

# Pressure-Velocity Coupled Three-Dimensional CFD on a Massively Parallel Computer

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# Outline

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- **Pressure-velocity coupled formulation of Navier-Stokes equations**
- **Benchmark problem : 3-D lid driven cavity, differential heated cavity**
- **Multigrid with an Analytical Solution Accelerated (ASA) smoother**
- **3D Domain partition and scalability properties**
- **Application to linear stability analysis**
- **Conclusions**

# Incompressible N-S Equations – Numerical Challenge

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

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

- No separate equation for pressure
- No boundary conditions for pressure

# Incompressible N-S Equations – Numerical Challenge (Cont.)

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## approaches with pressure- velocity decoupling

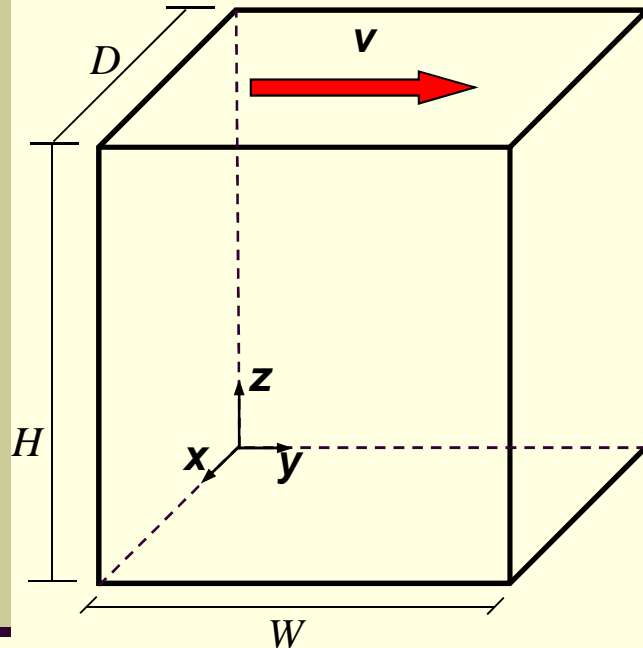
- ✓ High numerical robustness
- ✓ Low memory consumption
- ✗ Slow rate of numerical convergence
- ✗ Non-physical pressure field
- ✗ Not applicable for liquid – solid interface problems

## pressure–velocity coupled approaches

- ✓ High rate of numerical convergence
- ✓ The "most natural " way to solve N-S equations
- ✓ Calculated pressure is physical
- ✗ High memory consumption
- ✗ Not as numerically robust as pressure projection methods

# Benchmark Problems

## Lid-Driven Cubic Cavity



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

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

✓ Explicit non-linear terms treatment

$$(\mathbf{u}^n \cdot \nabla) \mathbf{u}^n$$

▪ Semi-Implicit non-linear terms treatment

$$(\mathbf{u}^n \cdot \nabla) \mathbf{u}^{n+1}$$

**Realistic Boundary Conditions:**

$\mathbf{u} = 0$  - at all static walls no slip/no penetration

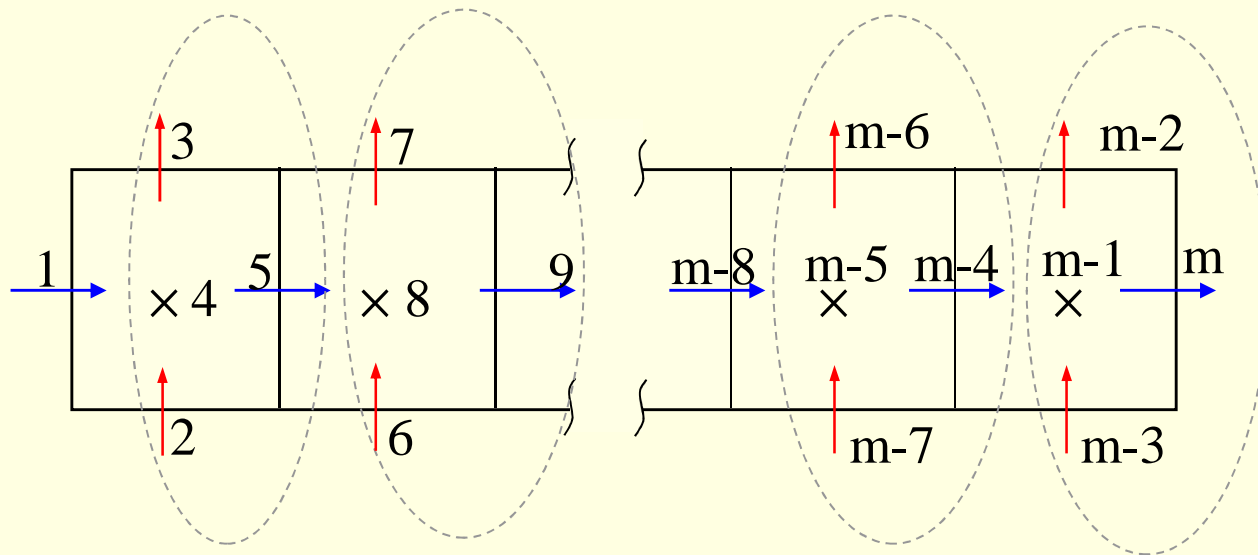
$\mathbf{u}|_{z=H/W} = \mathbf{v}$  - at the moving wall the flow velocity is equal to that of the moving wall itself

**No boundary condition for pressure is needed**

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

Zeng and Wesseling (1993) – CLGS:  
Horizontal (vertical) sweeping with  
horizontally (vertically) adjacent  
pressure linkage

Feldman and Gelfgat (2008) –  
**ASA**-CLGS: Horizontal (vertical) sweeping  
**without** horizontally (vertically) adjacent  
pressure linkage

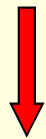


# CLGS and **ASA**-CLGS Efficiency Estimation for 2D

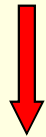
Zeng and Wesseling  
(1993) – CLGS:



Block 3-diagonal matrix  
or 7-diagonal matrix



LU decomposition



$\approx O(15M)$

Feldman and Gelfgat (2008) –  
**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)

