Performance of a DNS code on SX-Aurora TSUBASA

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Introduction

- Turbulence is fundamental phenomenon around our world.

- However, it is known that turbulence is an unsolved problem in classical physics.
  - One of Clay Mathematics Institute Millennium Prize problems.
    - *Is it possible to make a theoretical model to describe the behavior of a turbulent flow — in particular, its internal structures?*

- Direct numerical simulation (DNS) is one of useful means to tackle this difficult problem.

Difficulties in DNS of Turbulence

- Degree of freedom N^3 of turbulence is

$$N^3 \sim Re^{9/4}$$

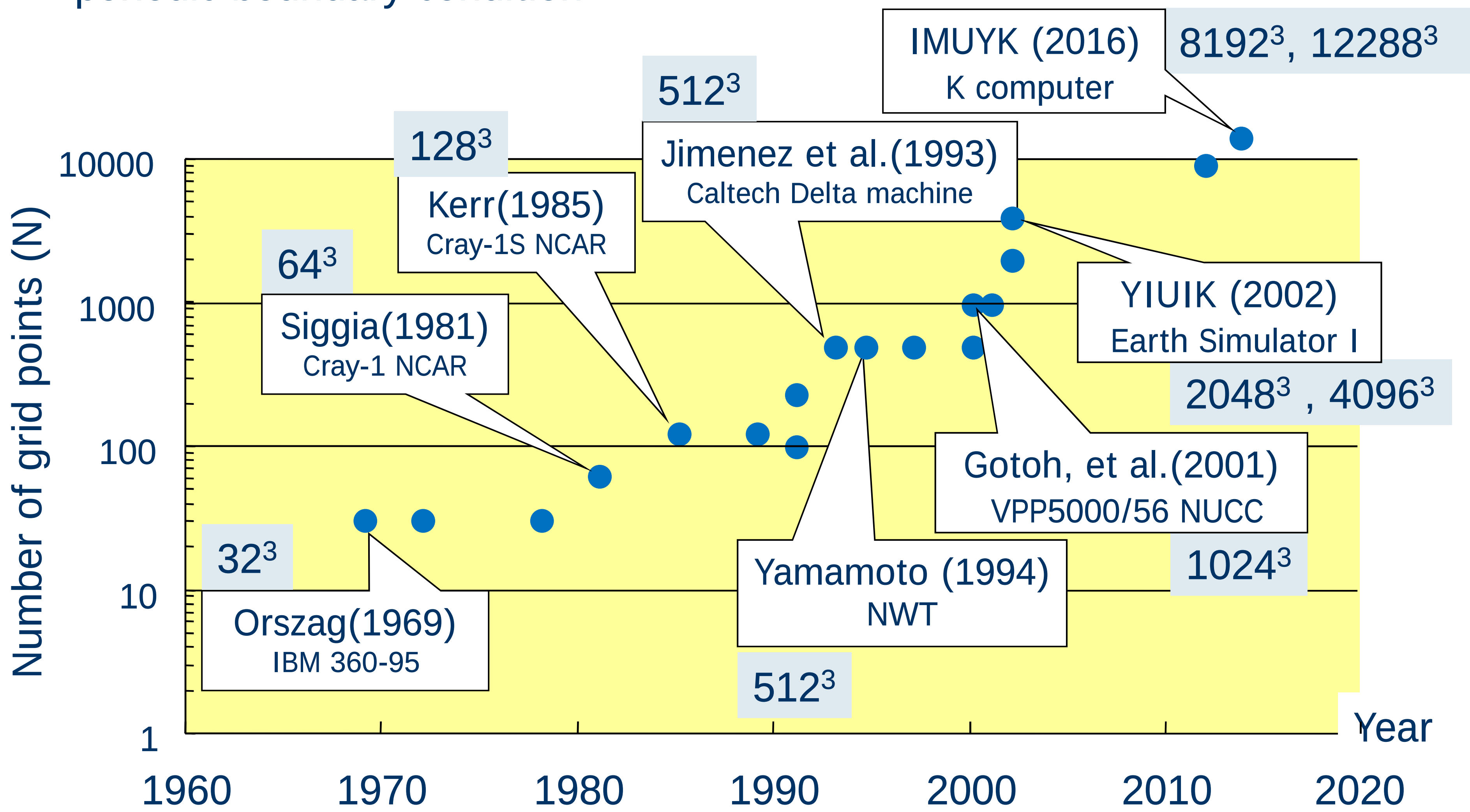
where Re is the Reynolds number.

