DNS of transition to turbulence in compressible mixing layer on heterogeneous computational clusters

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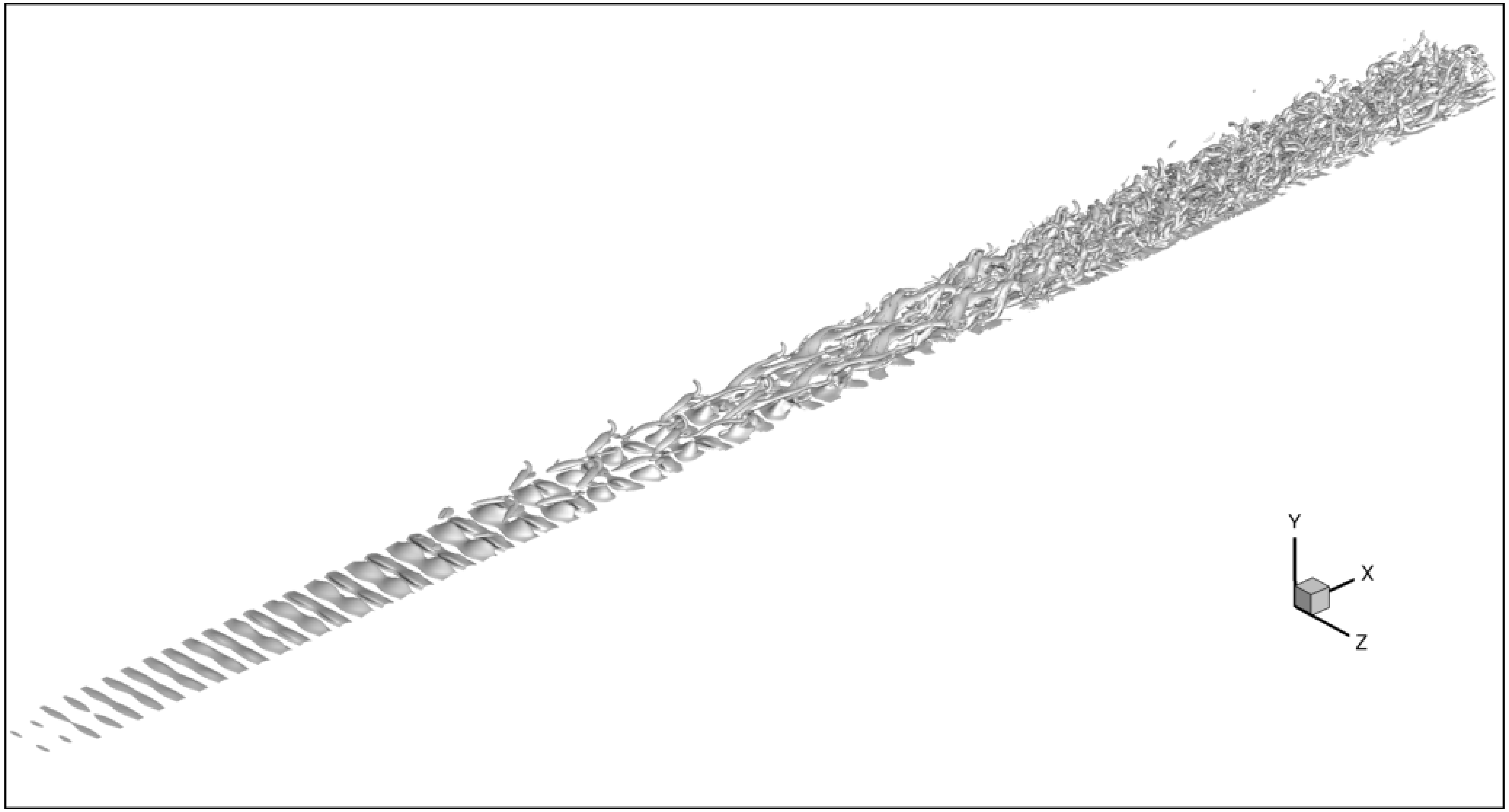
Motivation

- **Instability** of supersonic free shear flows is a **phenomenon of great importance** in a number of aerodynamic problems.
- Mechanisms of instability emergence on transition to turbulence in free shear flows also work in other flows with free boundaries, such as jets and wakes.
- Clear understanding of process going on in high-speed mixing layers has it own fundamental value as a **part of turbulence emergence problem**.
- Knowing characteristics of such flows is essential in many applied problems. For example, intensive sound radiation in jet, exhausting from engine nozzle into coflow.
- Direct numerical simulation of turbulent flows even at moderate Reynolds numbers requires **hundreds of hours** of computational time even **on high-performance computational clusters**.
- One of the reasonable ways to increase efficiency and reduce computational wall-clock time is to employ modern general-purpose graphics processing units (GPGPU) with high computational and data throughput.
- Usage of heterogeneous CPU-GPU systems is currently rapidly growing and **highly promising area of computing**.

DNS of transition to turbulence in supersonic flat plate boundary layer at M = 6



Nonlinear interaction of 1st and 2nd modes and onset of laminar-turbulent transition. Q criterion isosurface. Computational grid consists of 30 million grid cells.