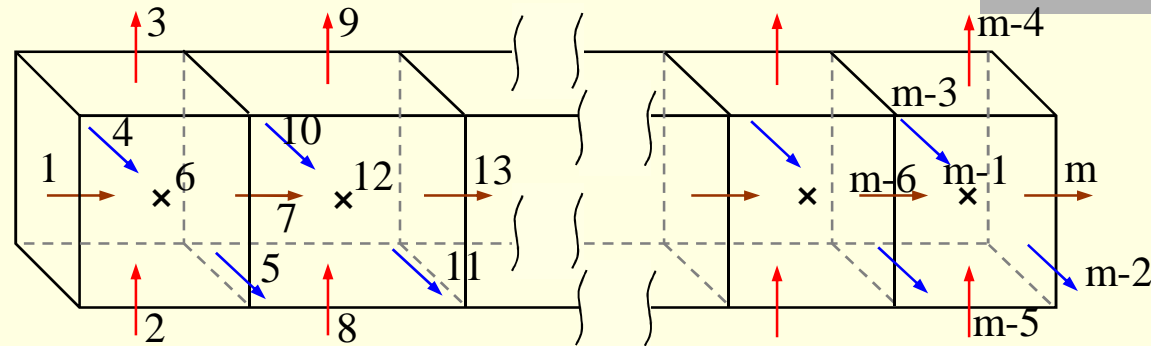


$\approx O(5M)$



# 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

$\approx O(5M)$

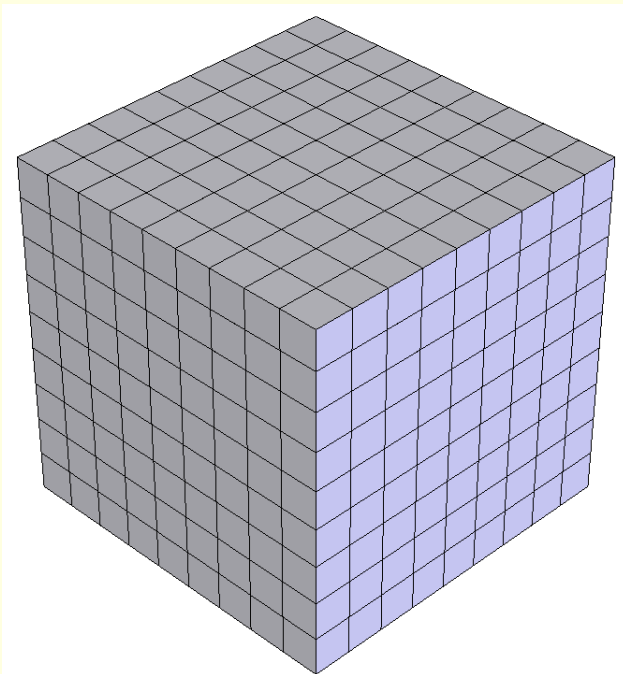


# Domain Partition for 3D Configuration

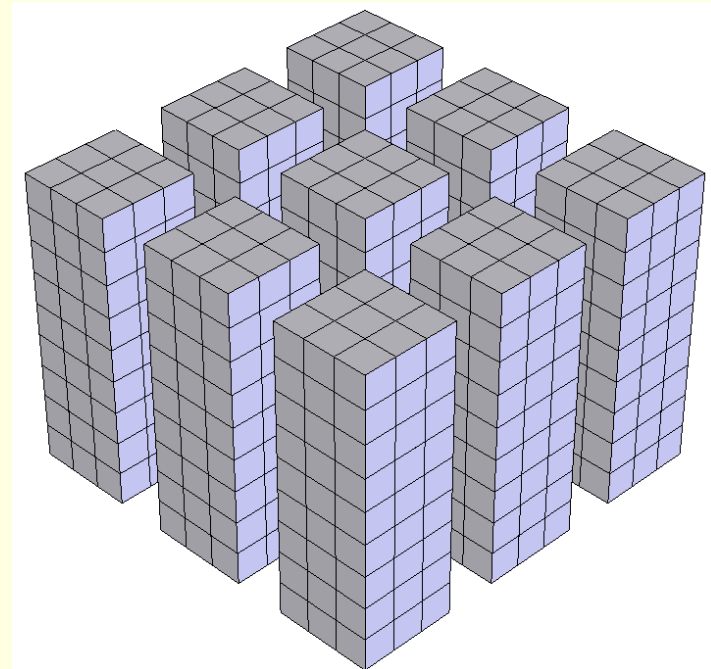
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Existence of **analytical solution** for the whole column allows for 2D virtual topology of 3D configuration.

