HPC Summer School
Computational Fluid Dynamics Simulation and its Parallelization

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Agenda

- **PART-I**

  Introduction of Application: 2D CFD Simulation

  ✓ Lecture

  ✓ Hands-on Practice

- **PART-II**

  Parallelization of the 2D CFD Simulation

  ✓ Lecture

  ✓ Hands-on Practice

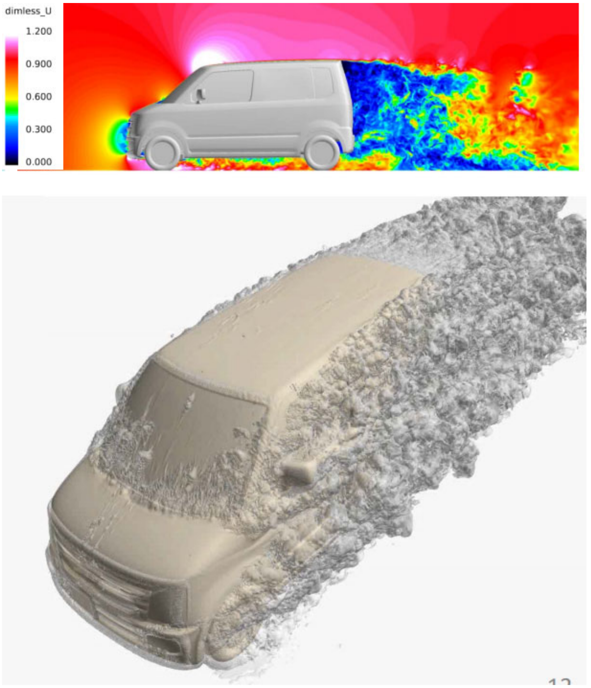
PART-I

Introduction of Application: 2D CFD Simulation

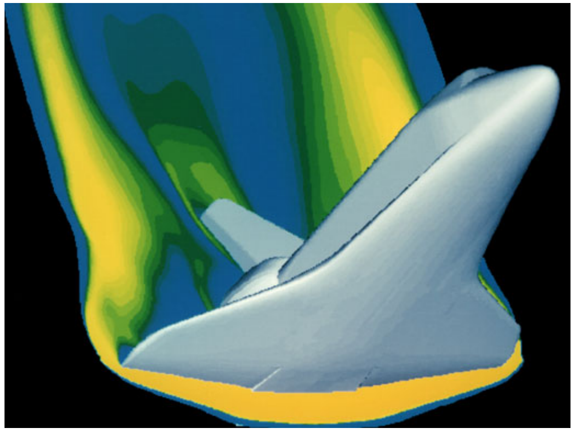
Introduction

Other example: simulation of COVID-19 droplets and aerosols
https://www.r-ccs.riken.jp/en/fugaku/research/covid-19/msg-en/

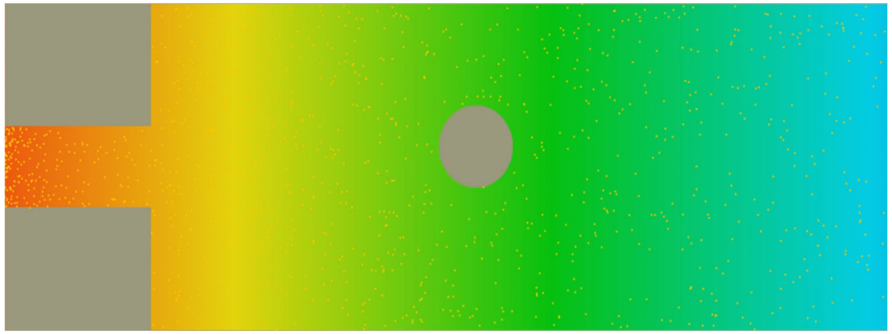
What is Computational Fluid Dynamics (CFD) simulation ?



Prediction of the Drag by 2.3 billion meshes.

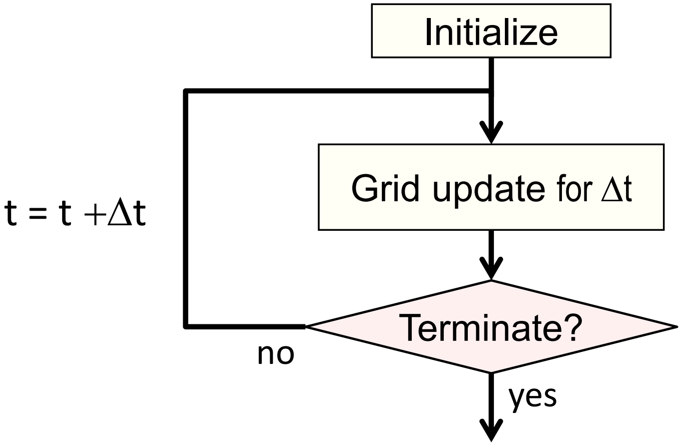


Simulation of high velocity air flow around the Space Shuttle during re-entry.



Simulation of 2D viscous flow with circular obstacle.

How to Compute Fluid Flow?



Initialize

Grid update for Δt

Terminate?

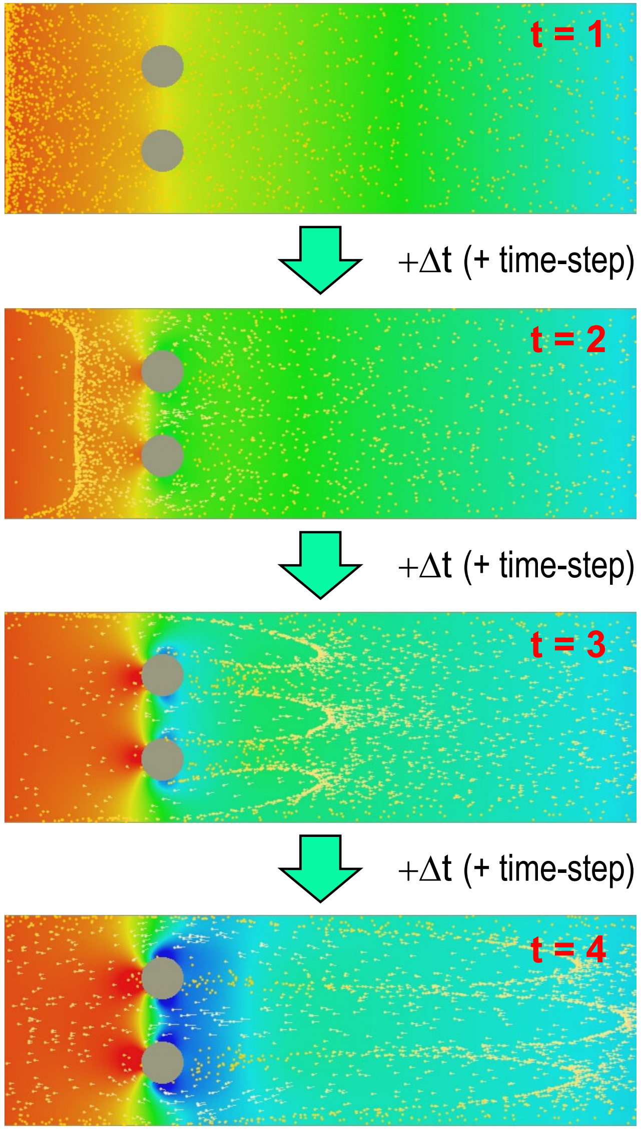
no

yes

t = t +Δt

Repeating grid update for Δt fluid change.

How to update?



Incompressive Viscous Fluid Flow

Governing Equations with partial differential equations

Equation of continuity
(incompressive flow)

$$\nabla V = 0$$

Navier–Stokes equations
(incompressive flow)

$$\frac{\partial V}{\partial t} + (V \cdot \nabla)V = -\nabla\varphi + \nu\nabla^2 V$$

V	velocity = (*u*, *v*)	$\nu \equiv {}^{\mu}/_{\rho}$	kinematic viscosity
P	pressure	$\varphi \equiv {}^{P}/_{\rho}$	
ρ	density		

Fractional-Step Method

1. Calculate **the tentative velocity** ***V**** **without the pressure-term.**

$$V^* = V^n + \Delta t \left\{ -(V^n \cdot \nabla) V^n + \nu \nabla^2 V^n \right\} \quad (1)$$

2. Calculate **the pressure field ϕ^{n+1}** **of the next time-step with** ***V**** **by solving the Poisson's equation.**

$$\nabla^2 \varphi^{n+1} = \frac{\nabla \cdot V^*}{\Delta t} \quad (2)$$

3. Calculate **the true velocity** V^{n+1} **of the next time-step with** ***V**** **and** ϕ.

$$V^{n+1} = V^* - \Delta t \nabla \varphi^{n+1} \quad (3)$$

Finite Difference Schemes

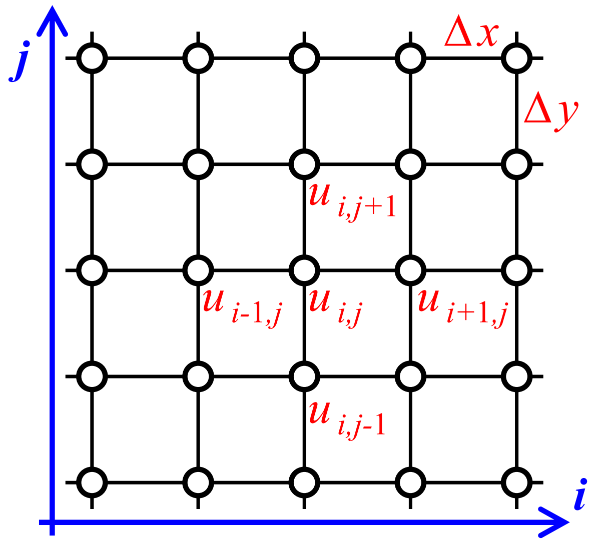
We can make discrete forms by substituting difference schemes.

$$\frac{du}{dx} \simeq \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

$$\frac{d^2u}{dx^2} \simeq \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2}$$

Central difference schemes

(=> Finite difference scheme)



2D collocate mesh

(Each grid point has all variables: u, v, ϕ.)

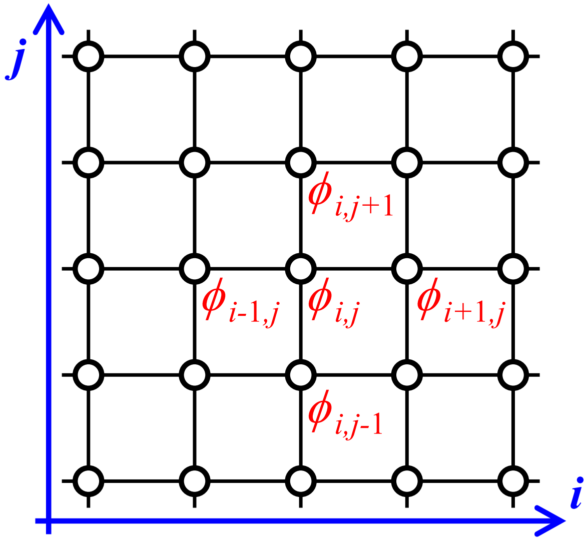
See "staggered mesh" for more advanced study.

Discrete Form of Step1

Step1 : Calculate the tentative velocity : *u*, v**

$$u^*_{i,j} = u_{i,j} + \Delta t \left\{ \begin{array}{c} -u_{i,j}\dfrac{u_{i+1,j}-u_{i-1,j}}{2\Delta x} - v_{i,j}\dfrac{v_{i,j+1}-v_{i,j-1}}{2\Delta y} + \\ NU\left(\dfrac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{(\Delta x)^2} - \dfrac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{(\Delta y)^2}\right) \end{array} \right\}$$

NU is kinematic viscosity.
A similar equation for v.

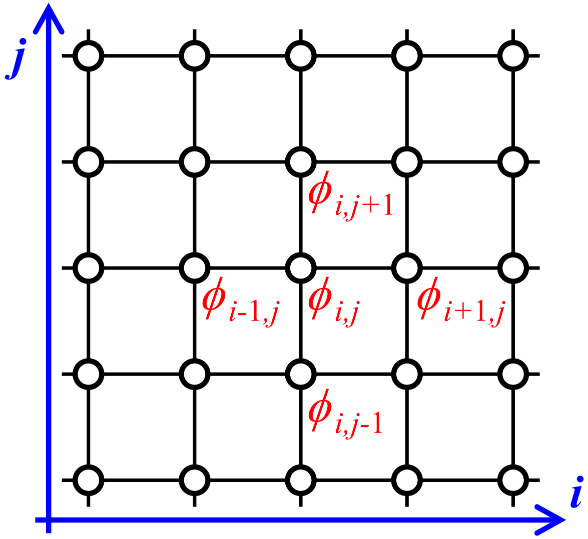


Discrete Form of Step2

Step2 : Calculate the pressure by Jacobi method.

Iterating phi’s update until residual met a certain condition.

$$\varphi'_{i,j} = \alpha\left(\frac{\varphi_{i+1,j} + \varphi_{i-1,j}}{(\Delta x)^2} + \frac{\varphi_{i,j+1} + \varphi_{i,j+1}}{(\Delta y)^2} - D_{i,j}\right)$$



where

$$\alpha = \frac{\Delta x^2 \Delta y^2}{2(\Delta x^2 + \Delta y^2)}$$

and

$$D_{i,j} = \frac{1}{\Delta t}\left(\frac{u^*_{i+1,j} - u^*_{i-1,j}}{2\Delta x} + \frac{v^*_{i,j+1} - v^*_{i,j-1}}{2\Delta y}\right)$$

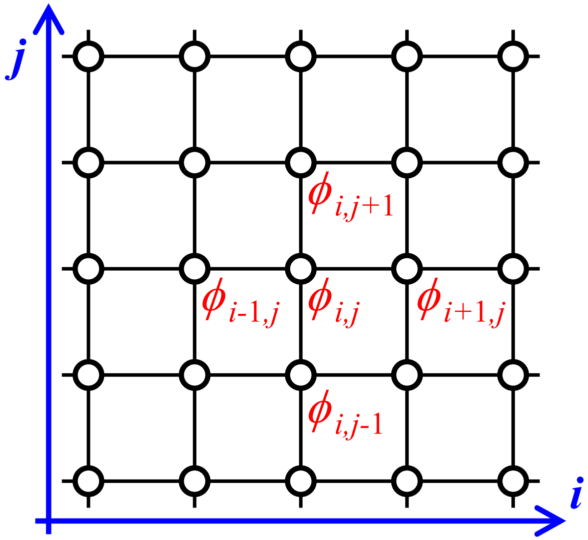
$D_{i,j}$ is referred to as **a source term** of Poisson’s equation.

