

A novel multigrid approach for solving incompressible Navier-Stokes equations on massively parallel supercomputers

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Outline

- **Concept and motivation**
- **Pressure-velocity coupled formulation of the Navier-Stokes equations**
- **Benchmark problems**
- **Analytical Solution Accelerated (ASA) smoother**
- **3D domain decomposition and scalability properties**
- **Application to the linear stability analysis**
- **Conclusions**

Target: *Incompressible Navier-Stokes equations*

Continuity: $\nabla \cdot \mathbf{u} = 0$

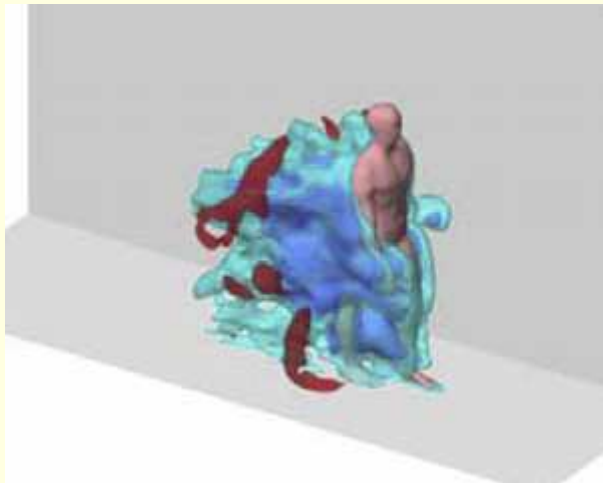
Momentum: $\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}$

- No separate equation for pressure
- No boundary conditions for pressure
- Assume: no simplifications possible

Concept: *Fixed structured grid* +
Pressure-velocity linked formulation

Curved boundaries on fixed grid:

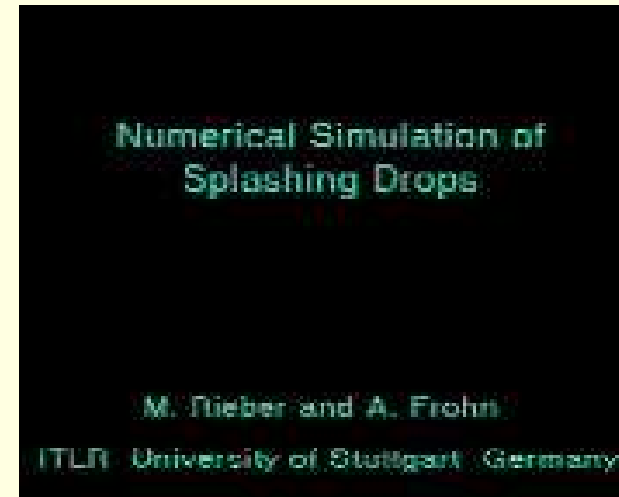
Immersed boundary approach
(Peskin, 1977)



Choi et al., 2007

Moving boundaries on fixed grid:

Volume-of-Fluid (Hirt & Nichols, 1981)
or **Level Set** (Osher, 1988) methods



Why not to decouple pressure and velocity ?

Pressure-velocity decoupling:

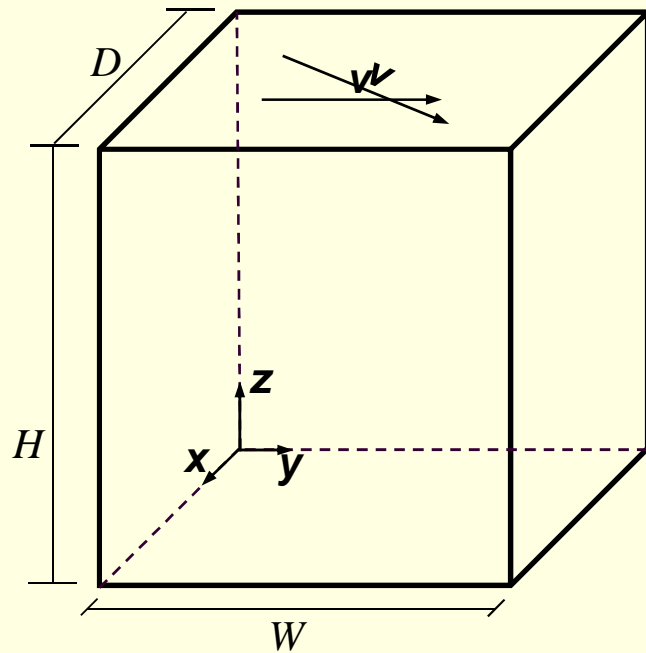
- ✓ Good robustness
- ✓ Low memory consumption
- ✗ Slow rate of convergence
- ✗ Non-physical pressure field
- ✗ Not applicable for liquid – solid interface problems

Pressure-velocity coupling:

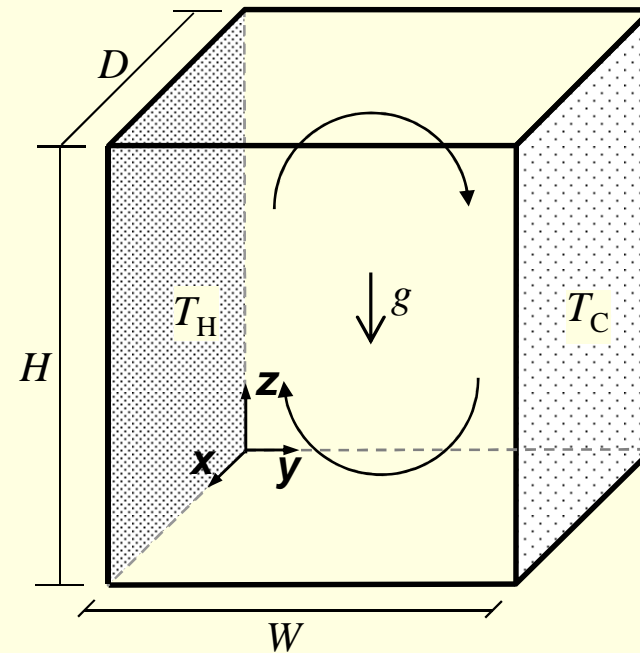
- ✓ Better convergence
- ✓ This is what the nature asks for
- ✓ The obtained pressure is physical
- ✗ High memory consumption
- ✗ Not as robust as decoupling methods

Benchmark Problems

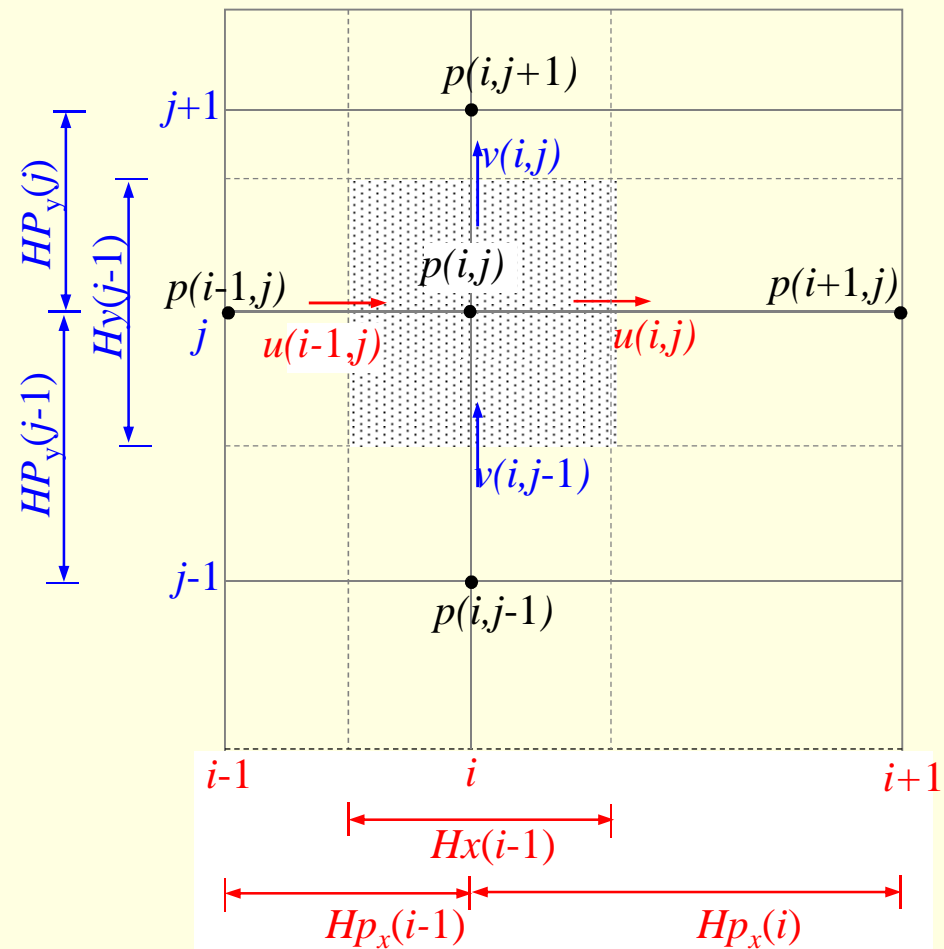
Lid-driven cubic cavity



Differentially heated cubic cavity



Staggered grid for finite volume method



The target: *efficient time-stepping*

To perform a time step \Leftrightarrow inverse of the *Stokes operator*

$$\begin{bmatrix} \frac{1}{\Delta t} - \frac{\Delta^{(u)}}{Re} & 0 & 0 & \partial_x \\ 0 & \frac{1}{\Delta t} - \frac{\Delta^{(v)}}{Re} & 0 & \partial_y \\ 0 & 0 & \frac{1}{\Delta t} - \frac{\Delta^{(w)}}{Re} & \partial_z \\ \partial_x & \partial_y & \partial_z & 0 \end{bmatrix} \begin{pmatrix} u \\ v \\ w \\ p \end{pmatrix} = \begin{pmatrix} f_u \\ f_v \\ f_w \\ 0 \end{pmatrix}$$

+ *boundary conditions for velocity*

+ *Dirichlet point for pressure*

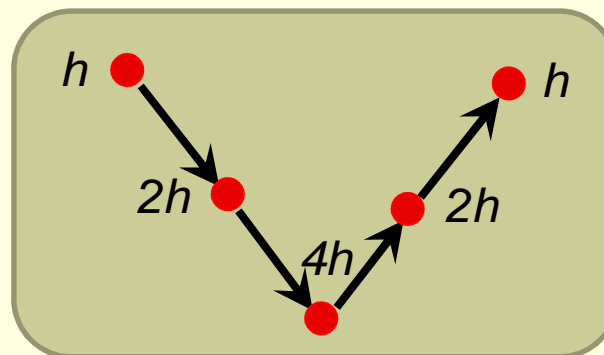
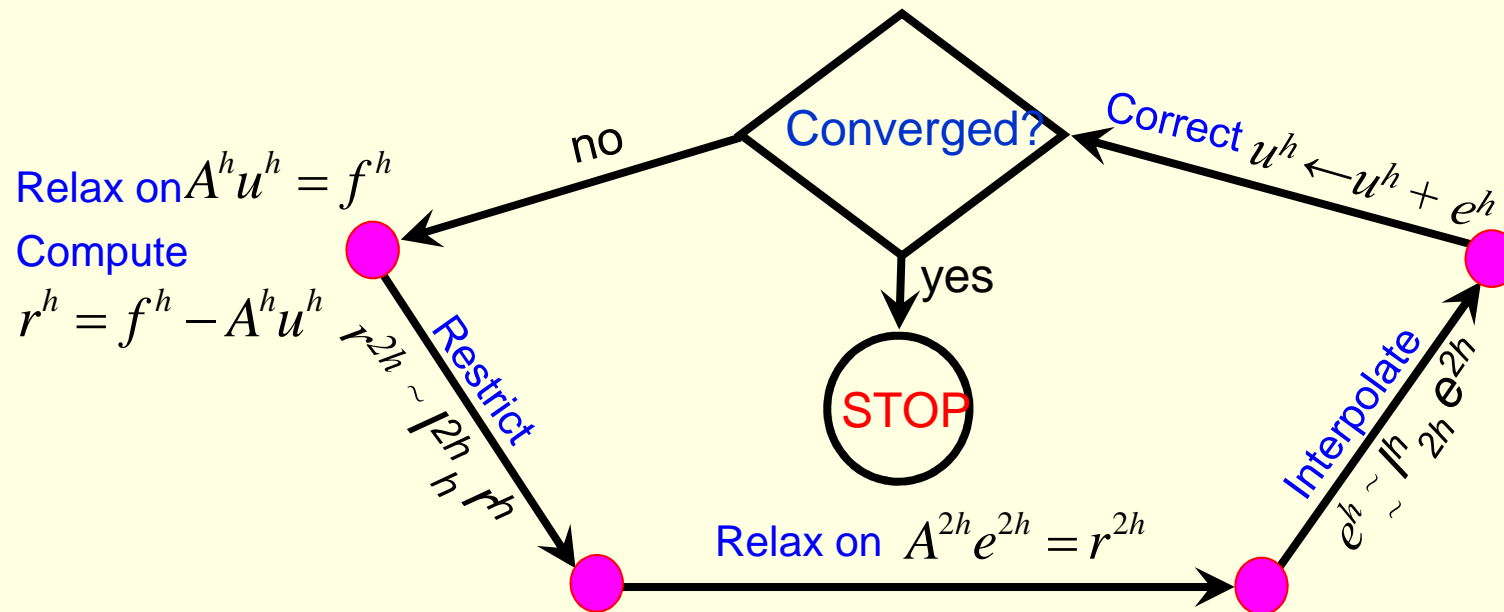
Stokes operator

