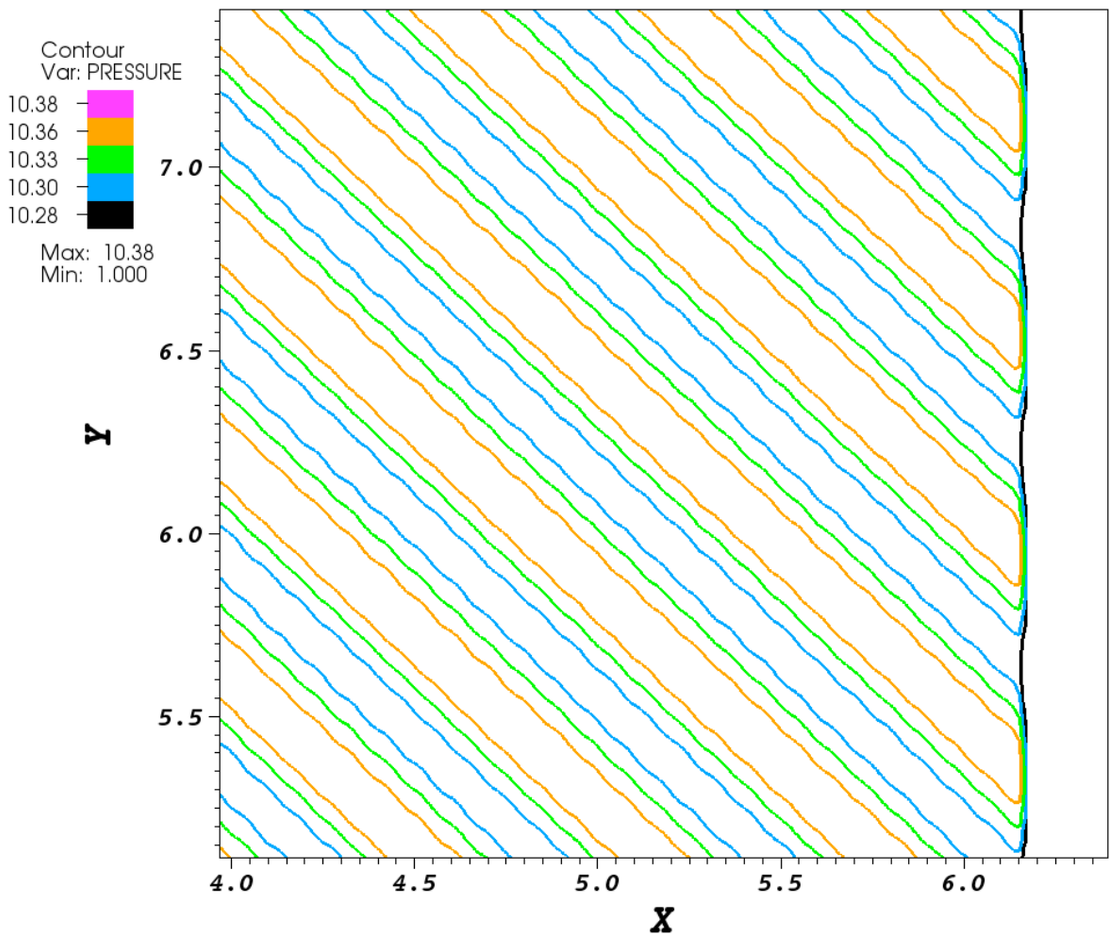
(b)