- It is known that huge amount of computational resources are required to obtain high Reynolds turbulent flow.

- Incompressible homogeneous isotropic turbulent flow in a box under periodic boundary condition is one of the canonical turbulent flows and the simplest flow which holds properties of turbulence.

History of Representative DNS

Incompressible homogeneous isotropic turbulence in a cube under periodic boundary condition



Aims of the study

- Evaluating the performance of a DNS code on SX-Aurora TSUBASA is necessary in considering if higher resolution DNSs are possible or not.
- We have measured the computation time of the vectorized DNS code as the first evaluation.
- I/O performance of checkpoint files in using off-loaded functions of SX-Aurora TSUBASA is also measured.

Turbulence in a box (Canonical turbulent flow)

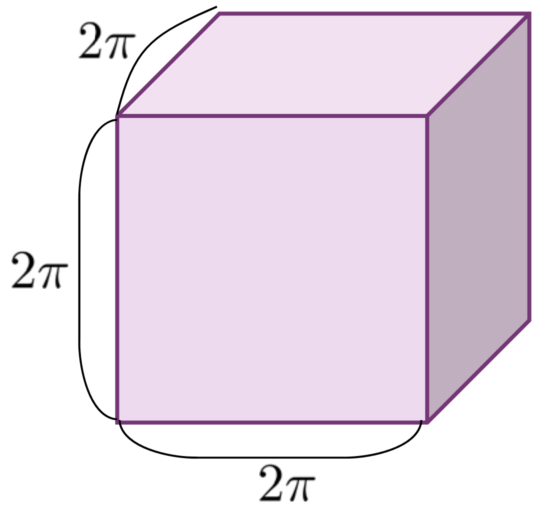
- Incompressible Navier-Stokes Equations under periodic boundary condition in a cube

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \nu \nabla^2 \boldsymbol{u} + \boldsymbol{f}$$

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

where,

$\boldsymbol{u} = (u_1, u_2, u_3)$	velocities,
p	pressure,
ν	kinematic viscosity, and
$\boldsymbol{f} = (f_1, f_2, f_3)$	external force.



Fourier Spectral Method (1/2)

- Fourier series expansion

$$u(x_j,t)=\sum_{k_3}\sum_{k_2}\sum_{k_1}\hat{u}_k(t)e^{\mathrm{i}k\cdot x_j}$$

where, $\hat{u}_k(t)=\frac{1}{N^3}\sum_{j_3}\sum_{j_2}\sum_{j_1}u(x_j,t)e^{-\mathrm{i}k\cdot x_j}$

- O.D.E. by discretizing with Fourier series expansion

$$\left(\frac{d}{dt}+\nu|\boldsymbol{k}|^2\right)\hat{u_i}(\boldsymbol{k})=\left(\delta_{ij}-\frac{k_ik_j}{|\boldsymbol{k}|^2}\right)\hat{h_j}(\boldsymbol{k})+\hat{f_i}(\boldsymbol{k})$$

where, $u_i(\boldsymbol{x})=\sum_{|\boldsymbol{k}|<K_c}\hat{u_i}(\boldsymbol{k})\exp(i\boldsymbol{k}\cdot\boldsymbol{x})$ Fourier series, and

$\boldsymbol{k}=(k_1,k_2,k_3)$ a wave number vector.

Fourier Spectral Method

- O.D.E. by Fourier Spectral method

$$\left(\frac{d}{dt}+\nu|\boldsymbol{k}|^2\right)\hat{u}_i(\boldsymbol{k})=\left(\delta_{ij}-\frac{k_i k_j}{|\boldsymbol{k}|^2}\right)\hat{h_j}(\boldsymbol{k})+\hat{f}_i(\boldsymbol{k})$$

- Non-linear terms are calculated by a spectral method.
  - Some techniques (phase shift & mode truncation techniques) are used in calculating non-linear terms for removing aliasing errors.

- Fourth-order Runge-Kutta-Gill method is adopted for time integration
  - Most of the calculation time is consumed in the Fast Fourier Transforms (FFT).