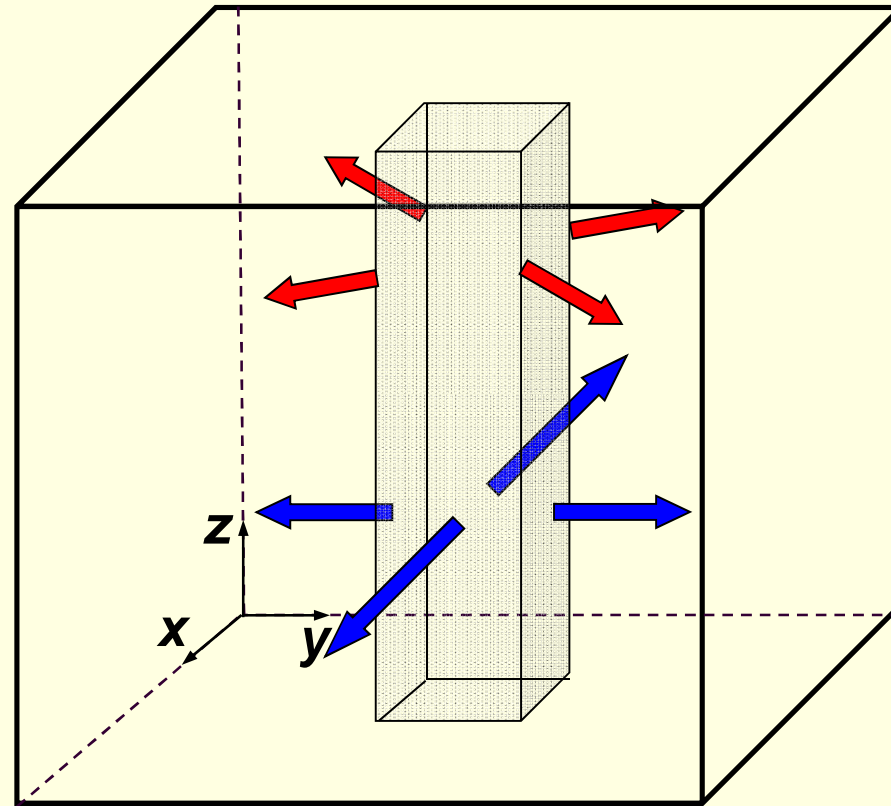
The whole domain





The partitioned domain



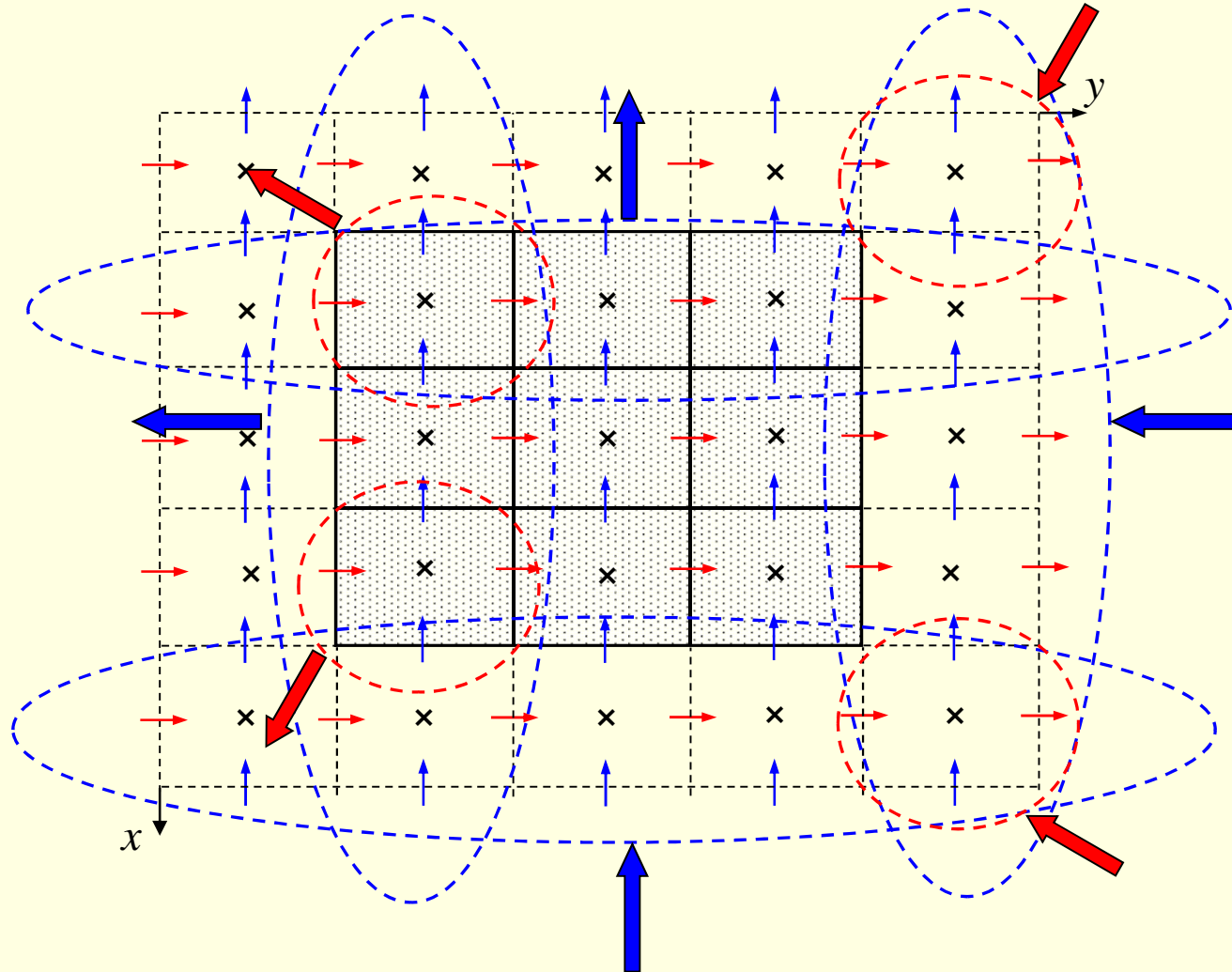
# Domain Partition for 3D Configuration ( Cont.)



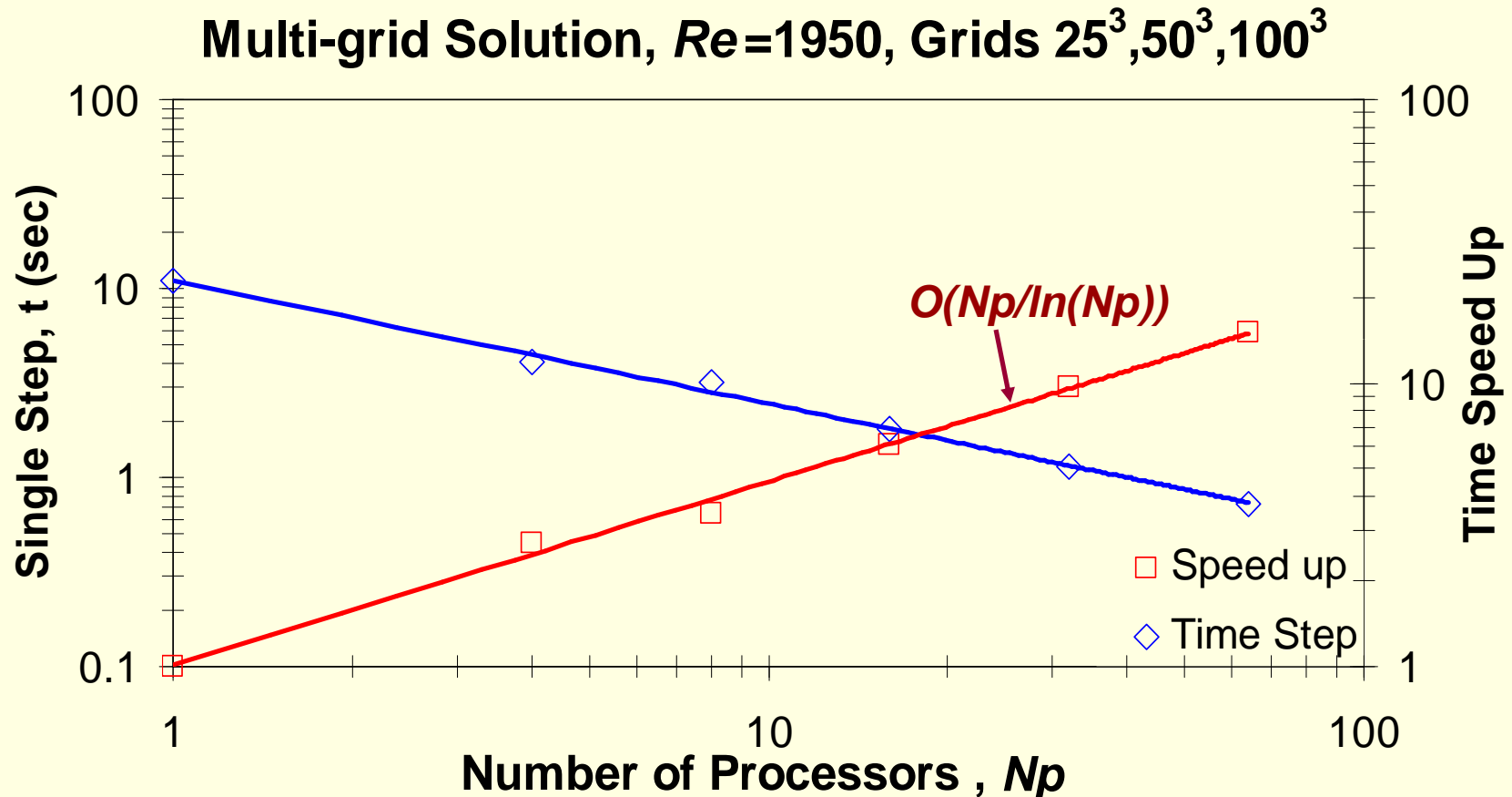
 All volumes located at the sub -volume faces exchange data with neighbors

