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Dynamic Discrete Ordinate Method in Solving Boltzmann Equation for Gas Flows

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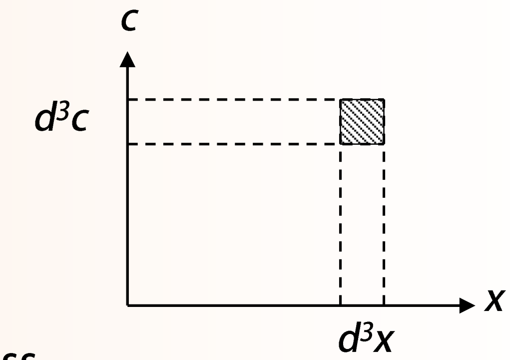
Outline

I. Boltzmann Equation
II. Discrete Ordinate Method (DOM)
III. Dynamic Discrete Ordinate Method (DDOM)
IV. Numerical Results and Validations
V. Massively Parallel Computation
VI. Conclusions

I. Boltzmann Equation

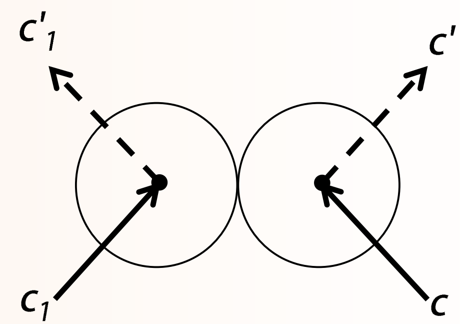
- Transport equation of velocity distribution function (*f*) of number density (*n*)

$$\int_{-\infty}^{+\infty} f\left(\vec{x},\vec{c},t\right) d^3c = n$$



- Assumptions on gas molecules
  - Identical spherical molecules with same mass
  - Dilute gas
  - Elastic collision:

$$\vec{c}+\vec{c}_1=\vec{c}\,'+\vec{c}_1\,' \quad ; \quad \vec{c}^{\,2}+\vec{c}_1^{\,2}=\vec{c}\,'^2+\vec{c}_1\,'^2$$



I. Boltzmann Equation

- Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{c}\frac{\partial f}{\partial \vec{x}} + \vec{F}\frac{\partial f}{\partial \vec{c}} = \Omega(f)$$

where the collision integral: $\Omega(f) = \int_{-\infty}^{+\infty} \left(f' f_1' - f\, f_1\right) g b\, db\, d\varepsilon\, d^3 c_1$

- Hydrodynamic moments

$$\rho = m\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f d^3 c \qquad \rho\vec{u} = m\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \vec{c} f d^3 c$$

$$\rho e = m\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \frac{1}{2}\left(\vec{c} - \vec{u}\right)^2 f d^3 c$$

($m = 1$ if particle mass is used as a unit scale to measure mass)

Equilibrium State

- Equilibrium velocity distribution function (Maxwellian)

$$f^{eq}(\vec{c}) = \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \exp\left\{-\frac{m}{2kT}\left[(\vec{c}-\vec{u})^2\right]\right\}$$

$$\Omega(f^{eq}) = 0$$

- Therefore, $\Omega = \nu(f^{eq} - f)$ is mathematically exact where the collision frequency is a function of *n* and *c*.

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Boltzmann Equation with BGK Model

- Bhatnagar-Gross-Krook (BGK) collision model:

$$\frac{\partial f}{\partial t}+\vec{c}\,\frac{\partial f}{\partial \vec{x}}+\vec{F}\,\frac{\partial f}{\partial \vec{c}}=\nu\left(f^{eq}-f\right)$$

$$f^{eq}\left(\vec{c}\right)=\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\exp\left[-\frac{m}{2kT}\left(\vec{c}-\vec{u}\right)^{2}\right]$$

- Coupling with hydrodynamic moments

$$Q_i=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\psi_i f d^3c \quad ; \quad Q_i=\left(\rho,\rho\vec{u},e\right) \quad ; \quad \psi_i=\left[1,\vec{c},\frac{1}{2}\left(\vec{c}-\vec{u}\right)^{2}\right]$$

- Leading to incorrect Prandtl number (*Pr*) when the collision frequency is taken as constant: $\mu=\frac{p}{\nu}$ $\quad \kappa=\frac{5}{2}\frac{k}{m}\frac{p}{\nu}$ $\quad \mathrm{Pr}=1$

Boltzmann BGK Equation in 2 and 1 Dimensions

- Defining $f_2(\vec{x},\vec{c}_2,t)=\int_{-\infty}^{+\infty} f(\vec{x},\vec{c}_2,c_3,t)\,dc_3$ and assuming $\frac{\partial f_2}{\partial x_3}=0$
- Integrating the 3-D BGK Boltzmann equation,

$$\frac{\partial f_2}{\partial t}+\vec{c}_2\frac{\partial f_2}{\partial \vec{x}_2}+\vec{F}\frac{\partial f_2}{\partial \vec{c}_2}=\nu\left(f_2^{eq}-f_2\right) \quad ; \quad f_2^{eq}(\vec{c}_2)=\left(\frac{m}{2\pi kT}\right)\exp\left[-\frac{m}{2kT}\left(\vec{c}_2-\vec{u}_2\right)^2\right]$$

$$Q_i=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\psi_i f_2 d^2c \quad ; \quad Q_i=\left(\rho,\rho\vec{u}_2,e\right) \quad ; \quad \psi_i=\left[1,\vec{c}_2,\frac{1}{2}\left(\vec{c}_2-\vec{u}_2\right)^2\right]$$

- Similarly, for 1-D Boltzmann equation,

$$\frac{\partial f_1}{\partial t}+c\frac{\partial f_1}{\partial x}+F\frac{\partial f_1}{\partial c}=\nu\left(f_1^{eq}-f_1\right) \quad ; \quad f_1^{eq}(c)=\left(\frac{m}{2\pi kT}\right)^{\frac{1}{2}}\exp\left[-\frac{m}{2kT}\left(c-u\right)^2\right]$$

$$Q_i=\int_{-\infty}^{+\infty}\psi_i f_1 dc \quad ; \quad Q_i=\left(\rho,\rho u,e\right) \quad ; \quad \psi_i=\left[1,c,\frac{1}{2}\left(c-u\right)^2\right]$$

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Boltzmann-BGK Equation Solvers

- Gas-Kinetic Scheme (GKS)
- Discrete Ordinate Method (DOM)
- Lattice Boltzmann Method (LBM)

II. Discrete Ordinate Method (DOM)

Basic Features of DOM

- Finite discrete velocity points

$$f\left(c_x, c_y, c_z\right) \Rightarrow \left[f_{1,1,1}, \dots, f_{\alpha,\beta,\gamma}, \dots, f_{N_x,N_y,N_z}\right]$$

- Splitting method

$$\frac{\partial f_{\alpha,\beta,\gamma}}{\partial t} + \vec{c}_{\alpha,\beta,\gamma} \frac{\partial f_{\alpha,\beta,\gamma}}{\partial \vec{x}_{\alpha,\beta,\gamma}} = \Omega_{\alpha,\beta,\gamma} \rightarrow \frac{\partial f_{\alpha,\beta,\gamma}}{\partial t} + \vec{c}_{\alpha,\beta,\gamma} \frac{\partial f_{\alpha,\beta,\gamma}}{\partial \vec{x}_{\alpha,\beta,\gamma}} = 0 \text{ and } \frac{\partial f_{\alpha,\beta,\gamma}}{\partial t} = \Omega_{\alpha,\beta,\gamma}$$