De-aliasing error technique: phase shift method

$$\hat{u}_i^s = \hat{u}_i \exp(i\boldsymbol{k} \cdot \boldsymbol{x}_s)$$

$$\boldsymbol{x}_s = (\pi/N, \pi/N, \pi/N)$$

Normal series

$\hat{u}_1(\boldsymbol{k}), \hat{u}_2(\boldsymbol{k}), \hat{u}_3(\boldsymbol{k})$

FFT^{-1} $\;u, v, w$ 3 times

$u_1(\boldsymbol{x}), u_2(\boldsymbol{x}), u_3(\boldsymbol{x})$

$u_i u_j$

uu, uv, uw, vv, vw, ww

FFT 6 times

$\widehat{u_i u_j}$

Phase shift series

$\hat{u}_1^s(\boldsymbol{k}), \hat{u}_2^s(\boldsymbol{k}), \hat{u}_3^s(\boldsymbol{k})$

FFT^{-1} 3 times

$u_1^s(\boldsymbol{x}), u_2^s(\boldsymbol{x}), u_3^s(\boldsymbol{x})$

$u_i^s u_j^s$

FFT 6 times

$\widehat{u_i^s u_j^s}$

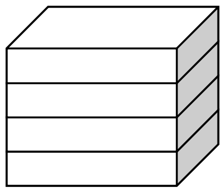
+

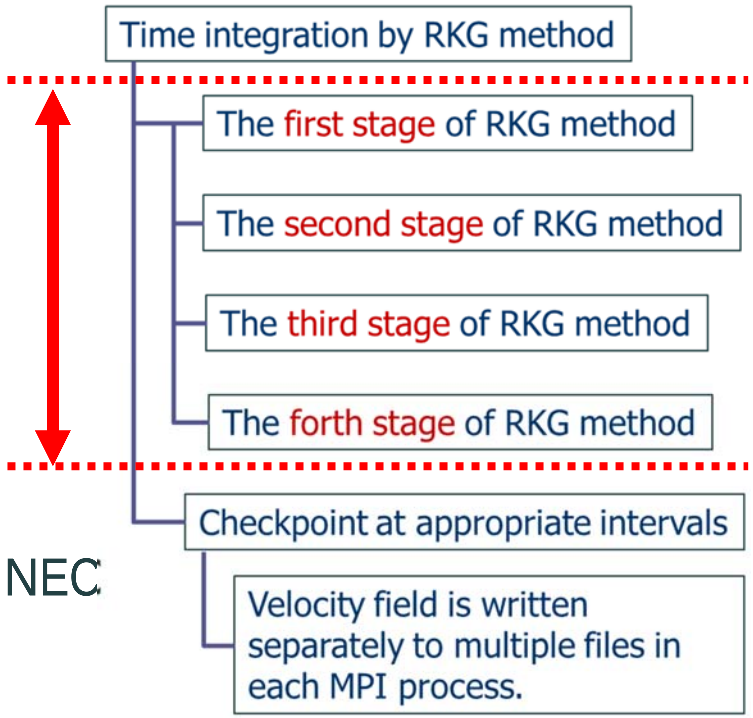
$\hat{h}_i(\boldsymbol{k})$

The number of FFTs to evaluate $\hat{h}_i(\boldsymbol{k})$ doubled.