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

# 3D Configuration- Data Exchange Principle



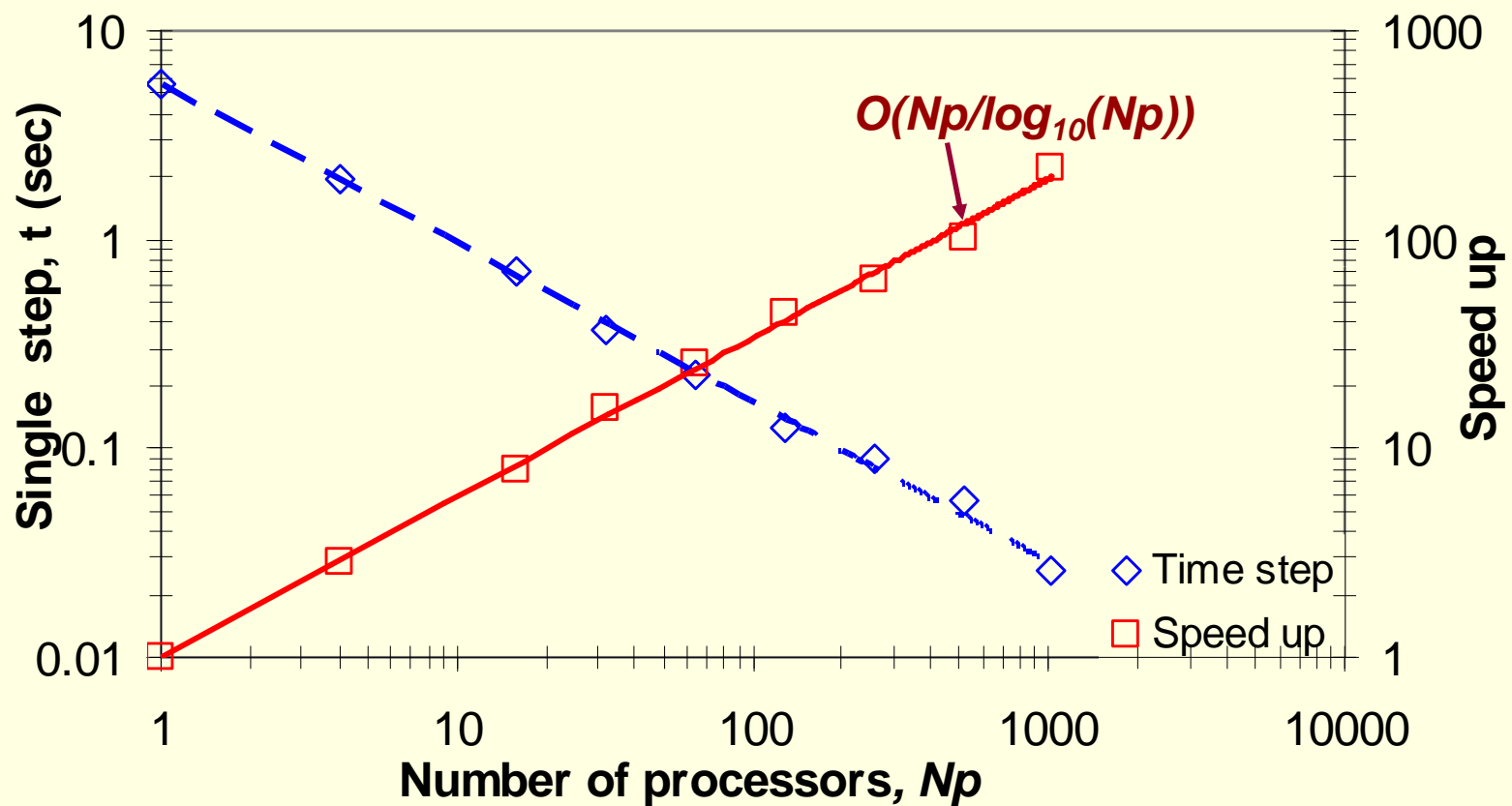
# Scalability Characteristics of Multi-Grid



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

# Scalability Characteristics of Single-Grid

Single-grid Solution,  $Re=1950$ ,  $100^3$  Grid



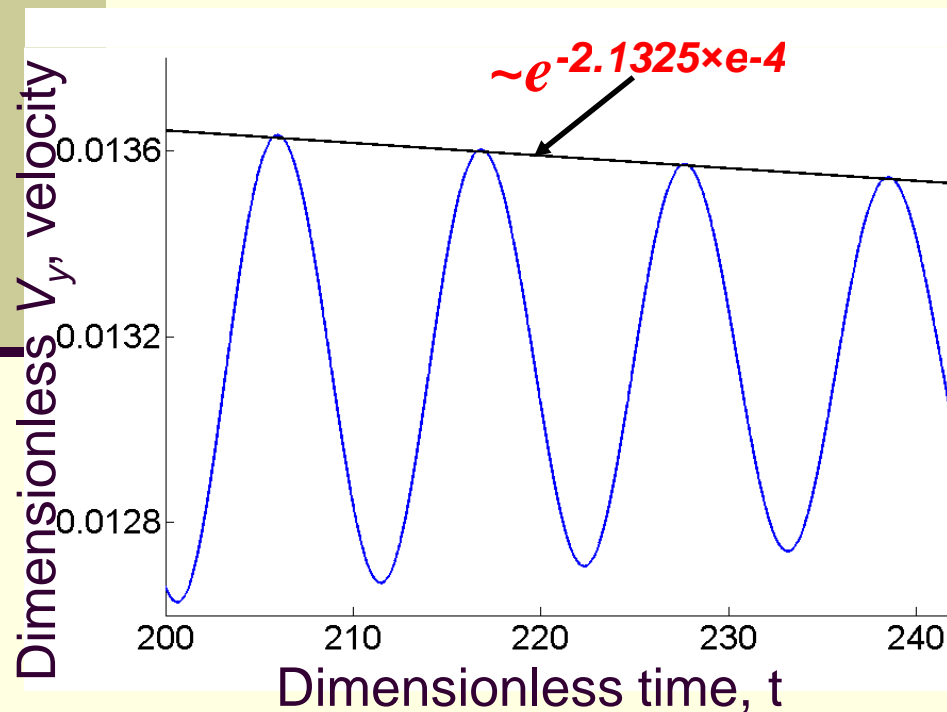
1024 CPU 25.7 msec per time step only 8 hours for  $10^6$  time steps