Problem Statement

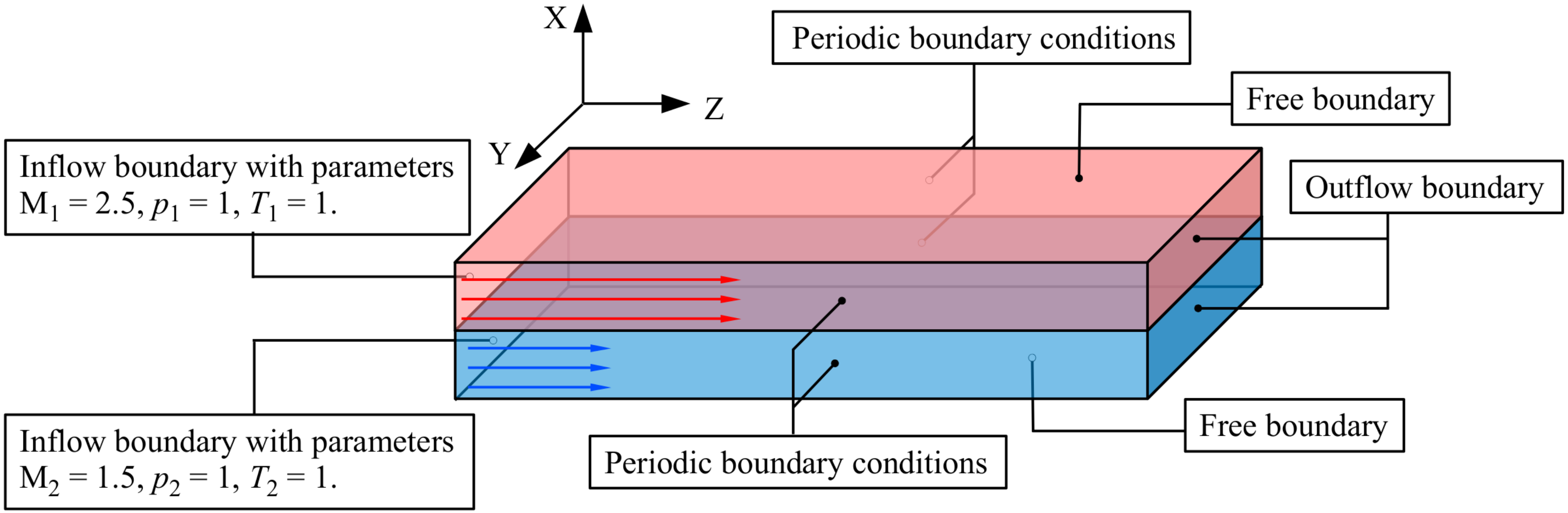


Fig. Computational domain sketch in the spatially evolving mixing layer problem.

- We simulate the growth of instability waves in a spatially evolving mixing layer.
- Two supersonic flows along Z axis with $M_1 = 2.5$ and $M_2 = 1.5$ Mach numbers.
- Temperatures and pressures are equal: $T_1 = T_2,\ p_1 = p_2$.
- Resulting convective Mach number $M_c = (U_1 - U_2)/(a_1+a_2) = 0.5$.
- On the inflow boundary step-like initial profile with time-dependent disturbances of transverse velocity U_x is imposed.

Governing Equations

In present work numerical simulations are performed by solving 3D unsteady compressible Navier-Stokes equations:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = \frac{1}{\mathrm{Re}} \left(\frac{\partial \mathbf{F}_v}{\partial x} + \frac{\partial \mathbf{G}_v}{\partial y} + \frac{\partial \mathbf{H}_v}{\partial z} \right)$$

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ u(E+p) \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ v(E+p) \end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ w(E+p) \end{pmatrix}$$

$$\mathbf{F}_v = (0,\ \tau_{xx},\ \tau_{xy},\ \tau_{xz},\ u\tau_{xx} + v\tau_{xy} + w\tau_{xz} - q_x)^T$$
$$\mathbf{G}_v = (0,\ \tau_{xy},\ \tau_{yy},\ \tau_{yz},\ u\tau_{xy} + v\tau_{yy} + w\tau_{yz} - q_y)^T$$
$$\mathbf{H}_v = (0,\ \tau_{xz},\ \tau_{yz},\ \tau_{zz},\ u\tau_{xz} + v\tau_{yz} + w\tau_{zz} - q_z)^T$$

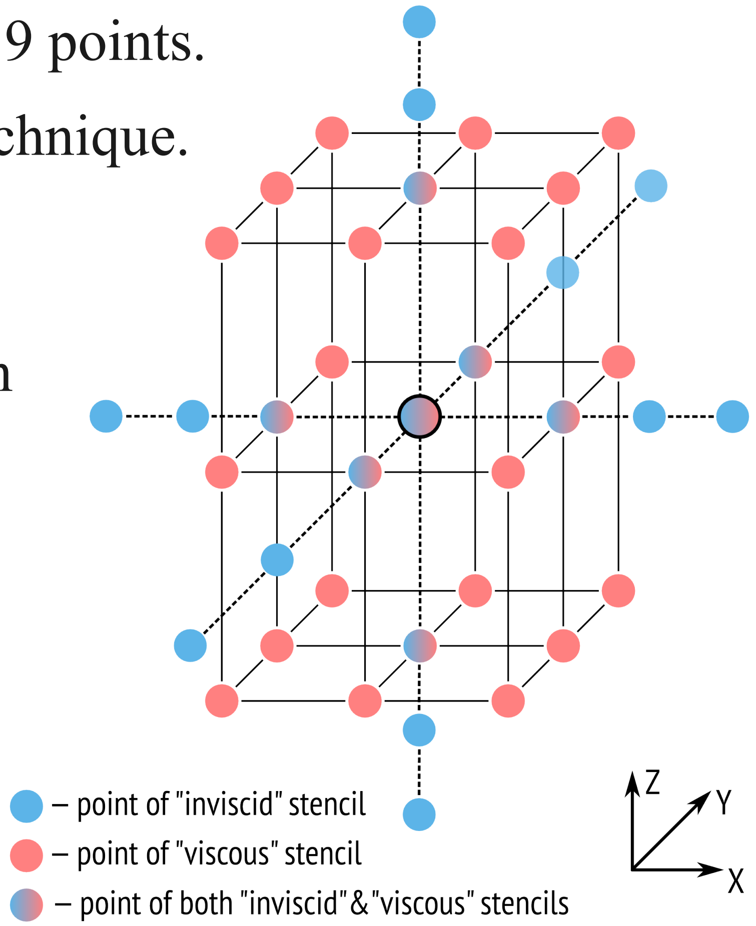
Here ρ is density, p is pressure, $\mathbf{u} = (u, v, w)$ is velocity vector,
E is total energy, $\mathbf{q}$ is heat flux vector and $\tau_{\alpha\beta}$ are viscous stresses.

Conservative variables vector is denoted as $\mathbf{Q}$.