Measurements of computation times

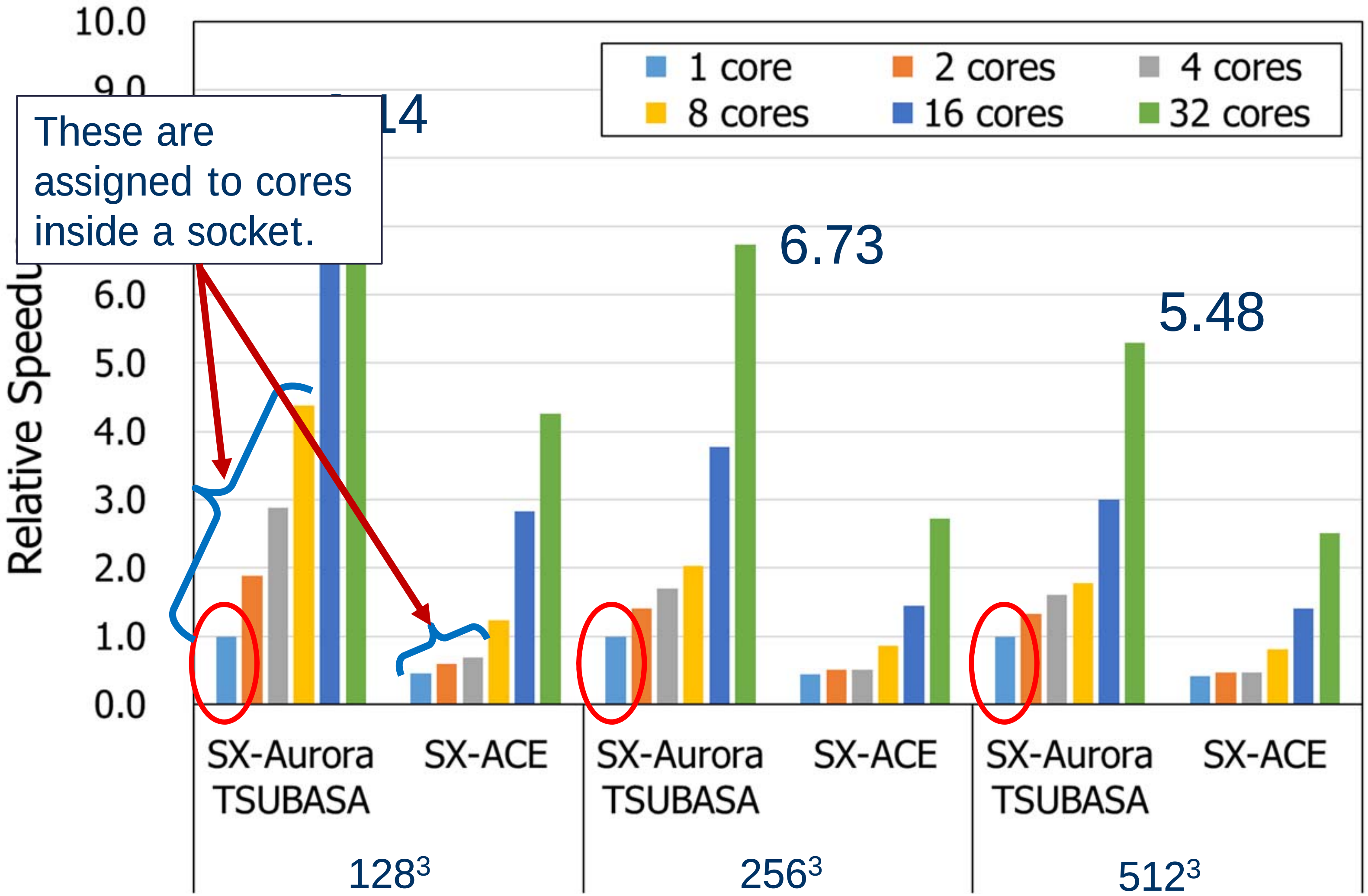
- Computation time for 1 time step of RKG integration was measured.
  - Code characteristics
    - Slab parallelization
    - 1 MPI process are allotted to a core
  - Grid sizes
    - $N^3=128^3$, 256^3, and 512^3