# Linear Stability Analysis for the Lid Driven Cavity

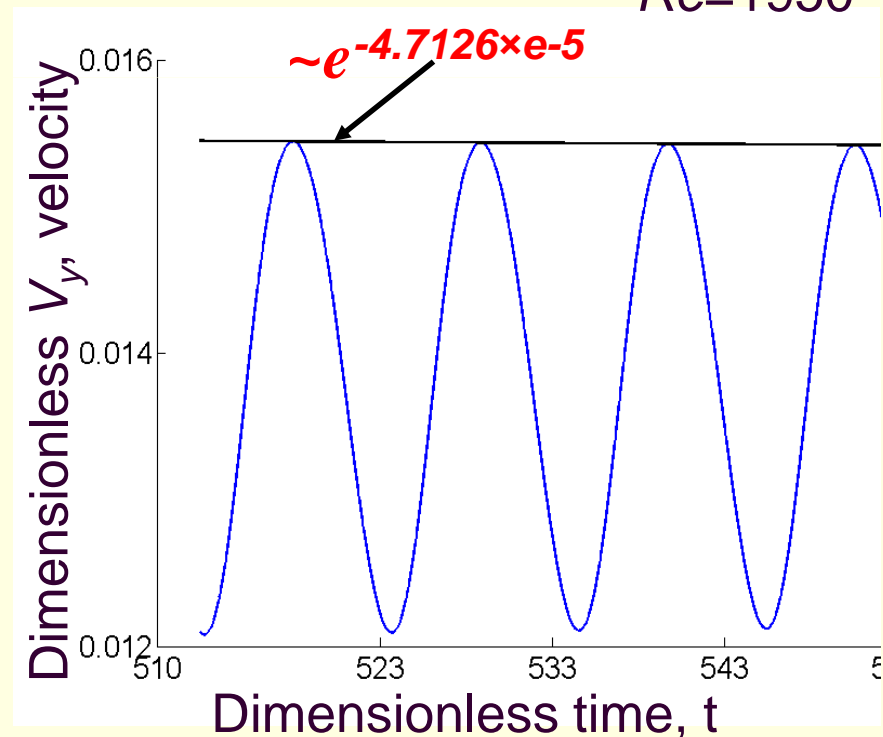
Dimensionless  $V_y$  velocity at the left corner of the middle plane  
(0.5, 0.1, 0.9),  $100^3$  Grid

Reynolds number is increasing

$Re=1900$



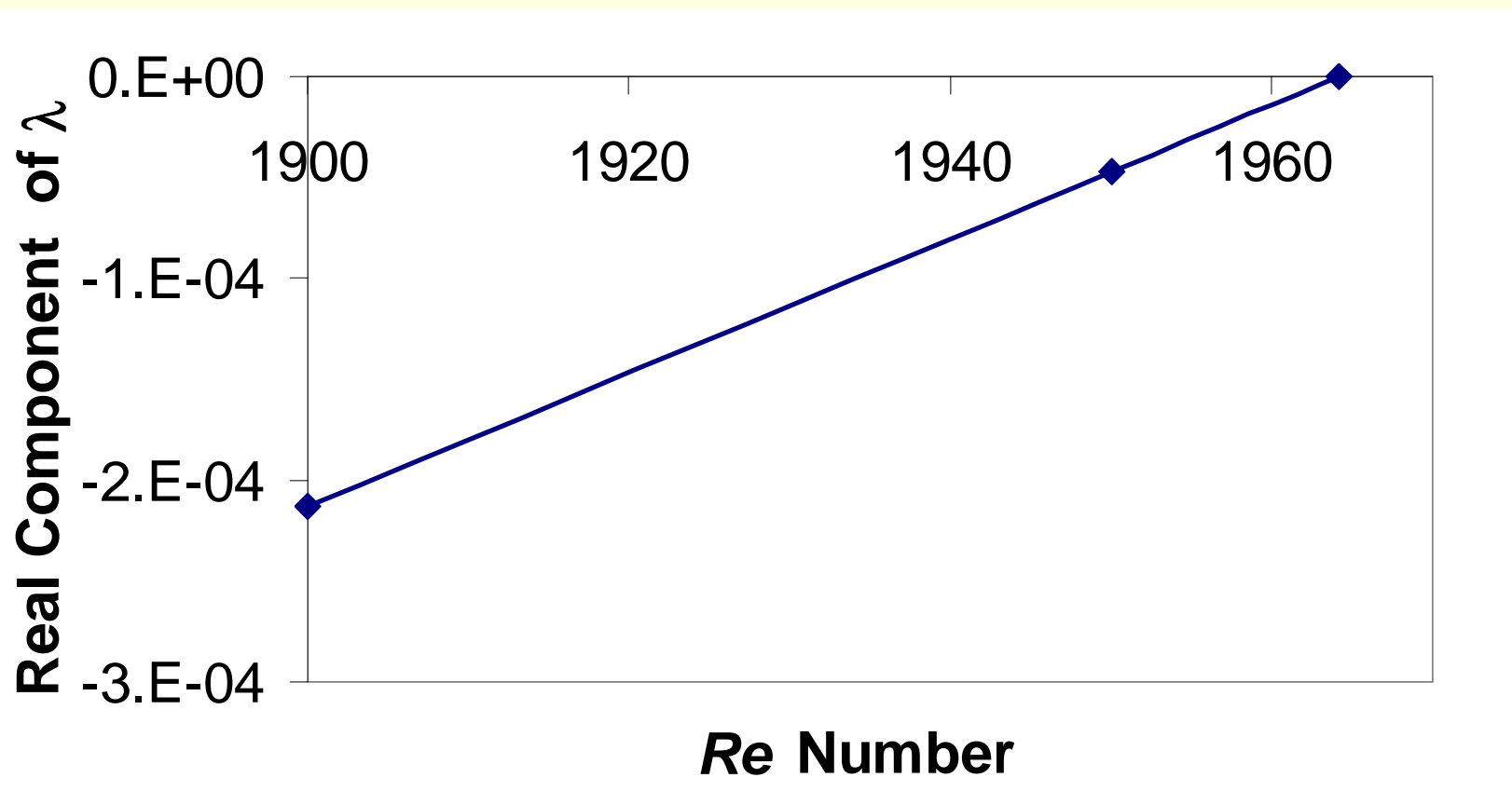
$Re=1950$



# Estimation of the critical $Re$ number for Hopf bifurcation

**100<sup>3</sup> Grid**

$Re_{cr} \approx 1964$



# Estimation of the critical $Re$ number for Hopf bifurcation (Cont.)

Grid	$Re=1900$	$Re=1925$	$Re_{cr}$	Richardson Extrapolation
$100^3$	$\lambda = -7.0256 \times 10^{-3}$ $\omega = 0.575$	$\lambda = -3.8756 \times 10^{-3}$ $\omega = 0.575$	1964	<b><math>Re_{cr} = 1917</math></b>  <b><math>Re_{cr} = 1916</math></b>
$150^3$	$\lambda = -4.3438 \times 10^{-3}$ $\omega = 0.575$	$\lambda = -1.2417 \times 10^{-3}$ $\omega = 0.575$	1935	
$200^3$	$\lambda = -3.3512 \times 10^{-3}$ $\omega = 0.575$	$\lambda = -2.8473 \times 10^{-4}$ $\omega = 0.575$	1927	