Discrete Form of Step3

Step3 : Calculate the true velocity of the next time-step

$$u_{i,j}^{true} = u_{i,j}^{*} - \Delta t \frac{(\varphi'_{i+1,j} - \varphi'_{i-1,j})}{2\Delta x}$$

$$v_{i,j}^{true} = v_{i,j}^{*} - \Delta t \frac{(\varphi'_{i,j+1} - \varphi'_{i,j-1})}{2\Delta y}$$

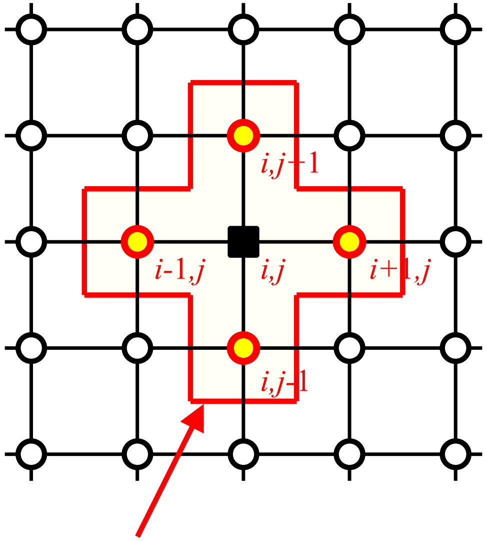


Stencil Computation

Common form in Steps 1, 2, and 3

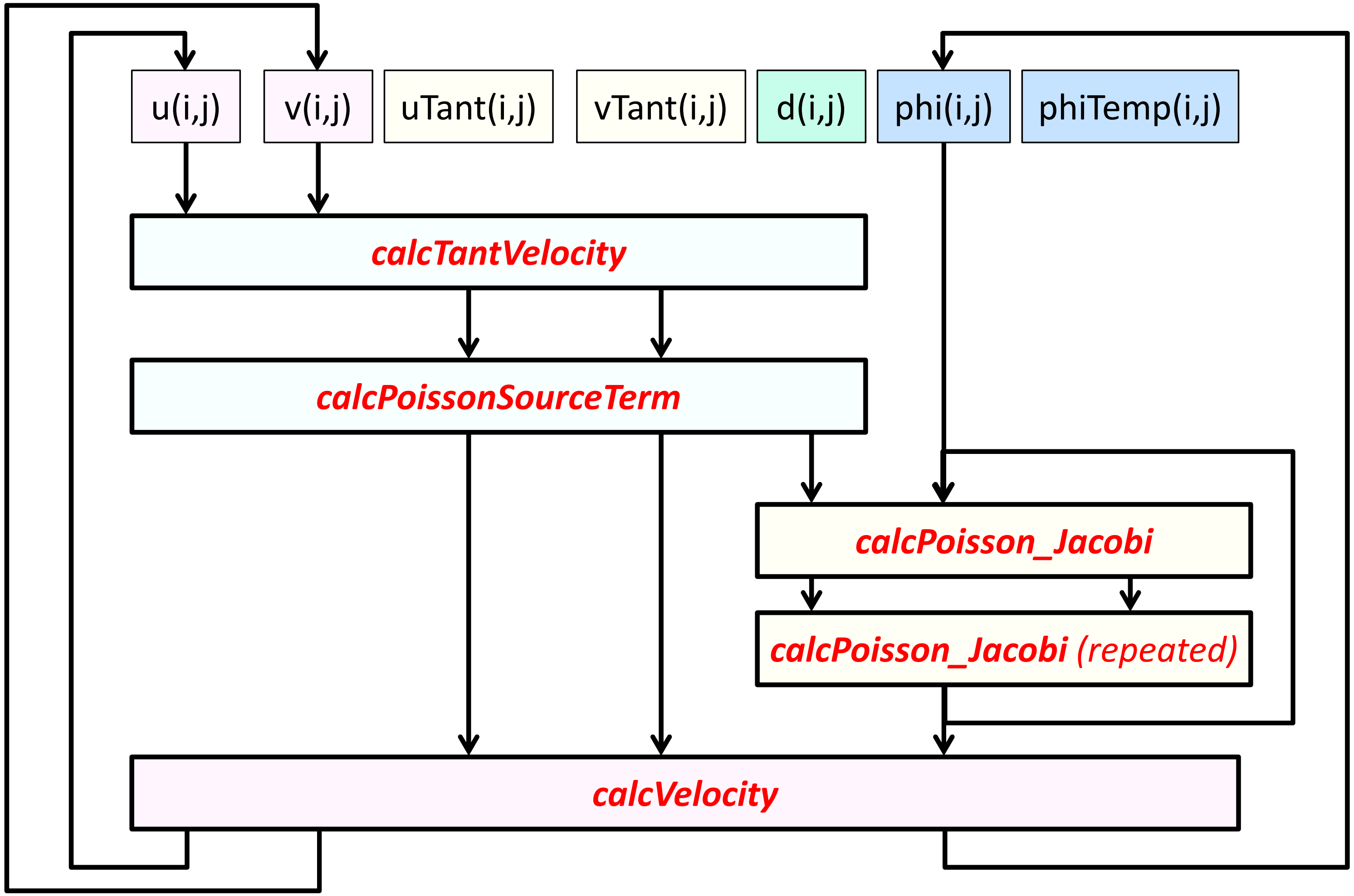
$$q_{i,j}^{new} = A + Bq_{i,j} + Cq_{i+1,j} + Dq_{i-1,j} + Eq_{i,j+1} + Fq_{i,j-1}$$

Each point is computed only with its adjacent points.



Stencil
(adjacent region of each point)

Data Dependency among Steps



Hands-on : Let’s read the codes!

```
login5$ pwd
        /home/ra020006/<your user ID>/
login5$ mkdir  programs_cfd
login5$ cd  programs_cfd
login5$ cp  /home/ra020006/data/program/serial_0824.tar.gz  ./
login5$ tar  zxvfp  serial_0824.tar.gz
login5$ cd  serial_0824/
login5$ ls
        cfd.cpp
        cfd.h
        main.cpp
        main.h
        stopwatch3.h
        Makefile
        README.txt
        scripts
```

You are in your home directory.

Create a work directory.

Copy and extract program files.

Source files – You modify them!
(program codes)

Rules for compilation with “make”

Information on how to compile, execute, etc.

Script programs for execution and visualization

Program Structure

- **Data structures (cfd.h)**
  - ✓ typedef struct array2D_ { … } array2D; // 2D array of a scalar value
  - ✓ typedef struct grid2D_ { … } grid2D; // 2D grid for fluid using multiple array2Ds

- **Functions for array2D**
  - ✓ void array2D_initialize(array2D *a, …); // Initialize 2D array : row x col
  - ✓ void array2D_resize(array2D *a, …); // Resize 2D array : row x col
  - ✓ void array2D_copy(array2D *a, …); // Copy src to dst (by resizing dst)
  - ✓ void array2D_clear(array2D *a, …); // Clear 2D array with value of v
  - ✓ void array2D_show(array2D *a, …); // Print 2D array in text
  - ✓ double linear_intp(array2D *a, …); // Get value with linear interpolation
  - ✓ inline int array2D_getRow(array2D *a, …); // Get size of row
  - ✓ inline int array2D_getCol(array2D *a, …); // Get size of col
  - ✓ inline double *at(array2D *a, …); // Get pointer at (row, col)
  - ✓ inline double L(array2D *a, …) // Look up value at (row, col)

Program Structure (cont'd)

- **Data structures (cfd.h)**
  - typedef struct array2D_ { … } array2D;   // 2D array of a scalar value
  - typedef struct grid2D_ { … } grid2D;   // 2D grid for fluid using multiple array2Ds

- **Functions for grid2D**
  - void grid2D_initialize(grid2D *g, ⋯);   // Initialize 2D grid (row x col) for CFD
  - void grid2D_calcTantVelocity(grid2D *g);   // Step 1 of Fractional-step method
  - void grid2D_calcPoissonSourceTerm(grid2D *g);   // Step 2 (Calculation of source terms)
  - void grid2D_calcPoisson_Jacobi(grid2D *g, , ⋯);   // Step 2 (Iterative solver : time-consuming)
  - void grid2D_calcVelocity(grid2D *g);   // Step 3
  - void grid2D_calcBoundary_Poiseulle(grid2D *g, , ⋯);   // Set boundary condition for top & bottom walls
  - void grid2D_calcBoundary_SqObject(grid2D *g, , ⋯);   // Set boundary condition for a square obstacle
  - void grid2D_outputAVEseFile(grid2D *g, , ⋯);   // Output a grid data to a file
  - inline int grid2D_getRow(grid2D *g);   // Get size of row
  - inline int grid2D_getCol(grid2D *g);   // Get size of col

main.{h, cpp}

main.h

```
/*
 * 2D fluid simulation based on Fractional-step method
 * Written by Kentaro Sano for
 * International Summer school, RIKEN R-CCS
 *
 * Version 2020_0919
 *
 * All rights reserved.
 * (C) Copyright Kentaro Sano 2018.6-
 *
 */
#ifndef ___MAIN_H___
#define ___MAIN_H___

#include <string.h>
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#include "cfd.h"
#include "stopwatch3.h"

int main(int argc,char** argv);
void fractionalStep_MainLoop(grid2D *g, int numTSteps);

#endif
```

main.cpp

```
#include "main.h"

int main(int argc,char** argv)
{
...
 tstep = 0;
 grid2D_initialize(&g, ROW, COL, PHI_IN, PHI_OUT);

 printf("======== Computation started for (%d x %d) grid with dT=%f.¥n", ROW, COL, DT);

 while(tstep < END_TIMESTEP) {
  time2.start();
  tstep_start = tstep;
  fractionalStep_MainLoop(&g, SAVE_INTERVAL);
  time2.stop();
  printf("[tstep=%5d to %5d] (%f sec) ", tstep_start, tstep, time2.get());
  grid2D_outputAVEseFile(&g, "AVEse", tstep, 240.0/grid2D_getRow(&g));
}

 time.stop();
 printf("======== Computation finished.¥n");
 printf("Time-step=%d : ElapsedTime=%3.3f sec¥n", tstep, time.get());

 return 0;
}

void fractionalStep_MainLoop(grid2D *g, int numTSteps)
{
 for (int n=0; n<numTSteps; n++) {
  grid2D_calcTantVelocity(g);
  grid2D_calcPoissonSourceTerm(g);
  grid2D_calcPoisson_Jacobi(g, TARGET_RESIDUAL_RATE);
  grid2D_calcVelocity(g);
  grid2D_calcBoundary_Poiseulle(g, PHI_IN, PHI_OUT);
  grid2D_calcBoundary_SqObject(g, OBJ_X, OBJ_Y, OBJ_W, OBJ_H);
  tstep++;
 }
}
```

cfd.h　　1 of 2

cfd.h

```
#ifndef ___CFD_H___
#define ___CFD_H___

#include <string.h>
...

// You can select one of the conditions.

//#define CONDITIONX
#define CONDITION0
//#define CONDITION1
//#define CONDITION2
//#define CONDITION3

//==========================================================
// Note: If you increase ROW&COL (then dX and dY decrease), you need
//      to decrease DT for CFL condition. Or simulation explodes.

#if defined CONDITIONX

//Flow condition X  (taking super long time)
#define ROW (2160)                      // cell resolution for row
#define COL (720)                       // cell resolution for column
#define DT  (0.0000075)                 // delta t (difference between timesteps)
#define NU  (0.0075)                    // < 0.01 for Karman vortices
#define JACOBIREP_INTERVAL (500)        // interval to report in Jacobi
#define END_TIMESTEP       (80000)      // tstep to end computation

#elif defined CONDITION0
```

```
...
#elif defined CONDITION1
...
#elif defined CONDITION2
...
#elif defined CONDITION3
...
#endif

#define TARGET_RESIDUAL_RATE (1.0e-2)  // Termination condition
#define SAVE_INTERVAL   JACOBIREP_INTERVAL  // Interval to save file
//==================================================================

#define HEIGHT 0.5                       // Grid Height is set a length of 0.5 (dimention-less length)
#define WIDTH (0.5*(double)ROW/(double)COL) // Width is calculated with the ratio of ROW to COL
#define DX    (WIDTH/(ROW-1))
#define DY    (HEIGHT/(COL-1))
#define DX2   (DX*DX)
#define DY2   (DY*DY)

// Boundary conditions for Poiseulle flow
#define U_IN (1.0)             // X velocity of inlet (incoming) flow (unused)
#define V_IN (0.0)             // Y velocity of inlet (incoming) flow (unused)
#define PHI_IN  (200.0)        // Pressure of inlet (incoming boundary)
#define PHI_OUT (100.0)        // Pressure of outlet (outgoing boundary)

// Rectangle object for internal boundary
#define OBJ_X  (ROW*0.25)    // X-center of object
#define OBJ_Y  (COL*0.5)     // Y-center of object
#define OBJ_W  (COL*0.2)     // Width (in x) of object
#define OBJ_H  (COL*0.30)    // Height (in y) of object

// Global variables
extern int tstep;            // time-step
```