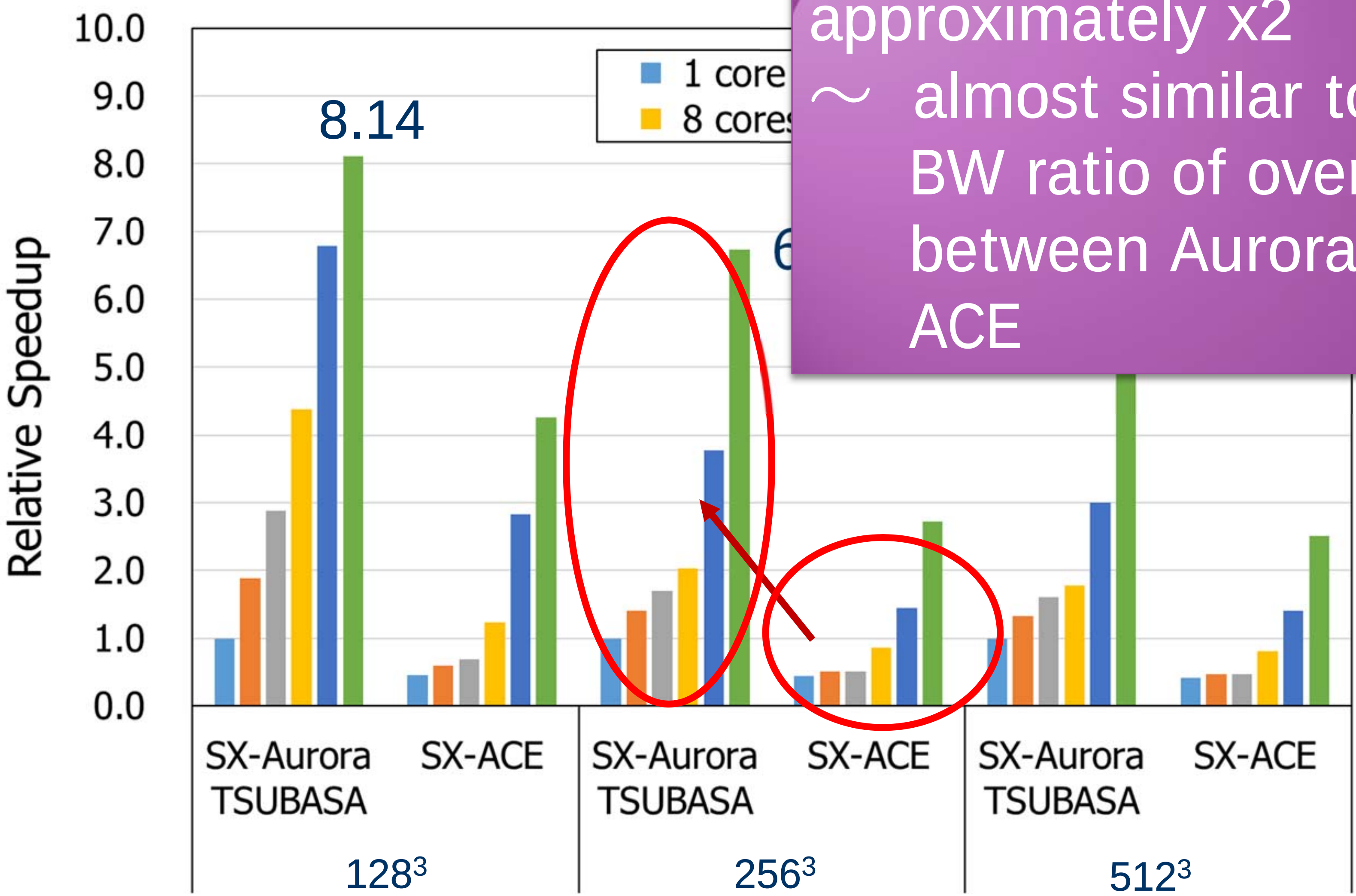


- Systems used in measurements
  - SX-Aurora TSUBASA@Tohoku Univ., and NEC
    - 1 core – 32 cores
  - SX-ACE@NEC
    - 1 core - 32 cores