Multigrid approach – a possible choice

- ✓ Low memory and CPU time consumption, $O(N)$
- ✓ Pressure-velocity coupling can be utilized
- ✓ Easily parallelized (by MPI or Open MP tools)
- ✗ Non-constant convergence rate
- ✗ Sophisticated programming is needed

Multigrid approach – the concept

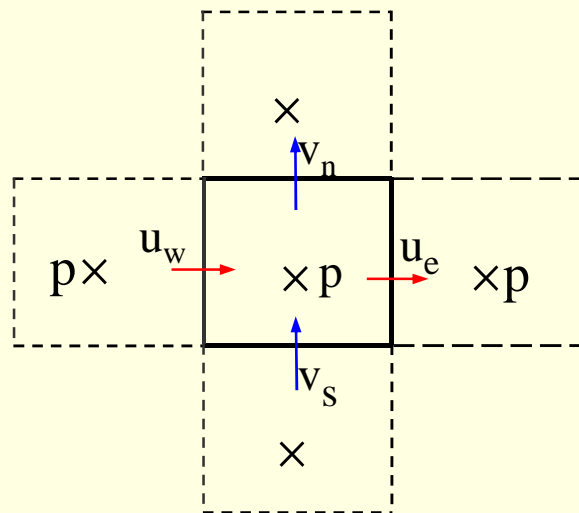
Typical Multigrid Cycle – Correction Scheme (CS)



V - cycle

Symmetrical coupled Gauss-Seidel smoothing operator (SCGS)

S.P. Vanka (1985) – analytical solution for a *single* finite volume



$$(u, v)^{\text{new}} = (u, v)^{\text{old}} + r_{(u,v)}(u, v)'$$

$$p^{\text{new}} = p^{\text{old}} + r_p p'$$

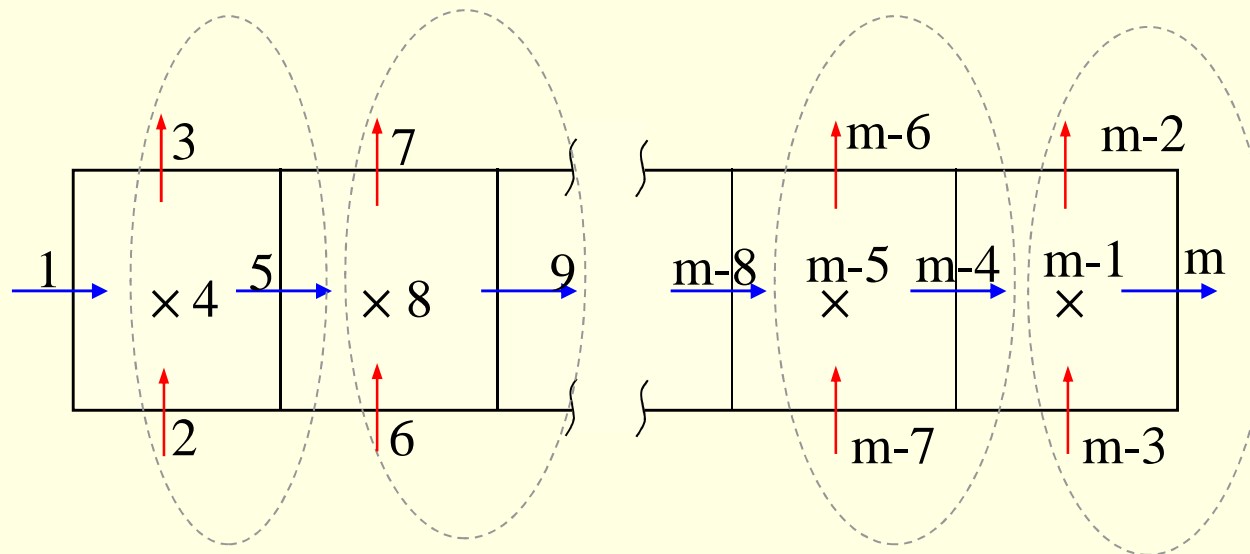
$$\begin{bmatrix} A_1 & 0 & 0 & 0 & A_2 \\ 0 & A_3 & 0 & 0 & A_4 \\ 0 & 0 & A_5 & 0 & A_6 \\ 0 & 0 & 0 & A_9 & A_{10} \\ A_7 - A_7 & A_8 & -A_8 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} u'_e \\ u'_w \\ v'_n \\ v'_s \\ p'_p \end{bmatrix} = \begin{bmatrix} R_{ue} \\ R_{uw} \\ R_{vn} \\ R_{vs} \\ R_{cp} \end{bmatrix}$$

for the Stokes operator and a constant time step A_i are constants and the 5×5 matrix can be inverted analytically

Accelerated Coupled Line Gauss-Seidel Smoother (ASA-CLGS) -2D

Zeng and Wesseling (1993) – CLGS: Horizontal (vertical) sweeping **with** horizontally (vertically) adjacent pressure linkage: **inverse of block – tri-diagonal matrix for single row (column)**

Feldman and Gelfgat (2009) – **ASA-CLGS**: Horizontal (vertical) sweeping **without** horizontally (vertically) adjacent pressure linkage: **analytical solution over single row (column)**



Accelerated coupled line Gauss-Seidel smoother (ASA-CLGS) -2D

Zeng and Wesseling (1993) – CLGS:

...

$$A_{i+1/2,j}^{(x)} u'_{i+1/2,j} + B_{i+1/2,j}^{(x)} p'_{i,j} = R_{i+1/2,j}^{(x)}$$

$$A_{i-1/2,j}^{(x)} u'_{i-1/2,j} - B_{i-1/2,j}^{(x)} p'_{i,j} = R_{i-1/2,j}^{(x)}$$

$$A_{i,j+1/2}^{(y)} v'_{ij+1/2} - B_{i,j+1/2}^{(y)} (p'_{i,j+1} - p'_{i,j}) = R_{i,j+1/2}^{(y)}$$

$$A_{i,j}^{(x)} (u'_{i+1/2,j} - u'_{i-1/2,j}) + A_{i,j}^{(y)} (v'_{i,j+1/2} - v'_{i,j-1/2}) = 0$$

...

Feldman and Gelfgat (2008) –

ASA-CLGS:

...

$$A_{i+1/2,j}^{(x)} u'_{i+1/2,j} + B_{i+1/2,j}^{(x)} p'_{i,j} = R_{i+1/2,j}^{(x)}$$

$$A_{i-1/2,j}^{(x)} u'_{i-1/2,j} - B_{i-1/2,j}^{(x)} p'_{i,j} = R_{i-1/2,j}^{(x)}$$

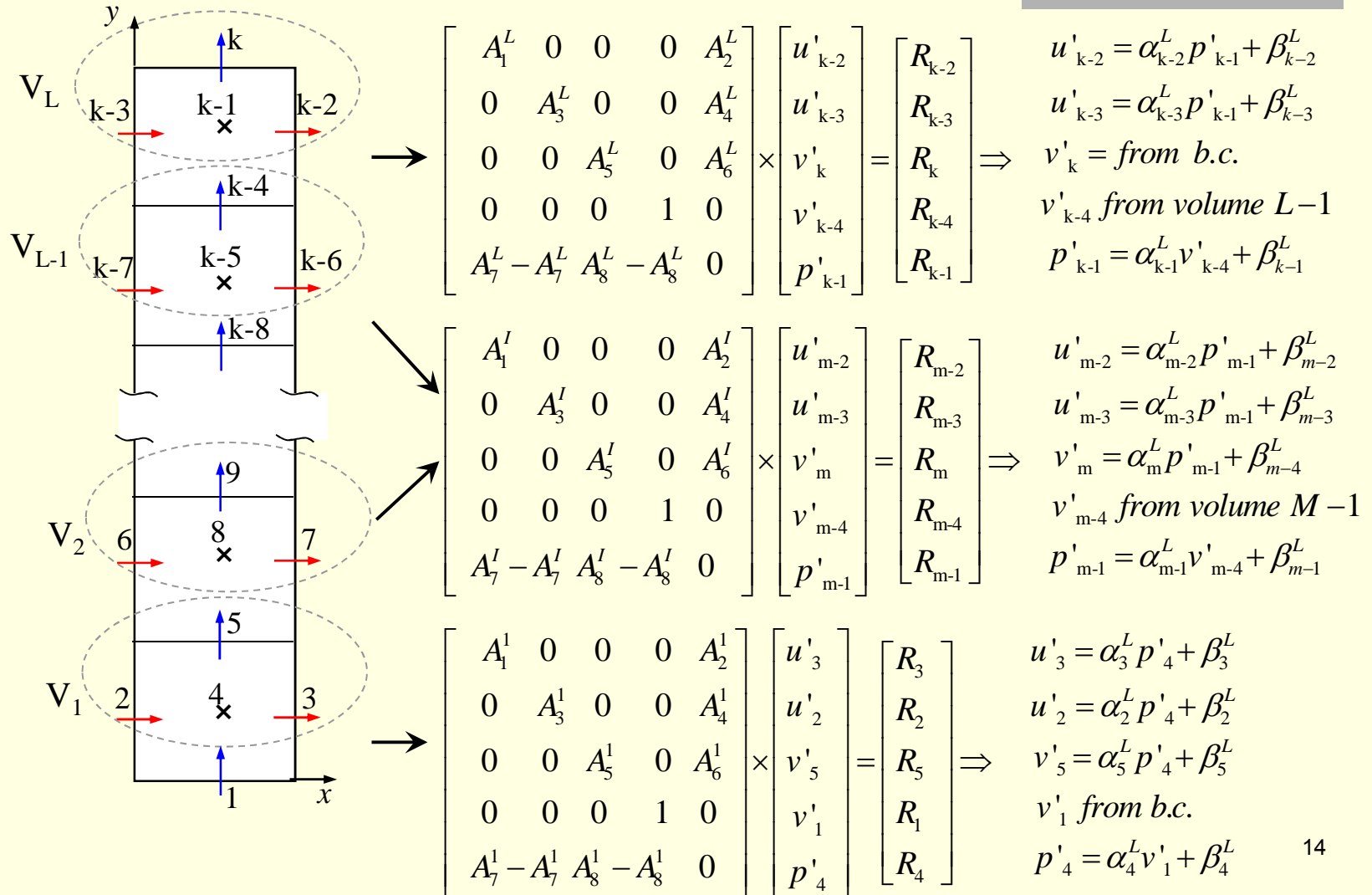
$$A_{i,j+1/2}^{(y)} v'_{ij+1/2} + B_{i,j+1/2}^{(y)} p'_{i,j} = \tilde{R}_{i,j+1/2}^{(y)}$$

$$A_{i,j}^{(x)} (u'_{i+1/2,j} - u'_{i-1/2,j}) + A_{i,j}^{(y)} (v'_{i,j+1/2} - v'_{i,j-1/2}) = 0$$

...