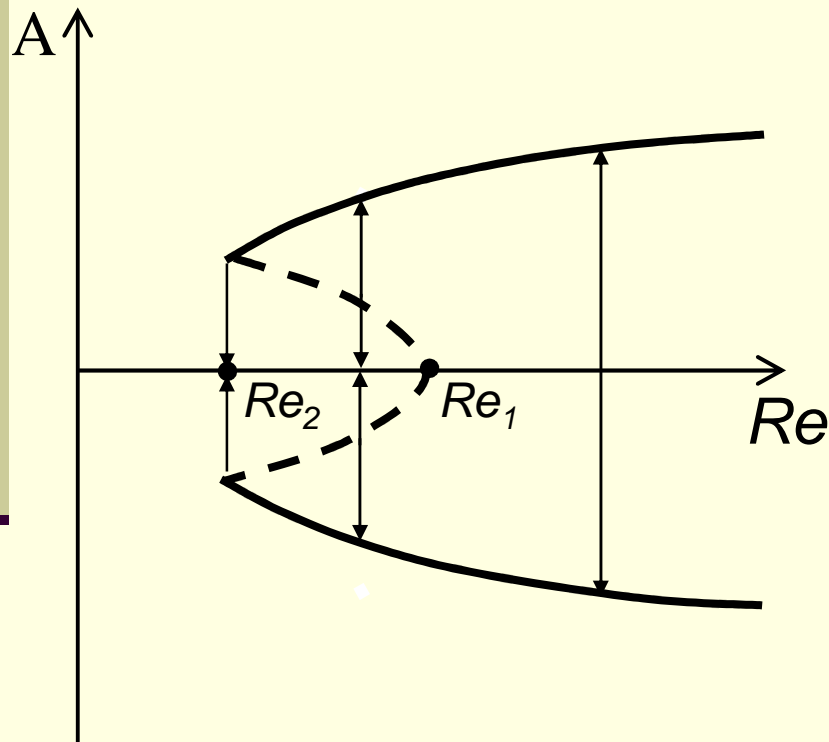
$$Re_{cr} = 1916$$

$$\omega_{cr} = 0.575$$



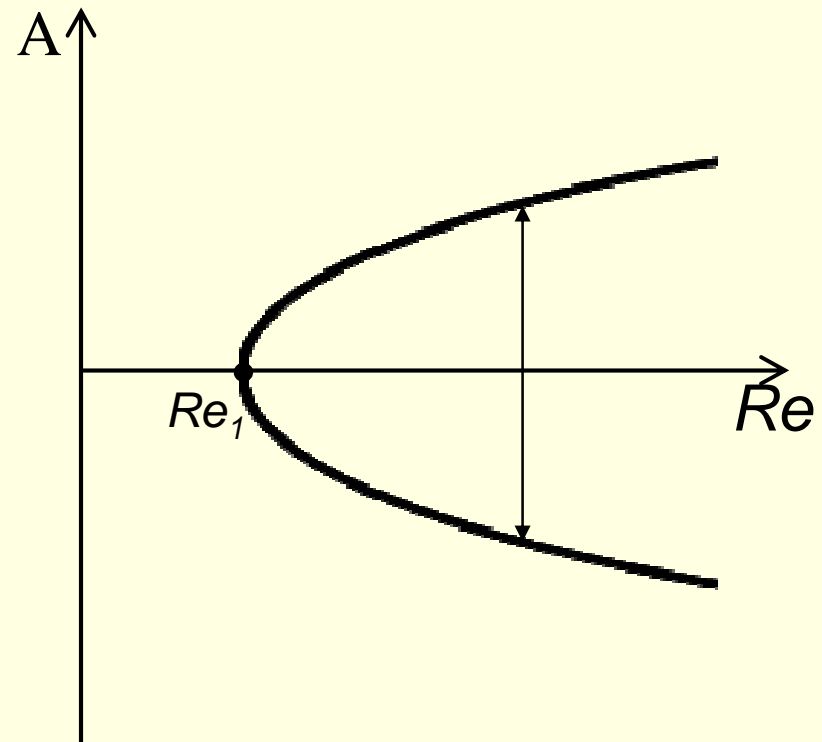
# Type of the obtained bifurcation

Subcritical



$Re_1$  → Hopf bifurcation  
 $Re_2$  → Saddle node bifurcation

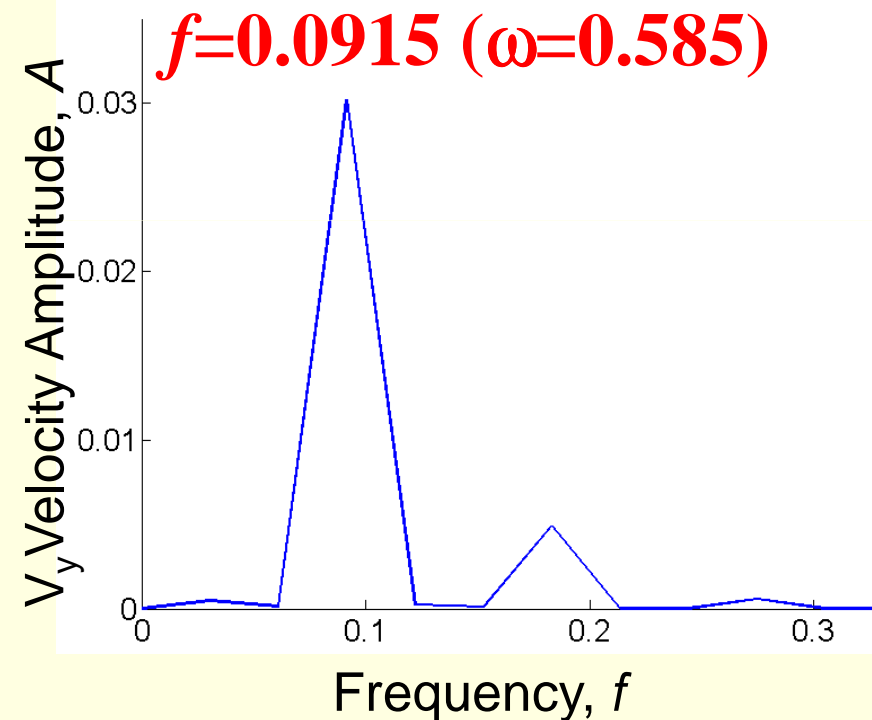
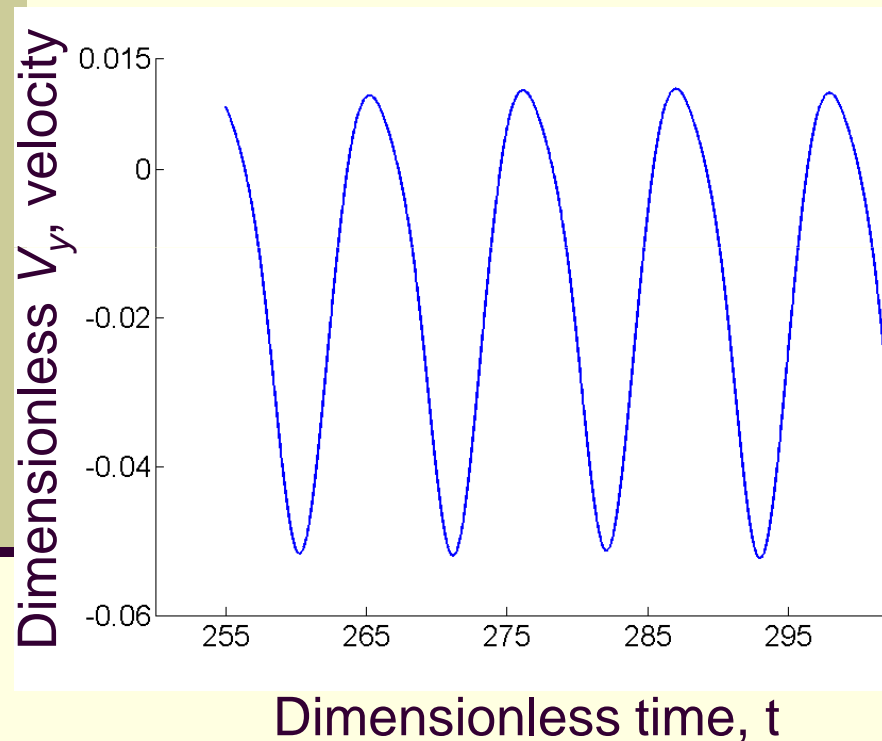
Supercritical