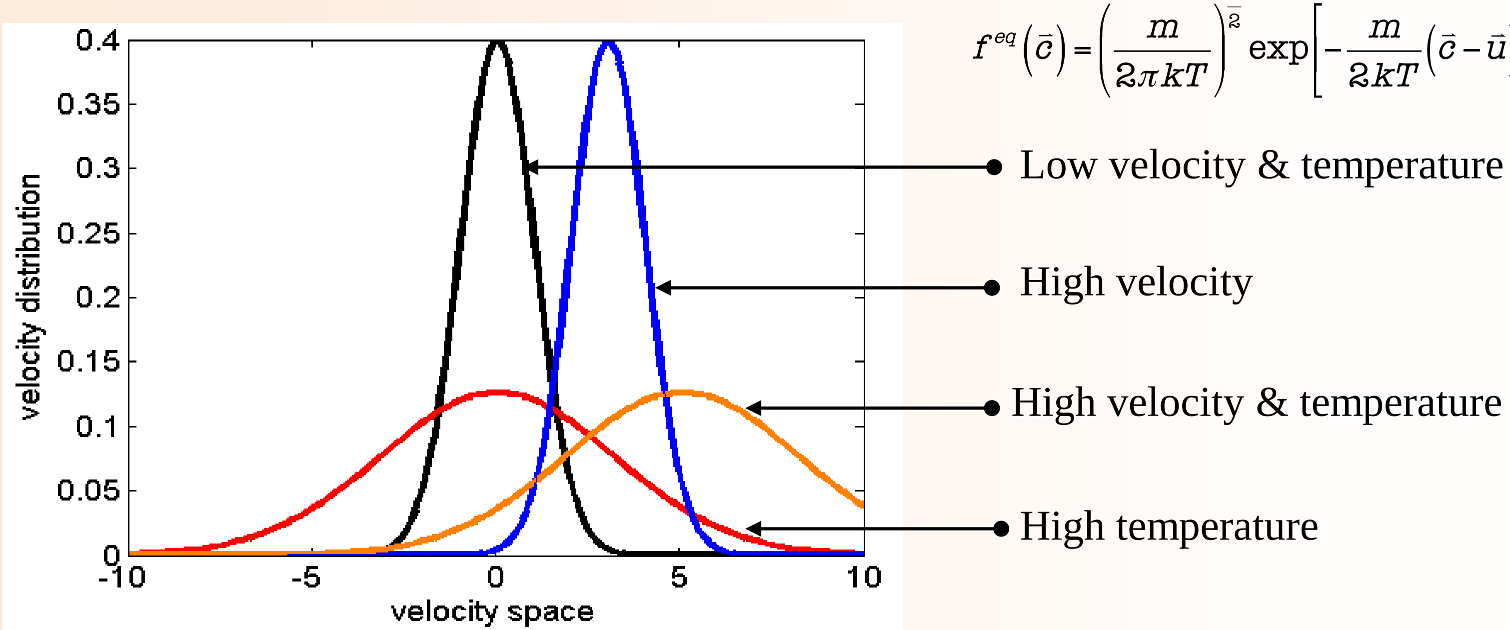
- Quadrature scheme

$$\iiint \psi_i f dc^3 \approx \sum_{\alpha=1}^{N_x} \sum_{\beta=1}^{N_y} \sum_{\gamma=1}^{N_z} W_{\alpha,\beta,\gamma} \left[\psi_i\left(c\right) f\left(c\right)\right]_{\alpha,\beta,\gamma}$$

Difficulties of Conventional DOM

- Difficulties encountered for high Mach number flows.
- High demand on computational resource due to large number of quadrature points needed to recover f^{eq}
- Sensitivity of the discrete point selection

$$f^{eq}(\vec{c}) = \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \exp\left[-\frac{m}{2kT}(\vec{c}-\vec{u})^2\right]$$



Objectives

- To develop a simple, robust, and efficient DOM solver
  - Reformulation: DOM with Dynamic Quadrature Scheme (DQS)
  - Code development
  - Code validation
  - Code speed enhancement
  - Code parallelization

III. Dynamic Discrete Ordinate Method

a. Dynamic Quadrature Scheme (DQS)

b. Transformed Moment Integral

c. Algorithm of Dynamic Discrete Ordinate Method (DDOM)

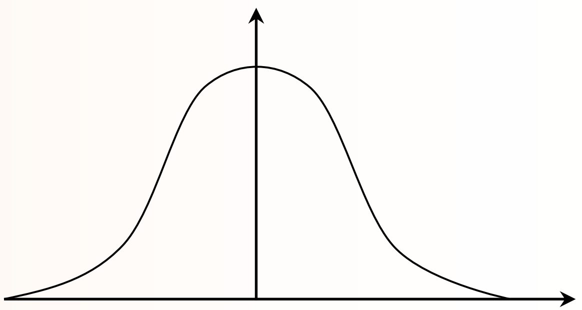
Dynamic Quadrature Scheme (DQS)

- Coordinate transformation of velocity space

$$\vec{\xi} = \frac{\vec{c} - \vec{u}}{\sqrt{2RT}}$$

- Gaussian profile

$$f \approx f^{eq} = G\left(\vec{\xi}\right) = \exp^{-\vec{\xi}^2}$$



- Gaussian-Hermite quadrature
  - Optimizing quadrature point distribution
  - Equivalency to the first-order Chapman-Enskog expansion
  - 3x3x3 quadrature points for recovery NSF equations for 3D case

$$Q = \iiint e^{-\vec{\xi}^2}\left(a_0 + \vec{a}_1\vec{\xi} + +\vec{a}_2\vec{\xi}^2 + \ldots\right)d\xi^3$$

$$Q = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} W_{i,j,k} P^{\alpha}_{i,j,k}\left(\vec{\xi}\right) + O\left(Kn^{\alpha}\right)$$

- Dynamic nature
  - $\vec{c}$ changing with time and space for fixed $\vec{\xi}$

Transformed Moment Integral

- Transformed moment integral

$$Q_i = \iiint \psi_i\left(\vec{\xi}\right) f\left(\vec{\xi}\right) \left\| \vec{\vec{J}} \right\| d\xi^3$$

- Gaussian-like integrand

$$Q = \iiint e^{-\xi^2} \left(b_0 + \vec{b}_1 \vec{\xi} + + \vec{b}_2 \vec{\xi}^2 + \ldots\right) d\xi^3$$

Algorithm of Dynamic Discrete Ordinate Method

- Similar to the algorithm of DOM
  - Solving BGK Boltzmann equation in physical velocity space
    - Collision
    - Advection
  - Calculating hydrodynamic moments in transformed velocity space
    - DQS
    - Error of $O(Kn^2)$ with 3 x 3 x 3 Gaussian-Hermite quadrature
  - Collision modeling
    - Viscous flow (Chapman-Enskog expansion)

$$f = f^{eq}\left(1+\phi\right) \quad \text{where} \quad \phi = -\frac{1}{\nu f^{eq}}\left(\frac{\partial f^{eq}}{\partial t} + \vec{c}\cdot\frac{\partial f^{eq}}{\partial \vec{x}}\right)$$

    - Inviscid flow

$$n \to \infty \setminus \qquad f = f^{eq}$$

IV. Numerical Results and Validations

a. Hardware/software configuration

b. One-dimensional Riemann problems

c. Two-dimensional problems

- Riemann problems
- Backward-step problem
- Shock-reflection problem
- Cavity flow problems

d. Performance comparison with Roe solver

Hardware/software configuration

- Dell T7400 with dual CPU of Intel Xeon 5482 @ 3.20GHz
- No any parallelization and optimization flag
- Fortran PGI 10.0