cfd.h　2 of 2

cfd.h

```
// Definition of data structure (grid and common variables)

// Data structure of 2D array (resizable)
typedef struct array2D_ {
  int row;              // ROW resolution of a grid
  int col;              // COL resolution of a grid
  double *v;            // Pointer of 2D array
} array2D;

// Member functions for array2D
void array2D_initialize(array2D *a, int row, int col);          // initialize 2D array : row x col
void array2D_resize(array2D *a, int row, int col);              // resize 2D array : row x col
void array2D_copy(array2D *src, array2D *dst);                  // copy src to dst (by resizing dst)
void array2D_clear(array2D *a, double v);                       // clear 2D array with value of v
void array2D_show(array2D *a);                                  // print 2D array in text
double linear_intp(array2D *a, double x, double y);             // get value ay (x,y)
                                                                // with linear interpolation
inline int array2D_getRow(array2D *a) { return (a->row); }      // get size of row
inline int array2D_getCol(array2D *a) { return (a->col); }      // get size of col
inline double *at(array2D *a, int i, int j)                     // get pointer at (row, col)
{
#if 0
  if ((i<0) || (j<0) || (i>=a->row) || (j>=a->col)) {
    printf("Out of range : (%d, %d) for %d x %d array in at(). Abort.¥n", i, j, a->row, a->col);
    exit(EXIT_FAILURE);
  }
#endif
  return (a->v + i + j * a->row);
}
inline double L(array2D *a, int i, int j) { return *(at(a,i,j)); }   // Look up value at (row, col)
```

```
// Data structure of 2D grid for fluid flow
typedef struct grid2D_ {
  array2D u, v, phi;          // velocity (u, v), pressure phi
  array2D phiTemp;            // tentative pressure (temporary for update)
  array2D uTant, vTant;       // tentative velocity (u, v)
  array2D d;                  // source term of a pressure poisson's equation
} grid2D;

// Member functions for grid2D
void grid2D_initialize(grid2D *g, int row, int col, double phi_in, double phi_out);
void grid2D_calcTantVelocity(grid2D *g);
void grid2D_calcPoissonSourceTerm(grid2D *g);
void grid2D_calcPoisson_Jacobi(grid2D *g, double target_residual_rate);
void grid2D_calcVelocity(grid2D *g);
void grid2D_calcBoundary_Poiseulle(grid2D *g, double phi_in, double phi_out);
void grid2D_calcBoundary_SqObject(grid2D *g, int obj_x, int obj_y, int obj_w, int obj_h);
void grid2D_outputAVEseFile(grid2D *g, char *base, int num, double scaling);
inline int  grid2D_getRow(grid2D *g) { return( array2D_getRow(&(g->u)) ); }
inline int  grid2D_getCol(grid2D *g) { return( array2D_getCol(&(g->u)) ); }

#endif
```

cfd.cpp 1 of 6

cfd.cpp

```
#include "cfd.h"

int    tstep; // time-step

// Member functions for array2D
void array2D_initialize(array2D *a, int row, int col)
{
  a->row = 0;
  a->col = 0;
  a->v   = (double *)NULL;
  array2D_resize(a, row, col);
  array2D_clear(a, 0.0);
}

void array2D_resize(array2D *a, int row, int col)
{
  if (a->v != (double *)NULL)  free(a->v);
  if ((row*col) <= 0)         a->v = (double *)NULL;
  else
    {
      a->v   = (double *)malloc(row * col * sizeof(double));
      a->row = row;
      a->col = col;

      if (a->v == NULL) {
        printf("Failed with malloc() in array2D_resize().?n");
        exit(EXIT_FAILURE);
      }
    }
}
```

```
void array2D_copy(array2D *src, array2D *dst)
{
  if ( (array2D_getRow(src) != array2D_getRow(dst)) ||
       (array2D_getCol(src) != array2D_getCol(dst)) )  array2D_resize(dst, src->row, src->col);
  for (int j=0; j<(dst->col); j++)
    for (int i=0; i<(dst->row); i++)  *(at(dst, i, j)) = L(src, i, j);
}

void array2D_clear(array2D *a, double v)
{
  for (int j=0; j<(a->col); j++)
    for (int i=0; i<(a->row); i++)  *(at(a, i, j)) = v;
}

void array2D_show(array2D *a)
{
  printf("2D Array of %d x %d (%d elements)¥n", a->row, a->col, a->row * a->col);
  for (int j=0; j<(a->col); j++)
    {
      printf("j=%4d :", j);
      for (int i=0; i<(a->row); i++) {
        printf(" %3.1f", *(at(a, i, j)));
      }
      printf("¥n");
    }
}
```

cfd.cpp 2 of 6

cfd.cpp

```
double linear_intp(array2D *a, double x, double y)
{
  int int_x  = (int)x;
  int int_y  = (int)y;
  double dx  = x - (double)int_x;
  double dy  = y - (double)int_y;
  double ret = 0.0;

  if ((x<0.0) || (y<0.0) || (x>=(double)(a->row - 1)) || (y>=(double)(a->col - 1))) {
    //printf("Out of range : (%f, %f) for %d x %d array in at(). Abort.¥n", x, y, a->row, a->col);
    //exit(EXIT_FAILURE);
    return ret;
  }

  ret = ((double)L(a, int_x  , int_y  )*(1.0-dx) + (double)L(a, int_x+1, int_y  )*dx)*(1.0-dy) +
        ((double)L(a, int_x  , int_y+1)*(1.0-dx) + (double)L(a, int_x+1, int_y+1)*dx)*dy;
  return ret;
}
```

```
// Member functions for grid2D
void grid2D_initialize(grid2D *g, int row, int col, double phi_in, double phi_out)
{
  array2D_initialize(&g->u,       row, col);
  array2D_initialize(&g->v,       row, col);
  array2D_initialize(&g->phi,     row, col);
  //array2D_initialize(&g->phiTemp, row+2, col+2); // for halo?
  array2D_initialize(&g->phiTemp, row, col);
  array2D_initialize(&g->uTant,   row, col);
  array2D_initialize(&g->vTant,   row, col);
  array2D_initialize(&g->d,       row, col);
  array2D_clear     (&g->u,       0.01);
  array2D_clear     (&g->v,       0.00);
  array2D_clear     (&g->phi,     0.0);
  array2D_clear     (&g->phiTemp, 0.0);
  array2D_clear     (&g->uTant,   0.00);
  array2D_clear     (&g->vTant,   0.00);
  array2D_clear     (&g->d,       0.0);

  // Initialize the pressure field with constant gradient
  array2D *a = &(g->phi);
  double row_minus_one = (double)array2D_getRow(a) - 1.0;
  for (int j=0; j<(a->col); j++)
    for (int i=0; i<(a->row); i++)
      *(at(a,i,j)) = phi_out * (double)i/row_minus_one +
                     phi_in  * (1.0 - (double)i/row_minus_one);

  // Update cells for boundary condition of Poiseulle flow
  grid2D_calcBoundary_Poiseulle(g, phi_in, phi_out);
}
```

cfd.cpp 3 of 6

cfd.cpp

```
void grid2D_calcTantVelocity(grid2D *g)
{
  array2D *u   = &(g->u);
  array2D *v   = &(g->v);
  array2D *uT  = &(g->uTant);
  array2D *vT  = &(g->vTant);
  int row_m_1  = array2D_getRow(u) - 1;
  int col_m_1  = array2D_getCol(u) - 1;
  int i, j;

#pragma omp parallel for private(i)
  for(j=1; j<col_m_1; j++)
    for(i=1; i<row_m_1; i++) {
      *(at(uT,i,j)) =
        L(u,i,j) + DT*(-L(u,i,j)*(L(u,i+1,j  ) - L(u,i-1,j  )) / 2.0 / DX
                  -L(v,i,j)*(L(u,i  ,j+1) - L(u,i  ,j-1)) / 2.0 / DY +
                   NU*( (L(u,i+1,j  ) - 2.0*L(u,i,j) + L(u,i-1,j  )) / DX2 +
                        (L(u,i  ,j+1) - 2.0*L(u,i,j) + L(u,i  ,j-1)) / DY2 ) );

      *(at(vT,i,j)) =
        L(v,i,j) + DT*(-L(u,i,j)*(L(v,i+1,j  ) - L(v,i-1,j  )) / 2.0 / DX
                  -L(v,i,j)*(L(v,i  ,j+1) - L(v,i  ,j-1)) / 2.0 / DY +
                   NU*( (L(v,i+1,j  ) - 2.0*L(v,i,j) + L(v,i-1,j  )) / DX2 +
                        (L(v,i  ,j+1) - 2.0*L(v,i,j) + L(v,i  ,j-1)) / DY2 ) );
    }
}
```

```
void grid2D_calcPoissonSourceTerm(grid2D *g)
{
  array2D *uT  = &(g->uTant);
  array2D *vT  = &(g->vTant);
  array2D *d   = &(g->d);
  int row_m_1  = array2D_getRow(uT) - 1;
  int col_m_1  = array2D_getCol(uT) - 1;
  int i, j;
#pragma omp parallel for private(i)
  for(j=1; j<col_m_1; j++)
    for(i=1; i<row_m_1; i++) {
      *(at(d,i,j)) = ((L(uT,i+1,j  ) - L(uT,i-1,j  )) /DX /2.0 +
                      (L(vT,i  ,j+1) - L(vT,i  ,j-1)) /DY /2.0) / DT;
    }
}
```

```
void grid2D_calcPoisson_Jacobi(grid2D *g, double target_residual_rate)
{
  int i,j,k=0;
  register double const1 = DX2*DY2/2/(DX2+DY2);
  register double const2 = 1.0/DX2;
  register double const3 = 1.0/DY2;
  double residual        = 0.0;
  double residualMax     = 0.0;
  double residualMax_1st = 0.0;
  array2D *phi           = &(g->phi);
  array2D *phiT          = &(g->phiTemp);
  array2D *d             = &(g->d);
  int row_m_1            = array2D_getRow(phi) - 1;
  int col_m_1            = array2D_getCol(phi) - 1;

  array2D_copy(&(g->phi), &(g->phiTemp));
```

cfd.cpp 4 of 6

cfd.cpp

```
#pragma omp parallel private(i,loc_residualMax, loc_residual)
 {
 do{ // Jacobi iteration

   // Loop to set phiTemp by computing with phi
#pragma omp for
   for(j=1; j<col_m_1; j++)
    for(i=2; i<row_m_1 - 1; i++)
     *(at(phiT,i,j)) = const1 * ( (L(phi,i+1,j  ) + L(phi,i-1,j  )) * const2 +
                            (L(phi,i  ,j+1) + L(phi,i  ,j-1)) * const3 - L(d,i,j));
#pragma omp barrier
#pragma omp single
   {
    k++;
    grid2D_calcBoundary_SqObject(g, OBJ_X, OBJ_Y, OBJ_W, OBJ_H);
    residualMax_prev = residualMax;
    residualMax = 0.0;
   }

   // Calculate residual
   loc_residualMax = 0.0;
#pragma omp for
   for(j=2; j<col_m_1 - 1; j++)
    for(i=2; i<row_m_1 - 1; i++) {
     loc_residual = fabs(L(phi,i,j) - L(phiT,i,j));
     if (loc_residualMax < loc_residual)  loc_residualMax = loc_residual;
    }
#pragma omp critical
    if (residualMax < loc_residualMax) residualMax = loc_residualMax;
#pragma omp barrier
#pragma omp single
    if (k == 1) residualMax_1st = residualMax;

  // Loop to set phi by computing with phiTemp
#pragma omp for
   for(j=1; j<col_m_1; j++)
    for(i=2; i<row_m_1 - 1; i++)
     *(at(phi,i,j)) = const1 * ( (L(phiT,i+1,j  ) + L(phiT,i-1,j  )) * const2 +
                           (L(phiT,i  ,j+1) + L(phiT,i  ,j-1)) * const3 - L(d,i,j));
```

```
#pragma omp barrier
#pragma omp single
   {
    k++;
    grid2D_calcBoundary_SqObject(g, OBJ_X, OBJ_Y, OBJ_W, OBJ_H);
   }

 } while ( fabs(residualMax - residualMax_prev) > (residualMax * target_residual_rate));
  } // #pragma omp parallel

 if ((tstep%JACOBIREP_INTERVAL) == 0)
    printf("> %4d iterations in Jacobi (tstep=%5d, residualMax=%f),  ", k, tstep, residualMax);
}


void grid2D_calcVelocity(grid2D *g)
{
 array2D *u   = &(g->u);
 array2D *v   = &(g->v);
 array2D *uT  = &(g->uTant);
 array2D *vT  = &(g->vTant);
 array2D *phi = &(g->phi);
 int row_m_1  = array2D_getRow(u) - 1;
 int col_m_1  = array2D_getCol(u) - 1;
 int i, j;

#pragma omp parallel for private(i)
 for(j=1; j<col_m_1; j++)
  for(i=1; i<row_m_1; i++) {
   *(at(u,i,j)) = L(uT,i,j) - DT/2/DX*( L(phi,i+1,j) - L(phi,i-1,j) );
   *(at(v,i,j)) = L(vT,i,j) - DT/2/DY*( L(phi,i,j+1) - L(phi,i,j-1) );
  }
}
```

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cfd.cpp

```
// Boundary conditions of outer cells for Poiseulle flow
void grid2D_calcBoundary_Poiseulle(grid2D *g, double phi_in, double phi_out)
{
  //      j
  // COL-1 A
  //      |  =>
  //      |  => flowing dir
  //      |  =>
  //    0 +----------> i
  //      0          ROW-1
  //
  // phi[i][j] : i for x direction, j for y direction
  // [0:ROW-1], inlet(left) boundary at i==1, outlet(right) boundary at i==(ROW-2)
  // [0:COL-1], top boundary at j==(COL-2), bottom boundary at j==1
  // One-cell boundary (one-cell most outer layer) is dummy cells for boundary condition.

  int i, i1, i2, j, j1, j2;
  array2D *u   = &(g->u);
  array2D *v   = &(g->v);
  array2D *phi = &(g->phi);
  int row      = array2D_getRow(u);
  int col      = array2D_getCol(u);

  j1 = 1; // bottom
  j2 = col-2; // top

#pragma omp parallel for
  for(i=0; i<row; i++) {
    *(at(u,i,j1))     = 0.0;
    *(at(v,i,j1))     = 0.0;
    *(at(v,i,j1-1))   = L(v,i,j1+1);
    *(at(phi,i,j1))   = L(phi,i,j1+1) - ((2.0*NU/DY)*L(v,i,j1+1));
    *(at(phi,i,j1-1)) = L(phi,i,j1);
```

```
    *(at(u,i,j2))     = 0.0;
    *(at(v,i,j2))     = 0.0;
    *(at(v,i,j2+1))   = L(v,i,j2-1);
    *(at(phi,i,j2))   = L(phi,i,j2-1) - ((2.0*NU/DY)*L(v,i,j2-1));
    *(at(phi,i,j2+1)) = L(phi,i,j2);
  }

  i1 = 1; // inlet(left, flow incoming)
  i2 = row-2; // outlet(right, flow outgoing)

#pragma omp parallel for
  for(j=1; j<col-1; j++) {
    // Pressure condition
    *(at(u,i1-1,j))   = L(u,i1+1,j);
    *(at(v,i1-1,j))   = L(v,i1+1,j);
    *(at(phi,i1,j))   = phi_in;
    *(at(phi,i1-1,j)) = L(phi,i1+1,j);
    // Pressure condition
    *(at(u,i2+1,j))   = L(u,i2-1,j);
    *(at(v,i2+1,j))   = L(v,i2-1,j);
    *(at(phi,i2,j))   = phi_out;
    *(at(phi,i2+1,j)) = L(phi,i2-1,j);
  }
}
```