SX-Aurora TSUBASA vs. SX-ACE



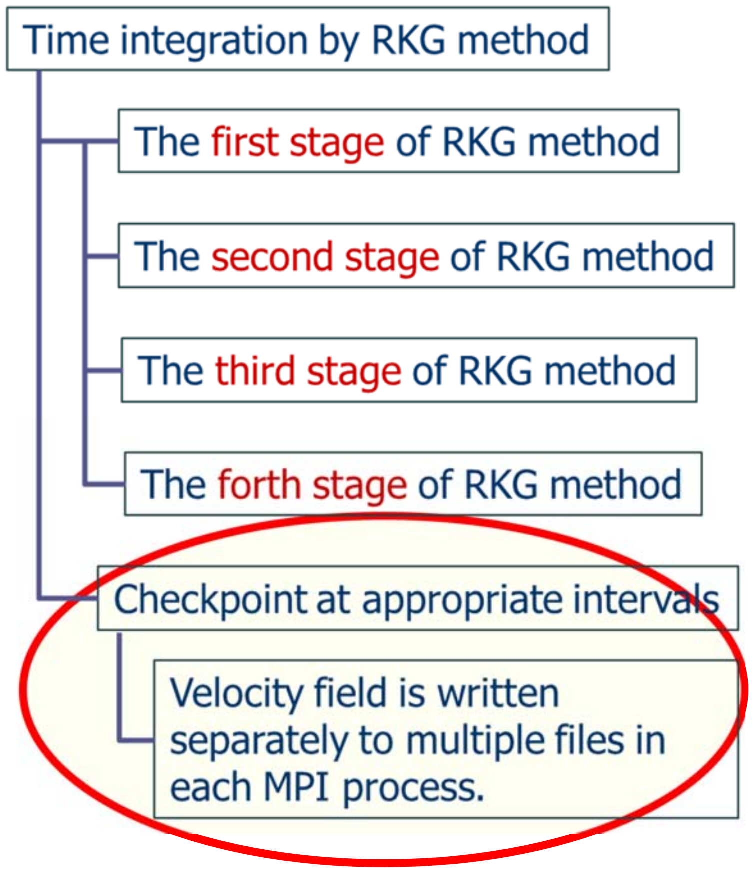
SX-Aurora TSUBASA vs. SX-ACE



approximately x2
～ almost similar to the BW ratio of over 2.0 between Aurora and ACE

I/O performance on off-loaded operations

- Several velocity fields in spectral space are kept as checkpoints at an appropriate time intervals so as to take statistics of turbulence.
  - Also, DNS can be restarted and continued at the last checkpointed velocity field.