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One-Dimensional Riemann Problems

- Shock tube problems

Initial conditions	p_l, ρ_l, u_l	p_r, ρ_r, u_r	t_{final}
Sod (subsonic)	1, 1, 0	0.1, 0.125, 0	0.18
Sjogreen (subsonic)	1.8, 1, -1	1.8, 1, 1	0.14
Sjogreen (supersonic)	0.4, 1, -2	0.4, 1, 2	0.14

Numerical setting	grid nos.	quad. pts.	$\Delta t/\Delta x$
	400	3	0.125

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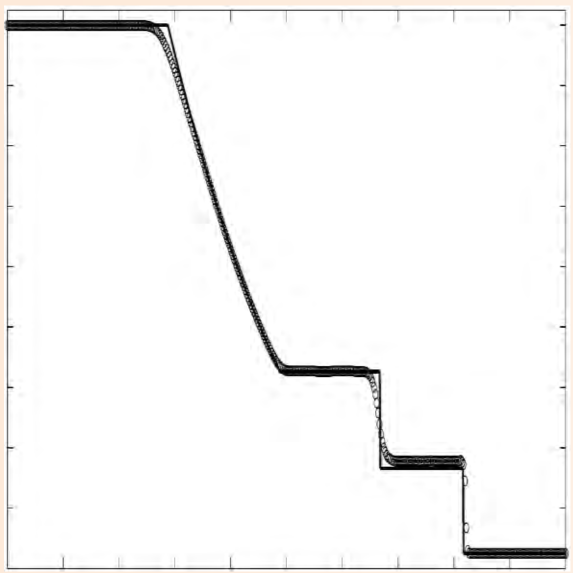
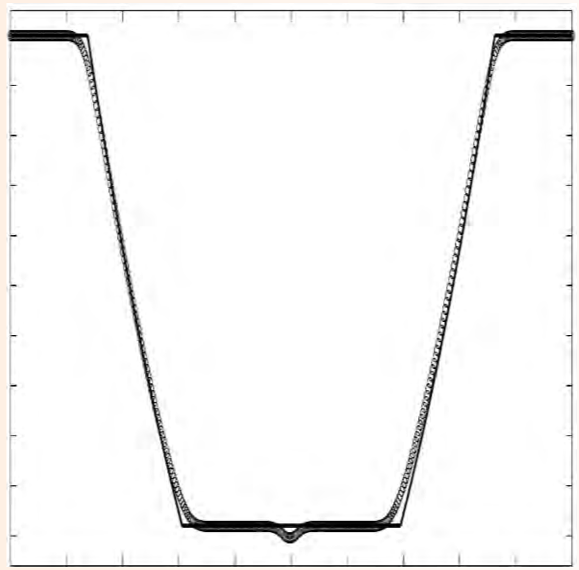
One-Dimensional Riemann Problems

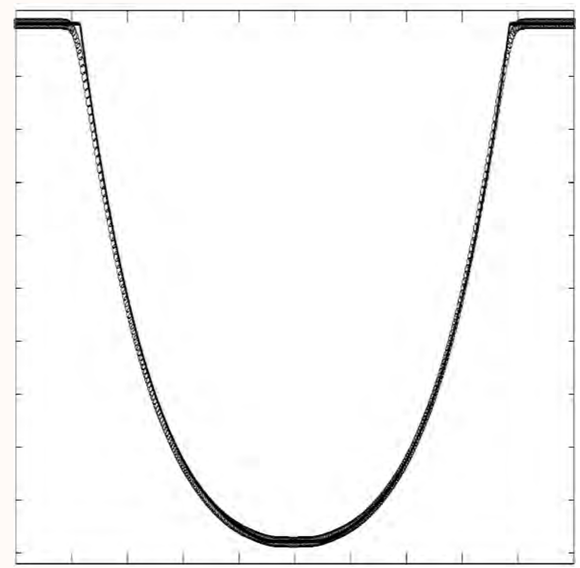
- Numerical result of density profile (reference to solid-line of exact solution)



Sod (subsonic)



Sjogreen (subsonic)



Sjogreen (supersonic)

One-Dimensional Riemann Problems

- 1-D speedup tests (with incomplete transformations)

DOM	DDOM-S	DDOM-P	DDOM
$\vec{\xi} = \vec{c}$	$\vec{\xi} = \vec{c} - \vec{u}$	$\vec{\xi} = \frac{\vec{c}}{\sqrt{2RT}}$	$\vec{\xi} = \frac{\vec{c} - \vec{u}}{\sqrt{2RT}}$

Sod (subsonic)	DOM	DDOM-S	DDOM-P	DDOM
Quad. Pts.	18	14	8	3
Speedup	1.00	0.88	1.45	4.27
Quad. Eff.	1.00	1.46	1.55	1.46

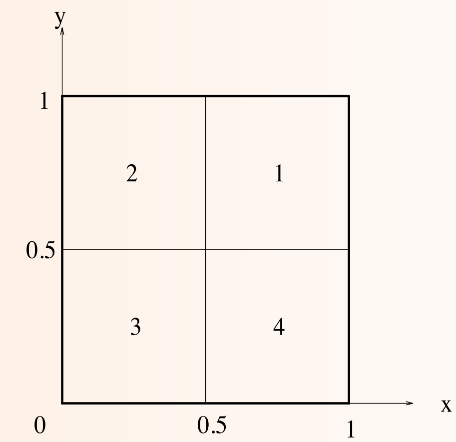
Sjogreen (supersonic)	DOM	DDOM-S	DDOM-P	DDOM
Quad. Pts.	20	24	14	3
Speedup	1.00	0.57	0.99	4.82
Quad. Eff.	1.00	1.46	1.42	1.38

Two-Dimensional Problems

- 2-D Riemann problem
- Backward-step problem
- Shock-reflection problem
- Cavity flow problem
- 2-D speedup tests

Two-Dimensional Problems

- 2-D Riemann problems

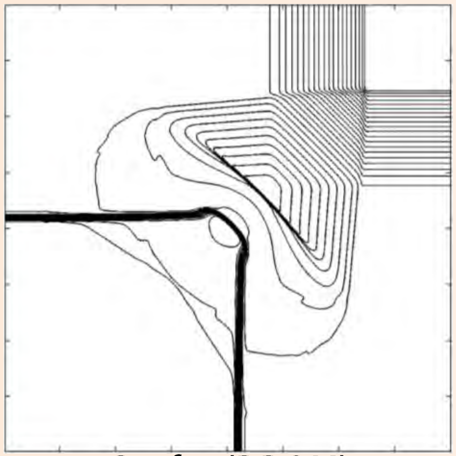


Initial conditions		left	right	t_{final}
Conf. 7 (subsonic) $[p, \rho, u, v]$	upper	0.4, 0.5197, -0.6259, 0.1	1, 1, 0.1, 0.1	0.25
	lower	0.4, 0.8, 0.1, 0.1	0.4, 0.5197, 0.1, -0.6259	
Conf. 15 (supersonic) $[p, \rho, u, v]$	upper	0.4, 0.5197, -0.6259, -0.3	1, 1, 0.1, -0.3	0.20
	lower	0.4, 0.8, 0.1, -0.3	0.4, 0.5313, 0.1, 0.4276	
Conf. 5 (supersonic) $[p, \rho, u, v]$	upper	1, 2, -0.75, 0.5	1, 1, -0.75, -0.5	0.23
	lower	1, 1, 0.75, 0.5	1, 3, 0.75, -0.5	