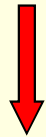
where $\tilde{R}_{i,j+1/2}^{(y)} = R_{i,j+1/2}^{(y)} + B_{i,j+1/2}^{(y)} p'_{i,j+1}$

Analytical solution over a column for ASA-CLGS smoother

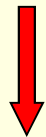


CLGS and ASA-CLGS efficiency estimation for 2D

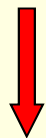
Zeng and Wesseling
(1993) – CLGS:



Block 3-diagonal matrix



Block – or 7-diagonal
Thomas algorithm



$\approx O(15M)$

Feldman and Gelfgat (2009) –
ASA-CLGS

(6-Diagonal Matrix)



$$p'_{k-1} = (c_1^L v'_{k-4} + R_{k-1}^L + \sum_{i=2}^4 c_i^L R_{k-i}^L) / c_5^L$$



$$\begin{bmatrix} v'_5 \\ u'_2 \\ u'_3 \end{bmatrix} = \begin{bmatrix} c_6^1 \\ c_7^1 \\ c_8^1 \end{bmatrix} \times p'_4 + \begin{bmatrix} c_9^1 R_5^L \\ c_{10}^1 R_2^L \\ c_{11}^1 R_3^L \end{bmatrix}$$



$\approx O(5M)$

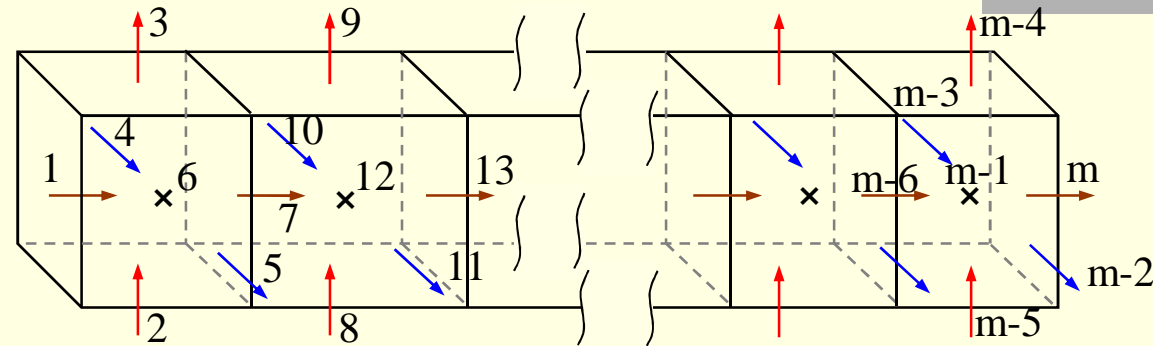
Thomas Algorithm
(3-Diagonal Matrix)



$\approx O(5M)$



ASA-CLGS -efficiency estimation for 3D



$$p'_p = (c_1^I w'_d + R_p^I + c_2^I R_e^I + c_3^I R_w^I + c_4^I R_n^I + c_5^I R_s^I + c_6^I R_d^I) / c_7^I$$

$$\begin{bmatrix} w'_d \\ v'_s \\ v'_n \\ u'_w \\ u'_e \end{bmatrix} = \begin{bmatrix} c_8^I \\ c_9^I \\ c_{10}^I \\ c_{11}^I \\ c_{12}^I \end{bmatrix} \times p'_p + \begin{bmatrix} c_{13}^I R_d^I \\ c_{14}^I R_s^I \\ c_{15}^I R_n^I \\ c_{16}^I R_w^I \\ c_{17}^I R_e^I \end{bmatrix}$$

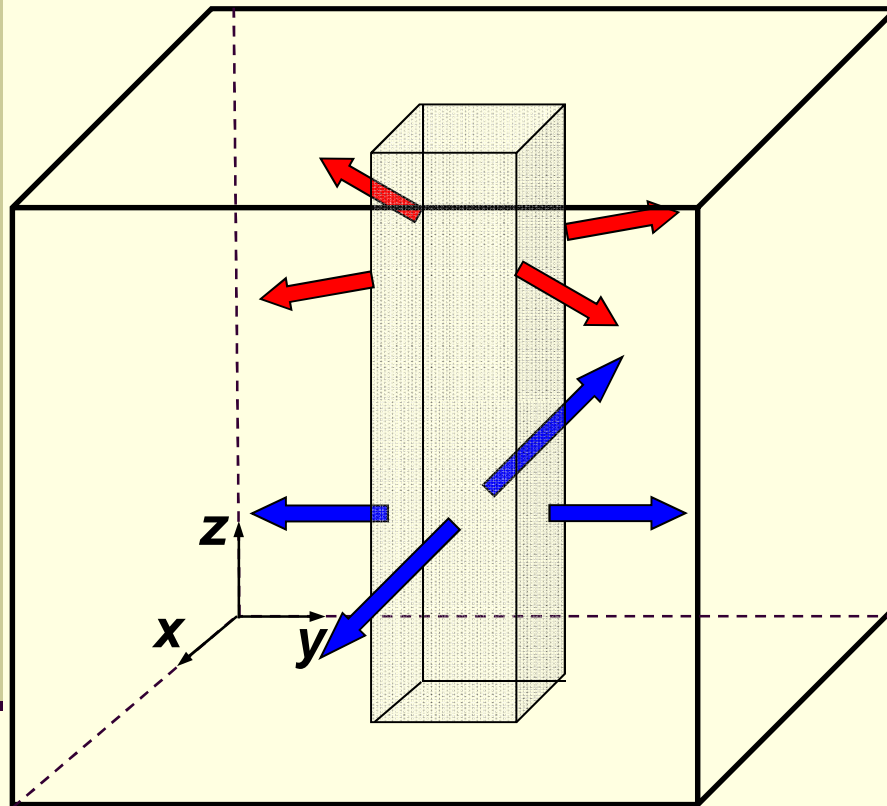
6 corrections for a single volume result in 17 multiplications and divisions and 11 summations

$$\approx O(5M)$$

Advantages and limitations of ASA-CLGS Approach

- ☑ There exists an analytical solution for the entire corrections row (column).
- ☑ Only $O(5M)$ operations are needed to obtain the entire row (column) corrections per one sweep for both **2D and 3D** geometries
- ☑ Effective for stretched grids.
- ☑ Effective for flows with a dominating direction
- ✗ Up to now applicable only for structured Cartesian grids.
- ✗ Slow convergence rate for large time steps

Domain decomposition for 3D configuration

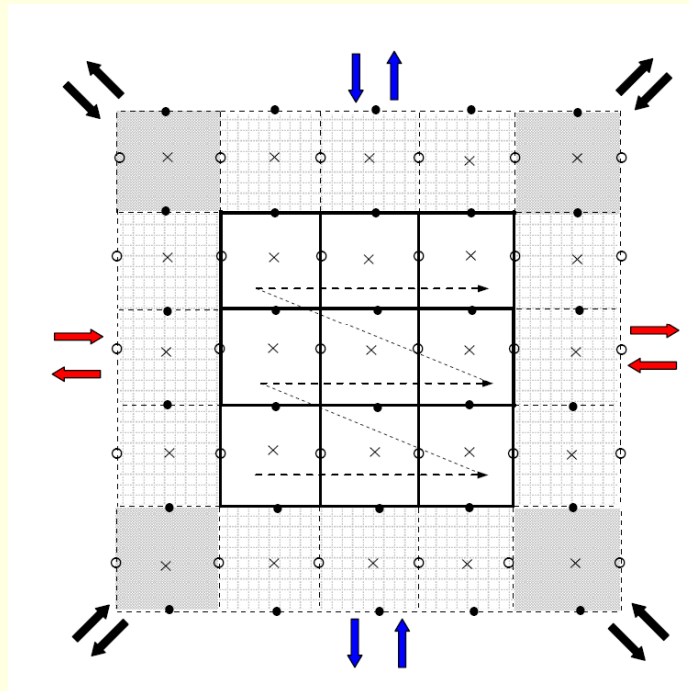


Existence of analytical solution for the whole column allows for 2D virtual topology of 3D configuration.

➡ All volumes located at the sub -volume faces exchange data with neighbors

➡ All volumes located at the **sub -volume vertical edges** exchange data with **diagonal** neighbors

3D Configuration: data exchange principle



○ v_y velocity

● v_x velocity

x pressure



2 processors
overlapping region



4 processors
overlapping region

Block relaxation on staggered grid



Simultaneous updating of $i, i+1$ and $j, j+1$ velocities



Dependence on velocity values located at the grid points $i, i\pm 1, i\pm 2, j, j\pm 1, j\pm 2$

The size of minimal redistributed sub-domain is 3×3

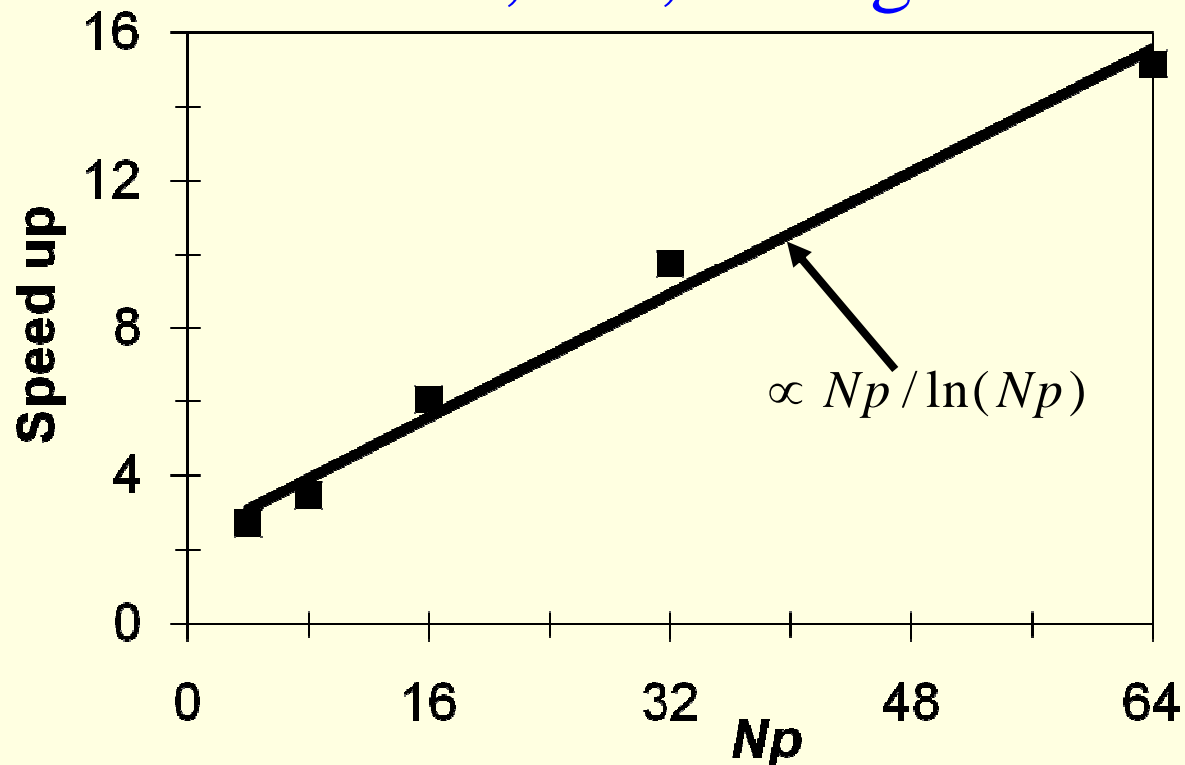


Critical points to enhance algorithm scalability

- **Blocking communication between neighboring processors (synchronous send-and-receive commands) .**
- **Explicit data communication between all neighbor processors , including the diagonal neighbors.**
- **Utilizing telescoping multigrid approach may cause problems in proper balancing on the finest grid, therefore blocking communication should be used.**
- **The decoupled energy equation is solved only on the finest grid by a simple Gauss-Seidel iteration.**