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cfd.cpp

```
void grid2D_calcBoundary_SqObject(grid2D *g, int obj_x, int obj_y, int obj_w, int obj_h)
{
 // j
 // A
 // |   +-+
 // |   |#|
 // |   |#|
 // |   +-+
 // |
 // +--------------> i
 //
 int i, i1, i2, j, j1, j2;
 int sta_i = (int)(obj_x - obj_w/2); // pos of left surface
 int end_i = (int)(sta_i + obj_w);   // pos of right surface
 int sta_j = (int)(obj_y - obj_h/2); // pos of bottom surface
 int end_j = (int)(sta_j + obj_h);   // pos of top surface

 array2D *u    = &(g->u);
 array2D *v    = &(g->v);
 array2D *phi  = &(g->phi);
 array2D *phiT = &(g->phiTemp);

 i1 = sta_i;  // left surface of the obstacle
 i2 = end_i;  // right surface of the obstacle

for(j=sta_j; j<=end_j; j++) {
   *(at(u,i1,j))     = 0.0;
   *(at(v,i1,j))     = 0.0;
   *(at(u,i1+1,j))   = L(u,i1-1,j);
   *(at(phi,i1,j))   = L(phi,i1-1,j) + ((2.0*NU/DX)*L(u,i1-1,j));
   *(at(phiT,i1,j))  = L(phi,i1,j);

   *(at(u,i2,j))     = 0.0;
   *(at(v,i2,j))     = 0.0;
   *(at(u,i2-1,j))   = L(u,i2+1,j);
   *(at(phi,i2,j))   = L(phi,i2+1,j) + ((2.0*NU/DX)*L(u,i2+1,j));
   *(at(phiT,i2,j))  = L(phi,i2,j);
 }
```

```
j1 = end_j;  // top surface of the obstacle
 j2 = sta_j;  // bottom surface of the obstacle

 for(i=sta_i+1;i<end_i;i++) {
   *(at(u,i,j1))     = 0.0;
   *(at(v,i,j1))     = 0.0;
   *(at(v,i,j1-1))   = L(v,i,j1+1);
   *(at(phi,i,j1))   = L(phi,i,j1+1) + ((2.0*NU/DY)*L(v,i,j1+1));
   *(at(phiT,i,j1))  = L(phi,i,j1);

   *(at(u,i,j2))     = 0.0;
   *(at(v,i,j2))     = 0.0;
   *(at(v,i,j2+1))   = L(v,i,j2-1);
   *(at(phi,i,j2))   = L(phi,i,j2-1) + ((2.0*NU/DY)*L(v,i,j2-1));
   *(at(phiT,i,j2))  = L(phi,i,j2);
 }
}
```

Hands-on :
Non (MPI)-parallelized CFD simulation

Note that the time consuming part is already parallelized by using OpenMP.
See “#pragma omp parallel private(i)” in grid2D_calcPoisson_Jacobi().

Compile and Execute Interactively

README.txt is also available for your reference.

Enter interactive mode => Modify source files by editor => Compile => Execute

1. **Connect to Fugaku compute node in interactive mode.**

```
$ pjsub  --interact   -L rscgrp=int,node=1,elapse=0:30:00  --sparam wait-time=600 (–mpi proc=48)
$ ls
xxx yyy zzz.cpp … (check the same files exist as the login node)
```

This reserves 1 CPU (1 node) for 48 MPI processes. If you cannot enter the interactive mode due to resource allocation time-out, try "elapse=0:15:00"

2. **Modify source codes with an editor (emacs, vim, nano, etc.)**

```
$ emacs  -nw  xxx.yy
```

3. **Compile in interactive mode**

```
$ make
=======================================================================
= Compilation starts for solver_fractional.
=======================================================================
FCC   -O3 -I./  -o main.o -c main.cpp …
```

4. **Set the environmental variable and Execute**

Set the number of OpenMP thread 1 (or it might be more than 1).

```
$ source scripts/set_omp_num_threads.sh  1
$ ./scripts/do_execute_on_compnode.sh
============ Computation started with 1 OMP threads for (360 x 120) grid with dT=0.000050.
> 104 iterations in Jacobi (tstep=    0, residualMax=0.006943),  [tstep=    0 to   200] (9.219616 sec) > AVEse_000200.dat
…
>    8 iterations in Jacobi (tstep=24800, residualMax=0.066284),  [tstep=24800 to 25000] (3.236435 sec) > AVEse_025000.dat
============ Computation finished.
Time-step=20100 : ElapsedTime=275.298 sec
```

Elapsed time for entire execution

Computational results are in "sim_data/", which is automatically created by "do_execute_on_frontend.sh"

Speed up Execution by OpenMP

README.txt is also available for your reference.

```
$ source scripts/set_omp_num_threads.sh 48
Before: OMP_NUM_THREADS=1
After : OMP_NUM_THREADS=48

$ env | grep OMP_NUM
OMP_NUM_THREADS=48

$ ./scripts/do_execute_on_compnode.sh
============ Computation started with 48 OMP threads for (360 x 120) grid with dT=0.000050.
>  104 iterations in Jacobi (tstep=    0, residualMax=0.006943),  [tstep=    0 to   200] (0.389549 sec) > AVEse_000200.dat
…
>    8 iterations in Jacobi (tstep=24800, residualMax=0.066284),  [tstep=24800 to 25000] (0.219520 sec) > AVEse_025000.dat
============ Computation finished.
Time-step=20100 : ElapsedTime=54.113 sec
```

Set the number of OpenMP threads (Try 1, 2, 4, 8, ..., 48)

Check the present number of OpenMP threads

Please check whether the number is correct

Execute with OpenMP threads

- **Compile and execute with a different number of OpenMP threads**
  - ✓ 1, 2, 4, 8, 12, 24, 48 threads
- **How scalable is it?**
  - ✓ When 8 times more threads are used, is the exec time reduced to 1/8?

Num. of Thread	Execution time (s)
1	301.054
2	160.157
4	91.245
8	66.189
12	53.833
24	52.928
48	64.643

Execute with Batch-job Scheduler

README.txt is also available for your reference.

(Without entering the interactivenode, on a login node,)

```
$ pjsub  ./scripts/do_batchjob.sh
```

Input job script "./scripts/do_batchjob.sh" into a job queue.

```
$ pjstat
JOB_ID    JOB_NAME   MD ST  USER     START_DATE      ELAPSE_LIM          NODE_REQUIRE    VNODE  CORE V_MEM
7579453    do_batchjo NM RUN l00116   08/24 14:05:54< 0000:30:00           1               -      -    -
```

Check the status of my job queue.

You can watch the job queue every second by:
> watch -n 1 pjstat

```
$ pjdel 7579453
```

Delete a job in the queue.

Please use Batch-job mode especially for large-scale parallel execution.

- **Settings and executed program (script) are written in "do_batchjob.sh".**
  - ✓ You can edit them.
- **Standard output / error output are written into a file.**
  - ✓ such like do_batchjob.sh.7506695.out, do_job.sh.7506695.err
    (It sometimes takes time due to a loaded file system.)

```
$ cat scripts/do_batchjob.sh
#!/bin/sh

#PJM -L rscgrp=small
#PJM -L node=1
#PJM -L elapse=15:00
#PJM –S

NUM=48
export OMP_NUMBER_THREADS=$NUM

./scripts/do_execute_on_frontend.sh
```

= Max. execution time allowed

= output do_batchjob.sh.7794883.stats

= Set the number of threads for OpenMP

= executed program

Visualize Computational Results

README.txt is also available for your reference.

<Enter the interactive mode>

```
[(compute node) serial_0920]$ .  /vol0004/apps/oss/spack/share/spack/setup-env.sh
```

Set spack environment variable

```
[(compute node) serial_0920]$ spack  load  py-numpy
                              (spack  load  /v5kgevs)
[(compute node) serial_0920]$ spack  load  py-matplotlib
                              (spack  load  /ismoz3u)
```

Load some python library dependencies
Note: sometimes multiple version of the same library is installed
Use “spack load /(hash of the top library)” instead, e.g., spack load /v5kgevs

```
[(compute node) serial_0920]$ ./scripts/do_visualize.sh
Start visualization
rm: cannot remove '*.png': No such file or directory
Unable to parse the pattern
```

On the compute node, convert ./sim_data/*.dat to png files, and on login node, pop up an animation window. (X-window server is required, see how to setup X-windows slide.)

```
[(compute node) serial_0920]$ exit
```

Exit to login node, or use another terminal

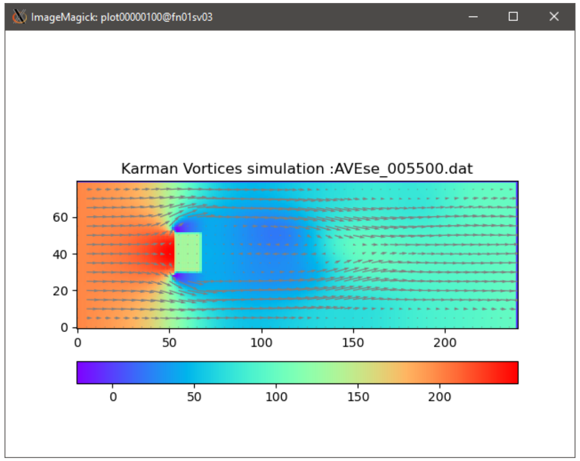
Install animate program on login node to play the simulation result as slideshow

```
[(login node) serial_0920]$ .  /vol0004/apps/oss/spack/share/spack/setup-env.sh
[(login node) serial_0920]$ spack  load  imagemagick
```

If these do not work, please try to logoff and login again.
It was confirmed to work with some login nodes,
login2, login5, and login6.

```
[(login node) serial_0920]$ cd  ./sim_data/
[(login node) serial_0920]$ animate -delay 10 *.png
```

A window will appear on your desktop. It will take few minutes to start because showing X-windows over the internet might be very slow.


ImageMagick: plot00000100@fn01sv03
Karman Vortices simulation :AVEse_005500.dat
60
40
20
0
0
50
100
150
200
0
50
100
150
200

Visualize Computational Results as mp4 File

Animation speed depends on network bandwidth between Fugaku and your PC.

If it is too slow or does not load, try the followings to make mp4 file

<Enter the interactive mode>

```
[(compute node) serial_0920]$ .  /vol0004/apps/oss/spack/share/spack/setup-env.sh

[(compute node) serial_0920]$ spack  load  py-numpy
                                            (spack  load  /v5kgevs)
[(compute node) serial_0920]$ spack  load  py-matplotlib
                                            (spack  load  /ismoz3u)
[(compute node) serial_0920]$ spack  load  ffmpeg
```

Load some python library dependencies and ffmpeg
Note: sometimes multiple version of the same library is installed
Use “spack load /(hash of the top library)” instead

```
[(compute node) serial_0915]$ ./scripts/do_make_mp4.sh
Start creation of mp4 file
Gtk-Message: 03:59:47.792: Failed to load module "canberra-gtk-module"
AVEse_000200.dat
AVEse_000400.dat
AVEse_000600.dat
...
[(compute node) serial_0915]$ ls  ./sim_data/*.mp4
./sim_data/plot-z-4.mp4
```

Generate the mp4 file

Then, download the generated mp4 file, and view it on your PC.   -->   See the next page.

How to Download Simulation Movie by SCP

Open a new terminal on your PC

```
[(your pc)]$ scp (your Fugaku account)@fugaku.r-ccs.riken.jp:(generated mp4 file) (destination on your PC)
```

Example:

```
[(your pc)]$ scp (your fugaku account)@fugaku.r-ccs.riken.jp:~/serial_0920/sim_data/plot-z-4.mp4 ~/
```

to download to home directory on mac/linux
OR

```
[(your pc)]$ scp (your fugaku account)@fugaku.r-ccs.riken.jp:~/serial_0920/sim_data/plot-z-4.mp4 /cygdrive/c/
```

to download to C drive on Windows PC with Cygwin

Play the downloaded mp4 file to see simulation result.

Change Simulation Parameters

- **You can select one of the predefined conditions in "cfd.h"**

```
// You can select one of the conditions.
//#define CONDITIONX
//#define CONDITION0
//#define CONDITION1
#define CONDITION2
//#define CONDITION3
```

✓ To select, uncomment another line.

- **Try to change the condition and run**

✓ How does the exec time change?

```
#if defined CONDITIONX   //Flow condition X  (taking super long time)
#define ROW (2160)                      // cell resolution for row
#define COL (720)                       // cell resolution for column
#define DT  (0.0000075)                 // delta t (difference between timesteps)
#define NU  (0.0075)                    // < 0.01 for Karman vortices
#define JACOBIREP_INTERVAL (500)        // interval to report in Jacobi
#define END_TIMESTEP      (80000)       // tstep to end computation

#elif defined CONDITION0   //Flow condition 0  (taking very long time)
#define ROW (1080)
#define COL (360)
#define DT  (0.000015)
#define NU  (0.0075)
#define JACOBIREP_INTERVAL (250)
#define END_TIMESTEP      (40000)

#elif defined CONDITION1   //Flow condition 1  (taking long time)
#define ROW (540)
#define COL (180)
#define DT  (0.000025)
#define NU  (0.0075)
#define JACOBIREP_INTERVAL (200)
#define END_TIMESTEP      (25000)

#elif defined CONDITION2   //Flow condition 2  (balanced condition for serial execution)
#define ROW (360)
#define COL (120)
#define DT  (0.00005)
#define NU  (0.0075)
#define JACOBIREP_INTERVAL (150)
#define END_TIMESTEP      (20000)

#elif defined CONDITION3   //Flow condition 3  (easy condition, fast execution)
#define ROW (180)
#define COL (60)
#define DT  (0.00005)
#define NU  (0.0075)
#define JACOBIREP_INTERVAL (100)
#define END_TIMESTEP      (16000)

#endif
```

360 x 120 grid
delta T = 0.00005
Interval for file save = 150
End of time step = 20000

We will start the afternoon session at 13:30 (JST) as scheduled.

This slide will be updated.
During the lecture of Module-2.

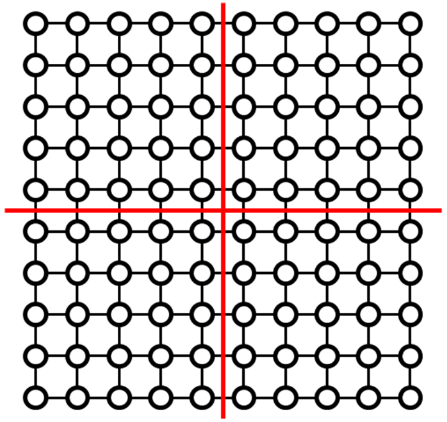
PART-II

Parallelization of the 2D CFD Simulation

Overview

- **Parallelization with "shared memory", which is done by OpenMP, is limited to a node.**
  - ✓ Many cores in multiple sockets share the same memory space.