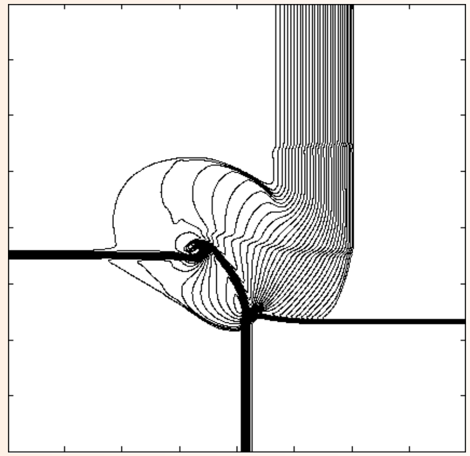
Numerical setting	grid nos.	quad. pts.	$\Delta t / \Delta x$
	400 x 400	2 x 2	0.125

Two-Dimensional Problems

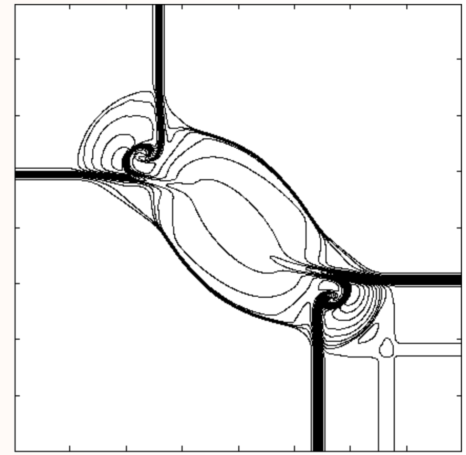
- Numerical result of density contours (reference to Riemann solver)



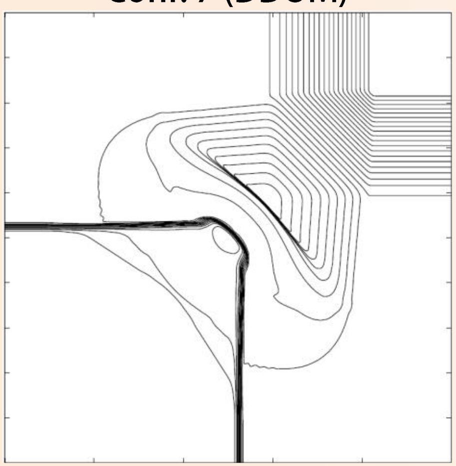
Conf. 7 (DDOM)



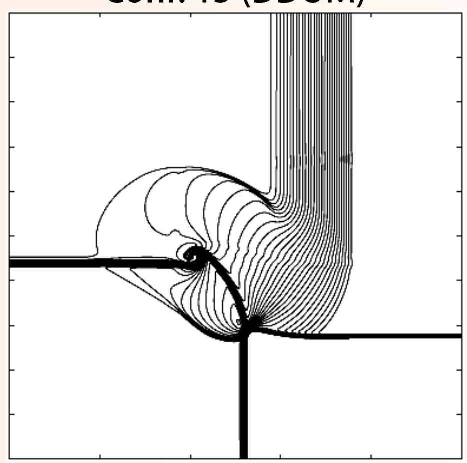
Conf. 15 (DDOM)



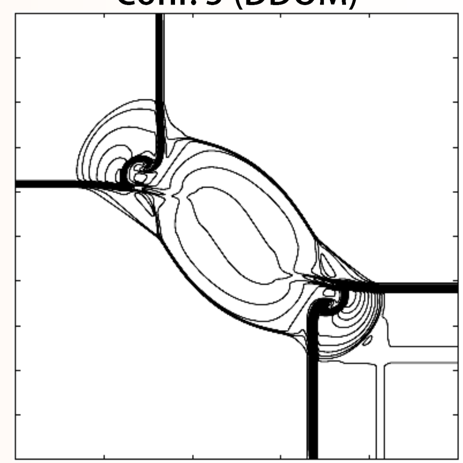
Conf. 5 (DDOM)



Conf. 7 [Lax and Liu (1998)]



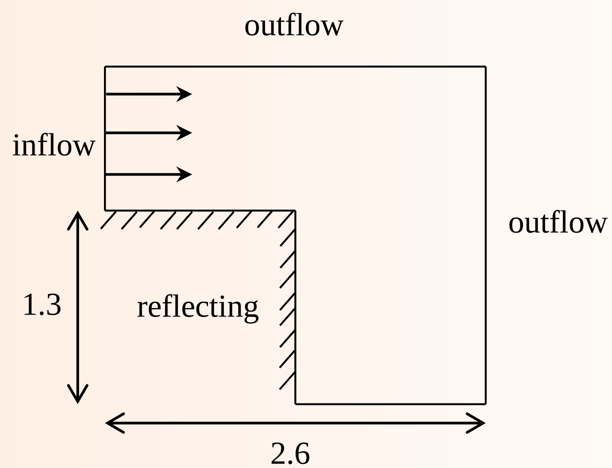
Conf. 15 [Lax and Liu (1998)]



Conf. 5 [Lax and Liu (1998)]

Two-Dimensional Problems

- Backward-step problem

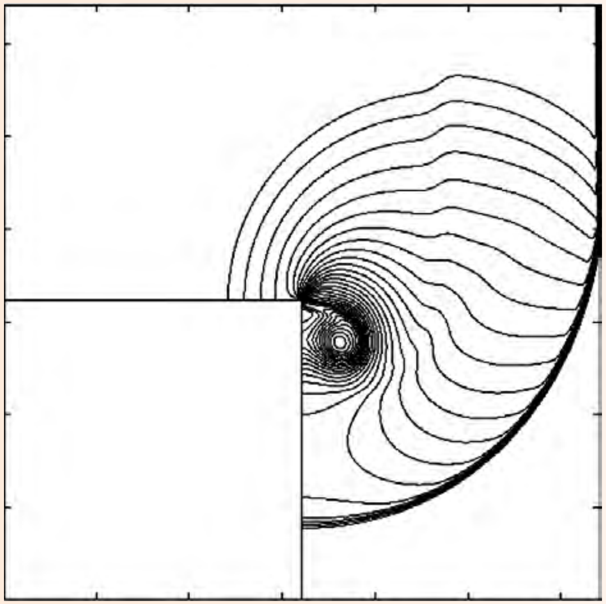


Initial conditions	p	ρ	u	v
inflow	2.4583	1.8620	0.8216	0
outflow	1	1	0	0

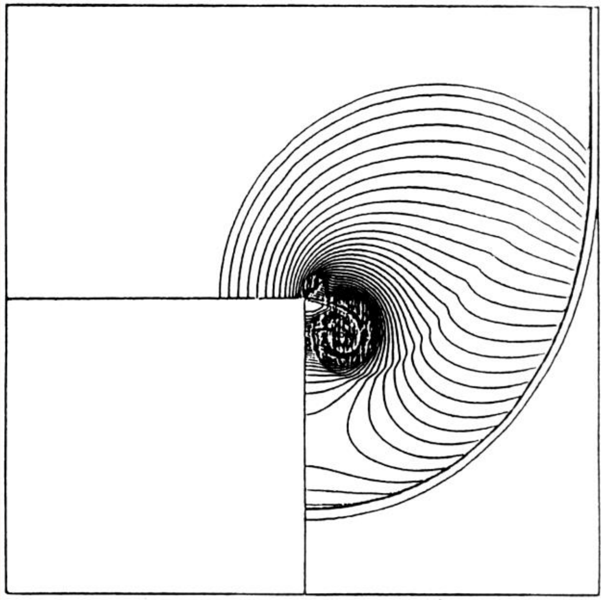
Numerical setting	grid. nos.	quad. pts.	$\Delta t/\Delta x$	t_{final}
	320 x 320	3 x 3	0.125	0.75

