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

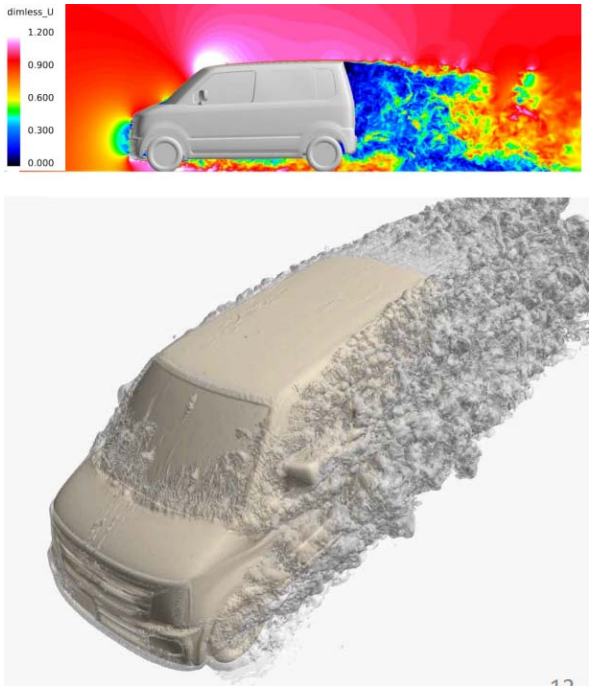
  ✓ Hands-on Practice

PART-I

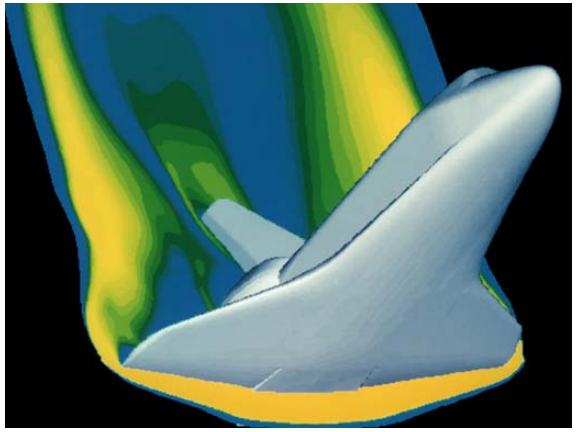
Introduction of Application: 2D CFD Simulation

Introduction

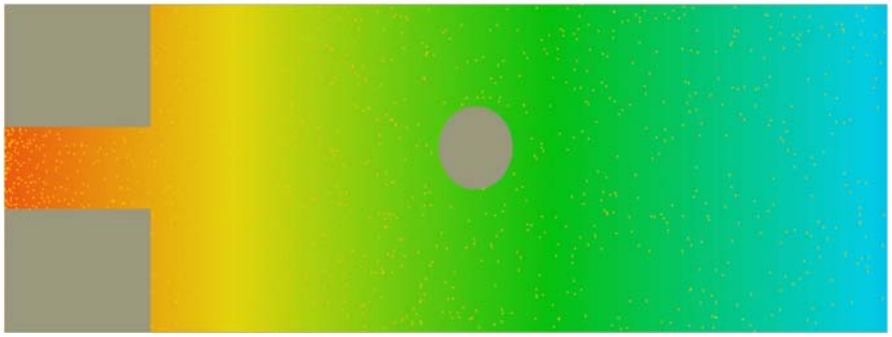
What is Computational Fluid Dynamics (CFD) simulation ?



Prediction of the Drag by 2.3 billion meshes.

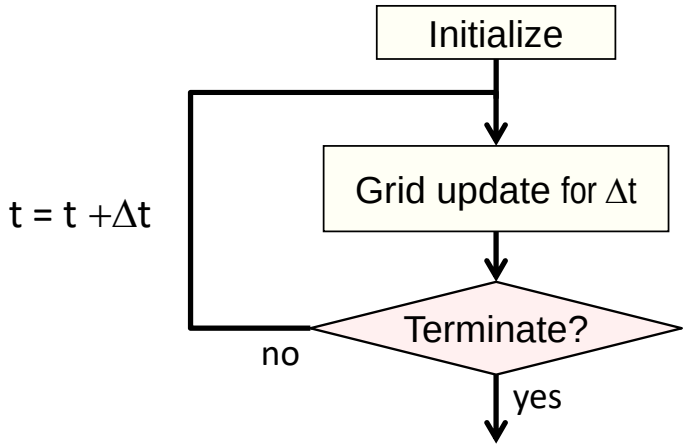


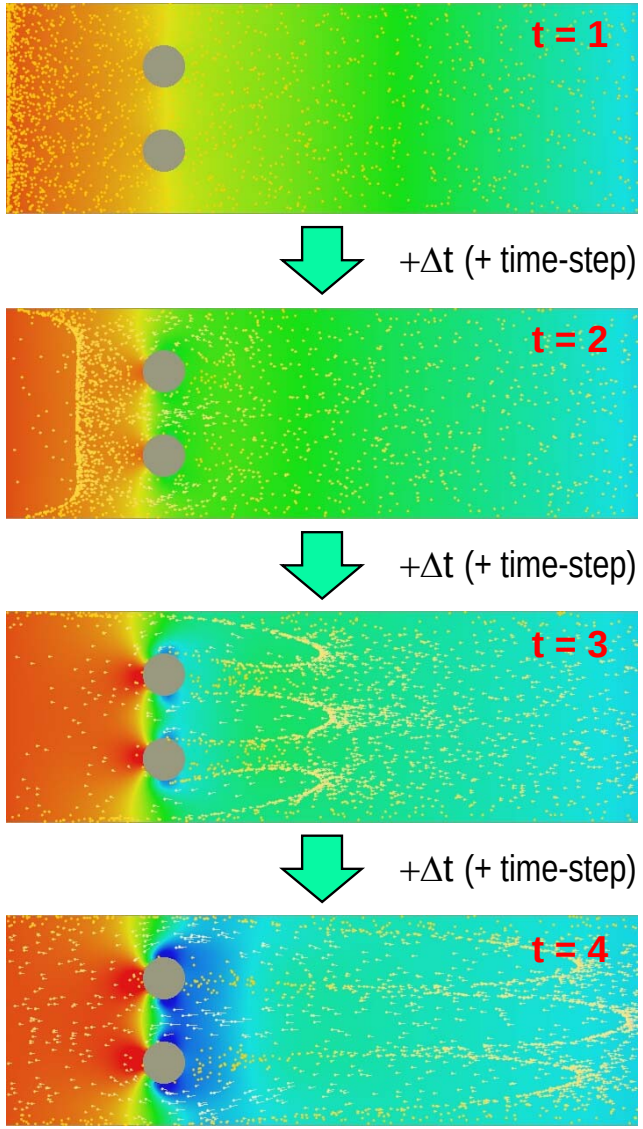
Simulation of high velocity air flow around the Space Shuttle during re-entry.