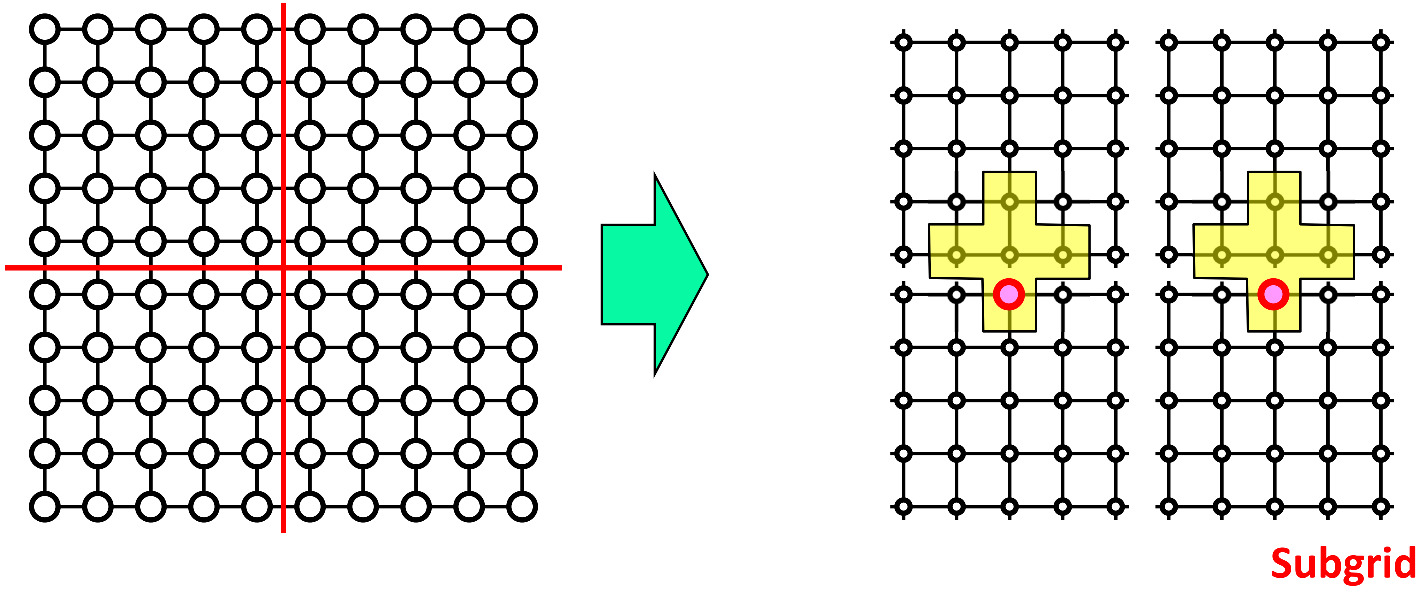
- **Scaling performance beyond a single node**
  - ✓ Parallelization with a distributed-memory nodes requires message passing.
  - ✓ One of the approaches to partition the entire computation is "**Domain Decomposition**."



- **Domain decomposition**
  - ✓ Decompose the computational grid to create sub-computation
  - ✓ Data communication and synchronization are performed when necessary.

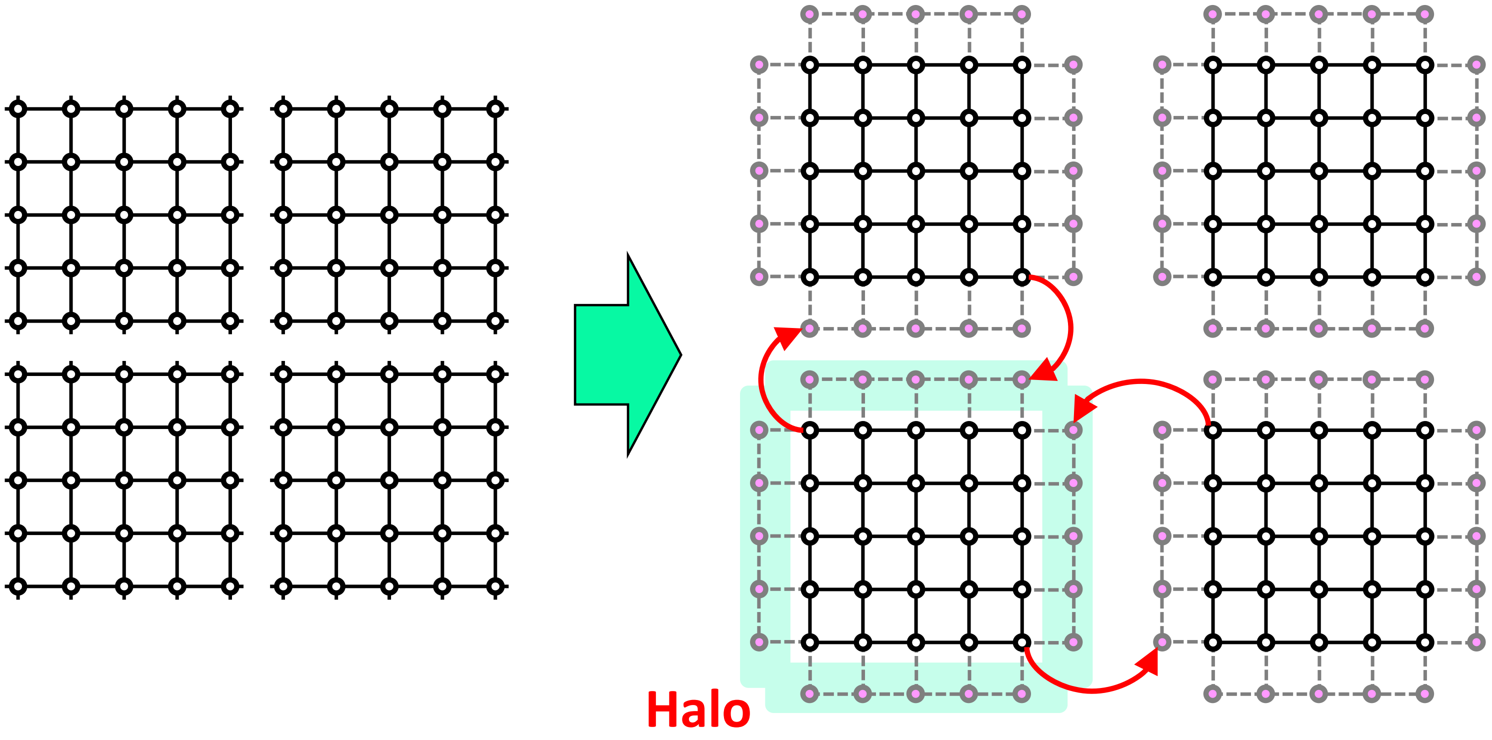
Parallel Computation w/ Domain Decomposition

- **Decompose the entire grid into subgrids**
  - ✓ Perform stencil computation with each subgrid in parallel
  - ✓ Exchange boundary data when necessary

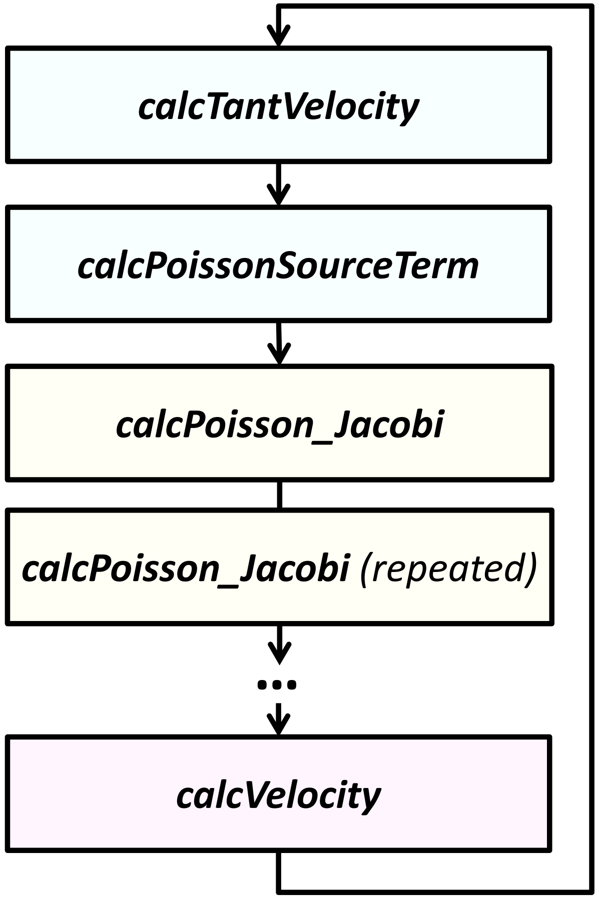


Exchanging Halo for Coarse Grain Communication

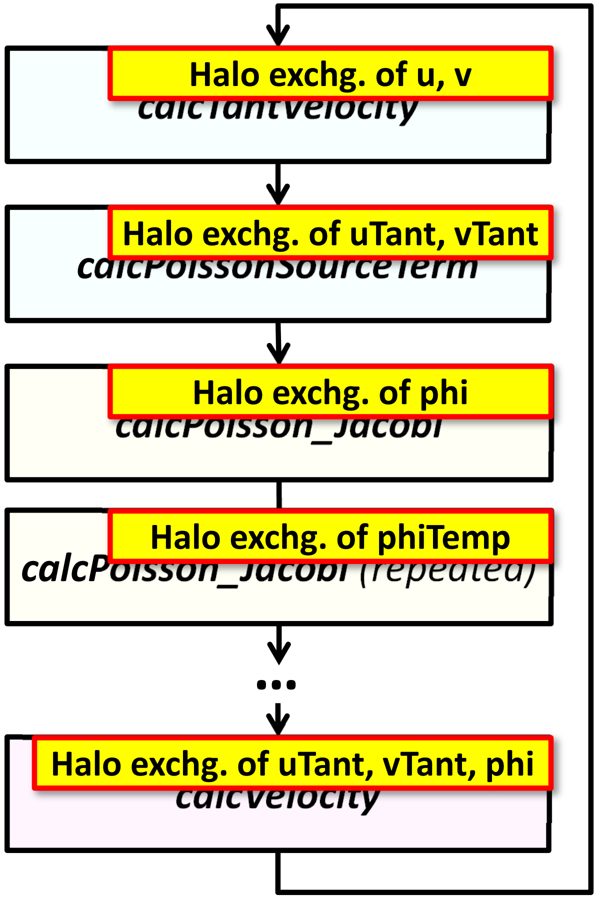
- **Halo : Overlapped boundary region**
  - ✓ Halo data are exchanged all at once in advance to the loop, so that no communication occurs during the loop.



Parallelization Overview



Serial program



MPI-parallel program

Let’s Read the parallelized Code!

```
@login1  cd  ~/programs_cfd
@login1  cp  /home/ra020006/data/program/parallel_complete_0910.tgz  ./
@login1  tar  zxvfp  parallel_complete_0910.tgz
@login1  cd  parallel_complete_0910/

@login1  ls
cfd.cpp
cfd.h
domain_decomp.cpp
domain_decomp.h
main.cpp
main.h
Makefile
README.txt
scripts
```

cfd.cpp, cfd.h: MPI parallelization is introduced.

domain_decomp.cpp, domain_decomp.h: New files.
Codes for subgrid management.

cfd.h

cfd.h

```
…
// Data structure of 2D array (resizable)
typedef struct array2D_ {
  int nx;                                          // NX resolution of a grid
  int ny;                                          // NY resolution of a grid
  double *v;                                       // Pointer of 2D array
  double *l_send, *r_send, *l_recv, *r_recv;       // Buffer for communicate
} array2D;
…
// Member functions for array2D
void array2D_initialize(array2D *a, int nx, int ny);     // initialize 2D array : nx x ny
void array2D_resize(array2D *a, int nx, int ny);         // resize 2D array : nx x ny
void array2D_copy(array2D *src, array2D *dst);           // copy src to dst (by resizing dst)
void array2D_clear(array2D *a, double v);                // clear 2D array with value of v
void array2D_show(array2D *a);                           // print 2D array in text
double linear_intp(array2D *a, double x, double y);      // get value at (x,y)
                                                         // with linear interpolation
inline int array2D_getNx(array2D *a) { return (a->nx); } // get size of nx
inline int array2D_getNy(array2D *a) { return (a->ny); } // get size of ny

inline double *at(array2D *a, int i, int j)              // get pointer at (nx, ny)
{
#if Debug
  if ((i<0-HALO) || (j<0-HALO) || (i>=a->nx+HALO) || (j>=a->ny+HALO)) {
    printf("Out of range : (%d, %d) for %d x %d array in at(). Abort.¥n", i, j, a->nx, a->ny);
    exit(EXIT_FAILURE);
  }
#endif
  return (a->v + i + j * (a->nx+2*HALO));
}
```

```
…
// Data structure of 2D grid for fluid flow
typedef struct grid2D_ {
  array2D u, v, phi;        // velocity (u, v), pressure phi
  array2D phiTemp;           // tentative pressure (temporary for update)
  array2D uTant, vTant;      // tentative velocity (u, v)
  array2D d;                 // source term of a pressure poisson's equation
} grid2D;
…

// Member functions for grid2D
void grid2D_initialize(grid2D *g, int nx, int ny, double phi_in, double phi_out, const info_domain mpd);
void grid2D_calcTantVelocity(grid2D *g, const info_domain mpd);
void grid2D_calcPoissonSourceTerm(grid2D *g, const info_domain mpd);
void grid2D_calcPoisson_Jacobi(grid2D *g, double target_residual_rate, const info_domain mpd);
void grid2D_calcVelocity(grid2D *g, const info_domain mpd);
void grid2D_calcBoundary_Poiseulle(grid2D *g, double phi_in, double phi_out, const info_domain mpd);
void grid2D_calcBoundary_SqObject(grid2D *g, int obj_x, int obj_y, int obj_w, int obj_h, const info_domain mpd);
void communicate_neighbor(array2D *a, const info_domain mpd);
void communicate_neighbor_debug(array2D *a, const info_domain mpd);
void grid2D_outputAVEseFile(grid2D *g, const char *base, int num, double scaling, const info_domain mpd);
inline int  grid2D_getNx(grid2D *g) { return( array2D_getNx(&(g->u)) ); }
inline int  grid2D_getNy(grid2D *g) { return( array2D_getNy(&(g->u)) ); }
```