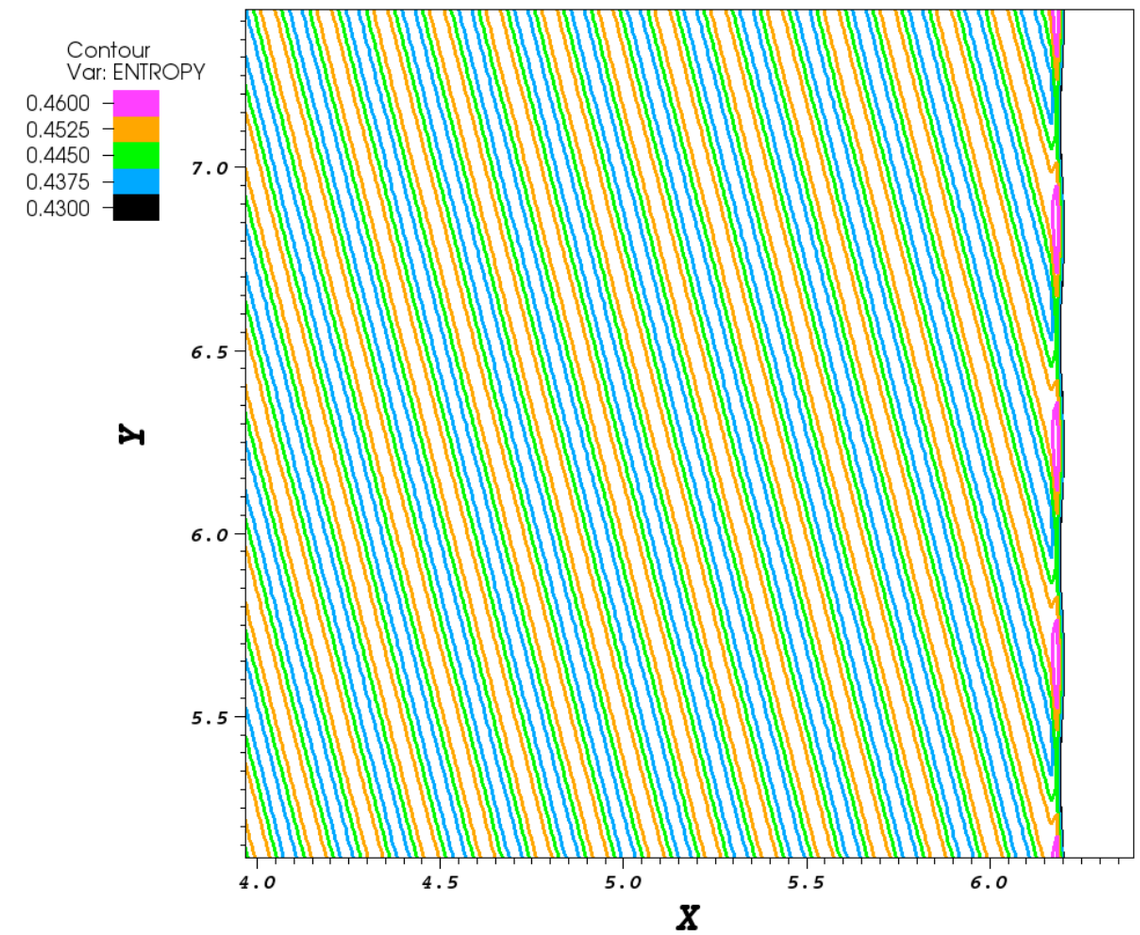
(d)

A 2D case

45 deg small amplitude entropy wave



Post shock pressure wave at 46.6 deg



Post shock entropy wave at 14.5 deg

Agrees with linear theory (McKenzie and Westphal, 1969)

What about GPU's ?

Why should GPU's be of interest here ?

- ✓ High arithmetic complexity of high-order methods
- ✓ Typically lots of work/degree of freedom
- ✓ Need for large and complex simulations

What makes performance complicated ?

- ✓ Dynamic nature of algorithm
- ✓ Essential differences in how elements are treated
- ✓ To use FFT's or not - tradeoff between
  - Long vectors decrease cost - O(NlogN)
  - Short vectors decreases WENO parts

GPU acceleration

Assume FFT's in all domains for sanity check

ND/NP	64	CPU	256	CPU	512	CPU
16	254	80	1822	2880	3750	12910
64	1018	1300	7873	46990	26891	211370
128	2049	5160	24088	187210	109084	851610
256	4900	20680	104405	750190	399708	3380060