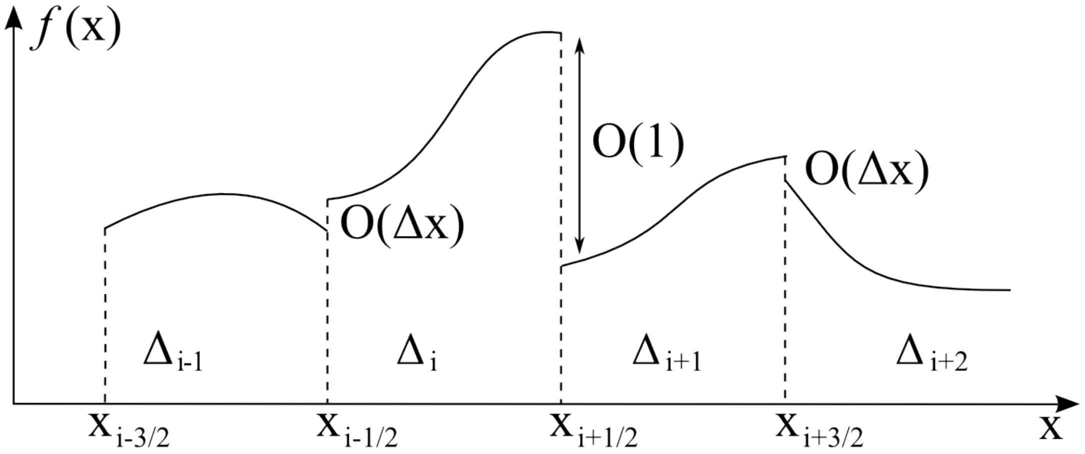
Vectors $\mathbf{F}$, $\mathbf{G}$ and $\mathbf{H}$ are inviscid fluxes, while $\mathbf{F}_v$, $\mathbf{G}_v$ and $\mathbf{H}_v$ are viscous fluxes.

Numerical Techniques

- For **convective** terms discretization high-resolution shock capturing WENO scheme of **5th order** by Shu & Oscher is used.
- For **diffuse** terms approximation central differences of **2nd order** are employed.
- Time advancement is performed with **explicit** four-stage low storage **4th order** Runge-Kutta-Gill scheme.
- Full stencil for both inviscid and viscous terms contains 39 points.
- Boundary conditions are imposed using the ghost cells technique.

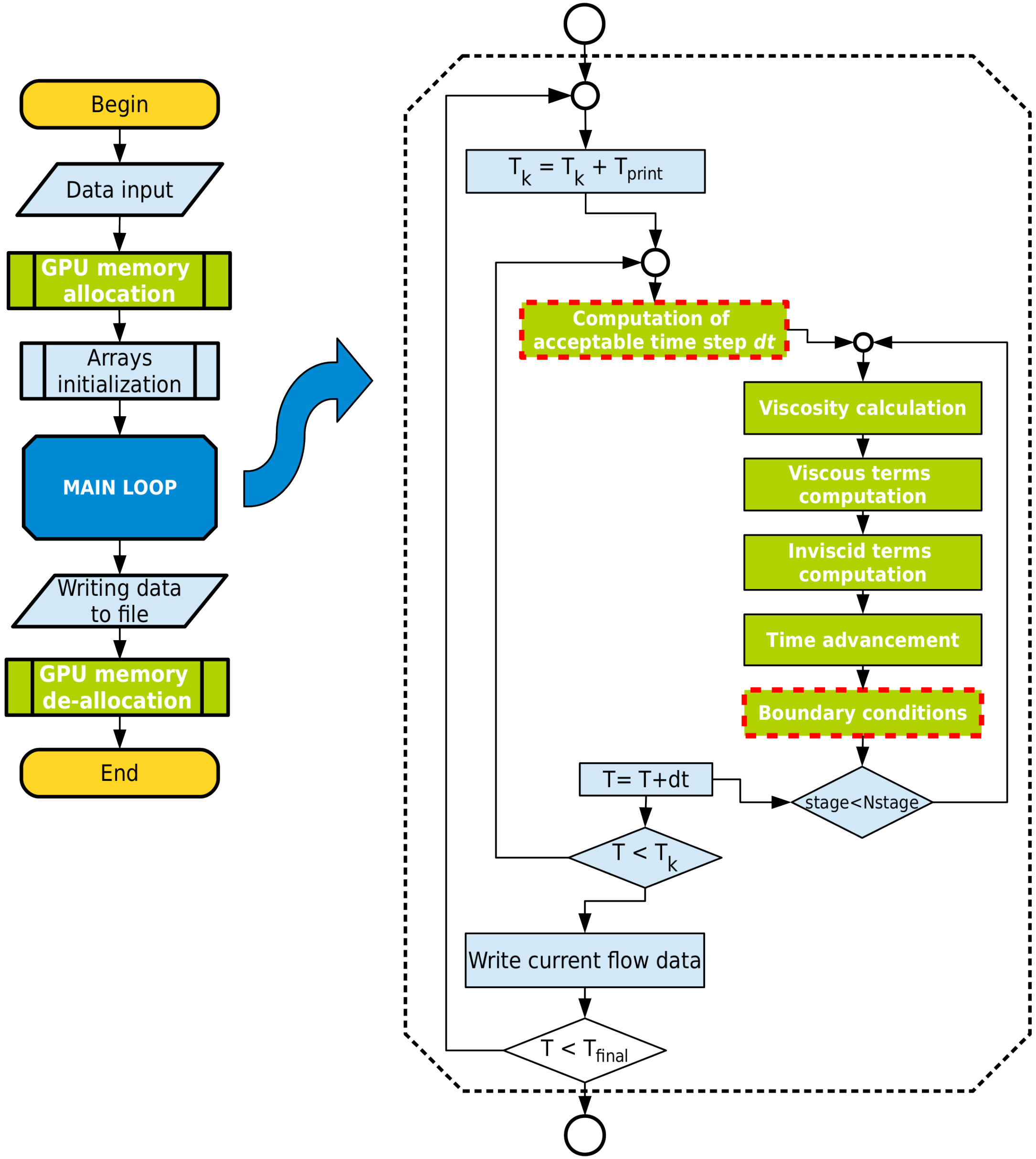


The main idea of WENO schemes is to use a piecewise polynomial reconstruction and avoid interpolation across discontinuities. WENO schemes use a convex superposition of the "candidate" stencils with adaptive coefficients.



$$TV(f^{n+1}) \leq TV(f^{n}) + O(\Delta x^{q})$$

Program Implementation



- CUDA 4/5 platform
- Multi-GPU capability
- Computational process is organized as consecutive calls of *kernels* (GPU-side functions) by main process, running on CPU
- Total memory requirements are about 300 bytes per cell for double-precision computations.

Fig. Flow chart of hybrid Navier-Stokes solver. CPU routines are colored light-blue color, GPU routines are marked with **green**.
Computational phases with MPI exchange have **red dashed frames**.