Simulation of 2D viscous flow with circular obstacle.

How to Compute Fluid Flow?





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.

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

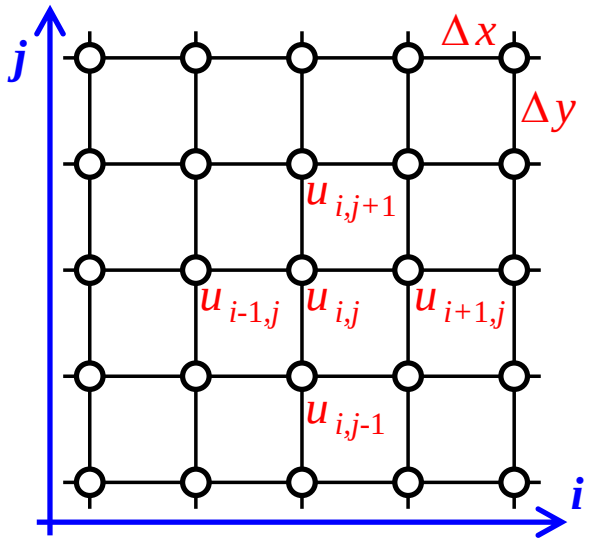
Finite Difference Schemes

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.)

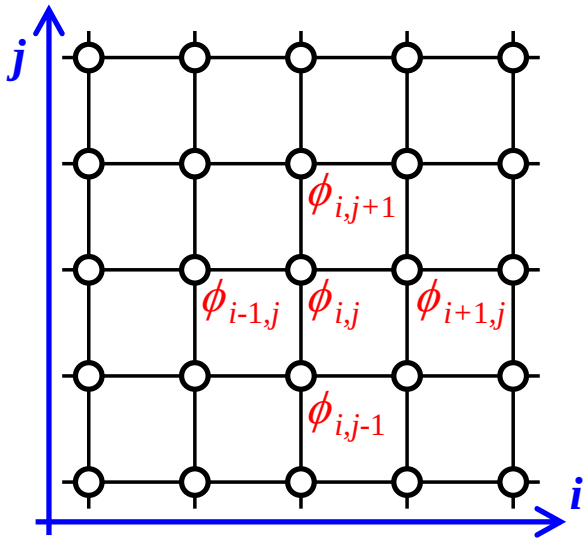
See “staggered mesh” for more advanced study.

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.

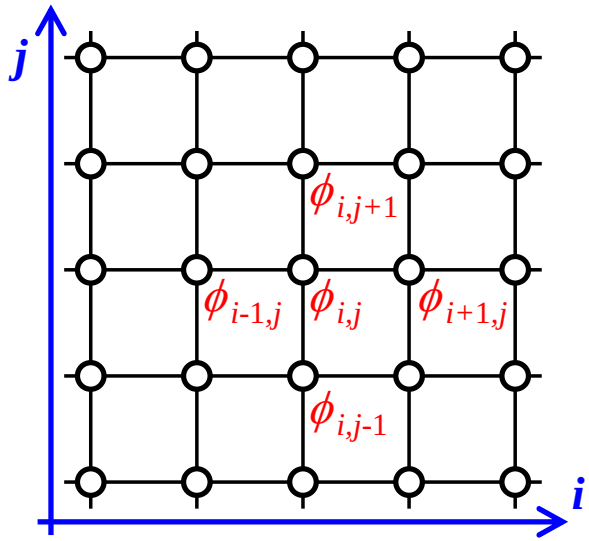
$$\varphi'_{i,j} = \alpha\left(\frac{\varphi_{i+1,j} + \varphi_{i-1,j}}{(\Delta x)^2} + \frac{\varphi_{i,j+1} + \varphi_{i,j+1}}{(\Delta y)^2} - D_{i,j}\right)$$

where

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

and

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



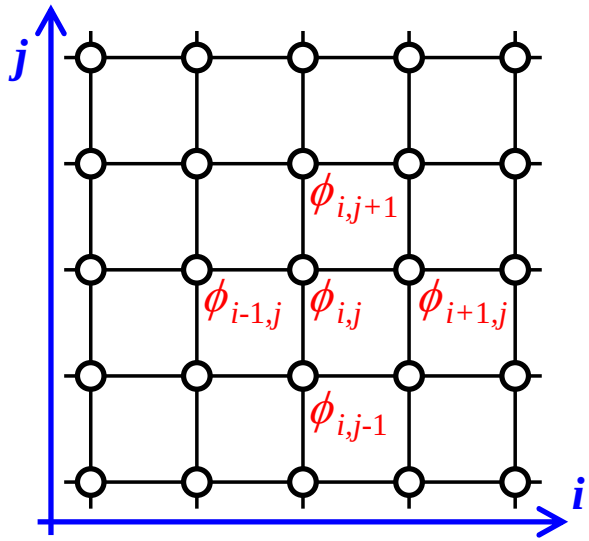
$D_{i,j}$ is referred to as **a source term** of Poisson's equation.