5-10 times is realistic - for large problems

Strategy for hybrid

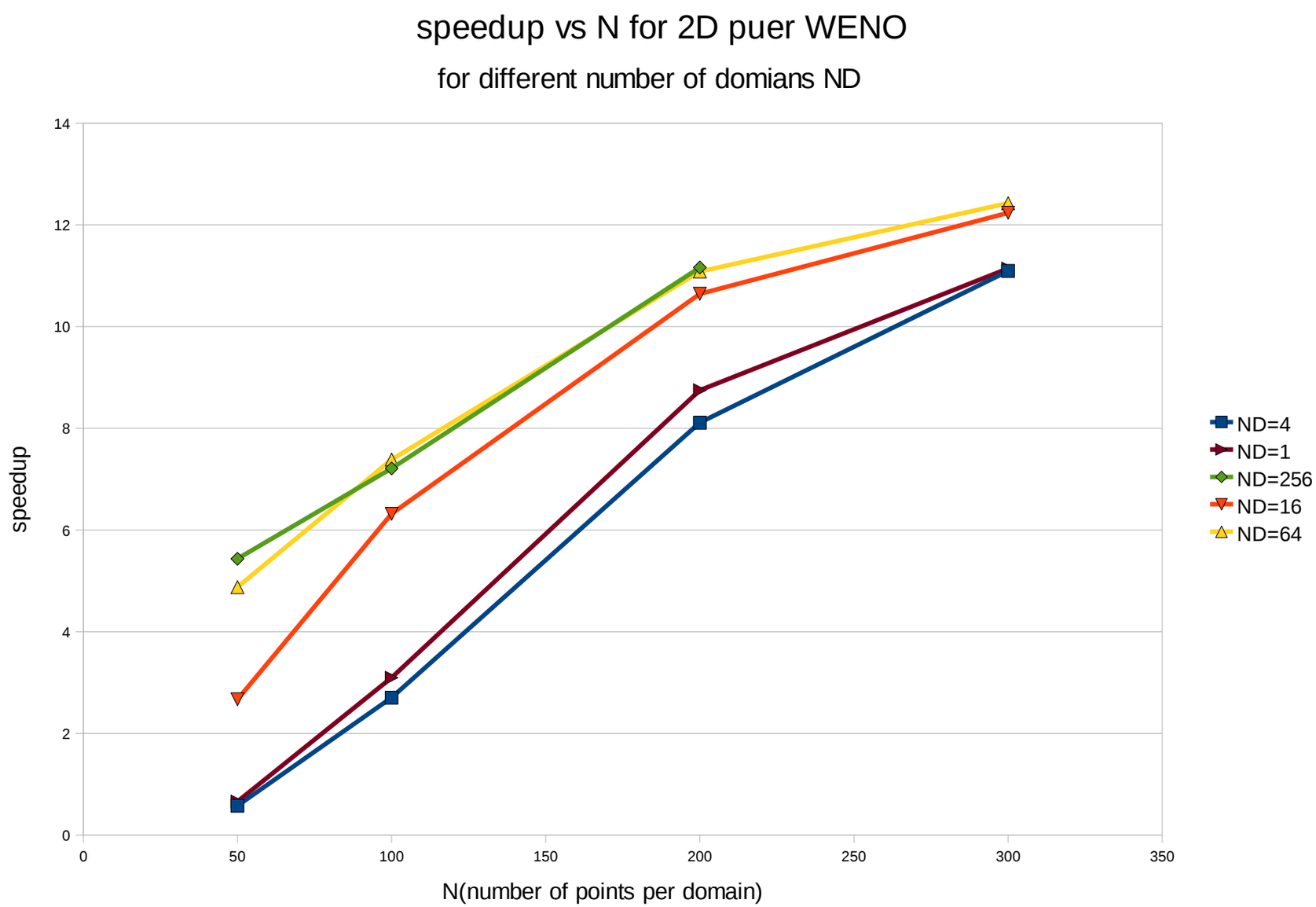
- ✓ Prepare all data and compute everywhere using CUFTT
- ✓ Filter and modify expansion coefficients
- ✓ Compute inverse FFT
- ✓ Identify WENO domains and recompute derivatives
- ✓ Update field values