Parallelization Scheme

- Data between GPUs is distributed via domain decomposition technique.
- Grid index is organized so that cells with the same i_z are in continuous memory segment
- **So** domain is divided into sub-domains along the Z-axis to **simplify data exchange** procedure and **reduce** number of temporary **exchange buffers**.
- Computations in each subdomain are performed in parallel using **CUDA**
- Within one computational node data exchange is carried out using **OpenMP** threads
- Inter-node exchange uses **MPI** library

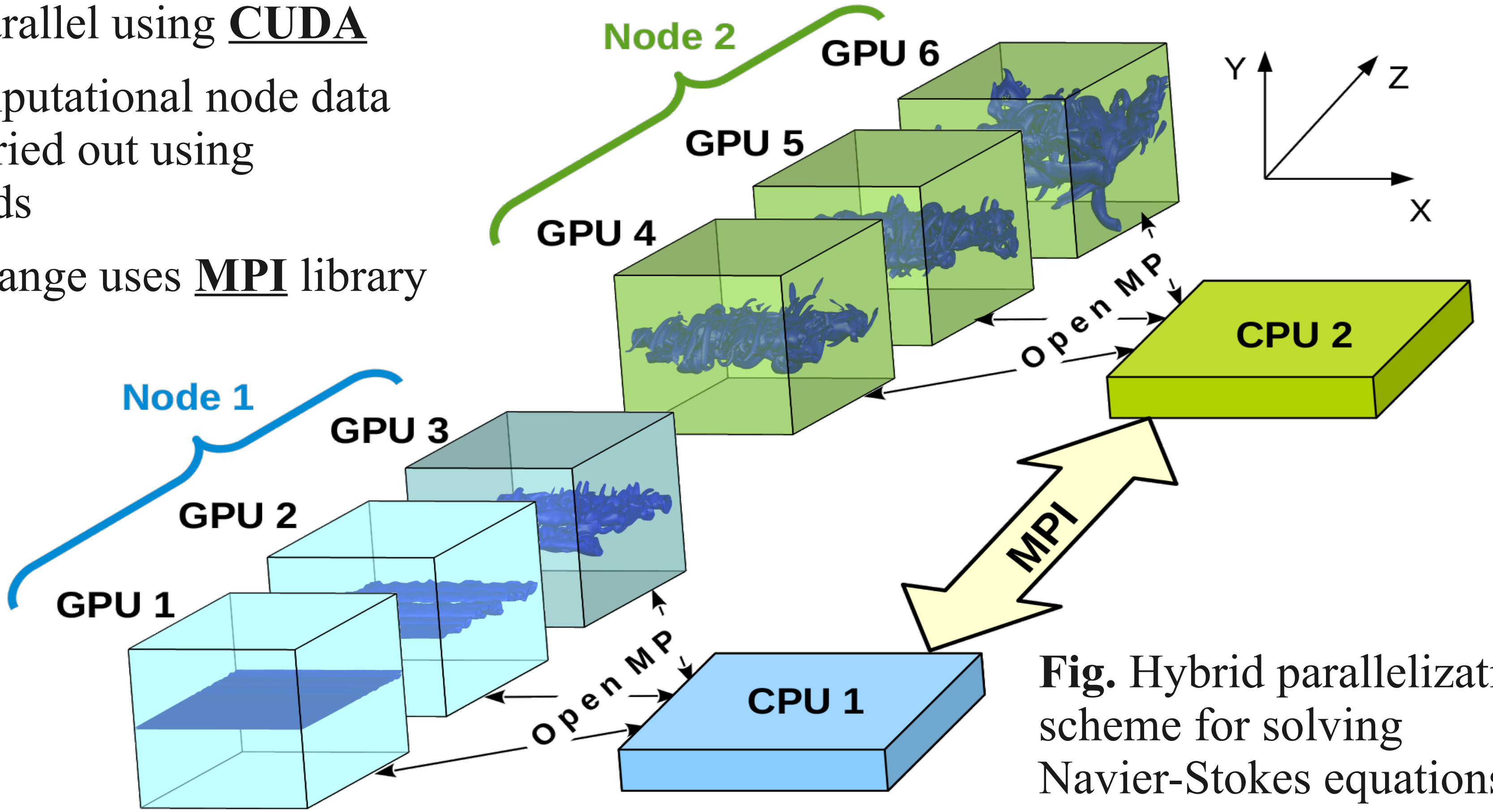
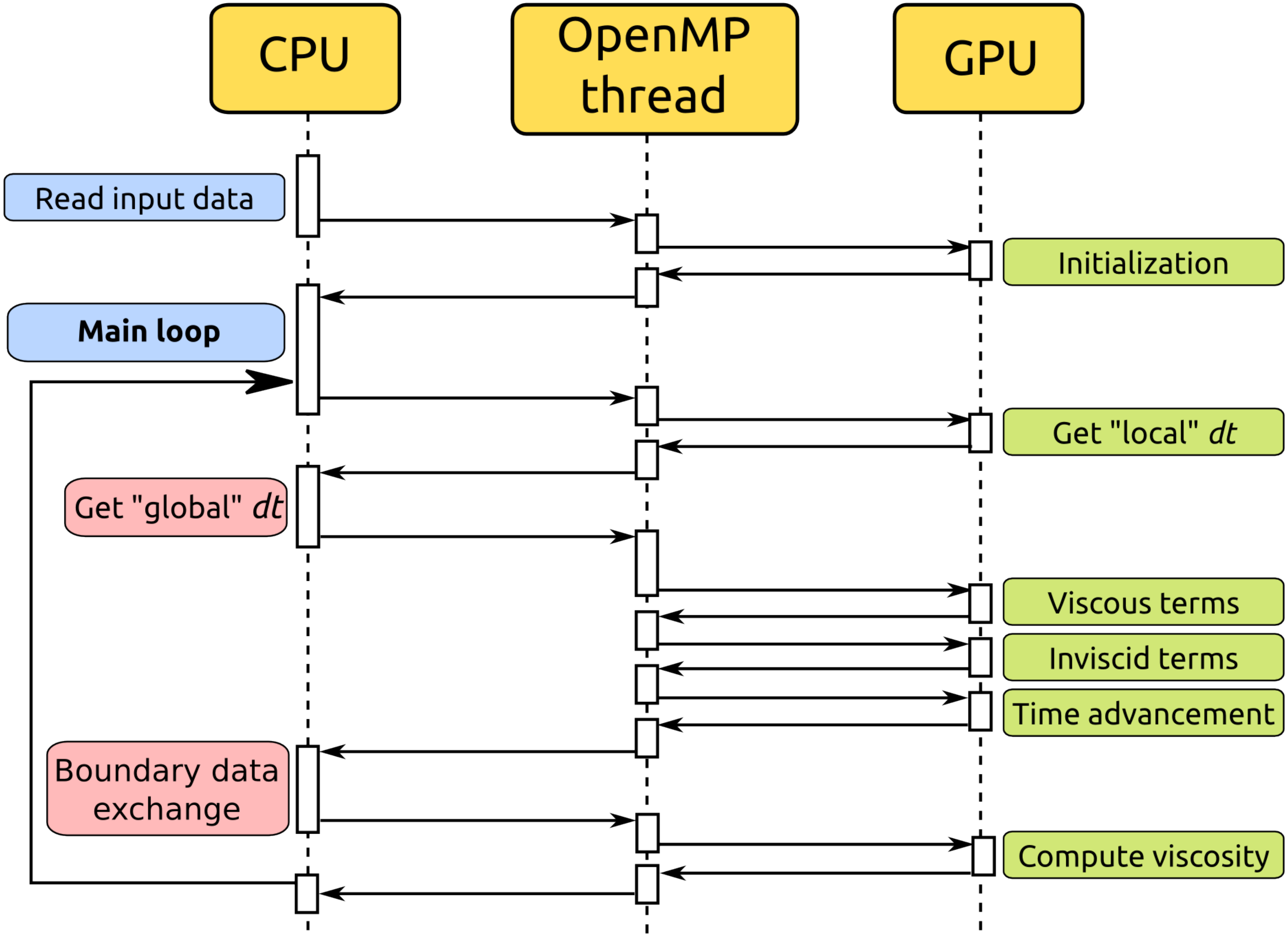