Discrete Form of Step3

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

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

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

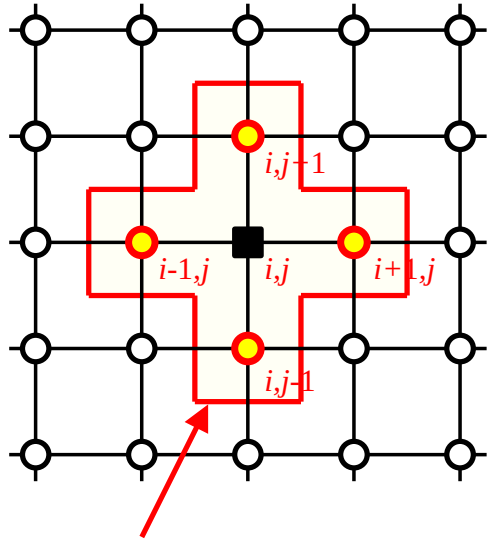


Stencil Computation

Common form in Steps 1, 2, and 3

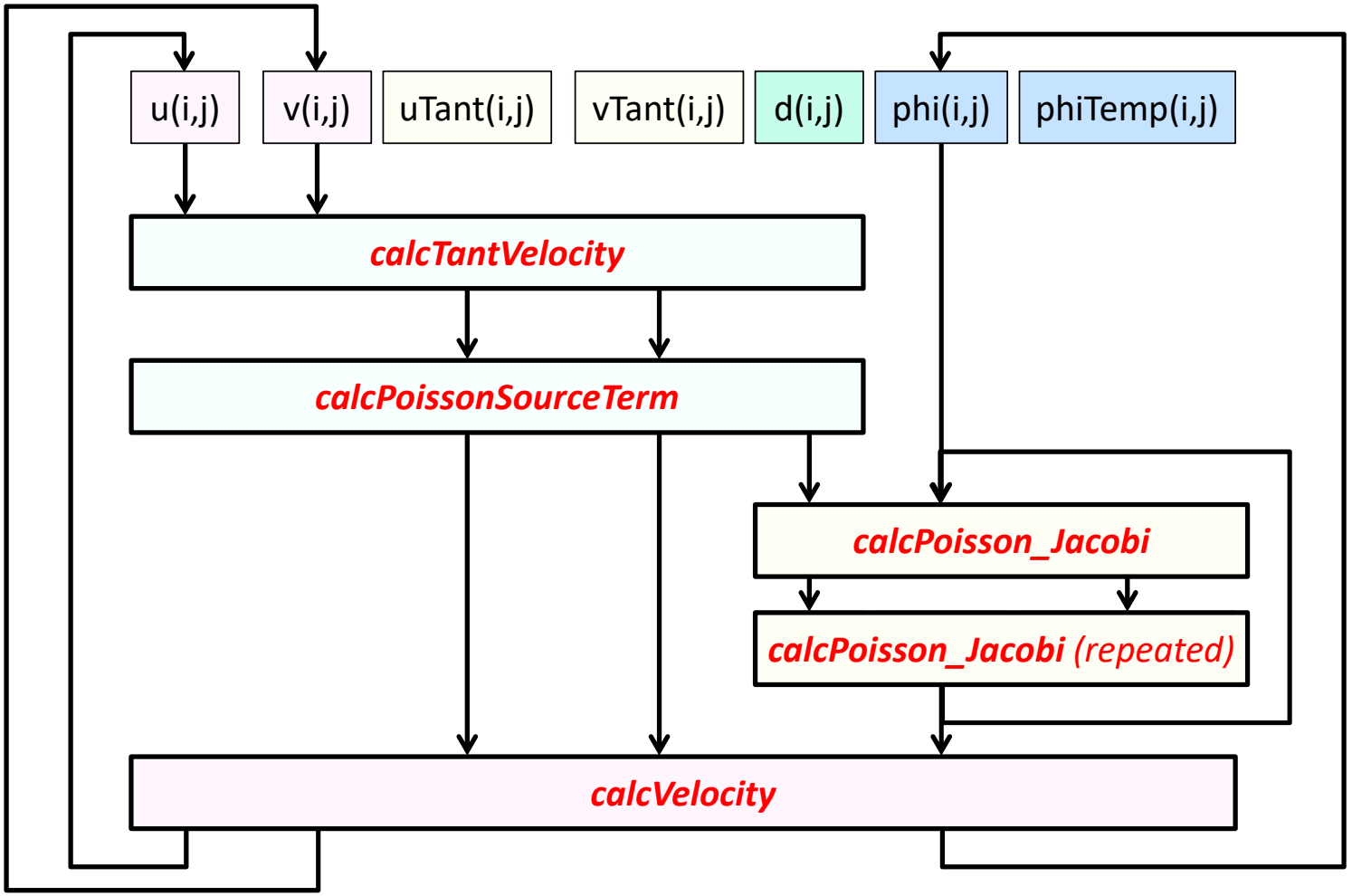
$$q_{i,j}^{new} = A + Bq_{i,j} + Cq_{i+1,j} + Dq_{i-1,j} + Eq_{i,j+1} + Fq_{i,j-1}$$

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!

```
@obcx02  cd
@obcx02  mkdir programs_cfd
@obcx02  cd programs_cfd
@obcx02  cp /work/gt57/t57004/share/serial_0920_final.tgz ./
@obcx02  tar zxvfp serial_0920_final.tgz
@obcx02  cd serial_0920/

@obcx02  ls
cfd.cpp
cfd.h
main.cpp
main.h
stopwatch3.h
Makefile
README.txt
scripts
```

Go to your home directory

Create work directory

Copy tgz archive of source files

Decompress it

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) );
  }
}
```

cfd.cpp 5 of 6

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.

```
[t57004@obcx04 serial_0920]$ ./scripts/do_clean.sh
rm -f solver_fractional  main.o cfd.o depend_c.inc depend_cpp.inc *.o *.dat *.sh.[eois]*
rm: cannot remove 'stdout.lst': No such file or directory
rm: cannot remove 'err': No such file or directory
```

Clean up previous compilation and computational results. (Recommended if you modified program.)

```
[t57004@obcx04 serial_0920]$ make
================================================================================
= Compilation starts for solver_fractional.
================================================================================
icc   -O3 -axCORE-AVX512 -align -qopenmp -no-multibyte-chars -ipo -I./ -o main.o -c main.cpp
icc   -O3 -axCORE-AVX512 -align -qopenmp -no-multibyte-chars -ipo -I./ -o cfd.o -c cfd.cpp
icc   -o solver_fractional main.o cfd.o -qopenmp -L./ -lm
main.cpp(4): remark #15009: main has been targeted for automatic cpu dispatch
...
```

Compile (OpenMP is already used here).

```
[t57004@obcx04 serial_0920]$ ./scripts/do_execute_on_frontend.sh
================ Computation started for (540 x 180) grid with dT=0.000025.
>  104 iterations in Jacobi (tstep=    0, residualMax=0.006943),  [tstep=    0 to   200] (0.879091 sec) > AVEse_000200.dat
...
>    6 iterations in Jacobi (tstep=24800, residualMax=0.073900),  [tstep=24800 to 25000] (0.312015 sec) > AVEse_025000.dat
================ Computation finished.
Time-step=25000 : ElapsedTime=120.261 sec
```

Execute program on a login server

Elapsed time for entire execution

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

```
[t57004@obcx04 serial_0920]$ ls
Makefile  README.txt  cfd.cpp  cfd.h  cfd.o  depend_cpp.inc  main.cpp  main.h  main.o  old  scripts  sim_data  solver_fractional  stopwatch3.h
```

Speed up Execution by OpenMP

README.txt is also available for your reference.

```
[t57004@obcx04 serial_0920]$ source scripts/set_omp_num_threads.sh 2
Before: OMP_NUM_THREADS=1
After : OMP_NUM_THREADS=2
```

Set the number of OpenMP threads (Try 1, 2, 4, 8, 16, ..., 56)

```
[t57004@obcx04 serial_0920]$ env | grep OMP_NUM
OMP_NUM_THREADS=2
```

Check the present number of OpenMP threads

```
[t57004@obcx04 serial_0920]$ ./scripts/do_execute_on_frontend.sh
...
================ Computation finished.
Time-step=25000 : ElapsedTime=120.261 sec
```

Execute with OpenMP threads

- **Compile and execute with a different number of OpenMP threads**
  - ✓ 1, 2, 4, 8, 16, 20, 28, 32, 48, 56
- **How scalable is it?**
  - ✓ When 8 times more threads are used, is the exec time reduced to 1/8?

Please do NOT run with many OMP threads frequently. Cores of frontend servers are Limited!

Execute with Batch-job Scheduler

README.txt is also available for your reference.