Two-Dimensional Problems

- Numerical result of density contours (reference to Riemann solver)



Backward-step (DDOM)



Backward-step [Takayama and Inoue (1991)]

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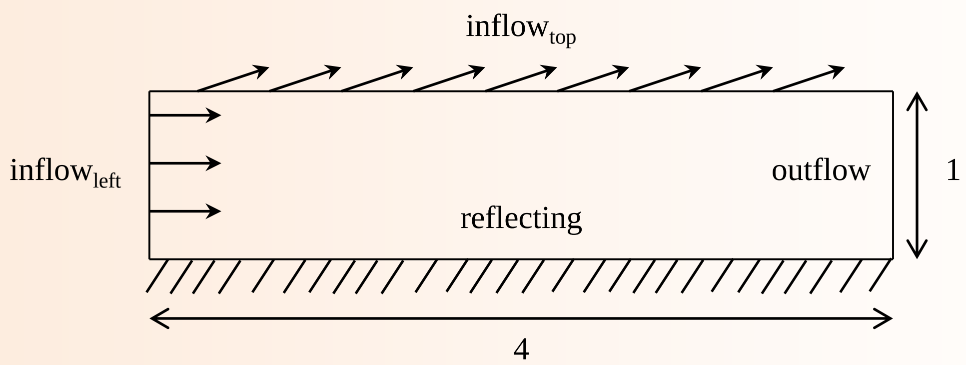
Two-Dimensional Problems

- Shock-reflection problem

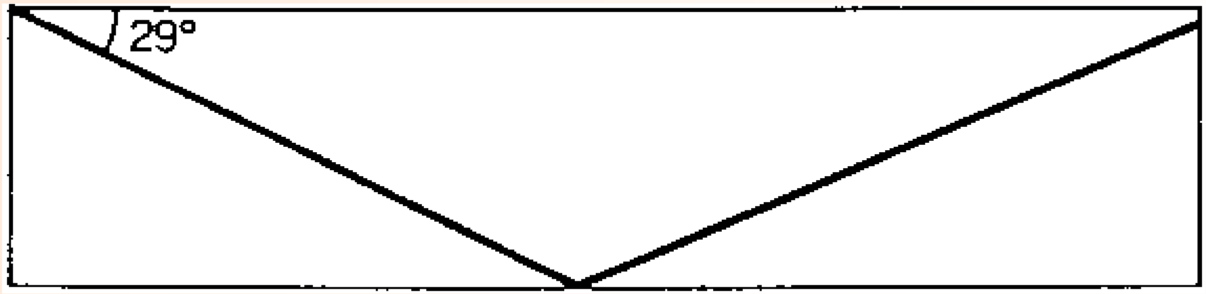


Boundary conditions	p	ρ	u	v
top	1.5282	1.69997	2.61934	0.50632
left	0.7143	1	2.9	0

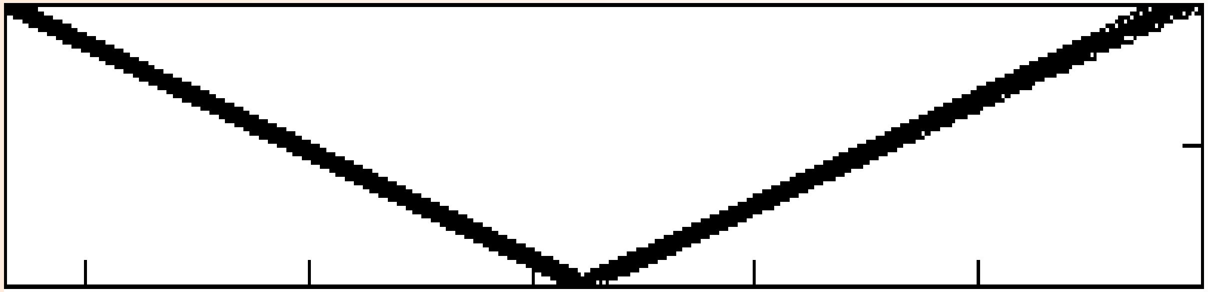
Numerical setting	grid. nos.	quad. pts.	$\Delta t/\Delta x$	t_{final}
	800 x 200	3 x 3	0.125	2.0

Two-Dimensional Problems

- Numerical result of pressure contours (reference to theoretical prediction)



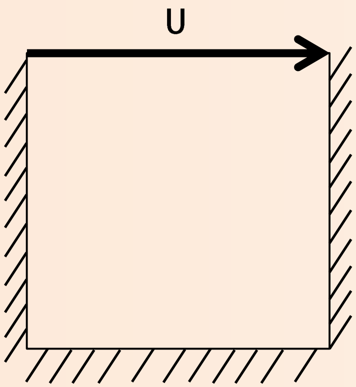
Shock-reflection [Colella (1987)]



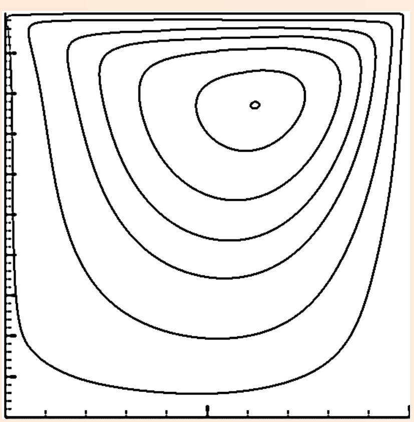
Shock-reflection (DDOM)

Two-Dimensional Problems

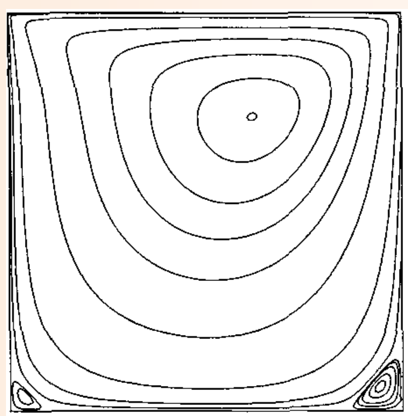
- Steady state solution of cavity flow (reference to LBM solver)



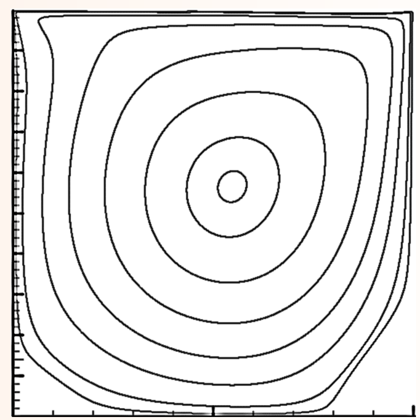
Re	Mach nos.	U_{top}	U_{side}	grid nos.	quad. pts.	$\Delta t/\Delta x$	t_{final}
100	0.15	0.1	0	502 x 502	3x3	0.3	¥
1,000	0.15	1	0	502 x 502	3x3	0.3	¥