$Re_1$  → Hopf bifurcation

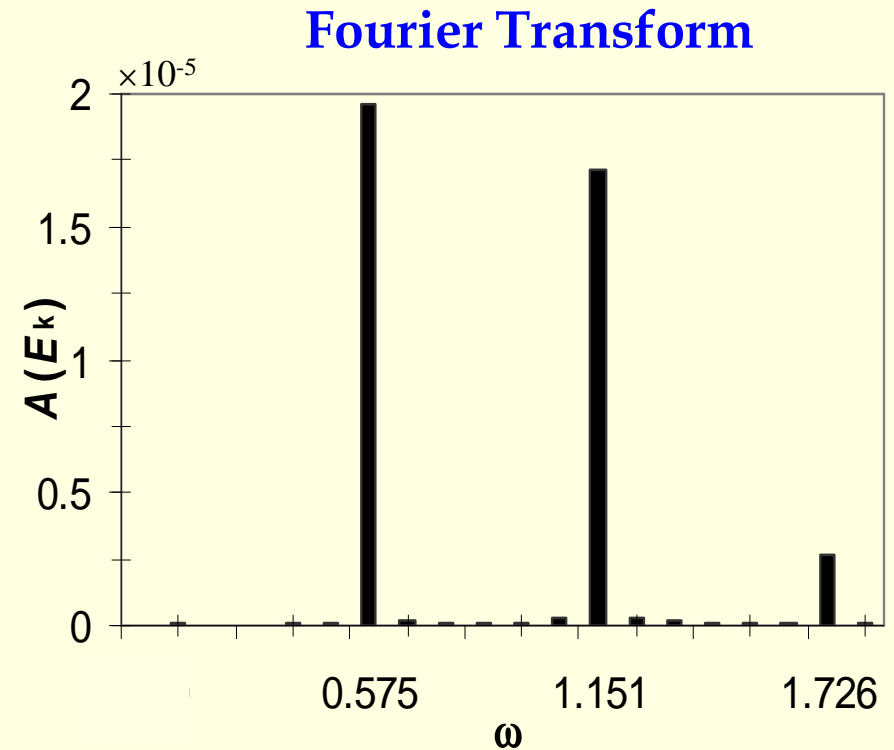
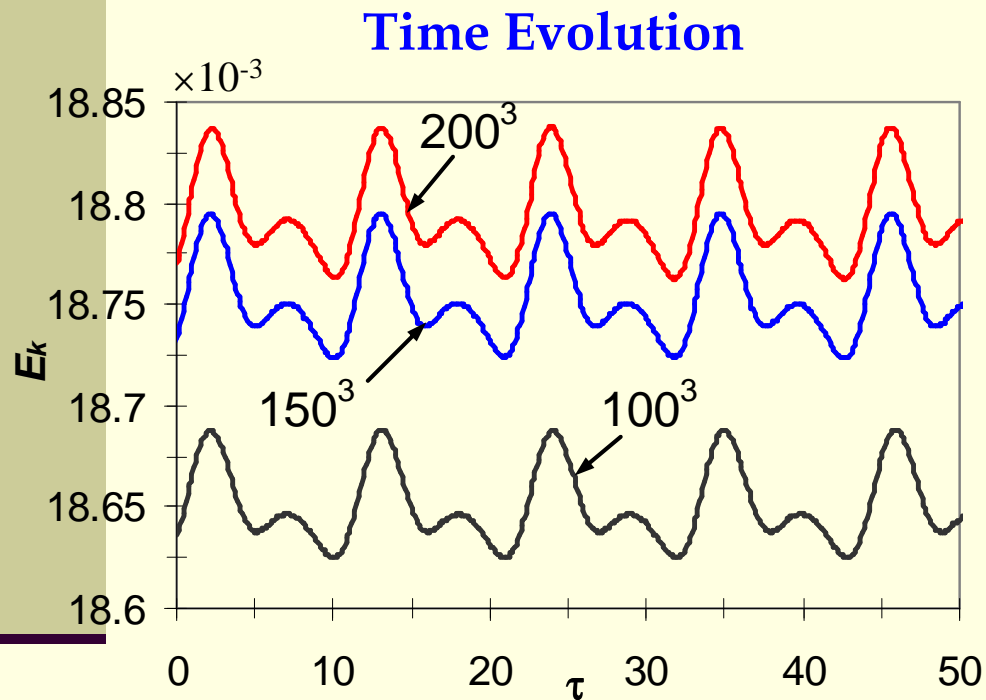
# The Character of the obtained bifurcation (Cont.)

Decreasing from  $Re=2000$   
leads to an oscillatory flow for  $Re=1950$



$Re_{cr}=1964$  is a subcritical Hopf bifurcation

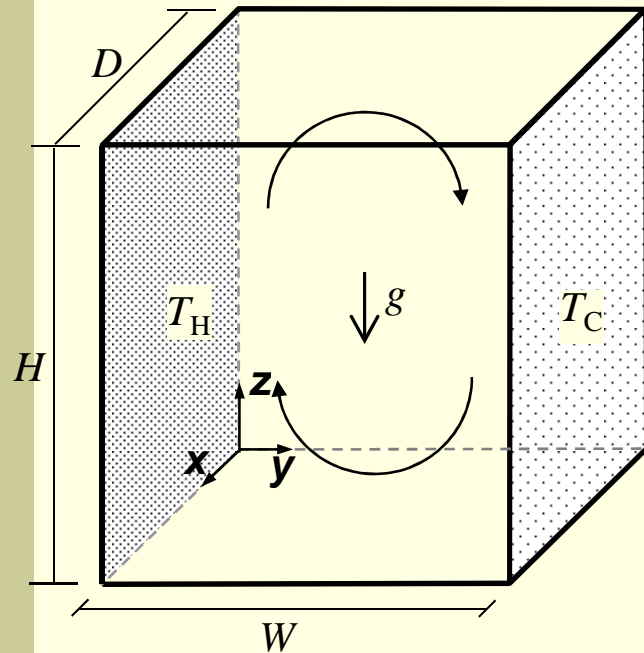
# The Flow Total Kinetic Energy



The maximum deviation between the kinetic energy values  
calculated on the  $152^3$  and  $200^3$  grids does not exceed 1%