Scalability characteristics of ASA-CLGS - multigrid approach

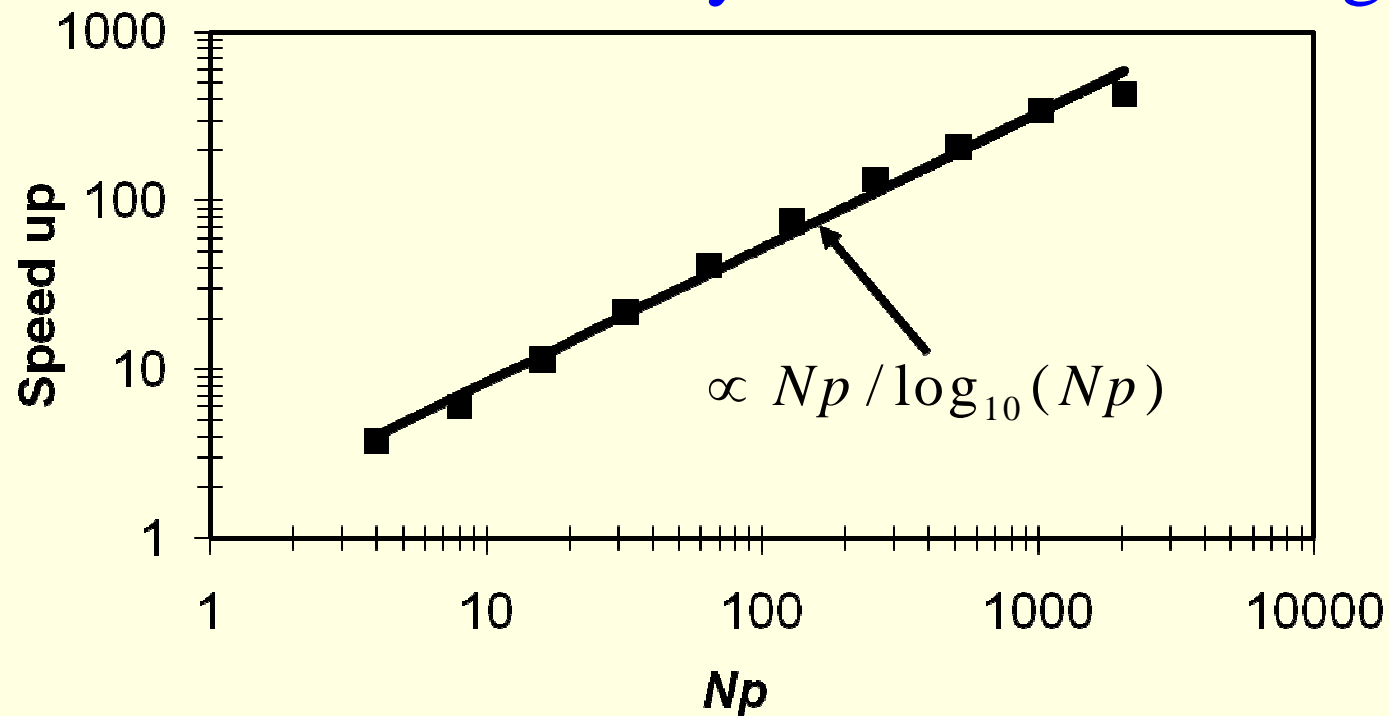
3D Lid driven cavity, $Re=1950$:
 25^3 , 50^3 , 100^3 grids



Number of CPU is restricted by the coarsest level ($8 \times 8 = 64$ CPU) 21

Scalability characteristics of ASA-CLGS – single grid approach

3D Lid driven cavity, $Re=1950$: 200^3 grid



2048 CPU applied on 200^3 grid \longrightarrow 57.4 msec per time step \longrightarrow
only 16 hours for 10^6 time steps

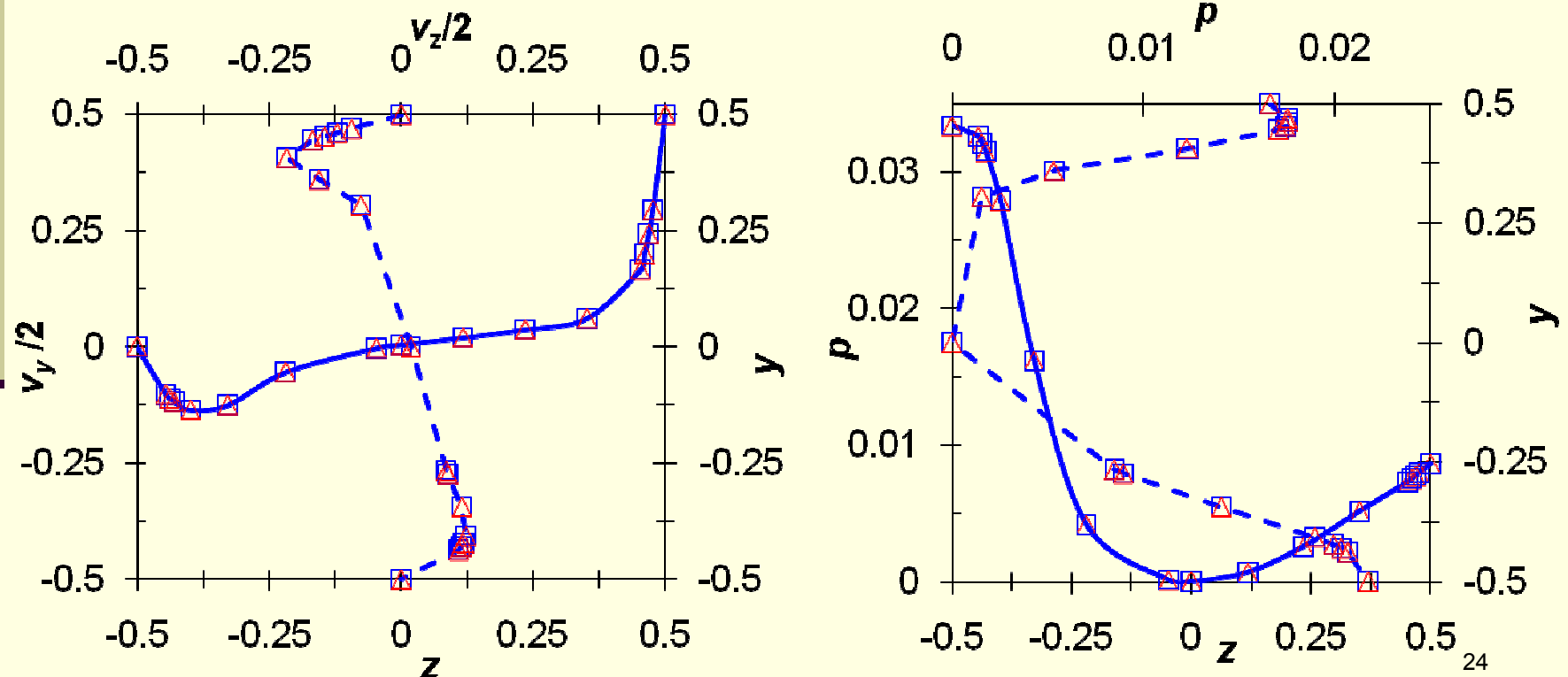
General solution strategies

- For a large number of processors the **single-grid** scalability is **significantly more efficient** than that of the multigrid.
- The efficiency of single-grid approach may be obliterated if **at two consecutive time steps** the velocity and/or pressure are **considerably different**. In this case a **relatively low amount** of involved cores will be compensated by a **high convergence rate** of the multigrid.
- Once a stable **asymptotic** regime is approached, the calculations can be performed on the single **finest grid only** with maximal possible number of CPU cores.

Verification: Lid-driven cavity, $Re=10^3$

ρ , v_y and v_z distribution along two centerlines

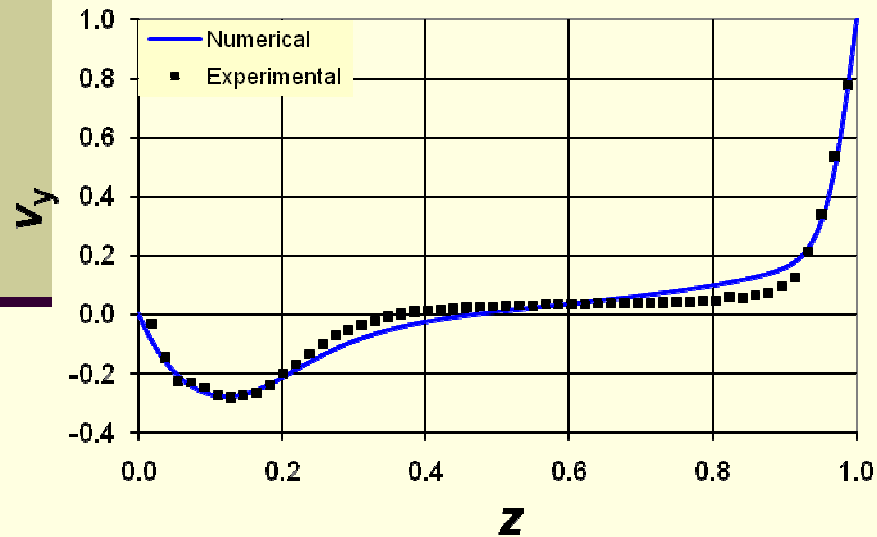
The present solution \triangle and the solution of Albensoeder and Kuhlmann (2005) \square



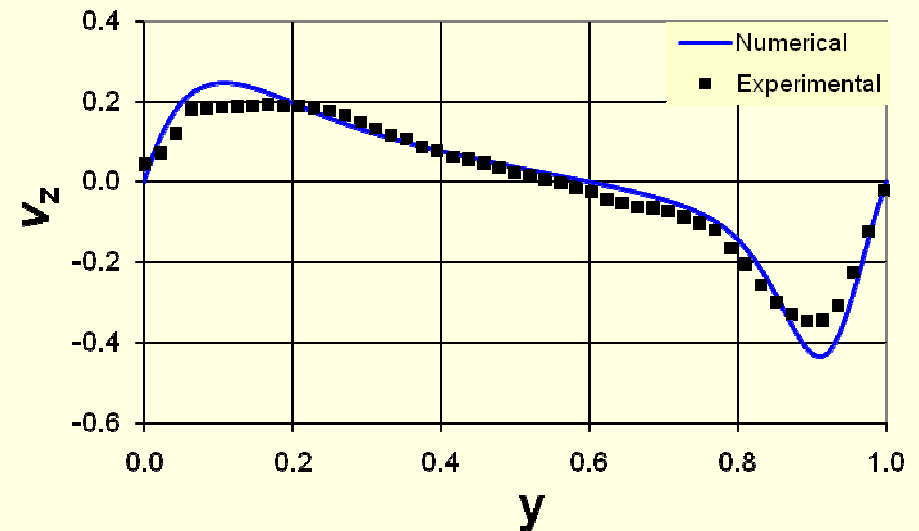
Validation: Lid-driven cavity, $Re=10^3$