```
[t57004@obcx04 serial_0920]$ pjsub  ./scripts/go1.sh
```

Input job script "./scripts/go1.sh" into a job queue.

```
[t57004@obcx04 serial_0920]$ pjstat
Oakbridge-CX scheduled stop time: 2020/09/25(Fri) 09:00:00 (Remain:  4days 16:18:35)
JOB_ID      JOB_NAME   STATUS  PROJECT  RSCGROUP      START_DATE       ELAPSE         TOKEN NODE
541501      go1.sh     QUEUED  gt57     lecture       --/-- --:--:--   00:00:00         -    1
```

Check the status of my job queue.

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

```
[t57004@obcx04 serial_0920]$ pjdel  541501
```

Delete a job in the queue.

Please use Batch-job mode mainly.

- **Settings and executed program (script) are written in "go1.sh".**
  - ✓ You can edit them.
- **Standard output / error output are written into a file.**
  - ✓ such like "go1.sh.o541501"
  - ✓ tail -f go1.sh.o541501 for watching the file

```
[t57004@obcx04 serial_0920]$ cat scripts/go1.sh
#!/bin/sh
#PJM -N "go1.sh"
##PJM -L rscgrp=lecture7
#PJM -L rscgrp=lecture
#PJM -L node=1
#PJM --omp thread=16
#PJM -L elapse=00:15:00
#PJM -g gt57
#PJM -j

export KMP_AFFINITY=granularity=fine,compact
./scripts/do_execute_on_frontend.sh
```

= OMP_NUM_THREADS

= Max. execution time allowed

= executed program

Visualize Computational Results

README.txt is also available for your reference.

```
[t57004@obcx04 serial_0920]$ ./scripts/do_visualize.sh
Start visualization
rm: cannot remove '*.png': No such file or directory
Unable to parse the pattern
```

Convert ./sim_data/*.dat to png files, and pop up an animation window for them. (X-window server is required on your PC.)

```
[t57004@obcx04 serial_0920]$ ./scripts/do_animate.sh
Start animation
```

Just animate png files existing in ./sim_data/

Animation speed depends on network bandwidth between OCBX machine and your home.

If it's too slow, try the followings to make mp4 file