# Benchmark Problems (Cont.)

## Differently Heated Rectangular and Cubic Cavity (Boussinesq Approximation)



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

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \sqrt{\frac{1}{\text{Gr}}} \nabla^2 \mathbf{u} + \theta \vec{e}_z$$

$$\frac{\partial \theta}{\partial t} + (\mathbf{u} \cdot \nabla) \theta = \frac{1}{\text{Pr} \sqrt{\text{Gr}}} \nabla^2 \theta$$

✓ Explicit Discretization

$$(\mathbf{u}^n \cdot \nabla) \mathbf{u}^n \quad (\mathbf{u}^n \cdot \nabla) \theta^{n+1}$$

▪ Semi-Implicit Discretization

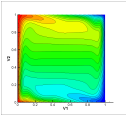
$$(\mathbf{u}^n \cdot \nabla) \mathbf{u}^{n+1} \quad (\mathbf{u}^n \cdot \nabla) \theta^{n+1}$$

Boundary Conditions:

$$\theta \Big|_{y=0} = 1, \quad \theta \Big|_{y=H/W} = 0 \quad \text{-isothermal vertical walls,} \quad \frac{\partial \theta}{\partial n} = 0 \quad \text{or} \quad \theta = 1 - y \quad \text{-horizontal and lateral walls}$$

$$\mathbf{u} = 0 \quad \text{-at all walls,}$$

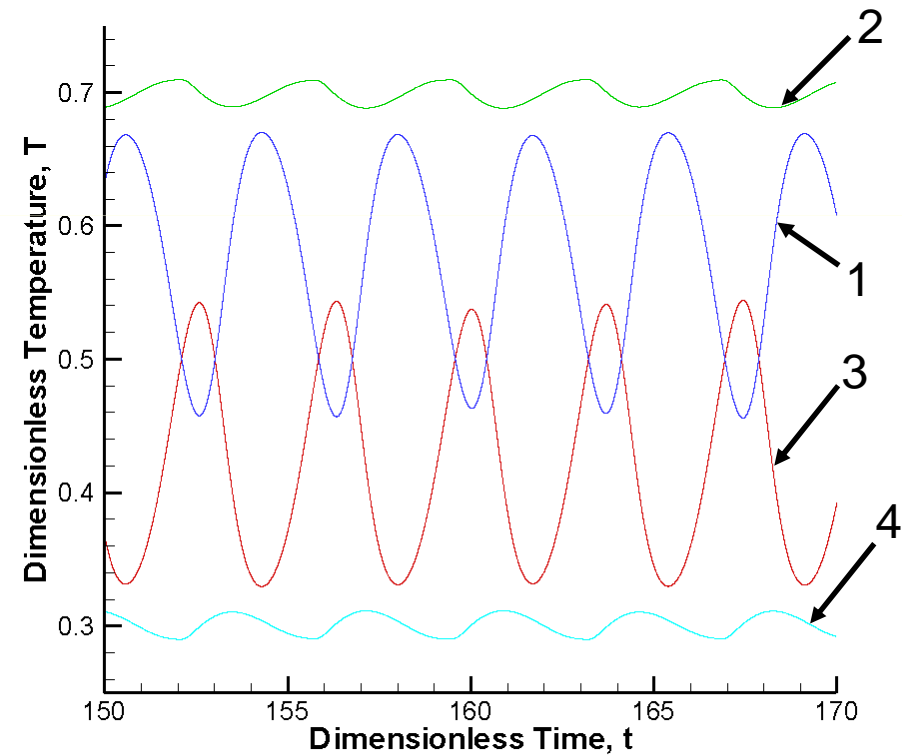
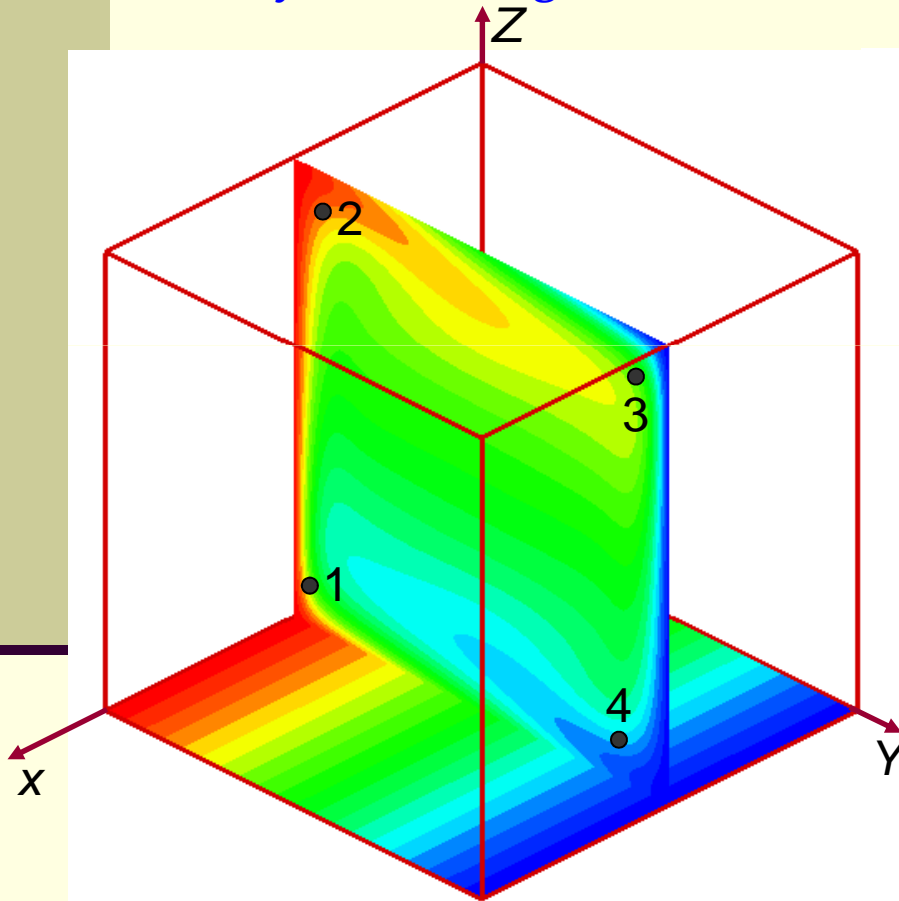
No boundary condition for pressure is needed



# Differentially Heated Cavity, $Gr=3.5 \times 10^6$

Perfectly conducting lateral walls

DNS results for midplane points



Central symmetry is preserved (opposite phases for opposite corners)

# Conclusions

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- ✓ An Accelerated Semi-Analytical Coupled Line Implicit Gauss-Seidel Smoother (**ASA-CLGS**) was developed and implemented for the solution of incompressible N-S equations.
- ✓ The Navier-Stokes equations are solved **without pressure-velocity decoupling**.
- ✓ The code was successfully parallelized for running on massively parallel supercomputers. **The overall obtained speed up reaches 200 for 1024 processors.**
- ✓ The multi- and single-grid approaches are scalable as  $O(Np/\ln(Np))$  and  $O(Np/\log_{10}(Np))$  respectively.
- ✓ The potential implementation of the developed parallelized time marching solver to the linear stability analysis was studied.