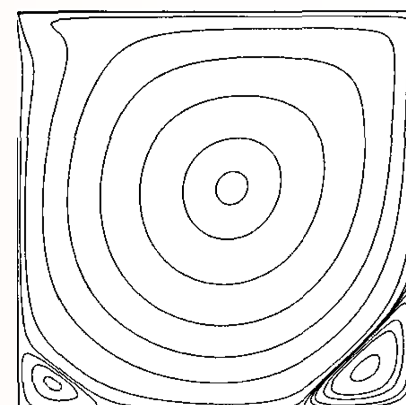
Re = 100 (DDOM)



Re = 100 [Hou et al.(1995)]



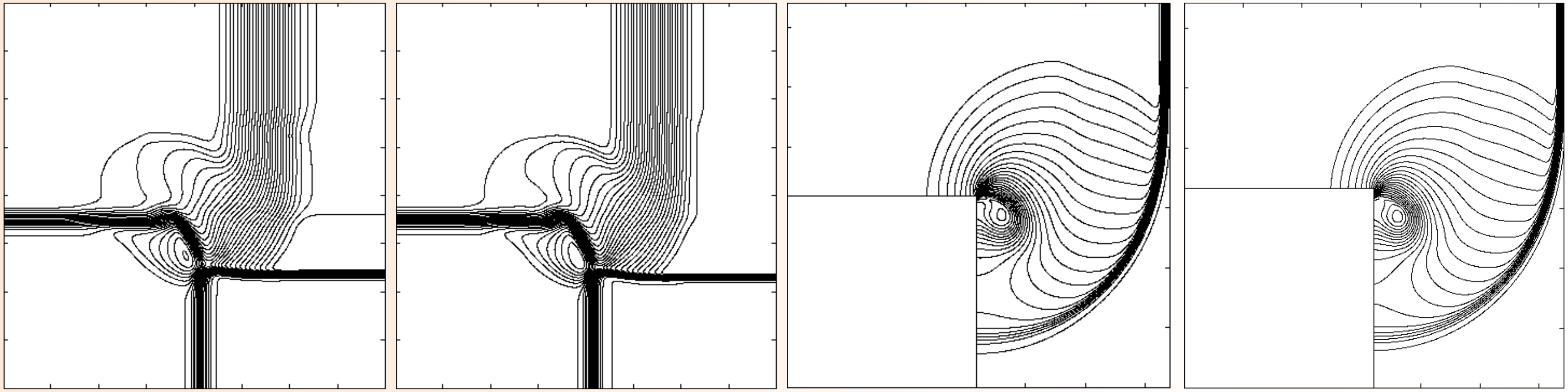
Re = 1,000 (DDOM)



Re = 1,000 [Hou et al.(1995)]

Two-Dimensional Problems

- 2-D speedup tests (Riemann and Backward-step problems)



Conf. 15 (DOM) | Conf. 15 (DDOM) | Backward-step (DOM) | Backward-step (DDOM)

Convergence rate	Quad. Pts.		Speedup	
	DOM	DDOM	DOM	DDOM
Riemann	256	4	1.00	20.09
Backward-Step	324	9	1.00	14.98

Performance Comparison with Roe Solver

- Roe solver by *CLAWPACK* (approximated Riemann solver)
  - Stable
  - Efficient
  - Low-numerical viscosity
- Enhanced DDOM solver
  - Inviscid flow model
  - Fast-scheme + Adaptive quadrature method

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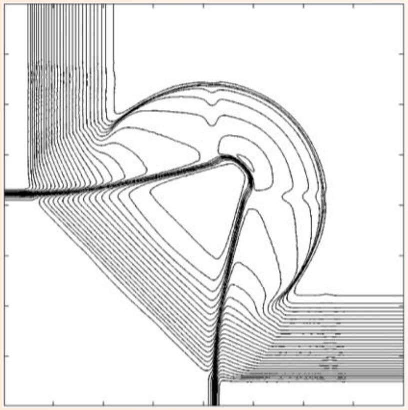
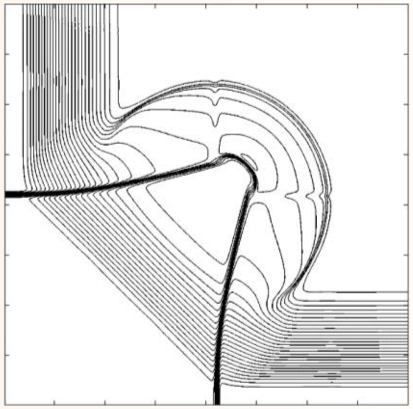
Performance Comparison with Roe Solver

- **Speedup tests** (Conf. 8 of 2D Riemann problem with 400 x 400 grids)



Enhanced DDOM

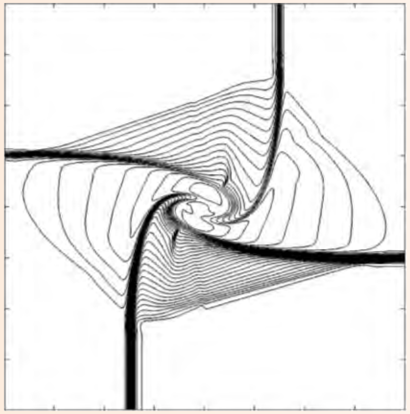


Splitting (Roe)

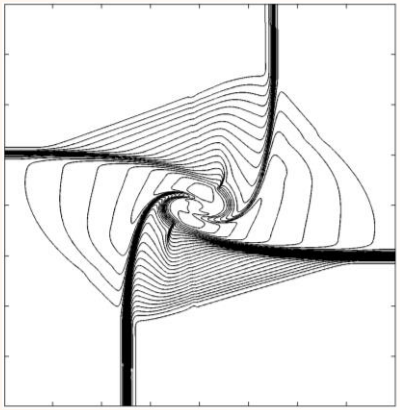
- DDOM is 14% faster than Roe Solver

Performance Comparison with Roe Solver

- **Speedup tests** (Conf. 6 of 2D Riemann problem with 400 x 400 grids)



Enhanced DDOM



Splitting (Roe)

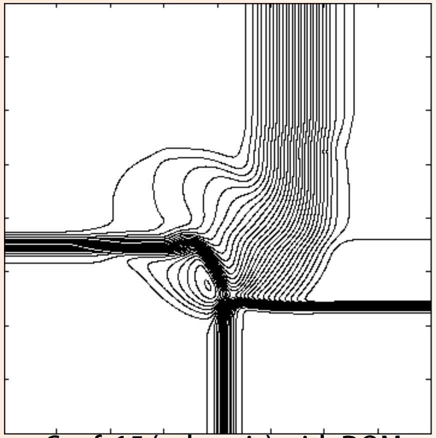
- DDOM is 14% faster than Roe Solver

Concluding Remarks on 2-D DDOM

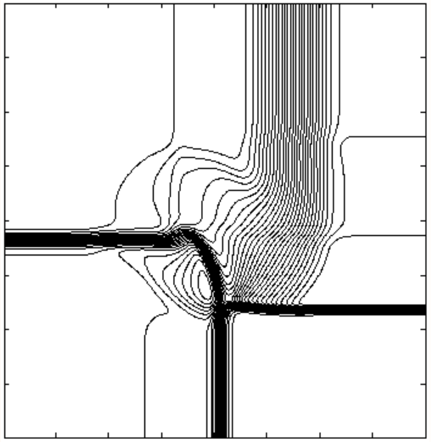
1. 2D-DDOM code is 20 times faster than conventional DOM.
2. Enhanced 2D-DDOM code is 14% faster than Roe solver.
3. With single CPU, real running time about 100 seconds for the 2-D Riemann problems of very short time (0.3 second).
4. Estimated time, for 3-D Riemann problem with grid 400 x 400 x 400 and quadrature 3 x 3 x 3, will be about 33 hours.
5. Parallel computing is inevitable for practical 3-D DDOM simulations.