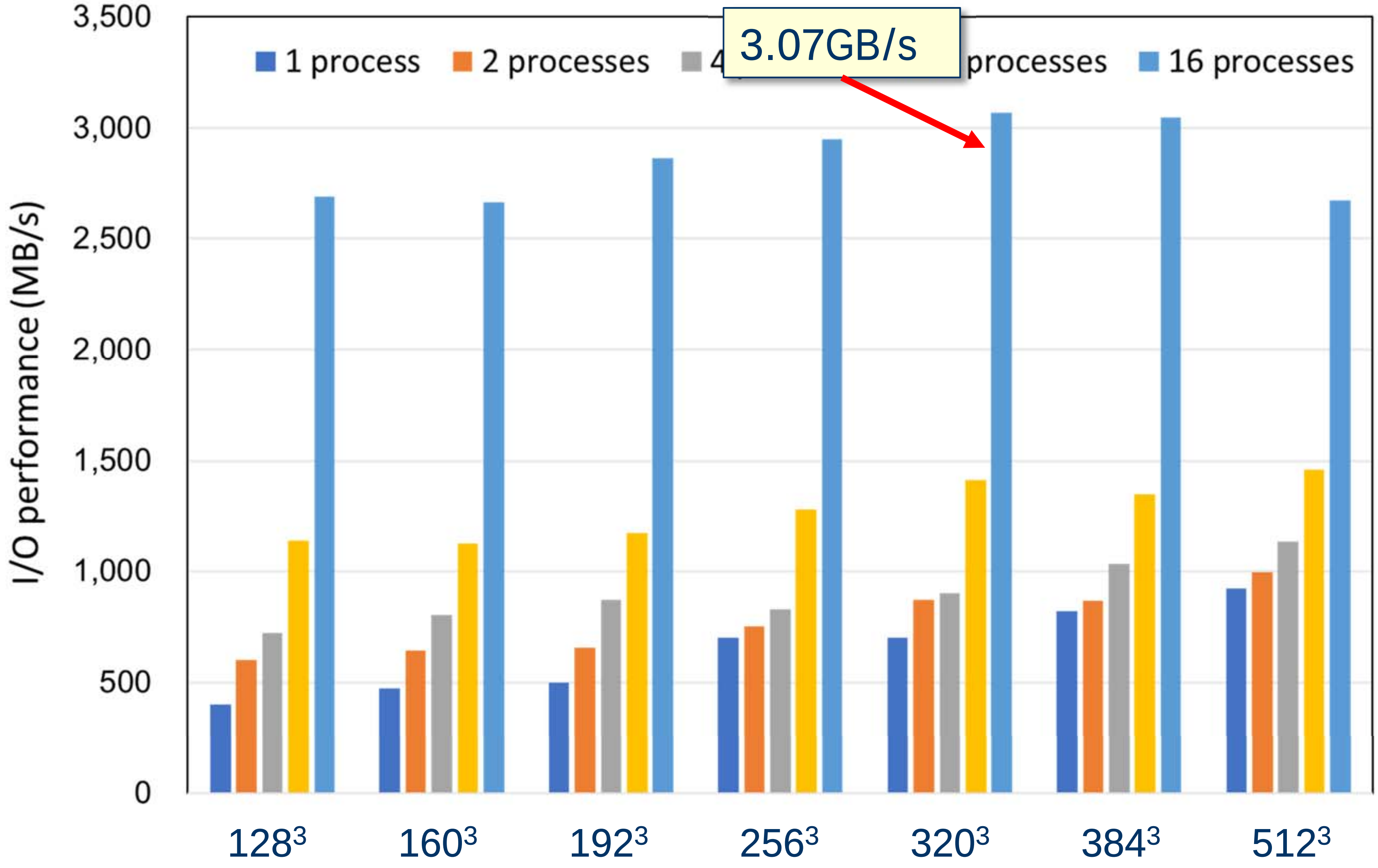


- Checkpoint files
  - Velocities at all grid points
  - Whole file size
    - 16 bytes (double precision complex variable)
      x (3 directions of velocities, u, v, and w)
      x (grid points/number of MPI parallel processes)
  - Number of files
    - Number of MPI parallel processes

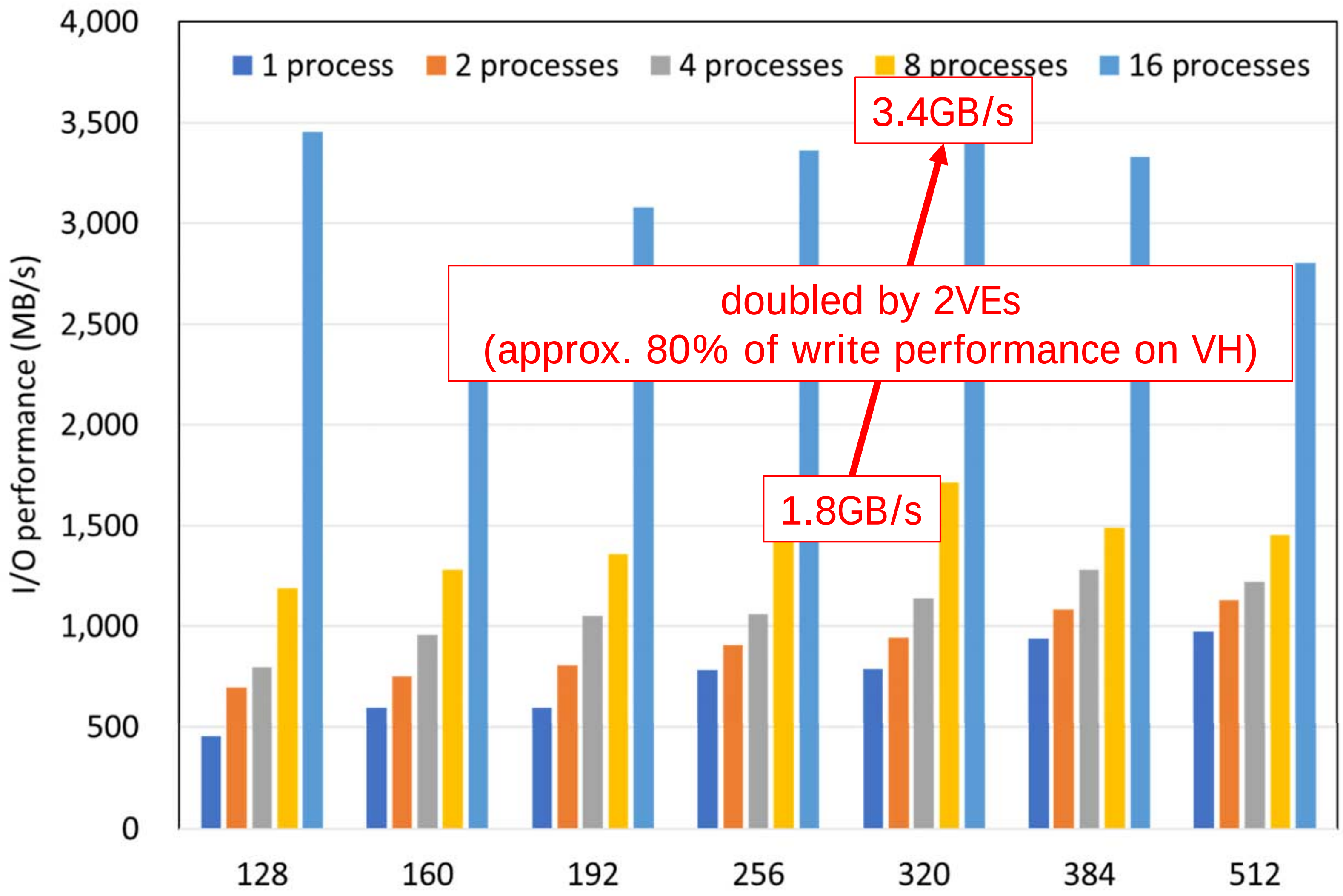
Measurement of reading and writing times of files