Comparison with experiments of A. Liberzon

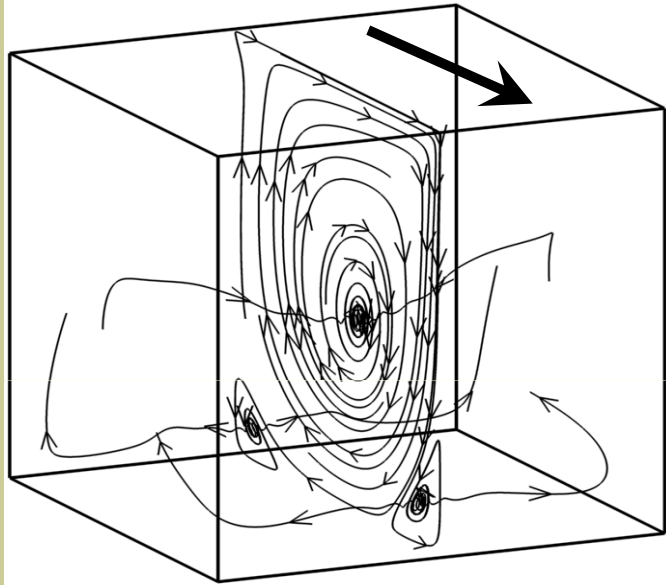
Dimensionless v_y velocity distribution along centerline in z direction ($x=0.5, y=0.5$)



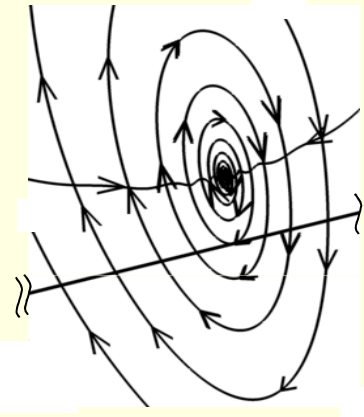
Dimensionless v_z velocity distribution along centerline in y direction ($x=0.5, z=0.5$)



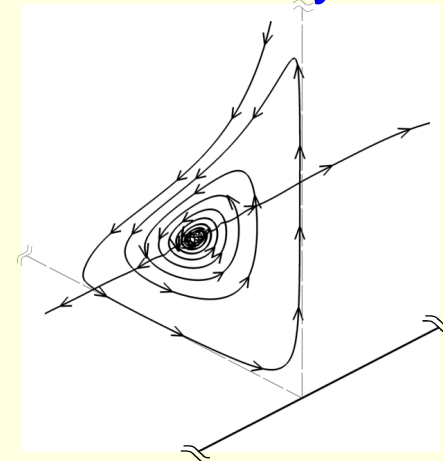
Steady flow in the cubic lid-driven cavity, $Re=1900$



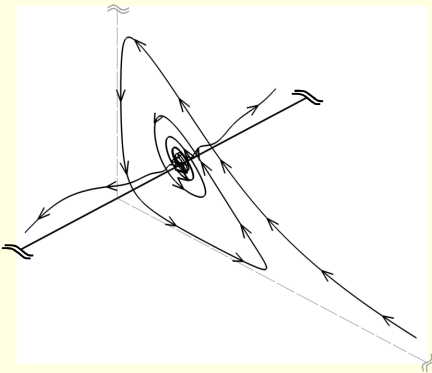
Primary eddy



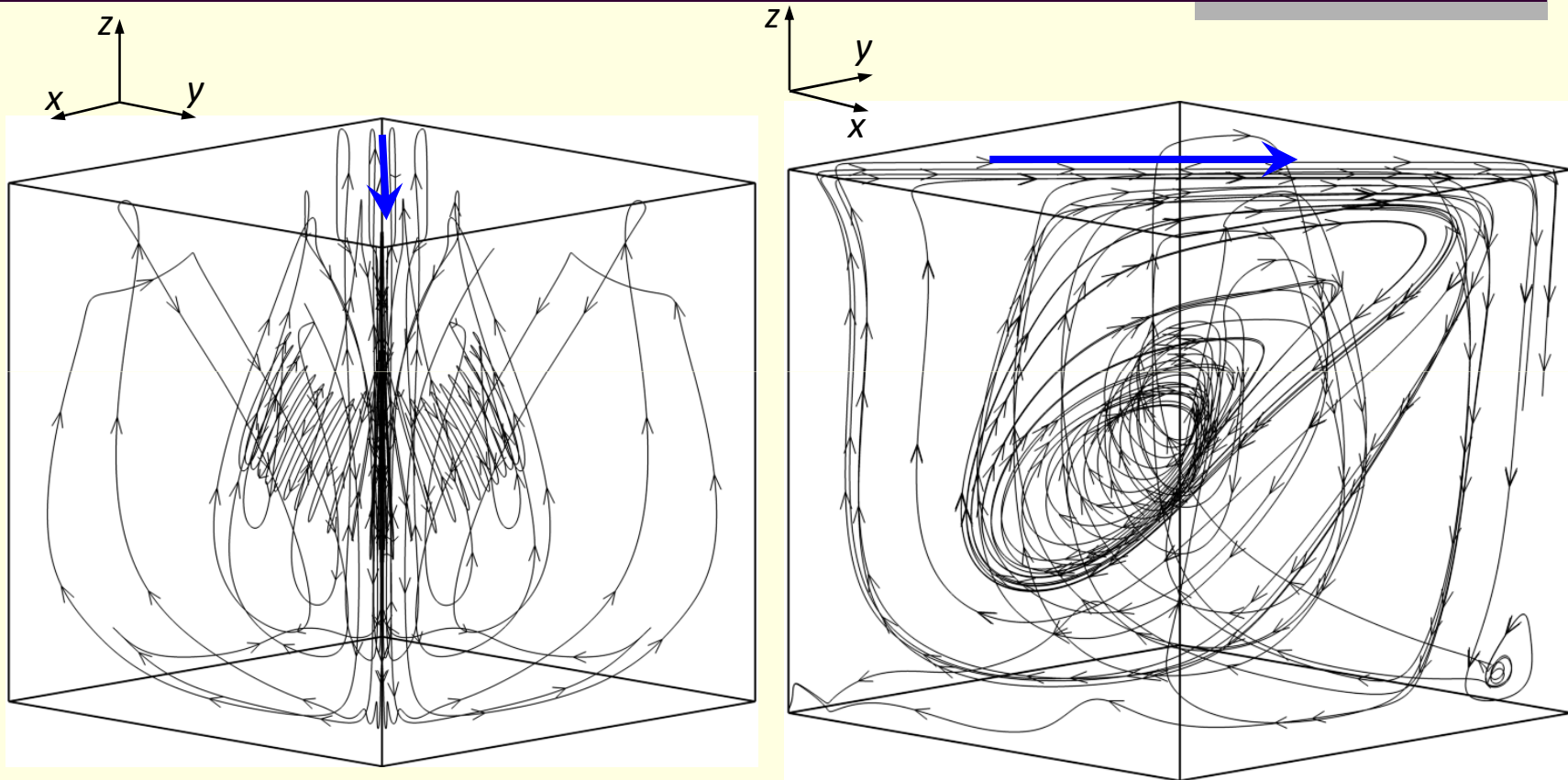
Secondary downstream eddy



Secondary upstream eddy



Lid-driven cavity with lid moving at 45° to the x axis, $Re=1000$.

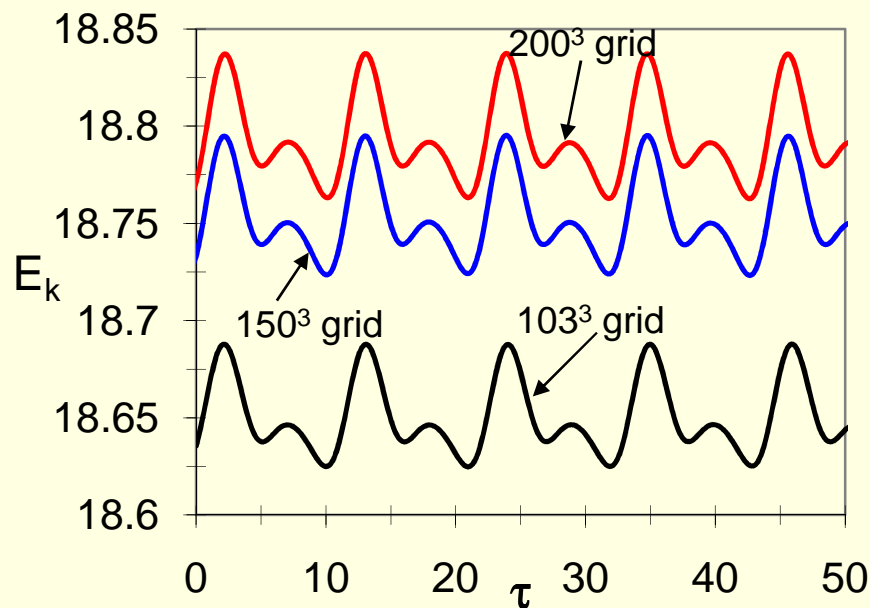


Reflection symmetric flow with respect to **diagonal** plane

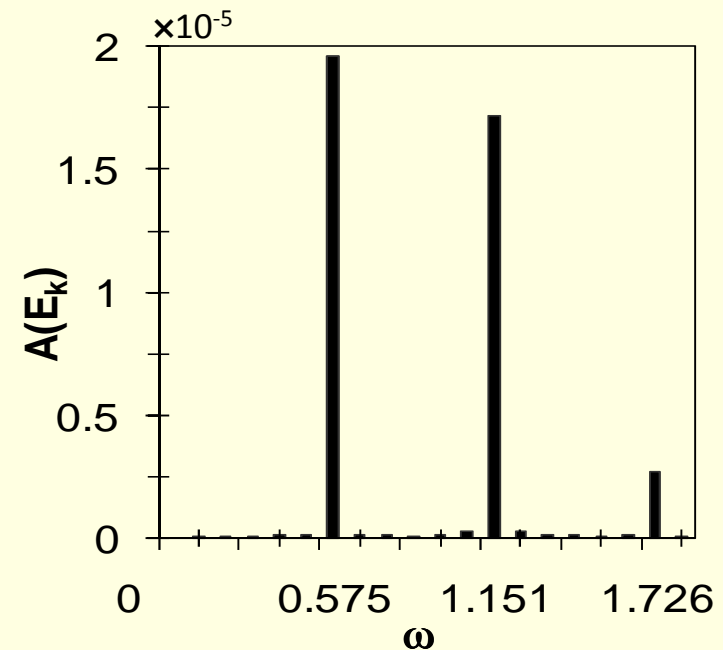
No evidence of the secondary **upstream** eddy

Oscillatory flow inside cubic lid-driven Cavity, $Re=1970$.

Time evaluation of the total kinetic energy, E_k



Fourier series of the total kinetic energy, E_k

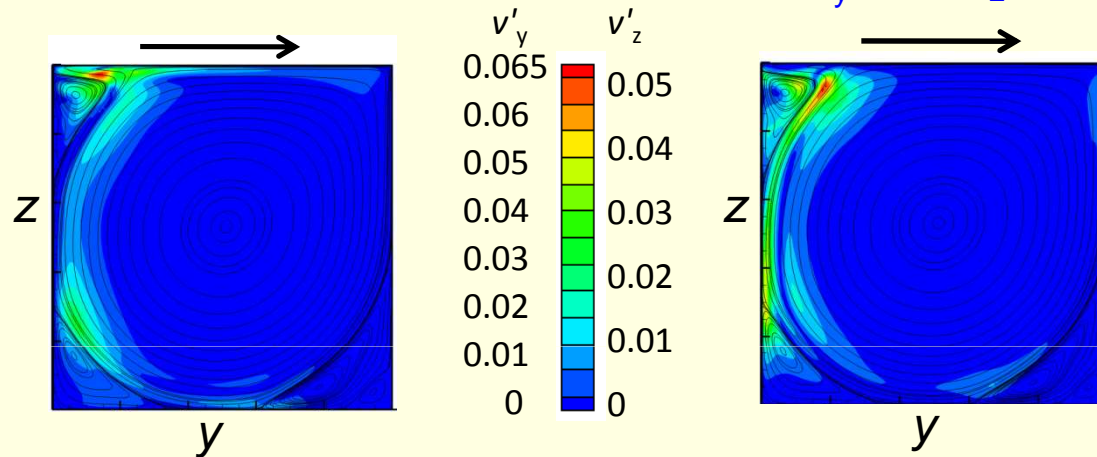


The period of oscillation remains grid-independent

The maximum deviation between the values calculated on 152^3 and 200^3 grids is less than 0.5%.