Preliminary 3-D Test Results

- Riemann problem with 400 x 400 x 10 grids



Conf. 15 (subsonic) with DOM



Conf. 15 (subsonic) with DDOM

- 200 times speedup

Conf. 15 (subsonic)	Quad. pts.	Speedup	Cost/step/grid(ms)
DDOM	2 x 2 x 2	232X	1.31
DOM	16 x 16 x 16	1X	304.

V. Massively Parallel Computation

a. Features of DDOM for parallelization

b. Methods of parallel computing

c. Hardware configuration

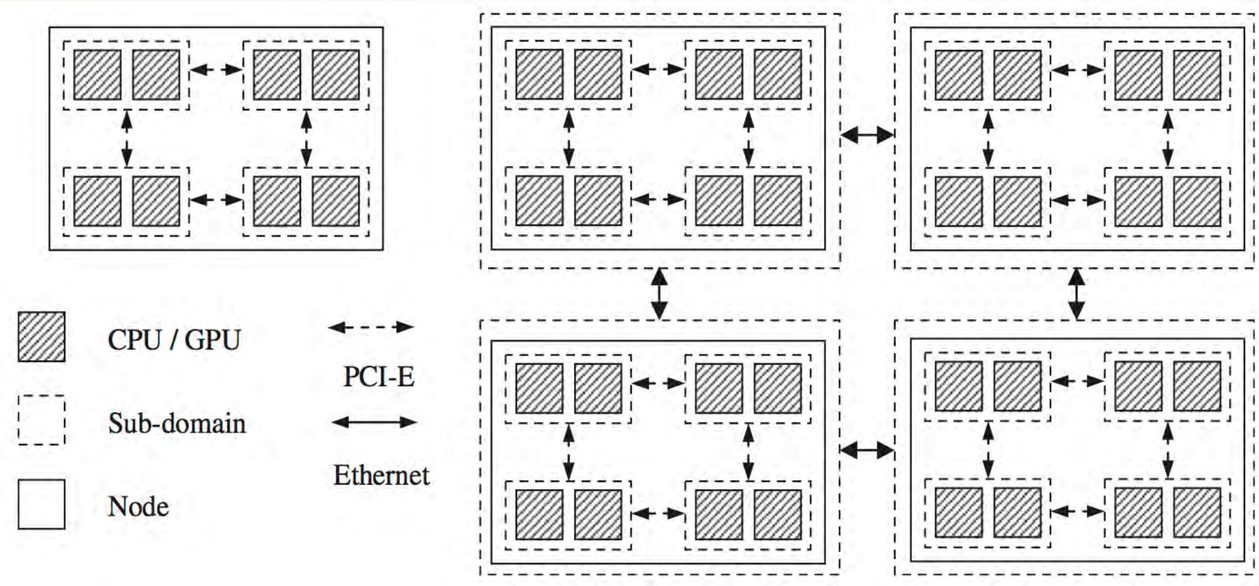
d. Performance tests

Features of DDOM for Parallelization

- Uncoupled features
  - Spatial space (*x*, *y*, and *z* grid system)
  - Velocity space (c_α, c_β and c_γ quadrature points)
- Data-localization
  - Nearby spatial and velocity space data
  - Low data accessing time
- Simple algebraic algorithm
  - No iteration
  - Only algebraic operation

Methods of Parallel Computing

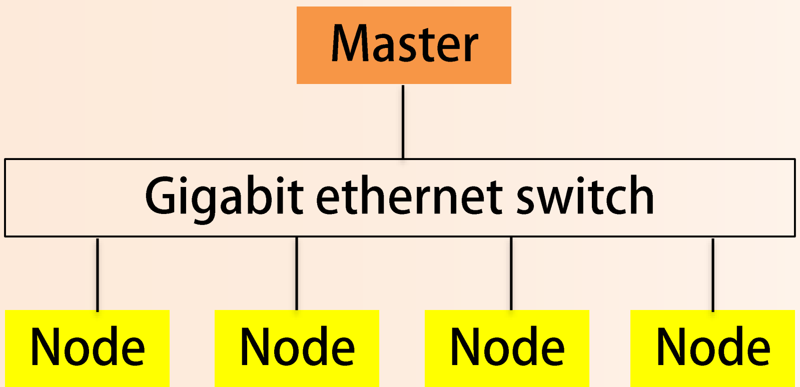
- Parallel programming methods
  - Domain decomposition
  - Parallel programs (OpenMP, MPI, CUDA)



Hybrid parallelism model

Hardware Configurations

- Beowulf cluster



Schematic of Beowulf cluster

Setup of Beowulf cluster

Platform	Device	Node	Core/Node	Processor/Core	Processor
Cluster	Intel W5590	8	2	4	64
Cluster	Nvidia GTX 460	2	2	336	1,344
	Intel W5590				

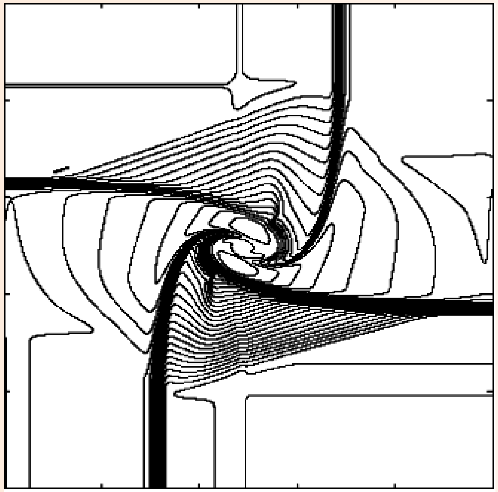
Test Problems and Settings

Test problems		Grid nos.	Quad. pts.	Scheme	Parallel-level
A	2-D Riemann	2,500 x 2,500	3 x 3	Standard	Thread
B	2-D Riemann*	640 x 640 x 44	3 x 3 x 3	Fast	Data
C	2-D Cavity flow	1,024 x 1,024	3 x 3	Standard	Data

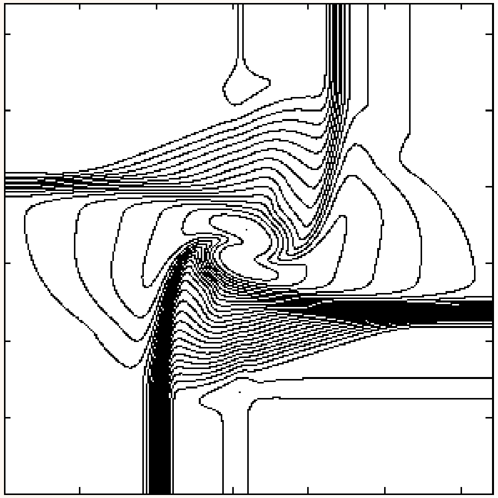
Test nos.	Program	Memory	Node	Core / GPU
A	OpenMP/MPI	Shared/Distributed	8	16 / 32 / 64
B	OpenMP/MPI/CUDA	Shared/Distributed	2	1 / 2 / 4
C	OpenMP/MPI/CUDA	Shared/Distributed	2	1 / 2 / 4

* 2-D Riemann problem calculated with 3D-DDOM code, where the gradient of the macroscopic variables in z-direction are given as zero.