GPU acceleration

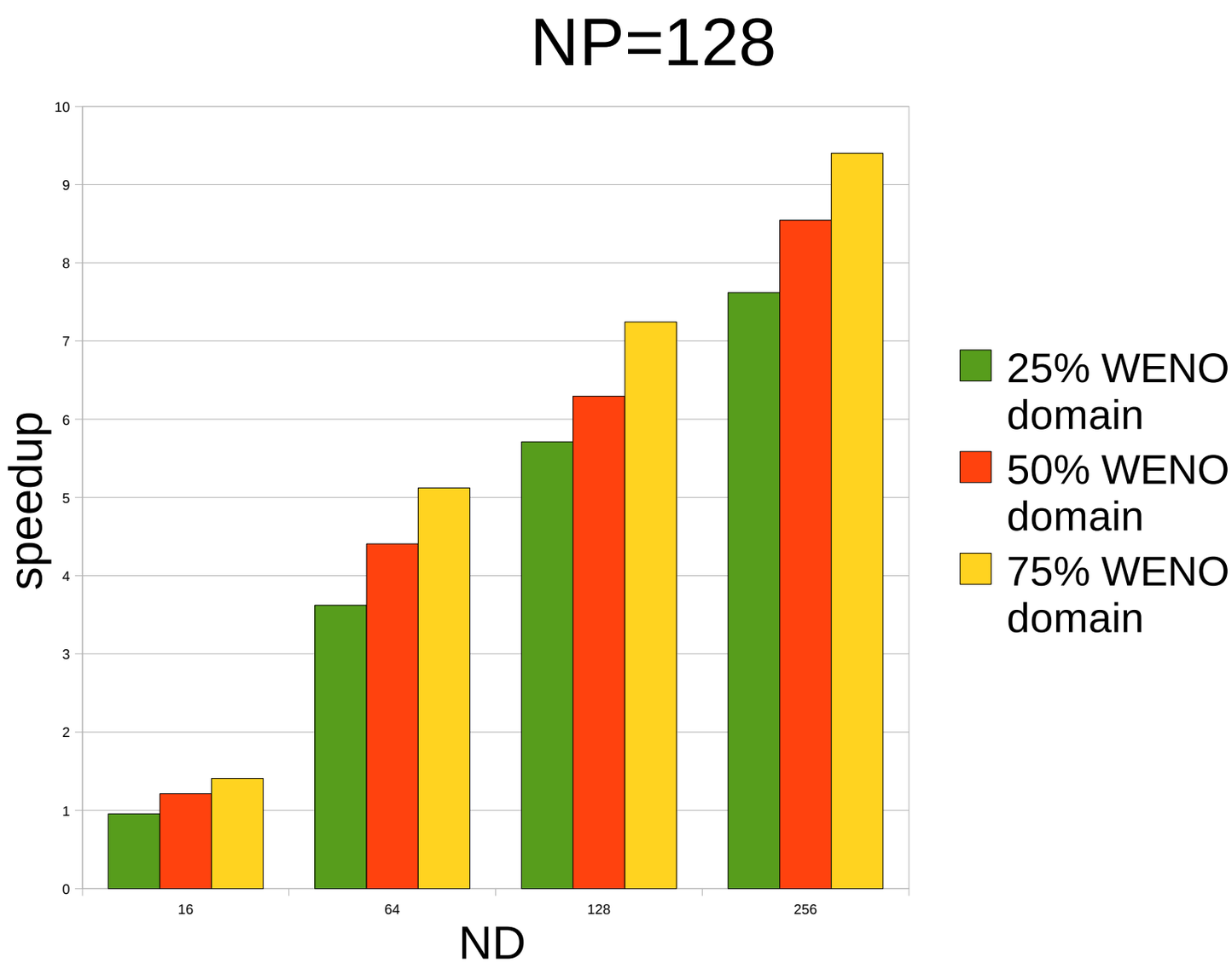
Considerations when going 2D/3D -

- ✓ Line-by-line or domain by domain ?
- ✓ Size of shared memory

WENO behaves

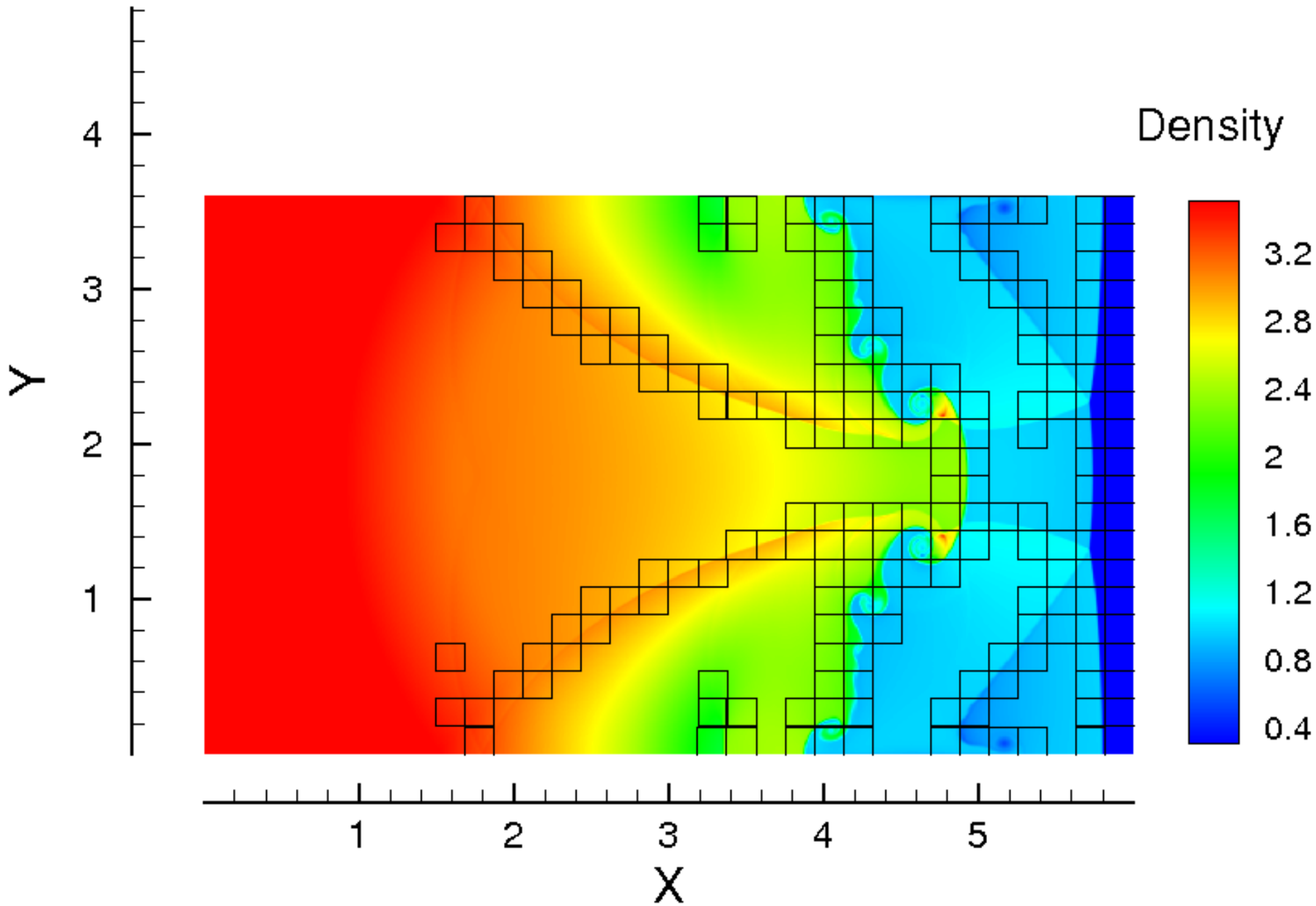


GPU acceleration



More work is better - good for 2D/3D