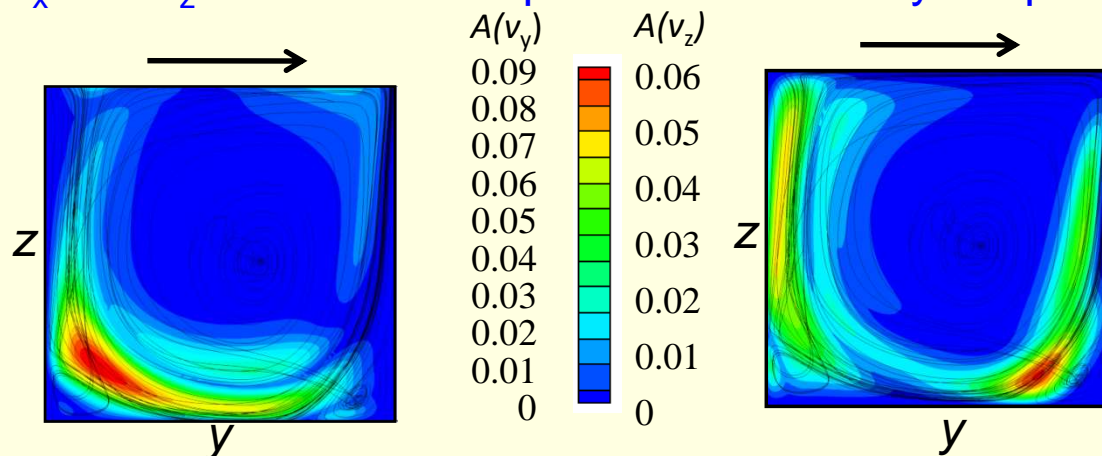
Oscillatory instability in 2D and 3D lid-driven cavities

2D absolute values of perturbations v'_y and v'_z , $Re=8700$



The maximum oscillations
for the both perturbations
are at the **same** place

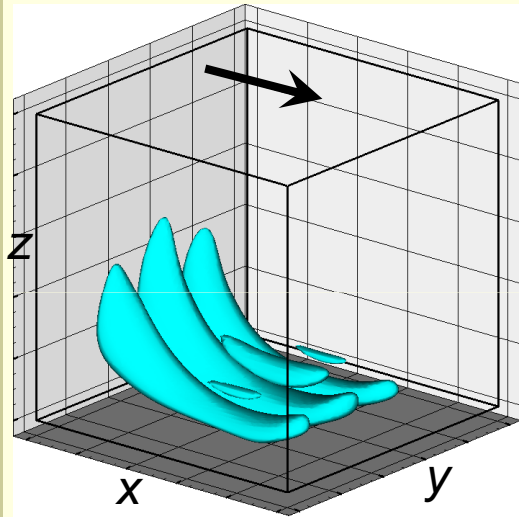
3D v_x and v_z oscillations amplitude at the cavity midplane, $Re=1970$



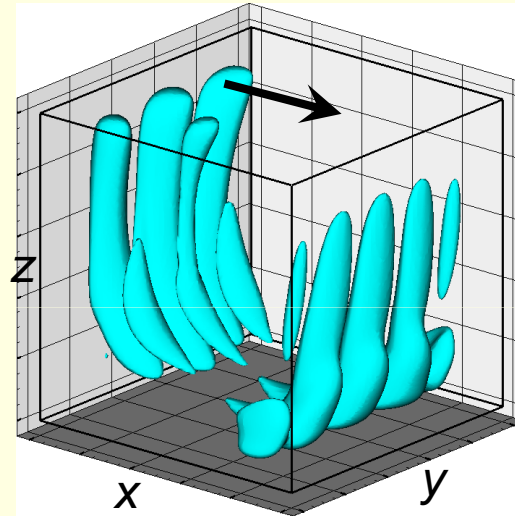
The maximum oscillations
for the velocity oscillations
are **not** at the **same** place

Iso-surface of oscillations amplitude

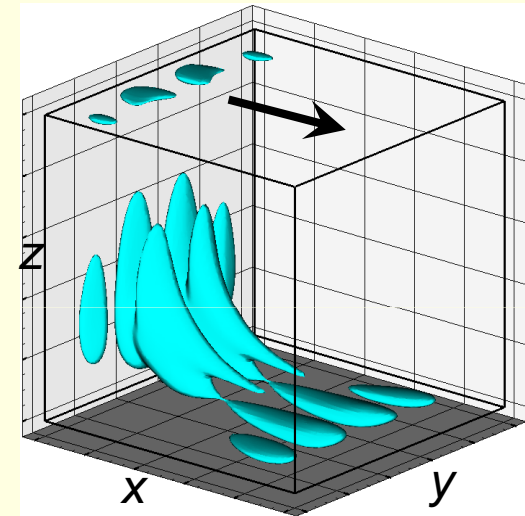
V_y component



V_z component



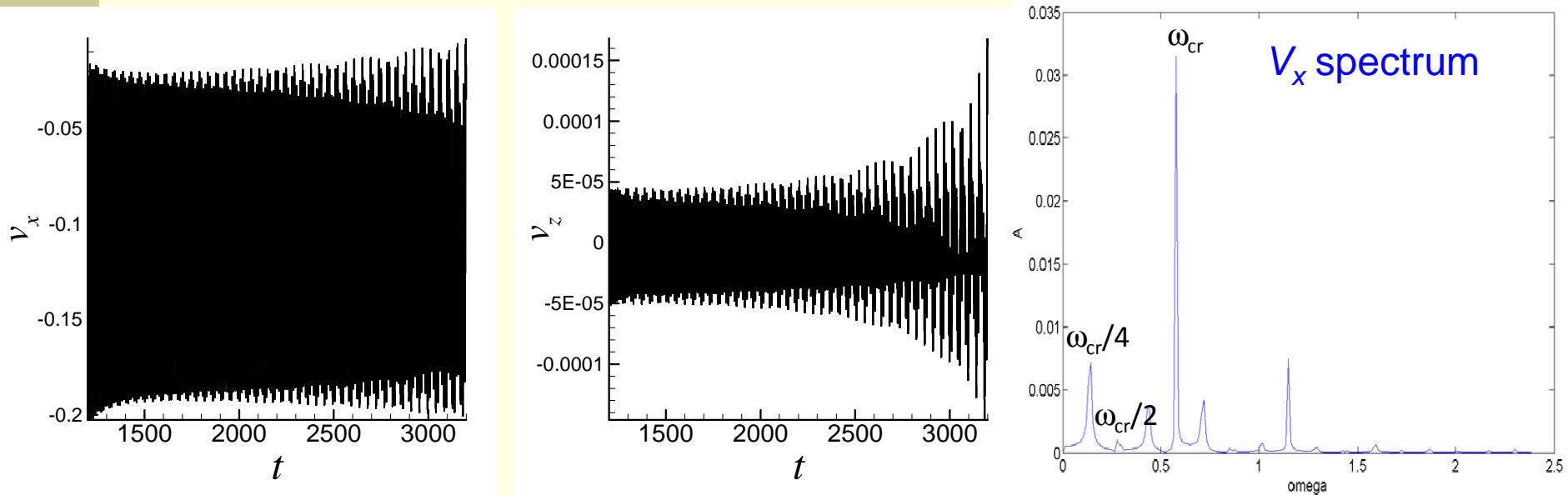
Spanwise V_x component



A decay of the amplitudes is observed when approaching
the no-slip **spanwise** boundaries

Subcritical Character of Bifurcation

Oscillations of x - and z - velocity components at the point $(-0.338, -0.338, 0)$



Calculation is performed on 104^3 grid at $Re=1945$ starting at $t=0$ from oscillatory state at $Re=1970$.

Estimation of Re_{cr} for subcritical Hopf bifurcation

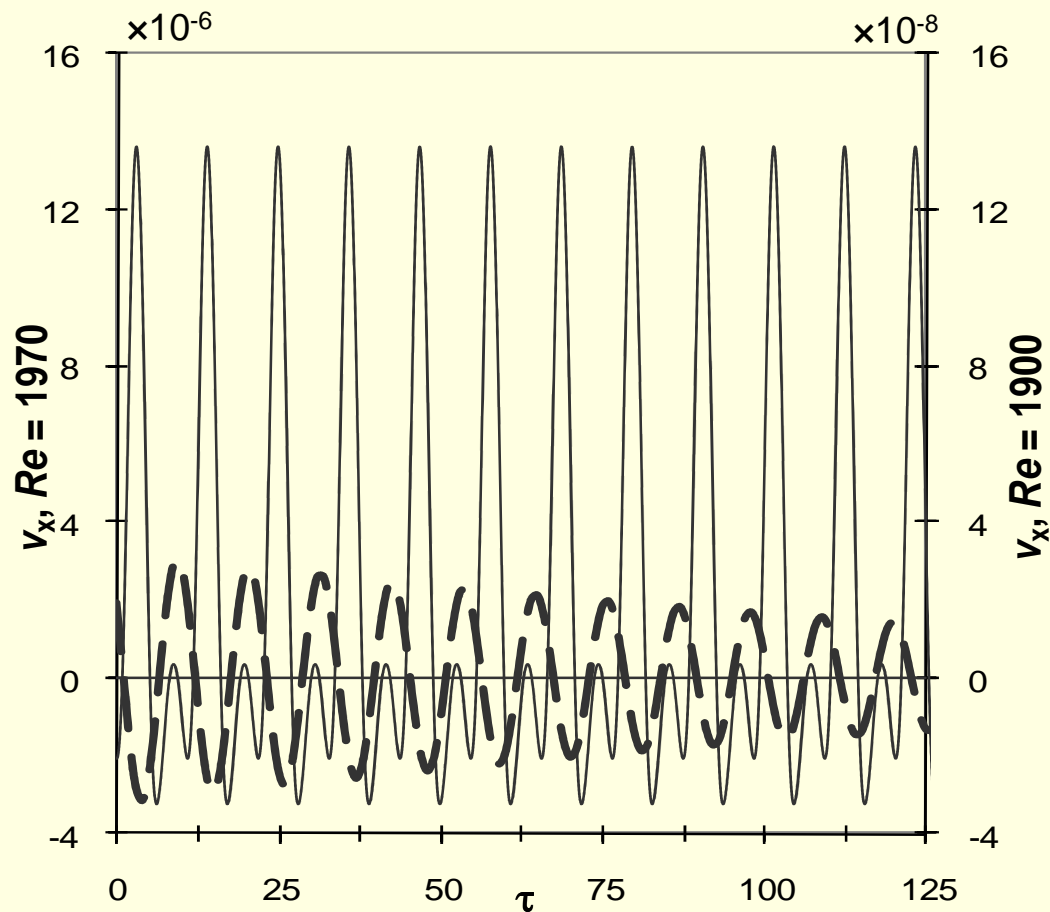
Oscillations of $f(t)$ decay $\sim \exp[(\lambda_r + i\omega)t]$, $\lambda_r < 0$

$$\lambda_r = \frac{\ln(A_k/A_{k-1})}{t_k - t_{k-1}} \quad A_k - k\text{-th maximum of an oscillatory signal}$$

Grid Resolution			Re_{cr}	Richardson Extrapolation
104 ³	$Re=1925$ $\lambda_r = -3.99 \times 10^{-3}$ $\omega=0.575$	$Re=1955$ $\lambda_r = -4.12 \times 10^{-4}$ $\omega=0.575$	1958	
152 ³	$Re=1900$ $\lambda_r = -4.41 \times 10^{-3}$ $\omega=0.575$	$Re=1925$ $\lambda_r = -1.44 \times 10^{-3}$ $\omega=0.575$	1937	$Re_{cr} \approx 1919$
200 ³	$Re=1900$ $\lambda_r = -3.36 \times 10^{-3}$ $\omega=0.575$	$Re=1925$ $\lambda_r = -2.81 \times 10^{-4}$ $\omega=0.575$	1927	$Re_{cr} \approx 1914$