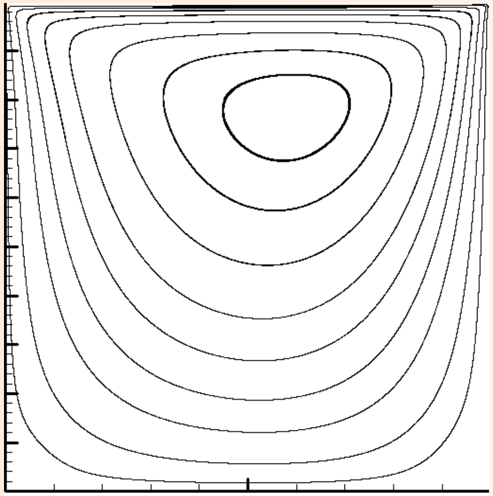
Preliminary Results of Parallel-DDOM



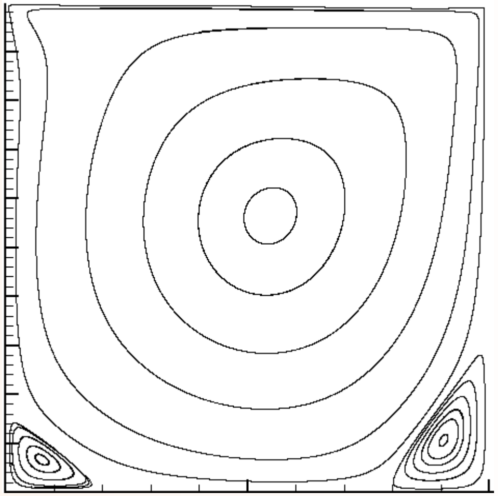
Test A, 2D DDOM (CPU)



Test B, 3D DDOM (GPU)



Test C, Cavity Flow at Re=100 by (GPU)



Test C, Cavity Flow at Re=1,000 by (GPU)

Parallel-DDOM Performance

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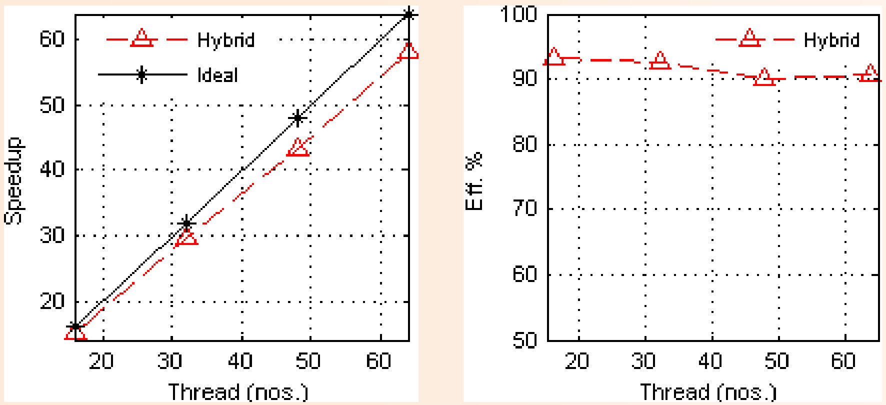
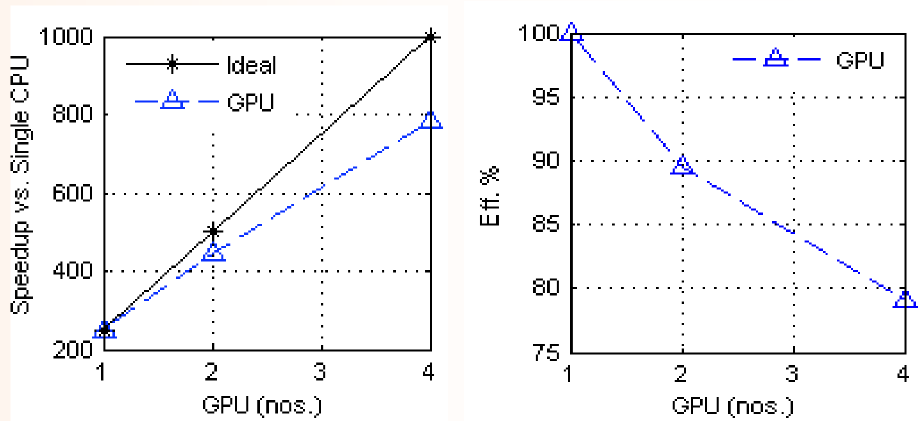
Test A with CPU-Cluster



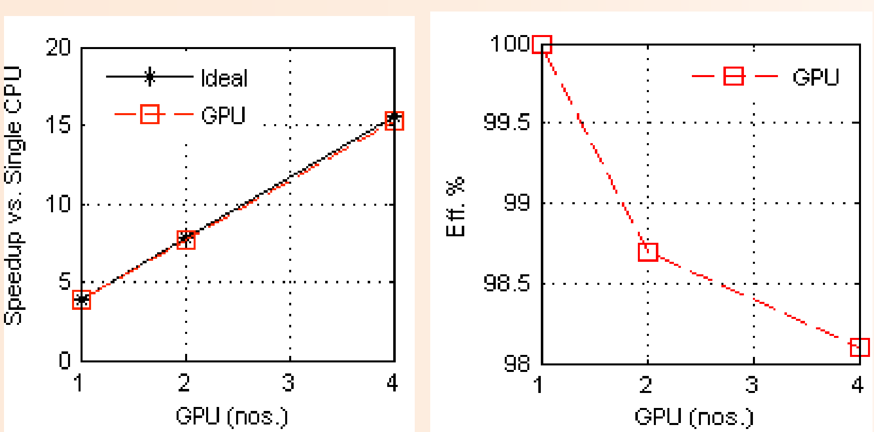
(2D Riemann | Δ OpenMP/MPI)

Test B with GPU-Cluster



(3D Riemann | Δ OpenMP/MPI/CUDA)

Test C with GPU-Cluster



(2D Cavity Flow | □ OpenMP/MPI/CUDA)

- Over 90% parallel efficiency of parallel-DDOM solver is achieved for CPU-cluster.
- Around 80 to 90 % parallel efficiency of parallel-DDOM solver is achieved for GPU-cluster.
- Parallel DDOM is a good candidate for parallel computing.

- **DDOM Code Summary**

Robust	Inviscid flow	✔
	Viscous flow	✔
	Incompressible flow	✔
	Compressible flow	✔

Efficient	Quadrature points	2x2x2 — 3x3x3 for 3D case
	Speedup over DOM	Around 20X for 2D case
	Performance	Efficiency as Roe solver

Scalable	Speedup by CPU cluster	Over 57X @ 90% parallel efficiency
	Speedup by GPU cluster	Over 780X @ 80% parallel efficiency

VI. Conclusions

1. DOM was reviewed to reveal its low-efficiency deficiency at high Mach number.
2. DQS was proposed and implemented to DOM, termed as DDOM, to resolve the deficiency of DOM.
3. One and two-dimensional DDOM codes were developed and tested to show the codes are robust applicable to different type of flows.

VI. Conclusions

4. The 1-D DDOM code is 5-times faster than conventional 1-D DOM code, and 20-times faster for 2-D DDOM code.
5. Further enhancement of the 2-D DDOM code achieved 14% faster than Roe solver.
6. Parallel 2-D and 3-D DDOM codes have been developed and preliminarily tested.
7. Over 90% parallel efficiency has been achieved with 64-CPUs cluster, and about 80 to 90% parallel efficiency with 4-GPUs cluster (780 times speedup).

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THANK YOU