Fig. Hybrid parallelization scheme for solving Navier-Stokes equations on multi-GPU configuration.

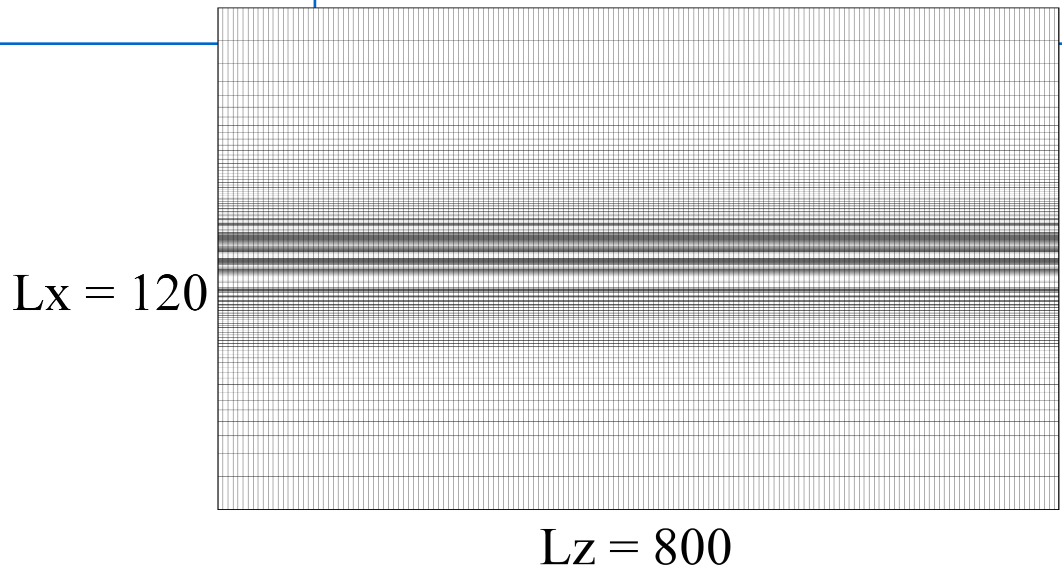
Computation Process Diagram



Mixing Layer Conditions

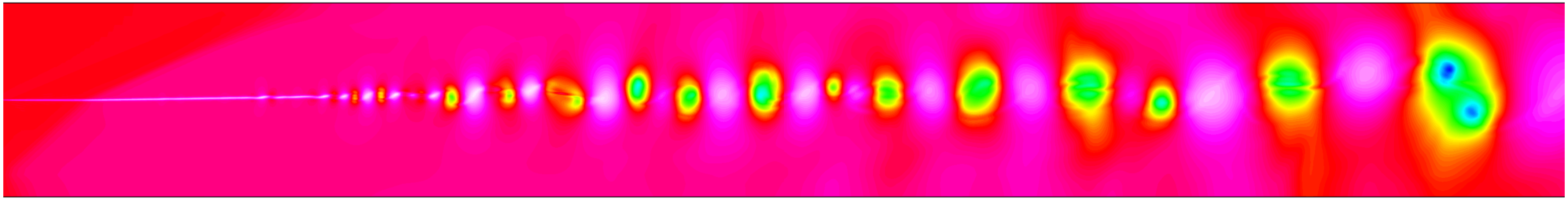
	2D	3D
Computational grid, $N_x \times N_y \times N_z$	$120\times3\times800 \approx 2.9\times10^5$ cells	$120\times120\times1200 \approx 1.7\times10^7$ cells
Inflow forcing	Disturbances of transverse velocity U_x, $u' = A\cos(\omega t - \alpha z)\exp(-x^2/\sigma^2)$, where $\omega = 0.68$, $\alpha = 0.34$	Disturbances of transverse velocity U_x, $u' = A\cos(\omega t - \alpha z)\exp(-x^2/\sigma^2)$- $\times$ $\times\{1 + \delta\sin(2\pi y/L_y)\}$, where $\omega = 0.68$, $\alpha = 0.34$
Computational resources	**1**×Nvidia GeForce 460GTX, 1Gb	**6**×Nvidia Tesla M2090, 6 Gb

- Values of frequency ω and wave number α corresponded to solution of linear stability problem with maximum growth rate.
- Mesh refined is near the centerline