Symmetry breaking during the transition from steady to oscillatory flow

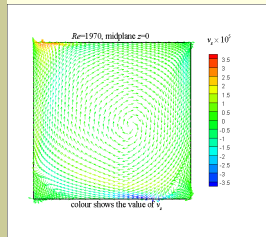
Time evolution of v_x component at a point $(-0.391, 0, 0.395)$ for $Re=1970$ (solid line), and $Re=1900$ (bold dashed line)



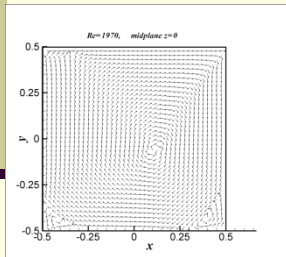
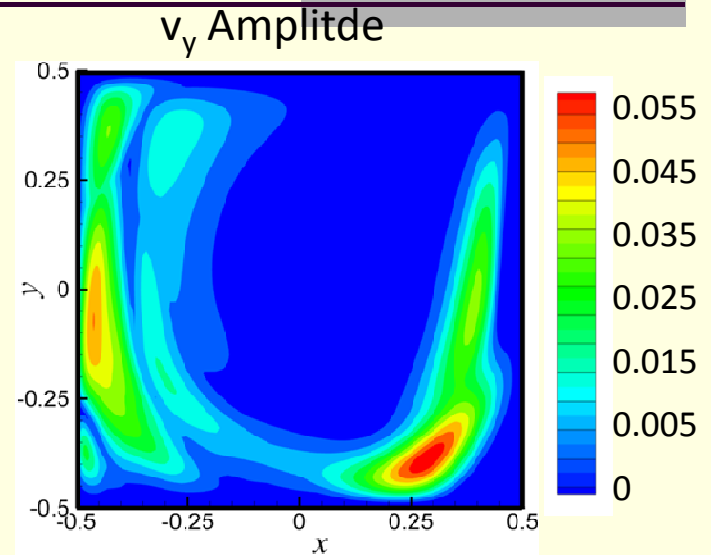
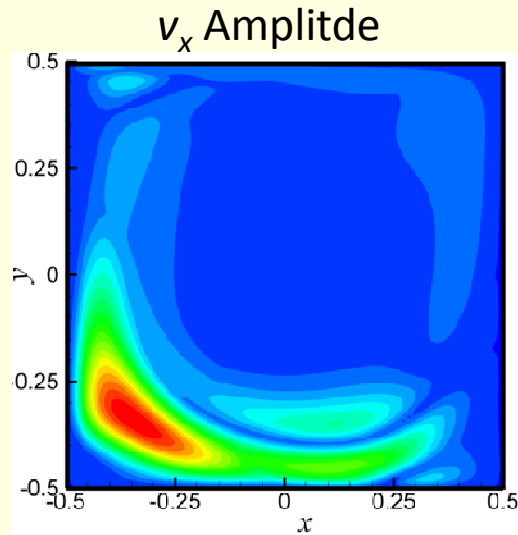
at $Re=1900$, oscillations converge to zero => no flow through the midplane.

non-zero average value of oscillations at $Re=1970$

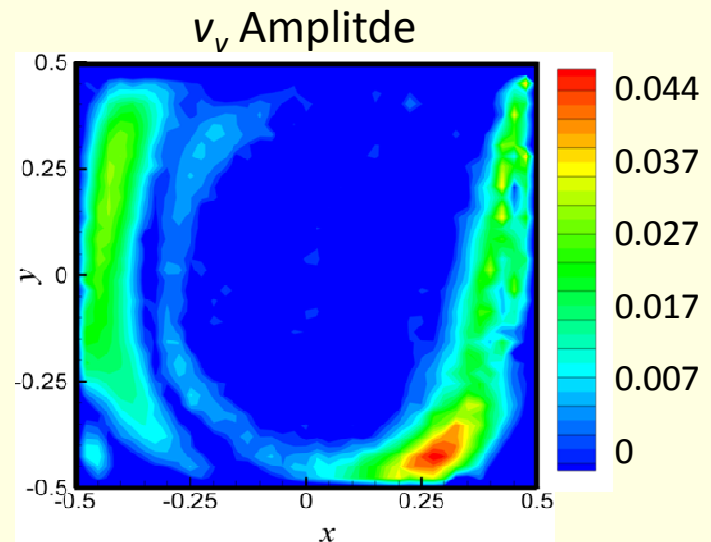
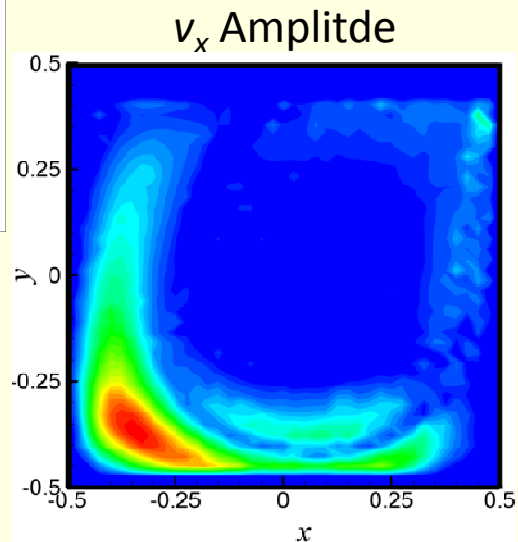
Maximal v_x and v_y Oscillation Amplitudes at the Cavity Mid-Plane



Numerical



Experimental



Lid-driven cavity – Summary

- ✓ Transition from steady to oscillatory state was studied by time-dependent three-dimensional computations on three successive grids of 104^3 , 152^3 and 200^3 nodes. **Grid independence** of the results was established.
- ✓ Present time-dependent computations showed that the oscillatory instability of lid driven flow in a cube with no-slip walls takes place at **$Re_{cr} \approx 1914$** with a dimensionless frequency **$\omega_{cr} = 0.575$** .
- ✓ The instability sets in via a **subcritical Hopf** bifurcation.
- ✓ The transition from steady to oscillatory state is followed by **breaking of the symmetry** with respect to the cavity midplane.

Verification: Differentially heated cavity

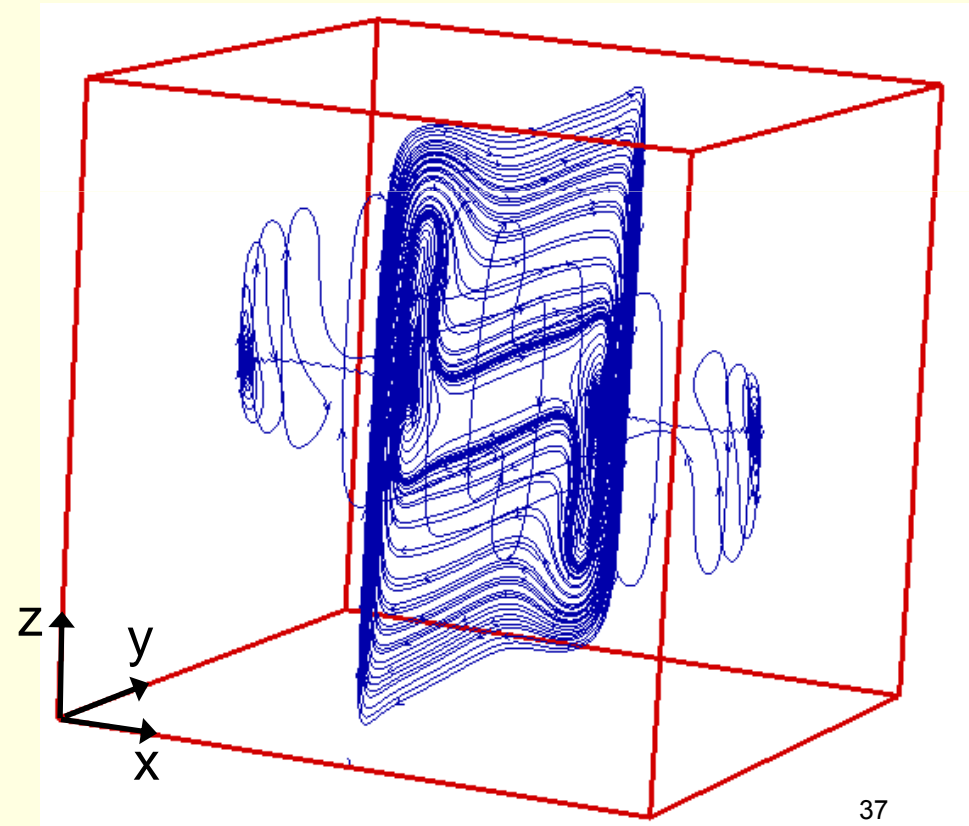
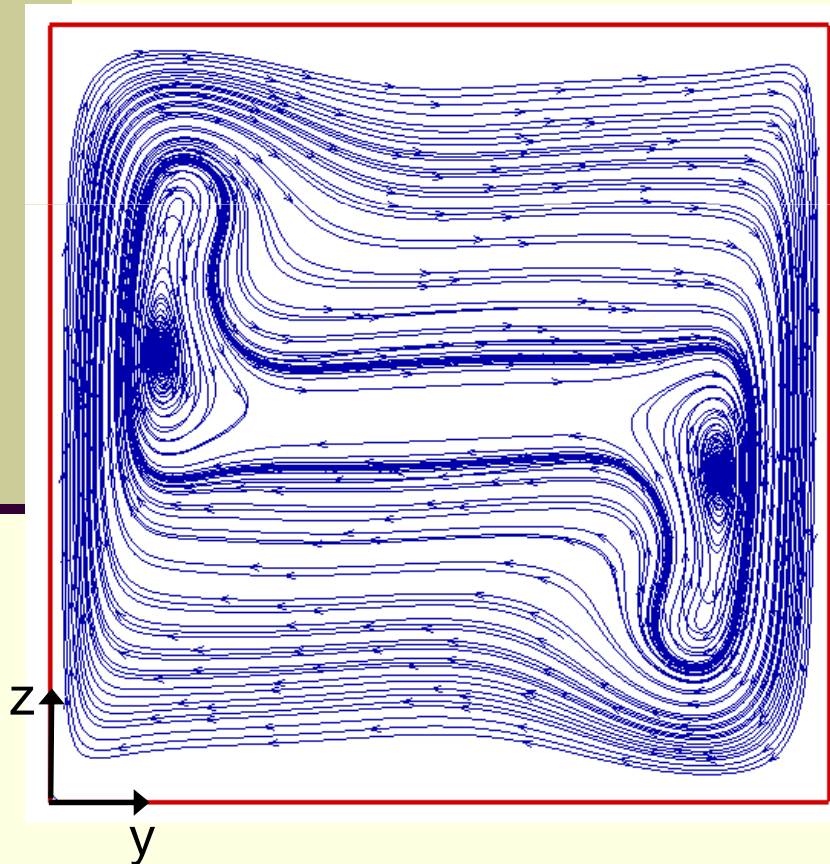
Comparison with Wakashima, 2004.
Adiabatic horizontal walls

	Ra=10 ⁴			Ra=10 ⁵			Ra=10 ⁶		
	Wakashima 120 ³	Present 100 ³	Dev. (%)	Wakashima 120 ³	Present 100 ³	Dev. (%)	Wakashima 120 ³	Present 100 ³	Dev. (%)
$u_{y \max}(z)$ (x=0.5,y=0.5)	0.1984 (0.825)	0.197 (0.825)	0.7	0.1416 (0.85)	0.1434 (0.85)	1.26	0.0811 (0.8603)	0.0802 (0.8605)	1.1
$u_{z \max}(y)$ (x=0.5,z=0.5)	0.2216 (0.177)	0.2202 (0.12)	0.6	0.2464 (0.068)	0.2464 (0.063)	0	0.2583 (0.0323)	0.2575 (0.0337)	0.3
Nu _{hot}	2.0624	2.0547	0.37	4.3665	4.3349	0.72	8.6973	8.7584	0.7
Nu _{cold}	-----	2.0547	-----	-----	4.3349	-----	-----	8.7584	-----