```
[t57004@obcx06 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
...
[t57004@obcx06 serial_0915]$ ls ./sim_data/*.mp4
./sim_data/plot-z-4.mp4
```

Then, download the mp4 file, and view it on your PC.

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
#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

PART-II

Parallelization of the 2D CFD Simulation

Overview

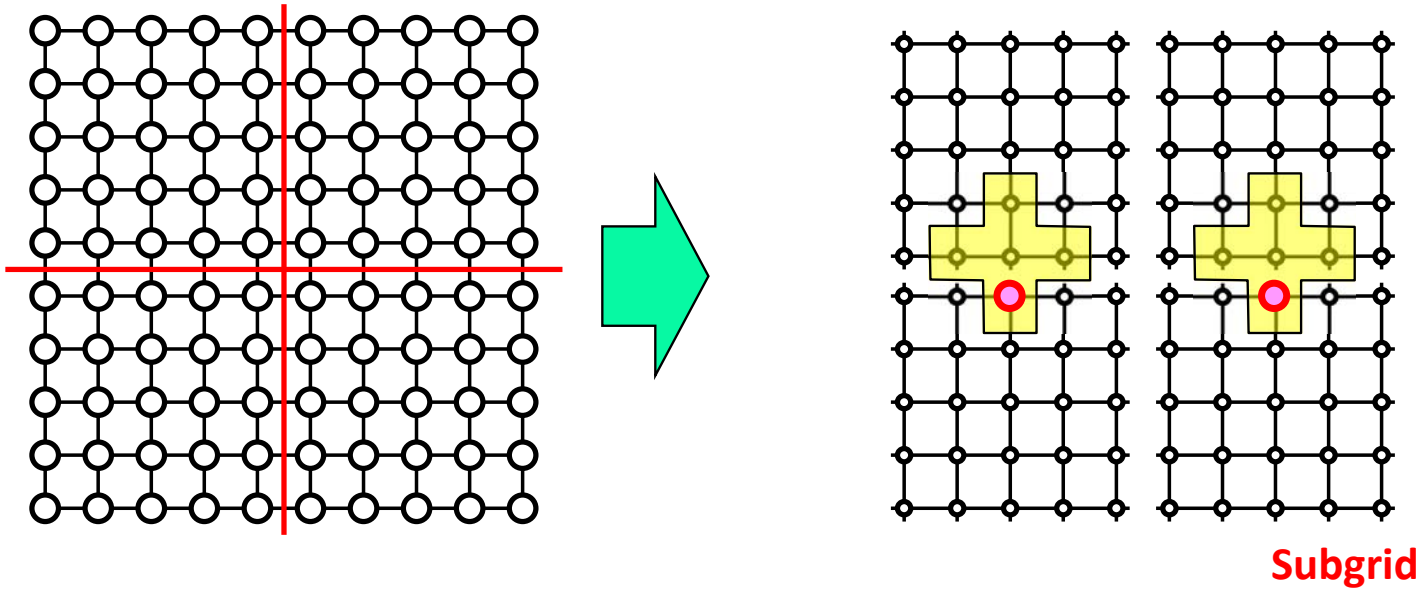
- **Parallelization with "shared memory", which is done by OpenMP, is limited to a node.**
  - ✓ Many cores in multiple sockets share the same memory space.

- **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.

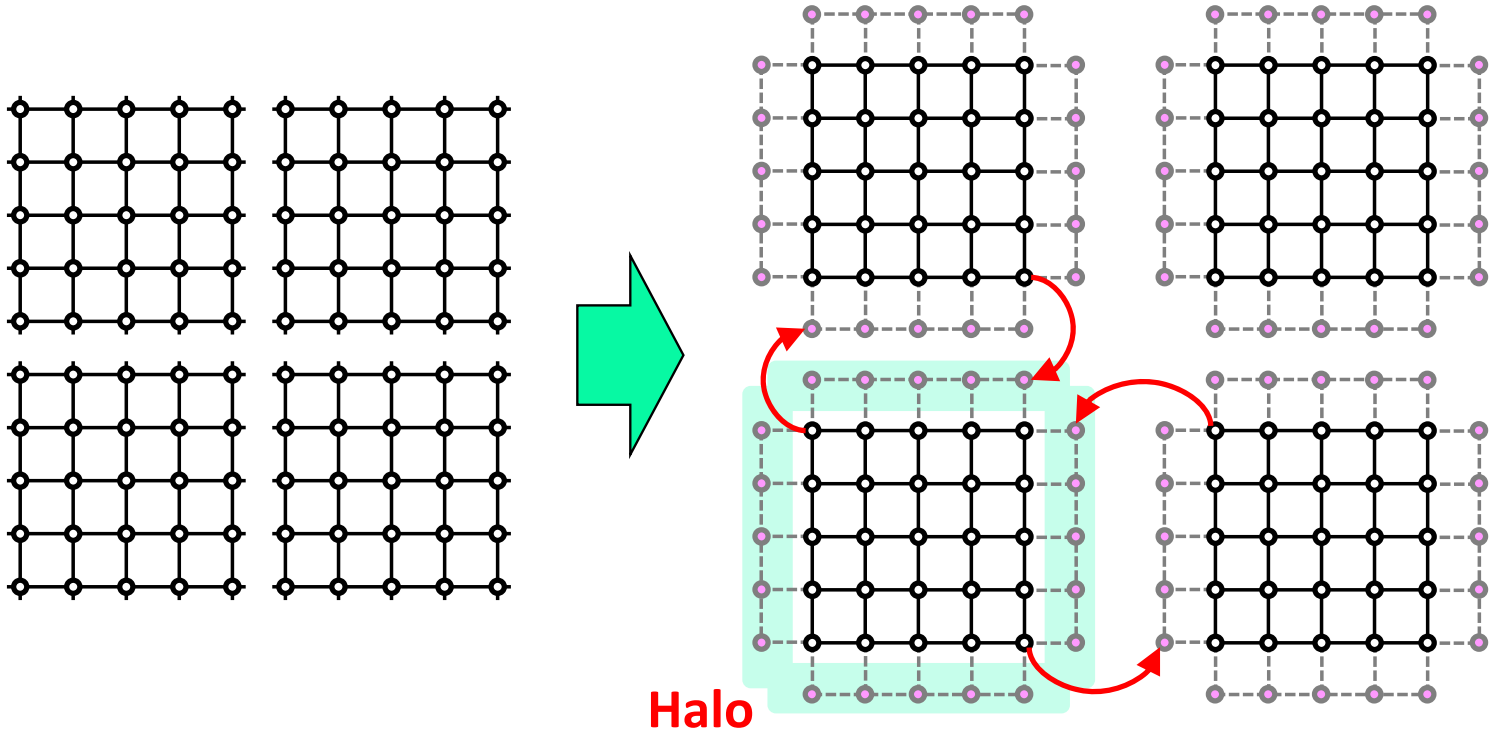
Parallel Computation w/ Domain Decomposition

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

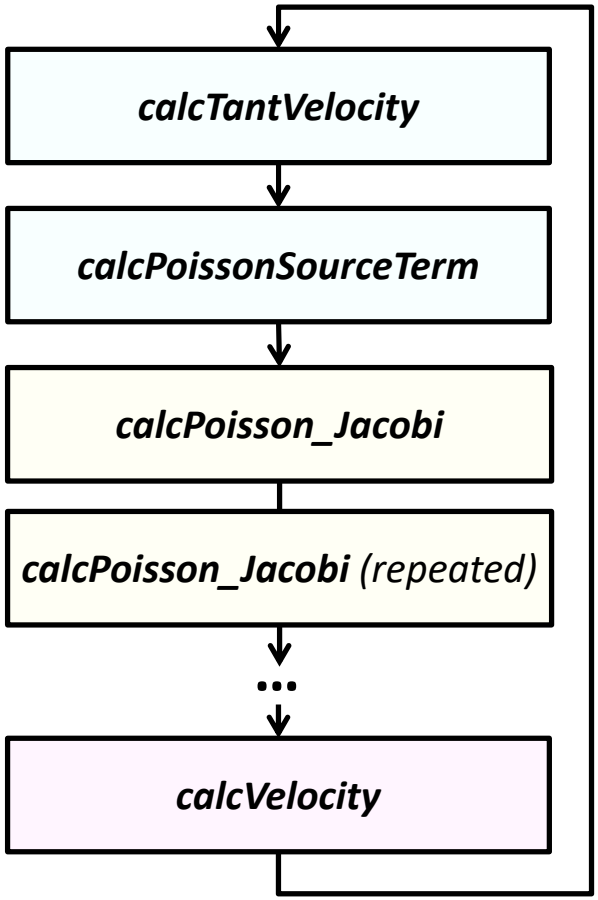


Exchanging Halo for Coarse Grain Communication

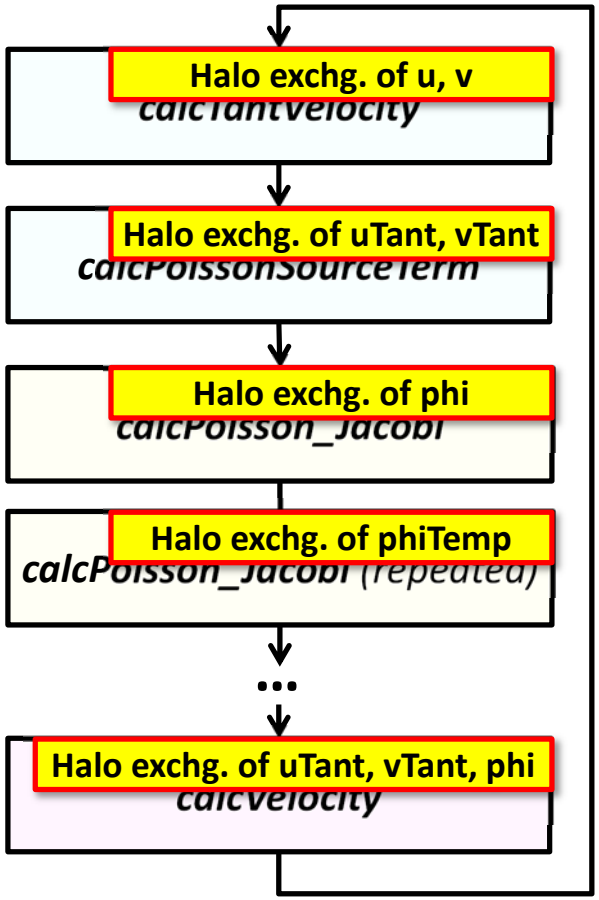
- **Halo : Overlapped boundary region**
  - ✓ Halo data are exchanged all at once in advance to the loop, so that no communication occurs during the loop.



Parallelization Overview



Serial program



MPI-parallel program

Let's Read the parallelized Code!