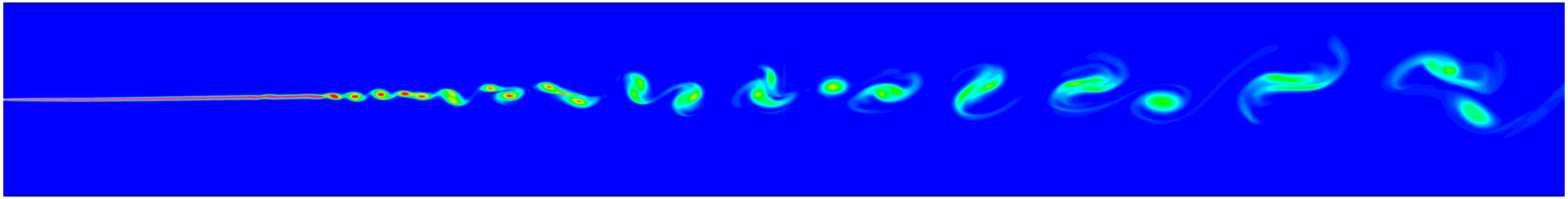


Mixing Layer 2D

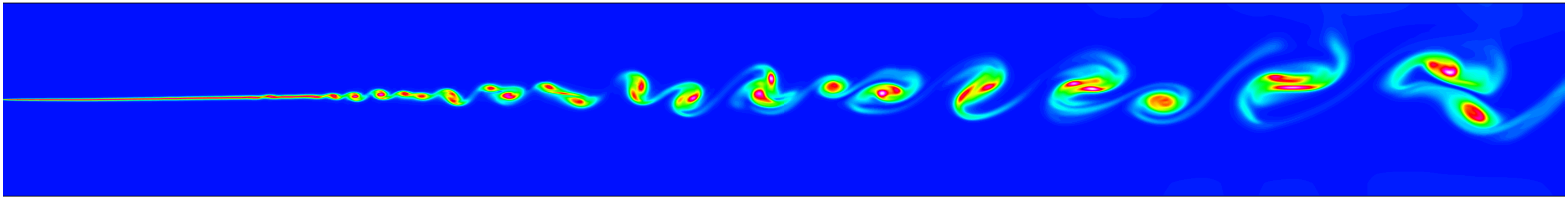
Temperature:



Vorticity magnitude:



Entropy:



Mixing Layer 3D

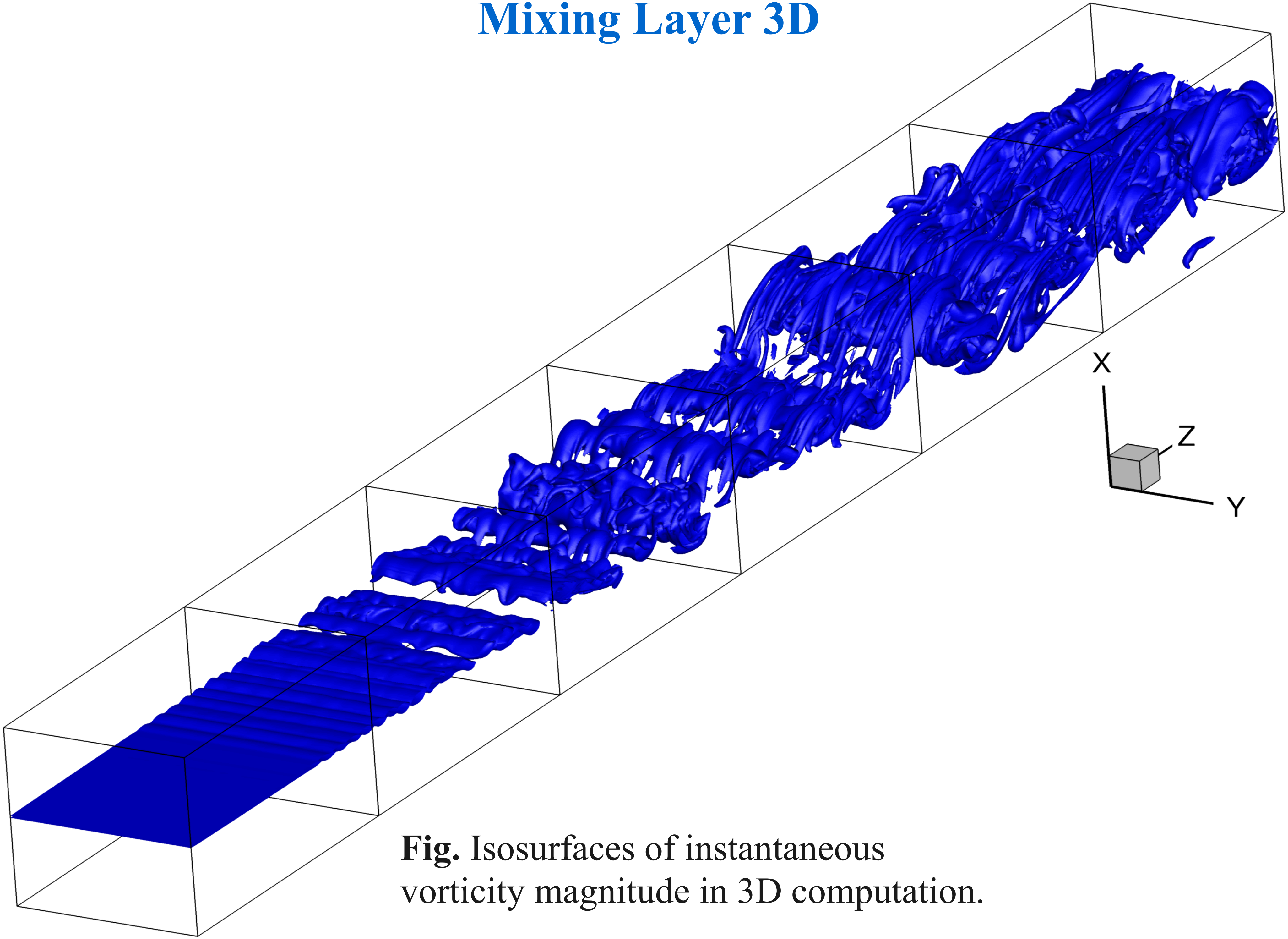


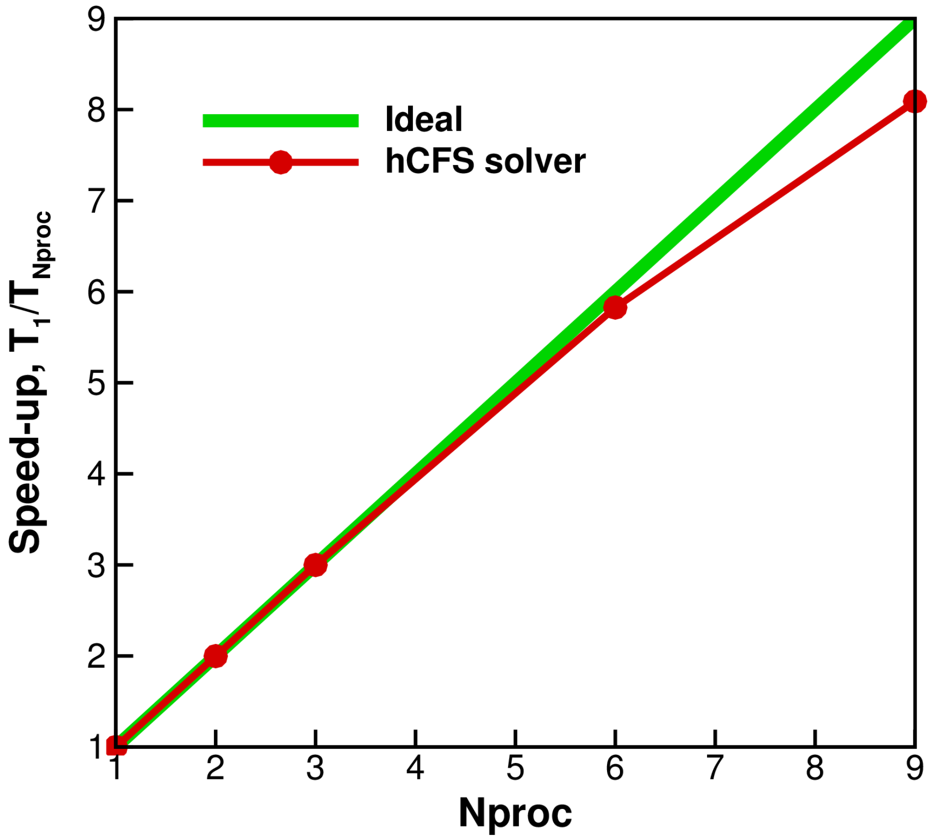
Fig. Isosurfaces of instantaneous vorticity magnitude in 3D computation.

Speed-up

Speed-up measurements were performed for a computational grid consisting of 120×120×1000=14.4 million nodes.

Efficiency for 9 GPU was about 90%.

Calculation of convective terms was the most expensive part of computation taking approximately 76% of total time while calculation of viscous terms took about 10% and interprocessor data exchange MPI another 10%.



Mean Flow Characteristics I

Numerical code was also used by research group at TsNIIMash to study spatially evolving 2D supersonic mixing layer with Mach numbers $M_1 = 2.87$, $M_2 = 1.17$ and convective Mach number $M_c = 0.86$. Computations were performed by **E.Yu. Kartseva**.

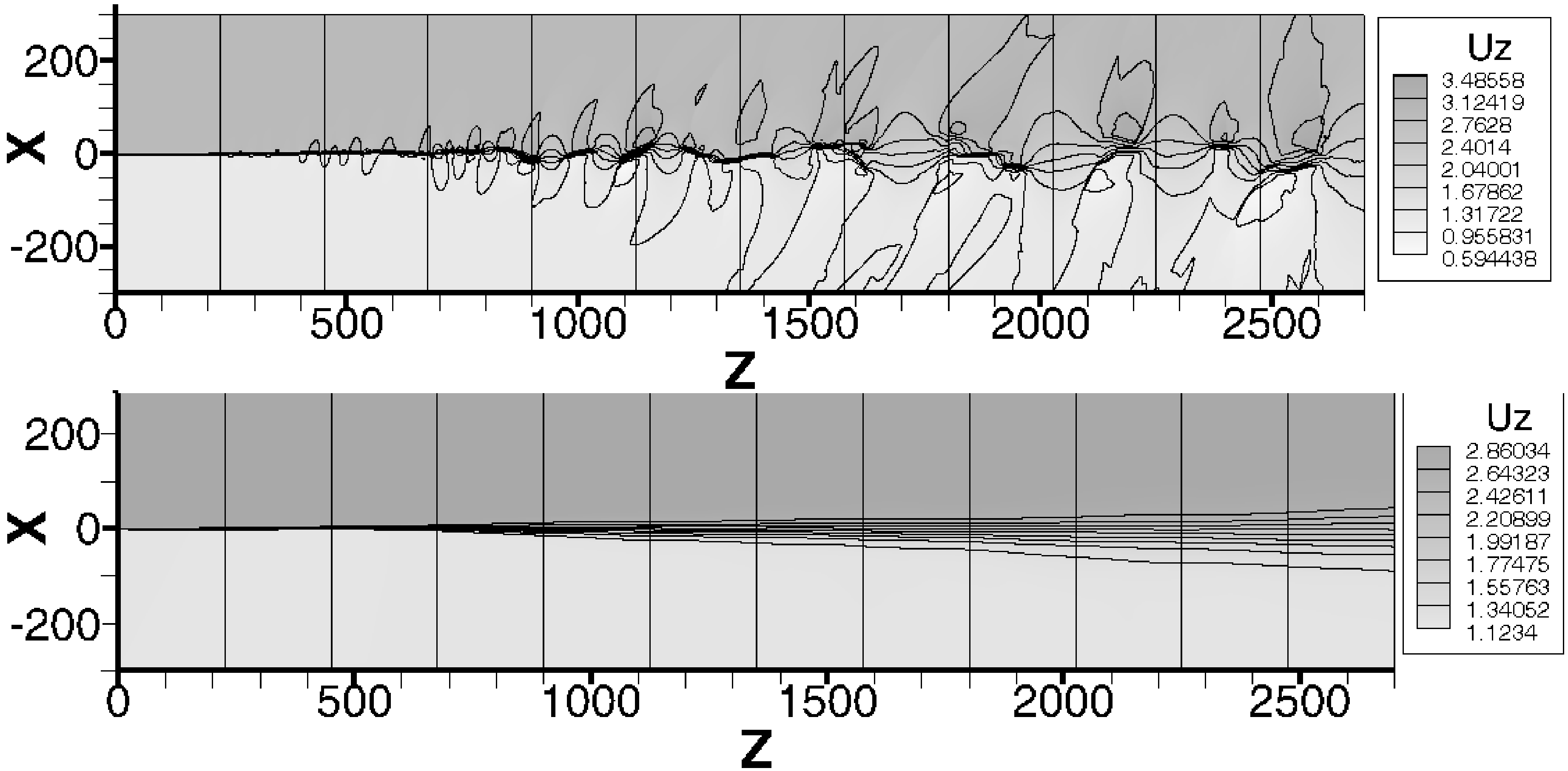


Fig. Instantaneous (top) and mean (bottom) flowfield of longitudinal velocity.