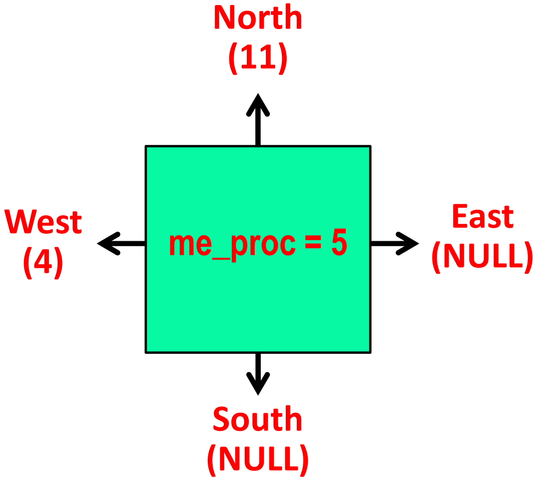
New file : domain_decomp.h

domain_decomp.h

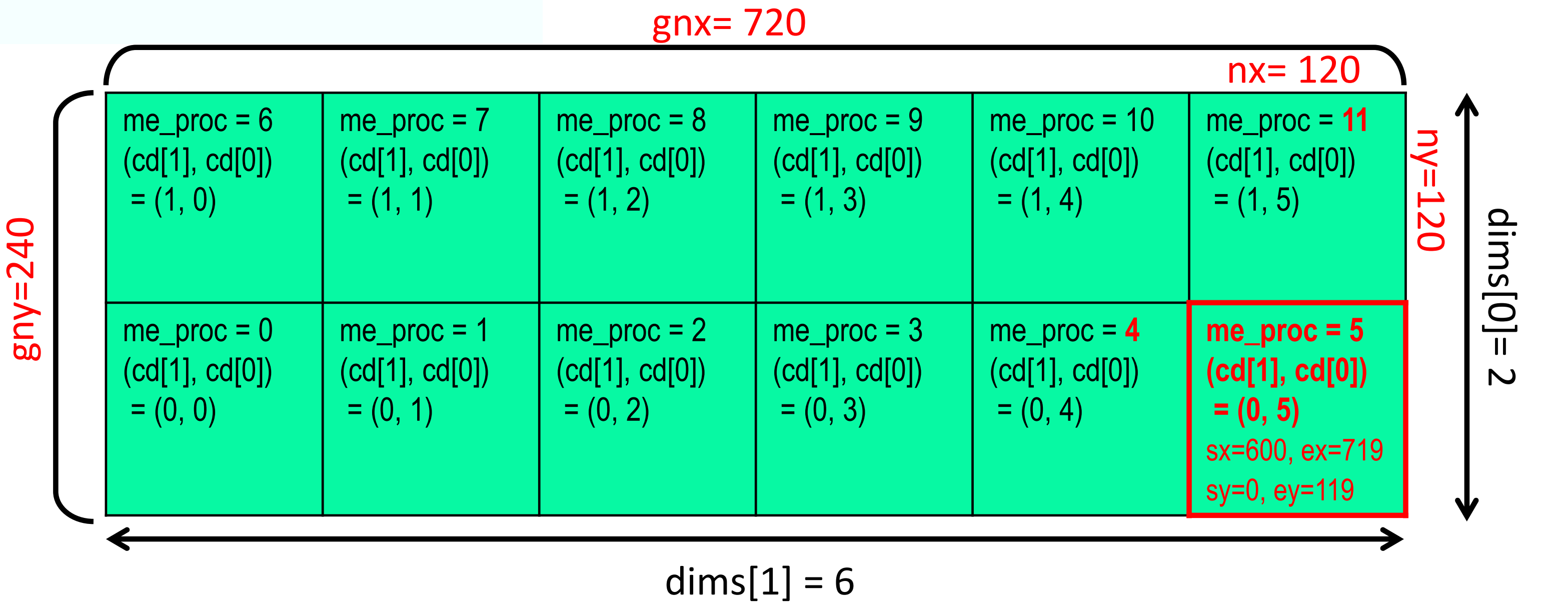
```
#ifndef ___DOMAIN_DECOMP_H___
#define ___DOMAIN_DECOMP_H___

#include <stdlib.h>
#include <math.h>
#include <mpi.h>
#include <stdio.h>

#define MCW MPI_COMM_WORLD

#define HALO (1)

//Data structure for mpi
typedef struct info_domain_ {
  int dims[2];                      //Dimension
  int coord[2];                     //Coord of me_proc
  int east, west, north, south;     //Neighbor procs ID
  int nx, ny, gnx, gny;             // (gnx, gny) : resolution of entire grid, (nx, ny) : resolution of each subgrid
  int sx, ex, sy, ey;               // start_x, end_x, start_y, end_y
} info_domain;

void info_domain_initialize(info_domain *mpd, const int num_procs, const int me_proc);
void calc_range(info_domain *mpd, const int nx, const int ny);

#endif
```

Details of Domain Decomposition

```
num_procs = 12                          // me_proc is 0 to 11.
dims[0] = sqrt(12/3) = 2                // num of subgrids
dims[1] = 12 / 2 = 6
In the case that me_proc == 5,
mpd->coord[1] = 5 % 6 = 5;              // coord of subgrid
mpd->coord[0] = 5 / 6 = 0;
mpd->east  = MPI_PROC_NULL              // No proc of adjacent subgrid
mpd->west  = me_proc - 1 = 4            //proc of adjacent subgrid
mpd->north = me_proc + mpd->dims[1] = 5 + 6 = 11
mpd->south = MPI_PROC_NULL
```



This is the case where n = 2, with 3*2^2 = 12 procs



me_proc = 6 (cd[1], cd[0]) = (1, 0)	me_proc = 7 (cd[1], cd[0]) = (1, 1)	me_proc = 8 (cd[1], cd[0]) = (1, 2)	me_proc = 9 (cd[1], cd[0]) = (1, 3)	me_proc = 10 (cd[1], cd[0]) = (1, 4)	me_proc = 11 (cd[1], cd[0]) = (1, 5)
me_proc = 0 (cd[1], cd[0]) = (0, 0)	me_proc = 1 (cd[1], cd[0]) = (0, 1)	me_proc = 2 (cd[1], cd[0]) = (0, 2)	me_proc = 3 (cd[1], cd[0]) = (0, 3)	me_proc = 4 (cd[1], cd[0]) = (0, 4)	**me_proc = 5** **(cd[1], cd[0])** **= (0, 5)** sx=600, ex=719 sy=0, ey=119

New file : domain_decomp.c

domain_decomp.c

```
void info_domain_initialize(info_domain *mpd, const int num_procs, const int me_proc)
{
  mpd->dims[0] = sqrt(num_procs / 3);
  mpd->dims[1] = num_procs / mpd->dims[0];
  if(mpd->dims[0] * mpd->dims[1] != num_procs){
    if(me_proc == 0) {
      printf("Number of processes is invalide. Please choose the valid condition.¥n");
      printf("Number of processes must be 3n^2¥n. (""n"" is arbitrary value.) ");
    }
    MPI_Abort(MCW, -1);
  }
  mpd->coord[1]  = me_proc % mpd->dims[1];
  mpd->coord[0]  = me_proc / mpd->dims[1];
  mpd->east      = mpd->coord[1]<mpd->dims[1]-1  ? me_proc+1              : MPI_PROC_NULL;
  mpd->west      = mpd->coord[1]>0               ? me_proc-1              : MPI_PROC_NULL;
  mpd->north     = mpd->coord[0]<mpd->dims[0]-1  ? me_proc+mpd->dims[1]   : MPI_PROC_NULL;
  mpd->south     = mpd->coord[0]>0               ? me_proc-mpd->dims[1]   : MPI_PROC_NULL;
}

void calc_range(info_domain *mpd, const int nx, const int ny)
{
  mpd->gnx = nx;
  mpd->gny = ny;
  mpd->nx = nx / mpd->dims[1];
  mpd->ny = ny / mpd->dims[0];
  mpd->sx = mpd->nx * mpd->coord[1];
  mpd->ex = mpd->nx * (mpd->coord[1]+1)-1;
  mpd->sy = mpd->ny * mpd->coord[0];
  mpd->ey = mpd->ny * (mpd->coord[0]+1)-1;
}
```

grid2D_calcTantVelocity()

cfd.c

```
void grid2D_calcTantVelocity(grid2D *g, const info_domain mpd)
{
  array2D *u   = &(g->u);
  array2D *v   = &(g->v);
  array2D *uT  = &(g->uTant);
  array2D *vT  = &(g->vTant);
  int i, j, sx, ex, sy, ey;

  sx = 0;                 if (mpd.west == MPI_PROC_NULL)     sx = 1;
  ex = array2D_getNx(u);  if (mpd.east == MPI_PROC_NULL)     ex = ex - 1;
  sy = 0;                 if (mpd.south == MPI_PROC_NULL)    sy = 1;
  ey = array2D_getNy(u);  if (mpd.north == MPI_PROC_NULL)    ey = ey - 1;

#pragma omp parallel for private(i)
  for(j=sy; j<ey; j++)
    for(i=sx; i<ex; i++) {
      *(at(uT,i,j)) =
                L(u,i,j) + DT*(-L(u,i,j)*(L(u,i+1,j  ) - L(u,i-1,j  )) / 2.0 / DX
                               -L(v,i,j)*(L(u,i  ,j+1) - L(u,i  ,j-1)) / 2.0 / DY +
                                NU*( (L(u,i+1,j  ) - 2.0*L(u,i,j) + L(u,i-1,j  )) / DX2 +
                                     (L(u,i  ,j+1) - 2.0*L(u,i,j) + L(u,i  ,j-1)) / DY2 ) );
      *(at(vT,i,j)) =
                L(v,i,j) + DT*(-L(u,i,j)*(L(v,i+1,j  ) - L(v,i-1,j  )) / 2.0 / DX
                               -L(v,i,j)*(L(v,i  ,j+1) - L(v,i  ,j-1)) / 2.0 / DY +
                                NU*( (L(v,i+1,j  ) - 2.0*L(v,i,j) + L(v,i-1,j  )) / DX2 +
                                     (L(v,i  ,j+1) - 2.0*L(v,i,j) + L(v,i  ,j-1)) / DY2 ) );
    }
  communicate_neighbor(uT, mpd);
  communicate_neighbor(vT, mpd);
}
```

Modify start_{x,y} and end_{x,y} for a sub-grid with Halo region

Exchange Halo with neighbor MPI processes (see Next Page).

communicate_neighbor() for Halo Exchange

Exchange Halo of Array u in Grid g by communicating data with adjacent subgrids.
Usage: communicate_neighbor(&g->u,   mpd);

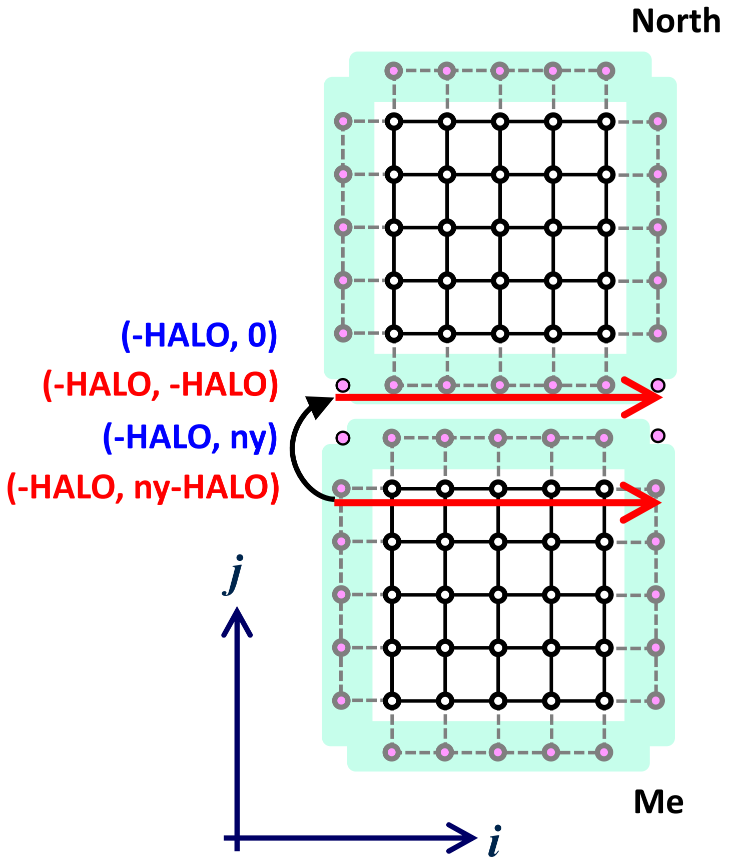
cfd.c

```
void communicate_neighbor(array2D *a, const info_domain mpd)
{
  int x, y, nx, ny;
  MPI_Status st;

  nx = array2D_getNx(a);
  ny = array2D_getNy(a);

 //Please read the code written here to understand MPI communications.
}
```

Hint to understand:

Row Halo (top and bottom) are continuously arranged in a memory while column Halo (left and right) are NOT. Since MPI_sendrecv() requires continuity for transferred data, you need to copy non-continuous data into some buffer before executing MPI_sendrecv() so that the copied data are continuous in the buffer.

You can use array2D's **double *l_send, *r_send, *l_recv, *r_recv;** as buffers for Halo communication.
Memory regions are allocated in array2D_resize().