At the constant y plane the average Nu number is
$$Nu_y = \int_0^1 \int_0^1 \left[\text{Pr} \sqrt{\text{Gr}} V \theta - \frac{\partial \theta}{\partial Y} \right] dX dZ$$

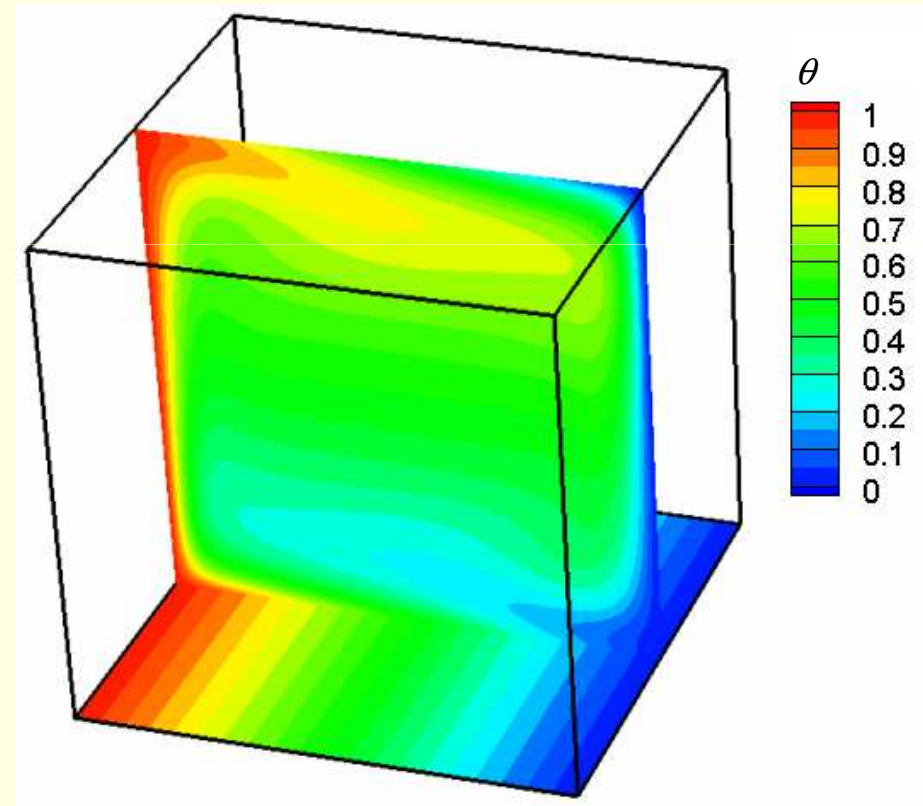
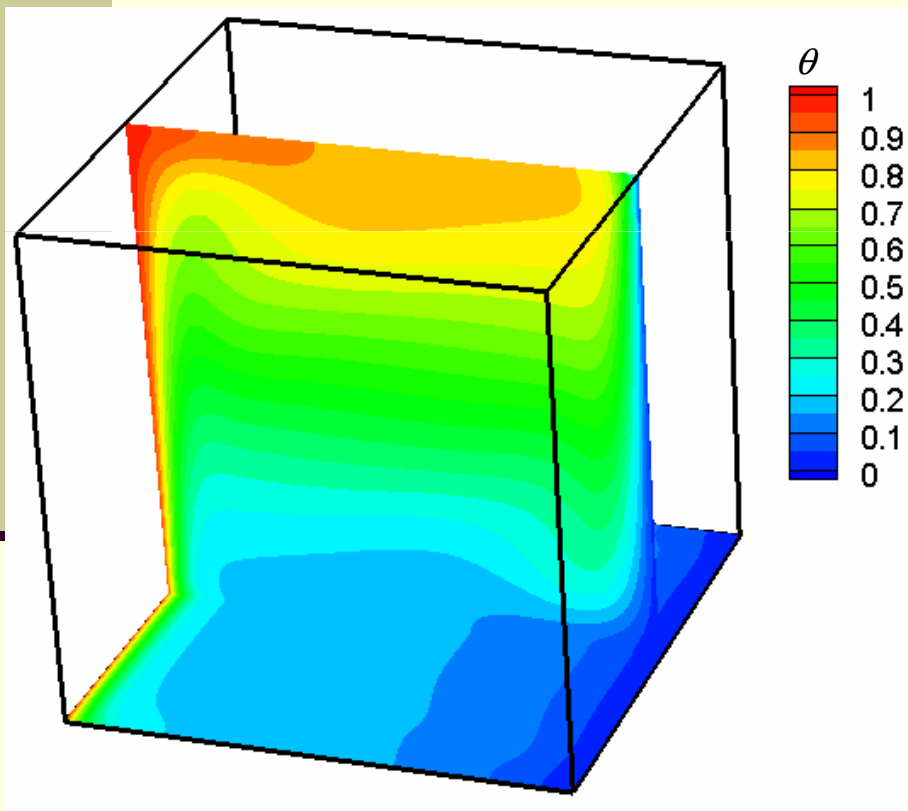
Steady flow visualization inside the cubic differentially heated cavity

Adiabatic horizontal walls, $Ra = 10^6$

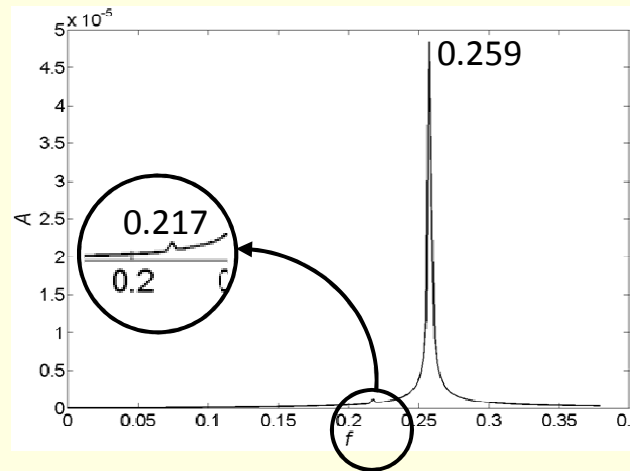
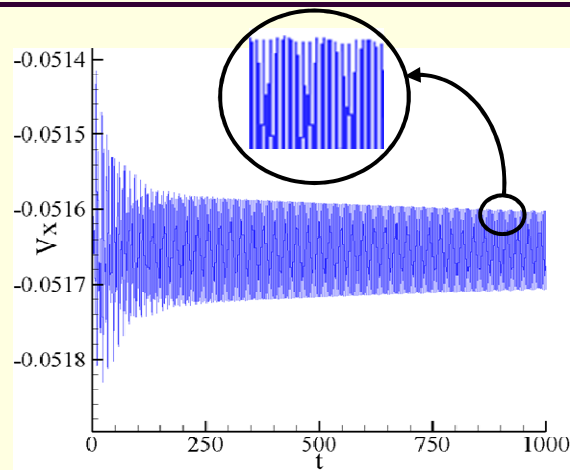


Temperature distribution in a laterally heated cubic cavity

Adiabatic and perfectly conducting horizontal walls, $Ra=10^6$



Ra_{cr} for Steady-Oscillatory Transition in a Differentially Heated Cavity, (104^3 grid)

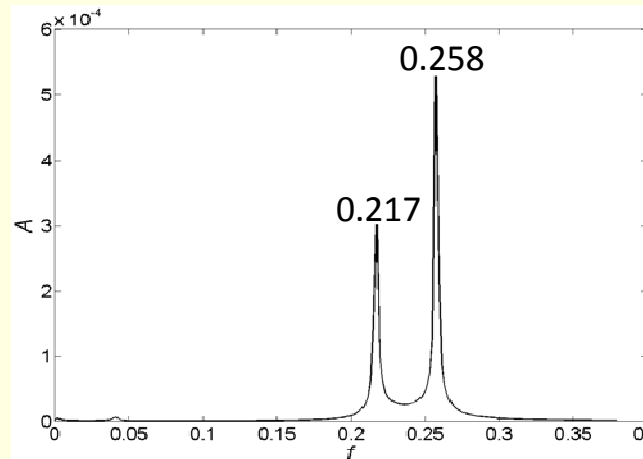
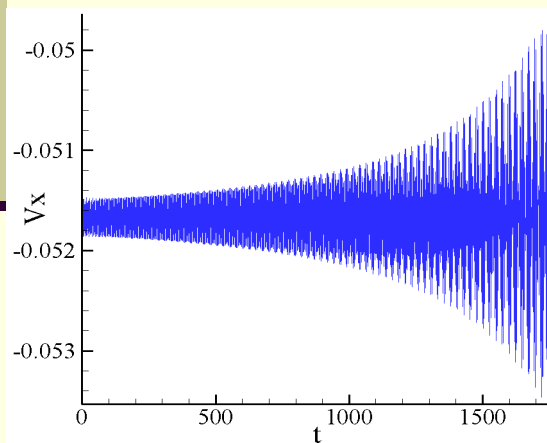


Convergence to Steady Flow

$$Ra = 3.05 \times 10^6$$

$$f = 0.259$$

10^6 time steps



Oscillatory Flow

$$Ra = 3.07 \times 10^6$$

$$f = 0.258$$

1.7×10^6 time steps

Experimental Results of Jones and Briggs, 1989 : $f_{cr} \approx 0.248$ $Ra_{cr} \approx 3.0 \times 10^6$

Differentially heated cavity – Summary

- ✓ The code was successfully **verified** on existing steady state benchmark solutions for the wide range of Ra numbers.
- ✓ Preliminary estimation of critical Gr number for the Hopf bifurcation on 103^3 grid was performed. The obtained result is well compared with existing experimental data.
- ✓ The **grid independence** should be established by use of finer grids.

Newton iteration with time-stepping

L.S. Tuckerman, 1999

$$(N_U + L)u = (N + L)U$$

$$U \leftarrow U - u$$

$$\underbrace{\left[(I - \Delta t L)^{-1} (I + \Delta t N_U - I) \right]}_{} u = \underbrace{\left[(I - \Delta t L)^{-1} (I + \Delta t N(U) - I) \right]}_{} U$$

Difference between two
consecutive linearized
time steps

Difference between two
consecutive time steps

For large Δt , $(I - \Delta t L)^{-1} \approx L^{-1}$, is a preconditioner for $N_U + L$

Linear stability analysis with time-stepping

L.S. Tuckerman, 1999

Inverse power method for the leading eigen value

$$u_{n+1} = (N_U + L)^{-1} u_n$$

$$\underbrace{\left[(I - \Delta t L)^{-1} (I + \Delta t N_U - I) \right]}_{\text{Difference between two consecutive linearized time steps}} u_{n+1} = \underbrace{(I - \Delta t L)^{-1}}_{\text{Difference between two consecutive time steps of the Stokes operator}} \Delta t u_n$$

Difference between two consecutive linearized time steps

Difference between two consecutive time steps of the Stokes operator

Good performance for 2D configuration

Still a challenge for 3D configuration

Conclusions

- ✓ A novel multigrid solver for time-dependent incompressible Navier-Stokes equations in pressure-velocity coupled formulation is developed and implemented.
- ✓ The characteristic CPU times consumed for a single time step per one node and per one CPU are of order 5×10^{-3} msec and 10^{-2} msec for 2D and 3D calculations, respectively.
- ✓ The approach performs well for time-dependent calculations with a small time step,
- ✓ Direct Newton and Arnoldi iterations needed for stability analysis require large time steps, which causes a slow convergence for 3D problems