- Reading and writing times of an instantaneous velocity field are measured by changing the number of MPI processes and the number of grid points.
  - 1, 2, 4, 8, and 16 MPI processes
  - $N=128^3$, 160^3, 192^3, 256^3, 320^3, 384^3, and 512^3
    - These numbers have factors of 2, 3, and 5 so that the Fast Fourier transforms can be applied.
    - File sizes for girds are 48MiB, 94MiB, 162MiB, 384MiB, 750MiB, 1296MiB, and 3072MiB in total, respectively. Each file is partitioned into some smaller ones according to the number of MPI processes.
- I/O system calls are off-loaded to the VH.

Read Performance (Read on VH off-loaded from VE)



Write Performance (Write on VH off-loaded from VE）



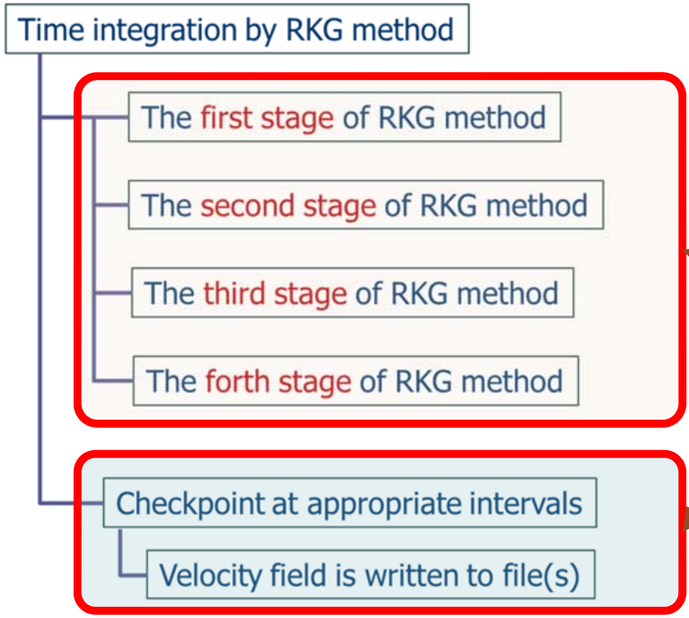
Further works (cont'd)

- Further optimization of the DNS code is required to obtain better performance.
  - Two separate arrays representing real parts and imaginary parts of complex Fourier coefficients are used in the original code so that higher performance is achieved on old-fashioned vector processors. These representations should be changed on present vector processors so as to hold real and imaginary parts contiguously on memory.
  - Bank conflicts were observed in the current code and should be improved.

- Hybrid implementation with OpenMP and MPI should be evaluated.

Further works

- Asynchronous I/O function has just implemented into VE operating system.
  - How to determine a checkpoint interval



When a checkpoint interval is taken to the same as the duration of some number of RKG time integration loops, these two parts can be overlapped by using double variables of velocity field.

- Checkpoint operations is possible to be hided behind the DNS computation.