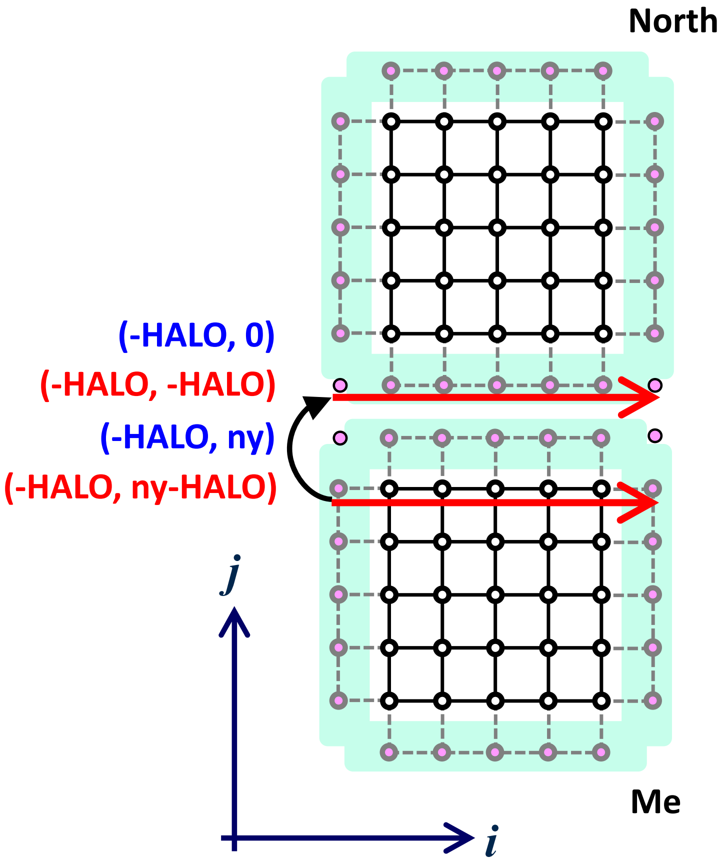


How to Implement Halo Exchange with MPI?

To obtain the top Halo of mine with south subgrid,

The row of (nx+2*HALO)*HALO cells starting at (-HALO, ny-HALO) should be sent to the bottom Halo of the south at (-HALO, **-HALO**).
  * The coordinate of origin in the subgrid is (0, 0)

The top Halo of mine starting at (-HALO, ny) should be received from the row of the south starting at (-HALO, -HALO).



Notice:
Think carefully about source and destination processes.

Sendrecv(….., north, ……, north, …)
  ← Is this right?
  Deadlock occurs?

Hands-on :

MPI-parallelized CFD simulation

Compile and Execute by Batch

```
$ ./scripts/do_clean.sh
...
$ make
==================================================================
= Compilation starts for solver_fractional.
==================================================================
...

$ pjsub  ./scripts/go3.sh
pjsub scripts/go3.sh
[INFO] PJM 0000 pjsub Job 541545 submitted.

$ pjstat
Oakbridge-CX scheduled stop time: 2020/09/25(Fri) 09:00:00 (Remain:  4days 13:59:26)

JOB_ID     JOB_NAME   STATUS  PROJECT  RSCGROUP      START_DATE       ELAPSE        TOKEN NODE
541552      go3.sh     RUNNING ra020006    small      09/20 19:00:06<   00:00:28         -    4

$ ls go3.sh.o*
go3.sh.o541501

$ less go3.sh.o541501
...

$ tail -f go3.sh.o541501
...
```

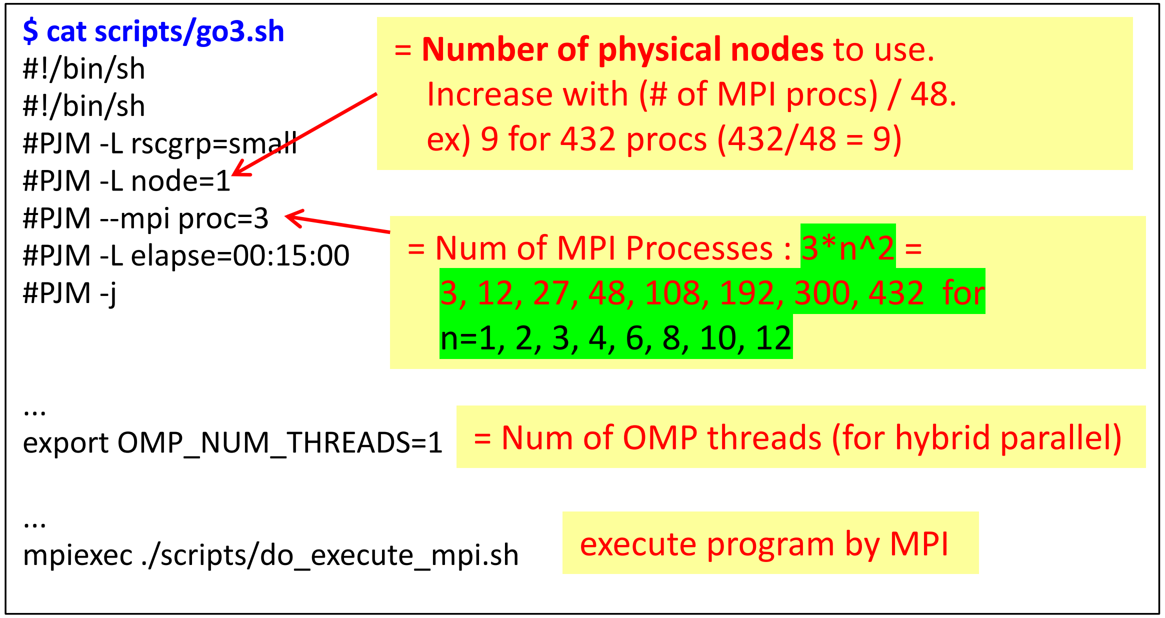
Input job script "./scripts/go3.sh" into a job queue.

Or, try "watch -n 1 pjstat"

If you want to kill a job,
> pjdel <Job ID>

Watch the N last lines added to the file.

Batch Job Script : go3.sh



```
$ cat scripts/go3.sh
#!/bin/sh
#!/bin/sh
#PJM -L rscgrp=small
#PJM -L node=1
#PJM --mpi proc=3
#PJM -L elapse=00:15:00
#PJM -j

...
export OMP_NUM_THREADS=1

...
mpiexec ./scripts/do_execute_mpi.sh
```

= **Number of physical nodes** to use.
Increase with (# of MPI procs) / 48.
ex) 9 for 432 procs (432/48 = 9)

= Num of MPI Processes : 3*n^2 =
3, 12, 27, 48, 108, 192, 300, 432 for
n=1, 2, 3, 4, 6, 8, 10, 12

= Num of OMP threads (for hybrid parallel)

execute program by MPI

```
$ less go3.sh.541501.1.0
me_proc: 0
Total dimension              : [2 x 6]
Coodrinate of me_proc        : [0 x 0]
Neighbor procs (E,W,N,S)     : 1, -1, 6, -1
Assigned mesh (nx,ny,gnx,gny) : 60, 60, 360, 120
Start & End mesh (sx,ex,sy,ey): 0, 59, 0, 59

============ Computation started with 3 MPI procs and 1 OMP
threads for (540 x 180) grid with dT=0.000025.
>  104 iterations in Jacobi (tstep=    0, residualMax=0.006943),  ...
>   14 iterations in Jacobi (tstep=  200, residualMax=0.005422),  ...
>   16 iterations in Jacobi (tstep=  400, residualMax=0.003904),  ...
...

Time-step=25000 : (MPI-Procs, ElapsedTime)=(3, 83.768 sec),
(MPI*OpenMP, Time)=(3, 83.768 sec)
```

- **Check the output file of MPI-parallel execution**
  - ✓ $ less go3.sh.541501.1.0
  - ✓ The last line show the execution time and the number of MPI processes.

Output of go3.sh

```
login1$ pjsub scripts/go3.sh
[INFO] PJM 0000 pjsub Job 7791871 submitted.
login1$ pjstat
JOB_ID      JOB_NAME    MD ST  USER     START_DATE      ELAPSE_LIM            NODE_REQUIRE     VNODE
CORE V_MEM
7791871     go3.sh      NM QUE 100122   -               0000:15:00            1                -
-    -
login1$ ls go3*
go3.sh.7791871.out
go3.sh.7791871.out.1.0
go3.sh.7791871.out.1.1
go3.sh.7791871.out.1.2
```

Output of MPI rank 0

When Job Queue is too busy, Let's use Interactive mode.

1. Connect to Fugaku compute node in interactive mode.

<< Reserve the max number of MPI process with (# of nodes) x 48. >>

```
$ pjsub  --interact   -L rscgrp=int,node=1,elapse=0:5:00  --mpi proc=48  --sparam wait-time=600
```

<< Specify the necessary # of nodes for your MPI parallel job. >>

```
$ pjsub  --interact   -L rscgrp=int,node=2,elapse=0:15:00 --mpi proc=96  --sparam wait-time=600
```

2. Set the environmental variable and Execute

```
$ source scripts/set_omp_num_threads.sh  1
$ ./scripts/go3.sh
```

Measure Exec Time without Saving Files

When you measure the elapsed time by excluding file-writing time, please

1) un-comment 53rd line and comment out the 54th line in Makefile.

2) un-comment 58th line and comment out the 59th line in Makefile.

```
else ifeq (${BASE_COMPILER},mpifccpx)
CFLAGS  = -Nclang -Kfast,openmp $(INCLUDE_DIR)
#CFLAGS  = -Nclang -Kfast,openmp $(INCLUDE_DIR) -DMEASURE_TIME
```

↓

```
else ifeq (${BASE_COMPILER},mpifccpx)
#CFLAGS  = -Nclang -Kfast,openmp $(INCLUDE_DIR)
CFLAGS  = -Nclang -Kfast,openmp $(INCLUDE_DIR) -DMEASURE_TIME
```

Then, read the last line of the output file:

```
Time-step=40000 : (MPI-Procs, Elapsed Time)=(3, 754.547 sec),  (MPI*OpenMP, Time)=(3, 754.547 sec)
```

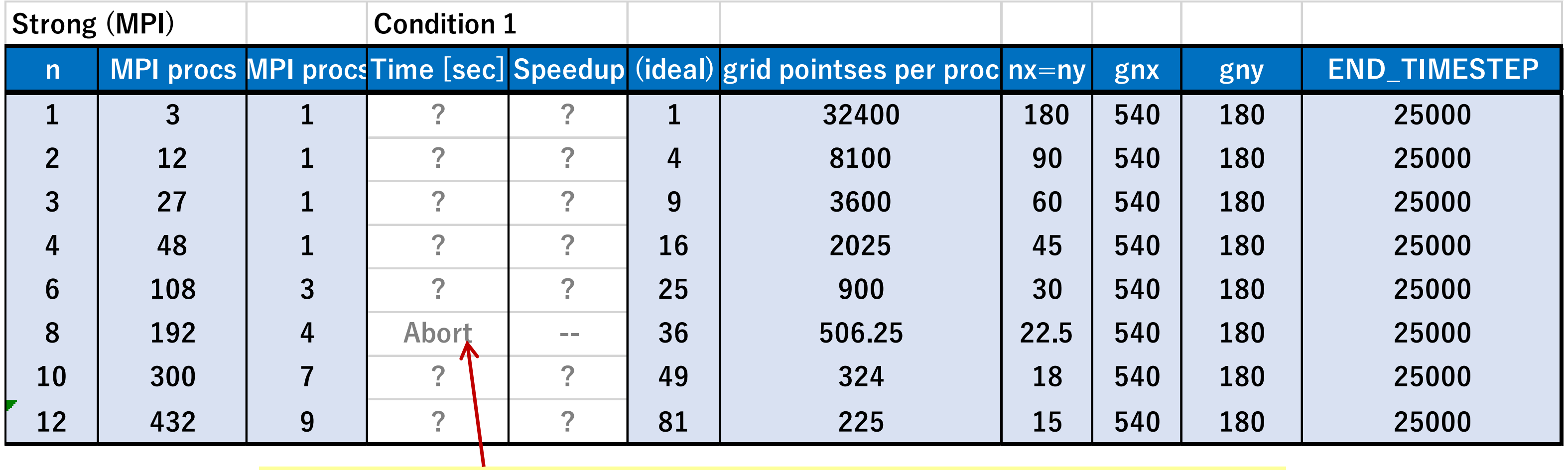
for MPI parallel

for OMP-MPI hybrid parallel

Observe Speedup by Changing #PJM --mpi proc

Strong scaling

- ✓ Parallel computation with 3n^2 MPI processes for **the same "entire" grid size**
- ✓ Measure execution time by changing n = 1, 2, 3, 4, ... 12 (3n^2 = 432)
  - ➢ Don't forget to **"un-comment 53rd line and comment out 54th line in Makefile to stop file output"**
  - ➢ Don't change the size of Grid (Use **Condition-1** in cfd.h)
- ✓ Fill out the table as bellow
- ✓ **Draw the graph: # of MPI processes vs. Speedup**



Strong (MPI)			Condition 1							
n	MPI procs	MPI procs	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
1	3	1	?	?	1	32400	180	540	180	25000
2	12	1	?	?	4	8100	90	540	180	25000
3	27	1	?	?	9	3600	60	540	180	25000
4	48	1	?	?	16	2025	45	540	180	25000
6	108	3	?	?	25	900	30	540	180	25000
8	192	4	Abort	--	36	506.25	22.5	540	180	25000
10	300	7	?	?	49	324	18	540	180	25000
12	432	9	?	?	81	225	15	540	180	25000

This cannot be executed due to some mismatch between the grid size and # of procs.

How to Make a Graph using "gnuplot"

graph_speedup.txt

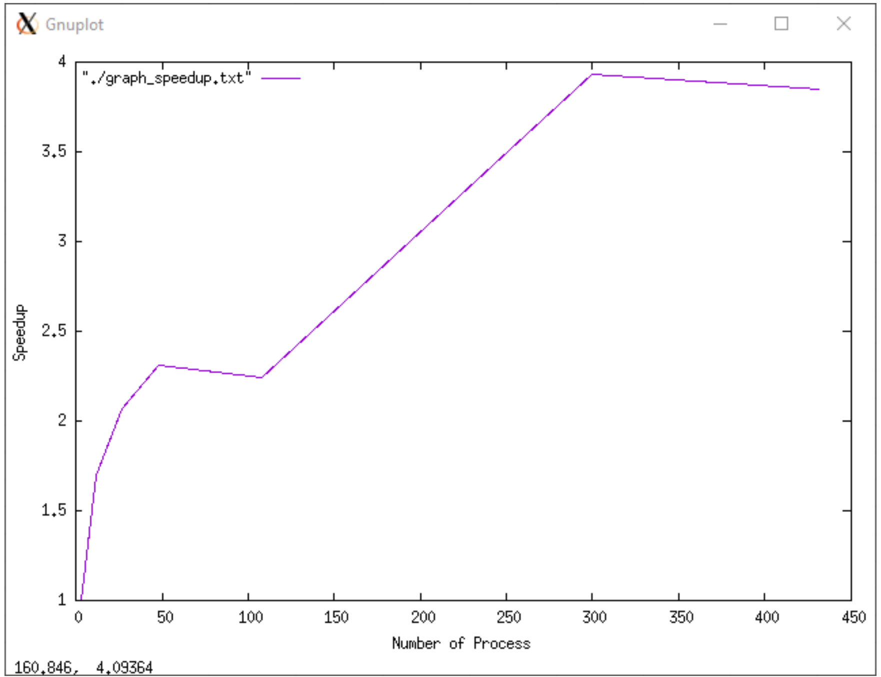
```
3     1.00
12    1.70
27    2.07
48    2.31
108  2.24
300  3.94
432  3.85
```

num of processes (x) speedup (y)

- ✓ create a data file with text editor (e.g., vim, emacs)
  - ➢ Write X-axis data in 1st column, Y-axis data in 2nd column
  - ➢ insert a space between the columns
- ✓ execute gnuplot in your terminal & type following commands

```
login2$ . ~/../data/spack/share/spack/setup-env.sh
login2$ spack load gnuplot
login2$ gnuplot
G N U P L O T
Version 5.2 patchlevel 8    last modified 2019-12-01
…
Terminal type set to 'x11'
gnuplot> set xlabel 'the number of processes'
gnuplot> set ylabel 'speedup’
gnuplot> set key top left
gnuplot> plot "./graph_speedup.txt" with line
```

For calculation,
you can use “bc –l” command (“-l” is of a small character of “–L”)



We will start the next session at 16:00

- We will end the today’s session as scheduled, and take a group photo at 17:20.