```
@obcx02  cd programs_cfd
@obcx02  cp /work/gt57/t57004/share/parallel_complete_0920_r1.tgz ./
@obcx02  tar zxvfp parallel_complete_0920_final.tgz
@obcx02  cd parallel_complete_0920/
@obcx02  ls
```

cfd.cpp
cfd.h

} MPI parallelization is introduced.

domain_decomp.cpp
domain_decomp.h

} New files.
Codes for subgrid management.

main.cpp
main.h
Makefile
README.txt
scripts

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)) ); }
```

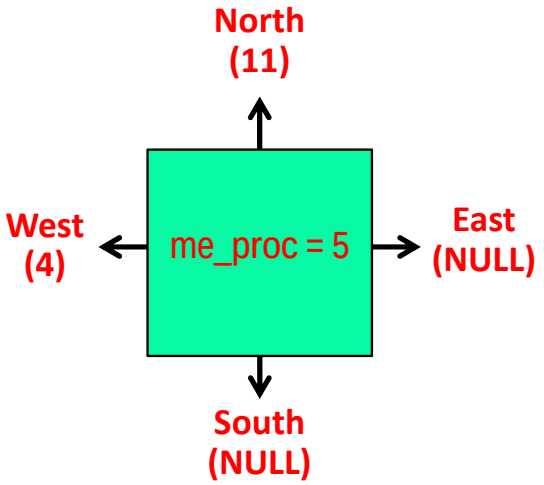
New file : domain_decomp.h

domain_decomp.h

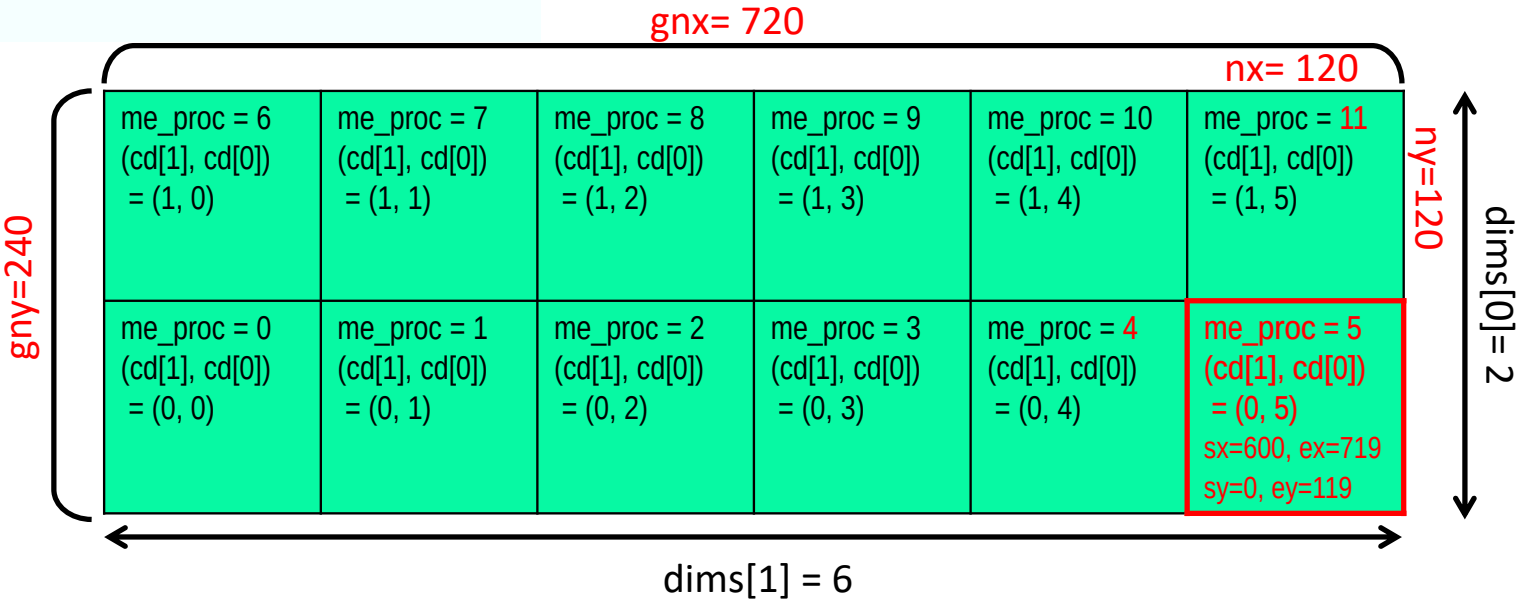
```
#ifndef ___DOMAIN_DECOMP_H___
#define ___DOMAIN_DECOMP_H___

#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



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

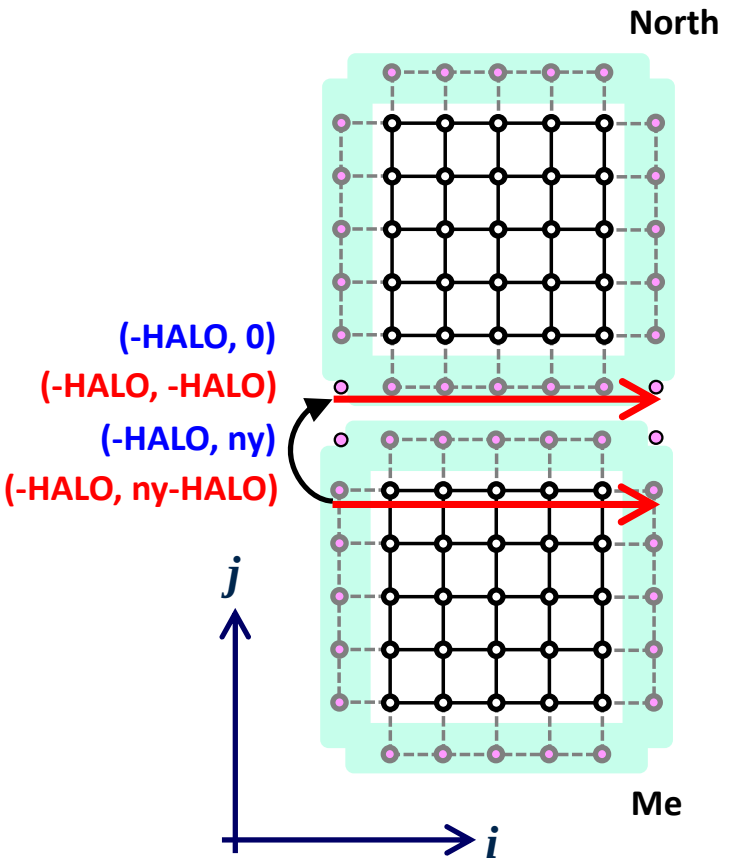
Exchange Halo of Array u in Grid g by communicating data with adjacent subgrids.
Usage: communicate_neighbor(&g->u, mpd);

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?

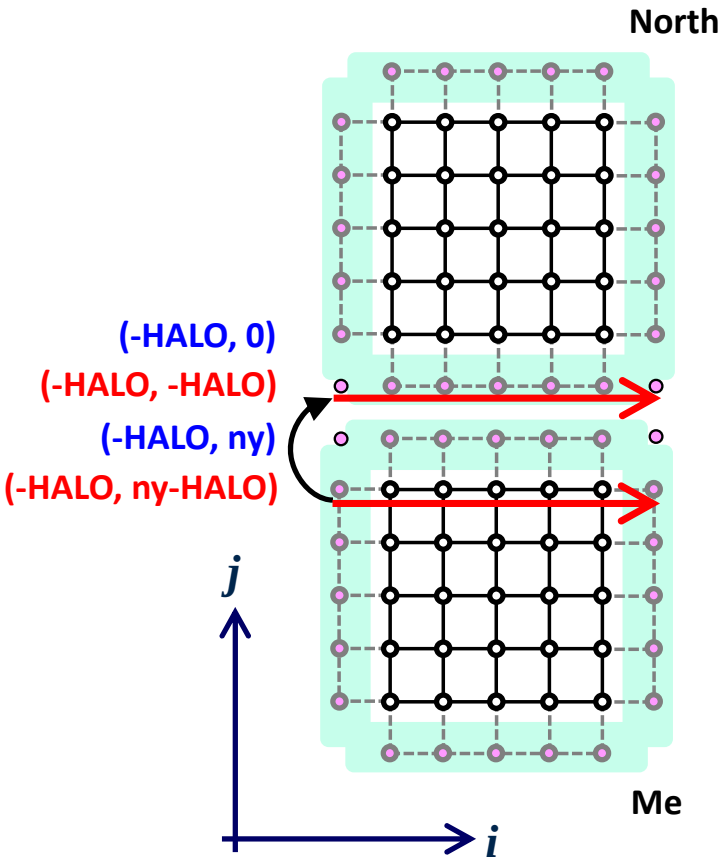
To obtain the top Halo of mine with south subgrid,

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