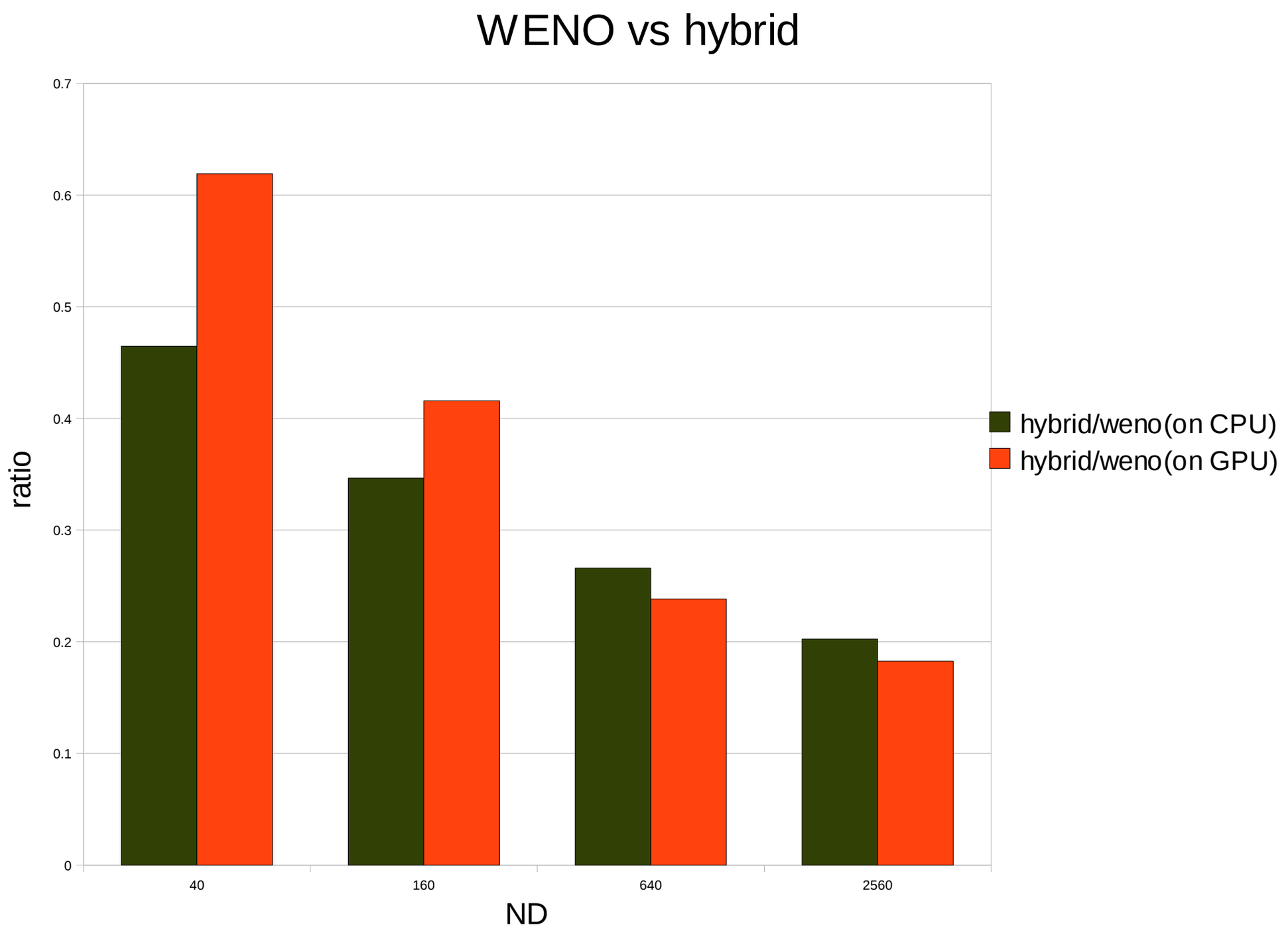
Putting it all together



Marked blocks are WENO blocks ~ 30%

GPU acceleration

Good behavior translates from CPU to GPU



Concluding remarks

On the algorithmic part

✓ Significant potential in hybrid FC-WENO schemes for complex multi-scale problems.
✓ Most core elements have been demonstrated.
✓ General geometries and increased physical complexity remains next challenge

Reasonable GPU acceleration is possible despite dynamic nature of method

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... or come see me