- **By the time, please create the table and the graph for speedups.**
  - Speedup for n = (Time of baseline w/ 3 procs) / (Time with 3n^2 procs)

- **When you create the graph, please upload it to Slack.**
  - ✓ I recommend you to submit multiple jobs by using copied (and edited) go3.sh scripts, and have a coffee ;-)

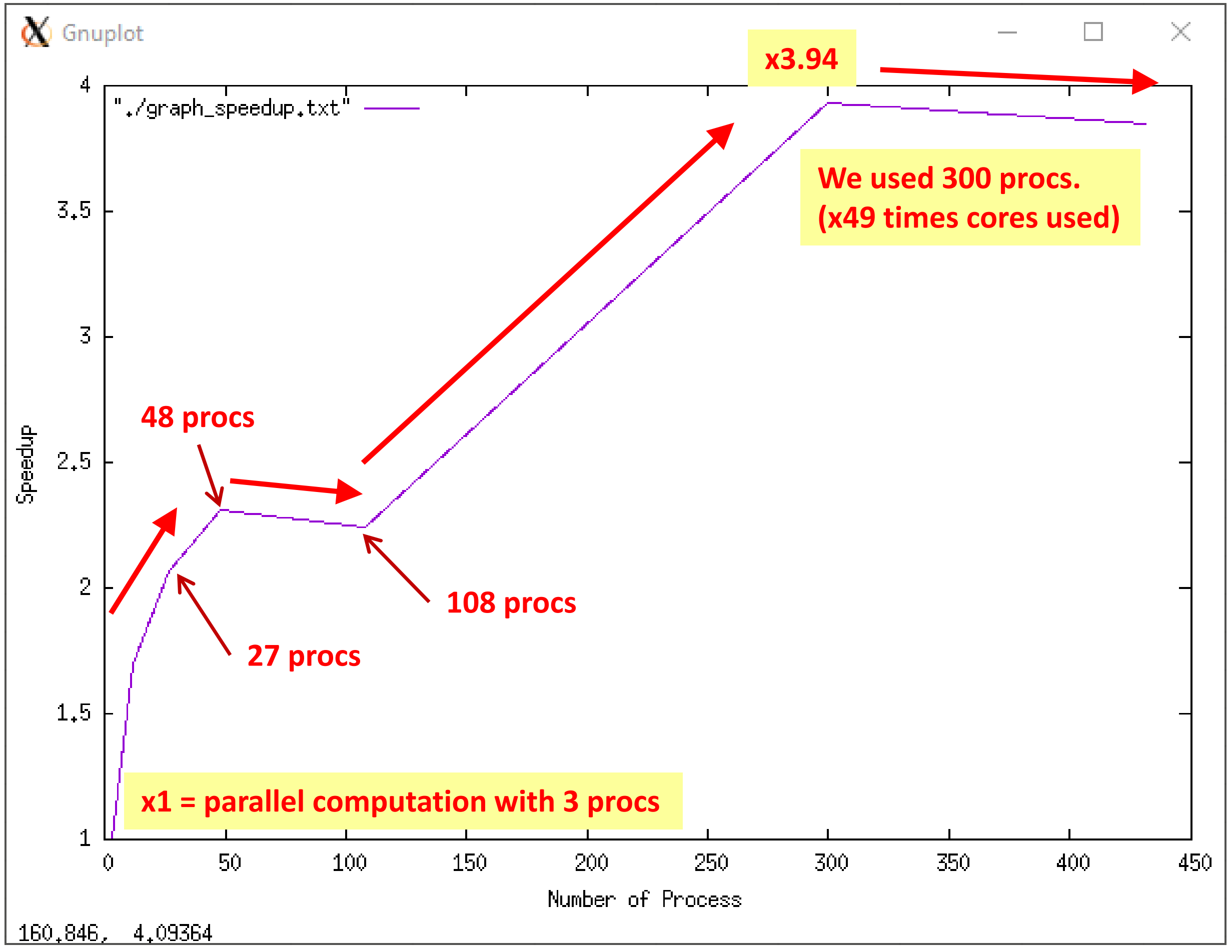
- **If you have time, please move onto the following slides by yourself.**

Question: Why Scalability is being limited as the number of MPI processes increases? What’s happen in strong scaling?

This slide will be updated.

During the lecture of Module-2

Why Speedup is just up to 3.94?



Results by Mr. / Ms. XXXX

Condition-1
MPI-parallel (no OpenMP)
Up to 432 cores

Observe Speedup by Changing Problem Size

The larger grid is used, the better speedup?

- ✓ Measure execution time and obtain speedups for Condition 1, 0, X
- ✓ Draw graphs against (MPI procs)
- ✓ How do Speedup change? And why?

Note: Computation of Condition X with 3 MPI procs takes more than 15 min. If you execute it, you need to increase "elapsed time" in go3.sh

Strong (MPI)			Condition 2							
n	MPI procs	Nodes	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
1	3	1	?	?	1	14400	120	360	120	20000
2	12	1	?	?	4	3600	60	360	120	20000
3	27	1	?	?	9	1600	40	360	120	20000
4	48	1	?	?	16	900	30	360	120	20000
6	108	3	?	?	25	400	20	360	120	20000
8	192	4	?	?	36	225	15	360	120	20000
10	300	7	?	?	49	144	12	360	120	20000
12	432	9	?	?	81	100	10	360	120	20000

Strong (MPI)			Condition 0							
n	MPI procs	MPI procs	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
1	3	1	?	?	1	129600	360	1080	360	40000
2	12	1	?	?	4	32400	180	1080	360	40000
3	27	1	?	?	9	14400	120	1080	360	40000
4	48	1	?	?	16	8100	90	1080	360	40000
6	108	3	?	?	25	3600	60	1080	360	40000
8	192	4	?	?	36	2025	45	1080	360	40000
10	300	7	?	?	49	1296	36	1080	360	40000
12	432	9	?	?	81	900	30	1080	360	40000

Strong (MPI)			Condition 1							
n	MPI procs	MPI procs	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
1	3	1	?	?	1	32400	180	540	180	25000
2	12	1	?	?	4	8100	90	540	180	25000
3	27	1	?	?	9	3600	60	540	180	25000
4	48	1	?	?	16	2025	45	540	180	25000
6	108	3	?	?	25	900	30	540	180	25000
8	192	4	Abort	--	36	506.25	22.5	540	180	25000
10	300	7	?	?	49	324	18	540	180	25000
12	432	9	?	?	81	225	15	540	180	25000

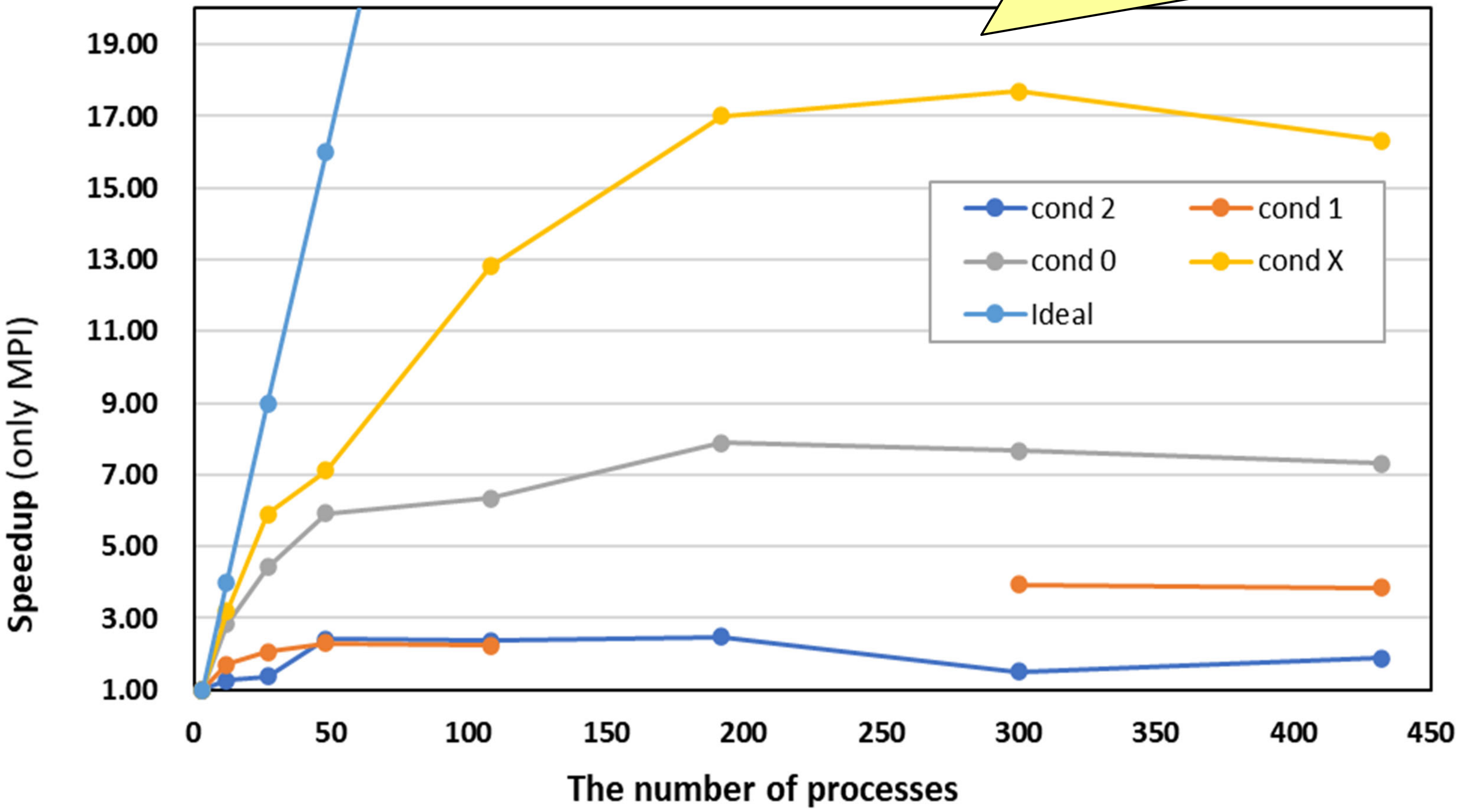
Strong (MPI)			Condition X							
n	MPI procs	MPI procs	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
1	3	1	?	?	1	518400	720	2160	720	80000
2	12	1	?	?	4	129600	360	2160	720	80000
3	27	1	?	?	9	57600	240	2160	720	80000
4	48	1	?	?	16	32400	180	2160	720	80000
6	108	3	?	?	25	14400	120	2160	720	80000
8	192	4	?	?	36	8100	90	2160	720	80000
10	300	7	?	?	49	5184	72	2160	720	80000
12	432	9	?	?	81	3600	60	2160	720	80000

This cannot be executed due to some mismatch between the grid size and # of procs.

Strong Scaling Example

What's happen in each case? (note: 1 proc = 1 core)

- # of procs = 3, 12, 27, 48, 108, 192, 300, 432
- CMG has 12 cores.
  1 CPU (1 node) has 48 cores (in 4 CMGs).
- More than 48 uses inter-node communication with Tofu.



Observe Speedup by Hybrid Parallel

If we combine OpenMP and MPI, how do speedups change?

- ✓ Edit go3.sh for `export OMP_NUM_THREADS=2, 4, 8`
- ✓ Draw graphs against (OMP*MPI threads)
- ✓ How do Speedup change? And why?

Strong (OMP&MPI) Condition X

OMP	n	MPI	Total	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
2	1	3	6	1030.56	1.00	1	518400	720	2160	720	80000
2	2	12	24	336.28	3.06	4	129600	360	2160	720	80000
2	3	27	54	202.59	5.09	9	57600	240	2160	720	80000
2	4	48	96	147.89	6.97	16	32400	180	2160	720	80000
2	6	108	216	110.43	9.33	25	14400	120	2160	720	80000
2	8	192	384								
2	10	300	600								
2	12	432	864								

Strong (OMP&MPI) Condition X

OMP	n	MPI	Total	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
4	1	3	12	650.52	1.00	1	518400	720	2160	720	80000
4	2	12	48	238.27	2.73	4	129600	360	2160	720	80000
4	3	27	108	163.99	3.97	9	57600	240	2160	720	80000
4	4	48	192	126.15	5.16	16	32400	180	2160	720	80000
4											
4											
4											
4											

Strong (OMP&MPI) Condition X

OMP	n	MPI	Total	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
8	1	3	24	635.67	1.00	1	518400	720	2160	720	80000
8	2	12	96	187.40	3.39	4	129600	360	2160	720	80000
8											
8											
8											
8											
8											
8											

More Advanced Exercise

- **Read the codes and optimize them to further speed up execution**
  - ✓ Find the optimum numbers for MPI procs and OMP threads; of best hybrid
  - ✓ Remove unnecessary codes
  - ✓ Reduce the number of barriers IF possible
  - ✓ Add OpenMP parallelization to functions that are not parallelized yet
- **Try more advanced modification for speedup**
  - ✓ Reduce the number of residual computation (this may change simulation results)
    - ➢ Now 1 residual computation per **2** Jacobi computations
    - ➢ What's happen if we have 1 residual computation per **4** Jacobi computations?
      (For speedup, we need to remove unnecessary "barrier", "critical", "single" sections)
- **Try what you propose to do …**
- **When you accomplish something interesting, please write it to Slack ch!**