```
[t57004@obcx04 parallel_0920]$ ./scripts/do_clean.sh
...
[t57004@obcx04 parallel_0920]$ make
================================================================================
= Compilation starts for solver_fractional.
================================================================================
...

[t57004@obcx04 parallel_0920]$ pjsub  ./scripts/go3.sh
pjsub scripts/go3.sh
[INFO] PJM 0000 pjsub Job 541545 submitted.

[t57004@obcx04 parallel_0920]$ 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 gt57     lecture       09/20 19:00:06<  00:00:28           -   4

[t57004@obcx04 parallel_0920]$ ls go3.sh.o*
go3.sh.o541501

[t57004@obcx04 parallel_0920]$ less go3.sh.o541501
...

[t57004@obcx04 parallel_0920]$ 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

```
[t57004@obcx04 parallel_0920]$ cat scripts/go3.sh
#!/bin/sh
#PJM -N "go3.sh"
##PJM -L rscgrp=lecture7
#PJM -L rscgrp=lecture
#PJM -L node=4
#PJM --mpi proc=12
#PJM --omp thread=1
#PJM -L elapse=00:15:00
#PJM -g gt57
#PJM -j
mpiexec.hydra -n ${PJM_MPI_PROC} ./scripts/do_execute_mpi.sh
```

= **Number of physical nodes** to use (max: 8)

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

= Num of OMP threads (for hybrid parallel)

execute program by MPI

- **Check the output file of MPI-parallel execution**
  - ✓ less go3.sh.o541501
  - ✓ The last line show the execution time and the number of MPI processes.

```
[t57004@obcx04 parallel_0920]$ less go3.sh.o541501
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

me_proc: 6
Total dimension           : [2 x 6]
Coodrinate of me_proc     : [1 x 0]
Neighbor procs (E,W,N,S)  : 7, -1, -1, 0
Assigned mesh (nx,ny,gnx,gny) : 60, 60, 360, 120
Start & End mesh (sx,ex,sy,ey): 0, 59, 60, 119

...

Writing to AVEse_019800.dat
Time-step=19800 :  36 iterations in Jacobi loop
Writing to AVEse_020000.dat
Time-step=20000 : ElapsedTime=26.402 sec
```

Measure Exec Time without Saving Files

When you measure the elapsed time by excluding file-writing time, please un-comment 37th line and comment out 36th line in Makefile.

```
      ifeq (${BASE_COMPILER},mpiicpc)
      CFLAGS  = -O3 -axCORE-AVX512 -align -qopenmp -no-multibyte-chars -ipo $(INCLUDE_DIR)
#     CFLAGS  = -O3 -axCORE-AVX512 -align -qopenmp -no-multibyte-chars -ipo $(INCLUDE_DIR) -DMEASURE_TIME
                ↓
      ifeq (${BASE_COMPILER},mpiicpc)
#     CFLAGS  = -O3 -axCORE-AVX512 -align -qopenmp -no-multibyte-chars -ipo $(INCLUDE_DIR)
      CFLAGS  = -O3 -axCORE-AVX512 -align -qopenmp -no-multibyte-chars -ipo $(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 grid size**
- ✓ Measure execution time by changing n = 1, 2, 3, 4, ... 12 (3n^2 = 432)
  - ➢ Don't forget to **"un-comment 37th line and comment out 36th line in Makefile."**
  - ➢ Don't change the size of Grid (Condition in cfd.h)
- ✓ Fill out the table as bellow
- ✓ **Draw the graph: # of MPI processes vs. Elapsed time**

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

How to Make a Graph using "gnuplot"

graph_speedup.txt

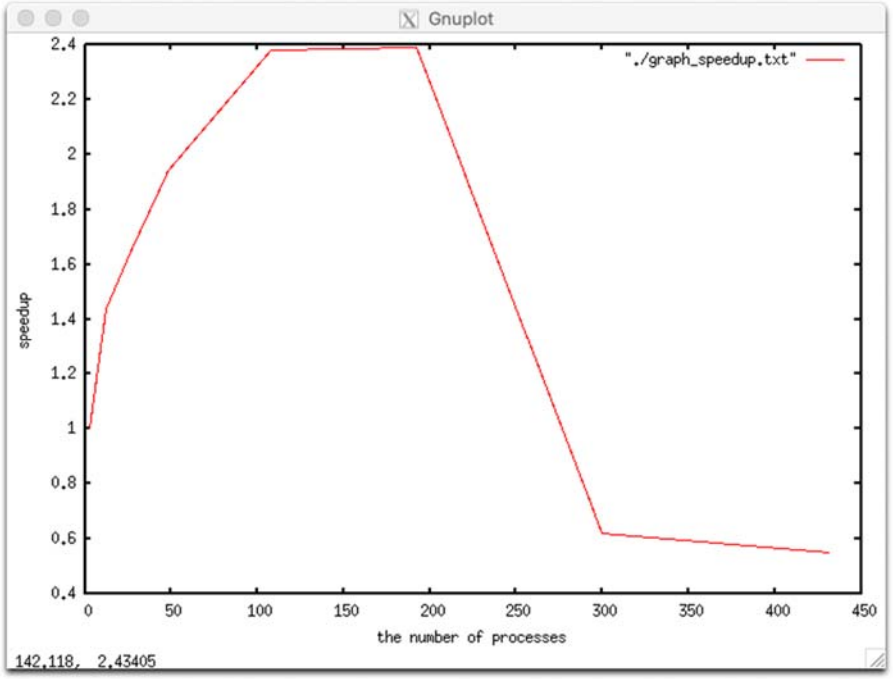
```
3     1.00
12    1.44
27    1.65
48    1.94
108   2.38
192   2.39
300   0.62
432   0.55
```

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