Mean Flow Characteristics II

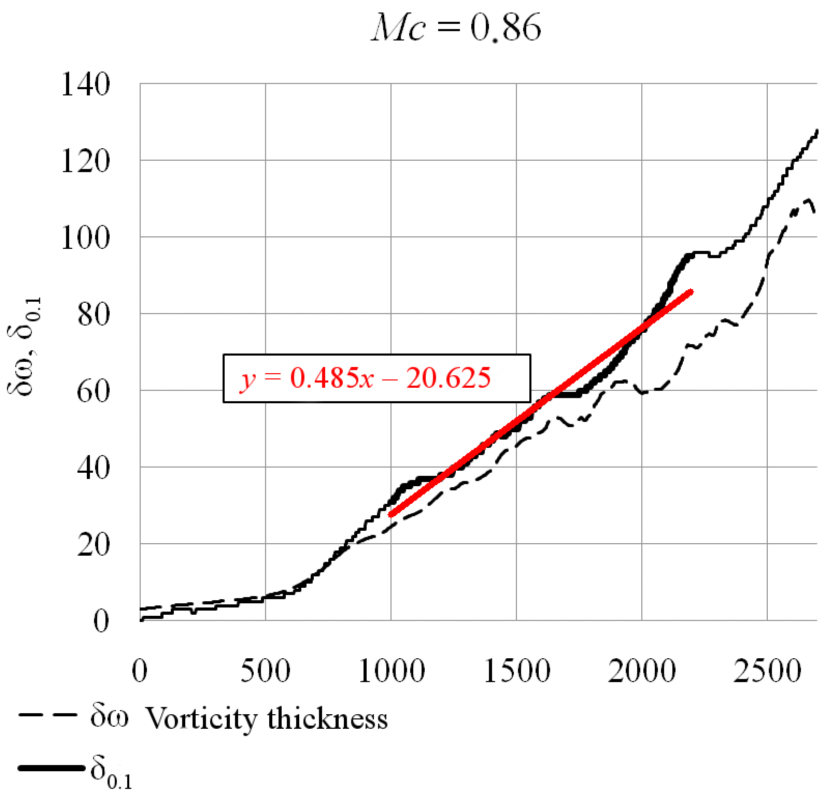


Fig. Mixing layer thickness as function of distance from the inflow boundary.

$$\delta_{\omega} = \frac{U_1 - U_2}{[\partial U / \partial x]_{\max}}$$

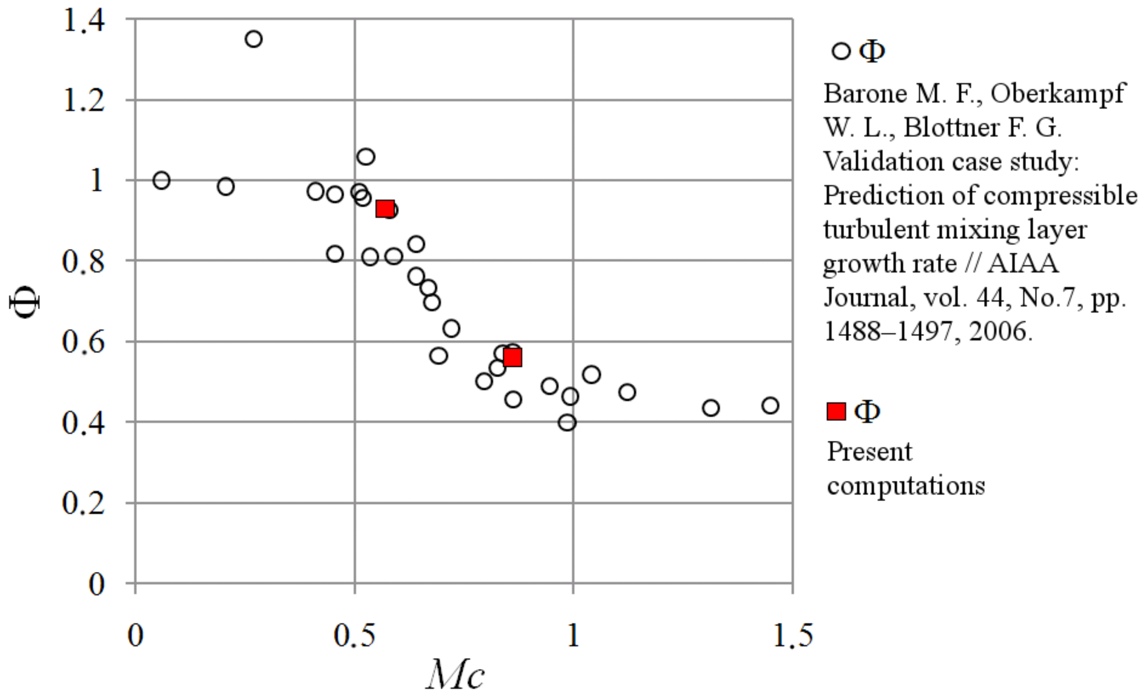


Fig. Ratio of compressible mixing layer spreading rate to incompressible mixing layer spreaing rate as function of convective Mach number.

$$\Phi = \frac{d\delta_{0.1} / dz}{\left(d\delta_{0.1} / dz\right)_i}$$

Conclusion and Further Work

- Multi-GPU code for solving unsteady compressible Navier-Stokes equations has been developed, verified and applied to numerical simulation of instability waves in supersonic mixing layer.
- Results of numerical simulation are in good agreement with linear theory and data, obtained by other researchers.
- Further work will include:
  - Optimization of WENO scheme implementation
  - Improving far-field boundary conditions
  - Numerical simulation of mixing layer development at supersonic convective Mach numbers
  - Adaptation of the code for DNS of the transition to turbulence in supersonic boundary layers.

Thank You for Your Attention