```
[t57004@obcx04 parallel_0920]$ gnuplot
G N U P L O T
Version 4.6 patchlevel 2    last modified 2013-03-14
...
Terminal type set to 'x11'
gnuplot> set xlabel 'the number of processes'
gnuplot> set ylabel 'speedup'
gnuplot> plot "./graph_speedup.txt" with line
```

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



Observe Speedup by Changing Problem Size

The larger grid, 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 or 12 MPI procs takes more than 15 min. If you execute it, you need to increase "elapsed time" in go3.sh

Strong — Condition 2

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

Strong — Condition 0

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

Strong — Condition 1

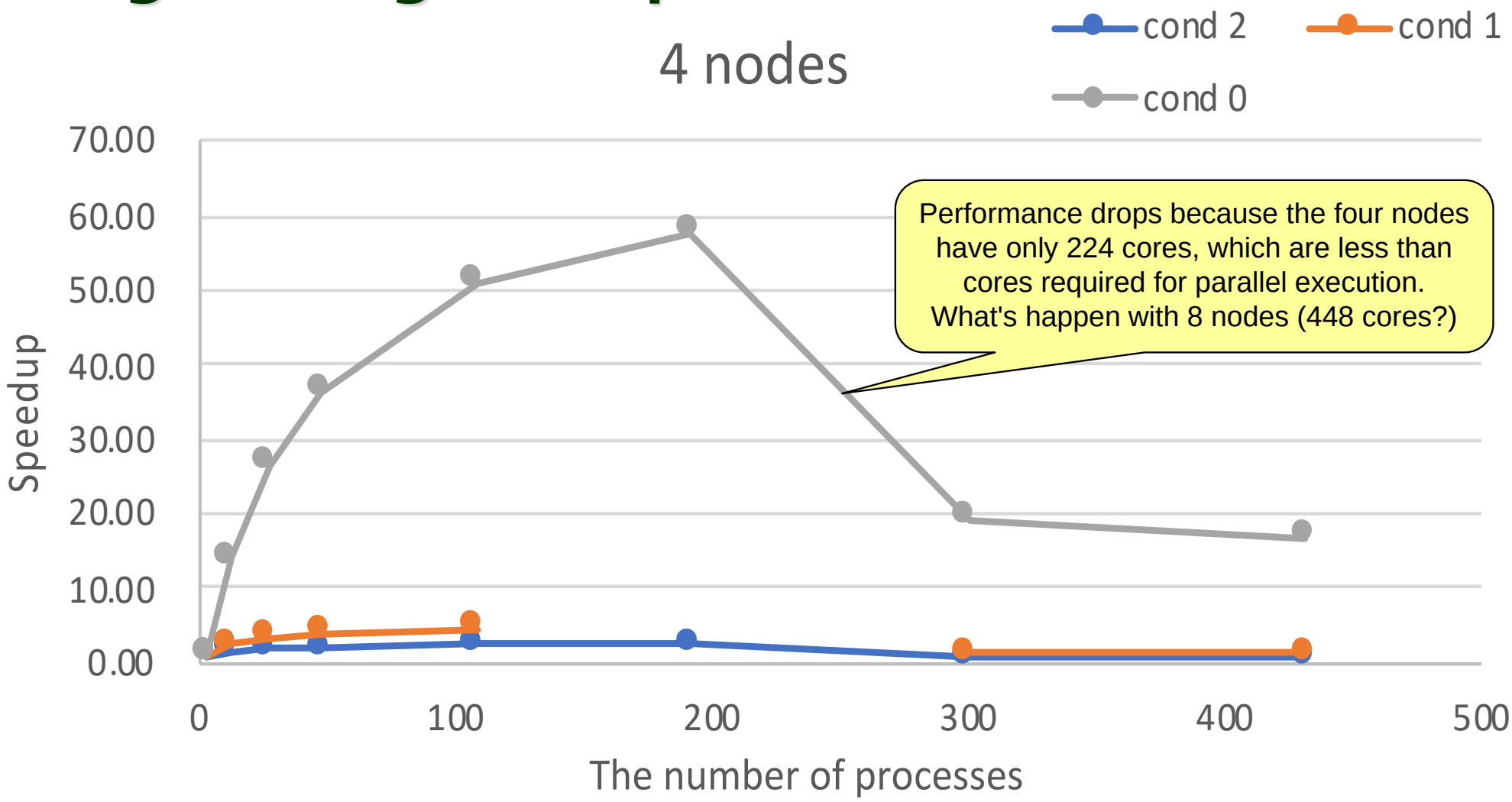
n	MPI procs	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
1	3	?	?	1	32400	180	540	180	25000
2	12	?	?	4	8100	90	540	180	25000
3	27	?	?	9	3600	60	540	180	25000
4	48	?	?	16	2025	45	540	180	25000
6	108	?	?	25	900	30	540	180	25000
8	192		?	36	506.25	22.5	540	180	25000
10	300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

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

Strong — Condition X

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

Strong Scaling Example



Observe Speedup by Hybrid Parallel

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

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

Strong (OMP & MPI)				Condition 0							
OMP	n	MPI	Total	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
2	1	3	6	?	?	1	129600	360	1080	360	40000
2	2	12	24	?	?	4	32400	180	1080	360	40000
2	3	27	54	?	?	9	14400	120	1080	360	40000
2	4	48	96	?	?	16	8100	90	1080	360	40000
2	6	108	216	?	?	25	3600	60	1080	360	40000
2	8	192	384	?	?	36	2025	45	1080	360	40000
2	10	300	600								
2	12	432	864								

Strong (OMP & MPI)				Condition 0							
OMP	n	MPI	Total	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
4	1	3	12	?	?	1	129600	360	1080	360	40000
4	2	12	48	?	?	4	32400	180	1080	360	40000
4	3	27	108	?	?	9	14400	120	1080	360	40000
4	4	48	192	?	?	16	8100	90	1080	360	40000
4	6	108	432	?	?	25	3600	60	1080	360	40000
4											
4											
4											

Strong (OMP & MPI)				Condition 0							
OMP	n	MPI	Total	Time [sec]	Speedup	(ideal)	grid pointses per proc	nx=ny	gnx	gny	END_TIMESTEP
8	1	3	24	?	?	1	129600	360	1080	360	40000
8	2	12	96	?	?	4	32400	180	1080	360	40000
8	3	27	216	?	?	9	14400	120	1080	360	40000
8	4	48	384	?	?	16	8100	90	1080	360	40000
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!**