CEE 618 Scientific Parallel Computing (Lecture 14)

Scalapack, Mixed OpenFOAM, and Others

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Linear System: $A \cdot x = B$, $x = ?$

```
-2.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   |-13.33| =  1.00
 1.00  -2.00   1.00   0.00   0.00   0.00   0.00   0.00   |-25.67| =  2.00
 0.00   1.00  -2.00   1.00   0.00   0.00   0.00   0.00   |-36.00| =  3.00
 0.00   0.00   1.00  -2.00   1.00   0.00   0.00   0.00   |-43.33| =  4.00
 0.00   0.00   0.00   1.00  -2.00   1.00   0.00   0.00   |-46.67| =  5.00
 0.00   0.00   0.00   0.00   1.00  -2.00   1.00   0.00   |-45.00| =  6.00
 0.00   0.00   0.00   0.00   0.00   1.00  -2.00   1.00   |-37.33| =  7.00
 0.00   0.00   0.00   0.00   0.00   0.00   1.00  -2.00   |-22.67| =  8.00
```

1. A is an 8-by-8 matrix and $b = [1, 2, 3, 4, 5, 6, 7, 8]^T$.
2. Task is to calculate $x = [-13.33, -25.67, \dots]^T$.
3. DGESV subroutine of LAPACK can be used for serial computing.
   - D: Double preicision
   - GE: GEneral
   - SV: factor the matrix and SolVe a system of equations

DGESV of LAPACK

SUBROUTINE DGESV(N, NRHS, A, LDA, IPIV, B, LDB, INFO)

```
-2.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   |-13.33| =  1.00
 1.00  -2.00   1.00   0.00   0.00   0.00   0.00   0.00   |-25.67| =  2.00
 0.00   1.00  -2.00   1.00   0.00   0.00   0.00   0.00   |-36.00| =  3.00
 0.00   0.00   1.00  -2.00   1.00   0.00   0.00   0.00   |-43.33| =  4.00
 0.00   0.00   0.00   1.00  -2.00   1.00   0.00   0.00   |-46.67| =  5.00
 0.00   0.00   0.00   0.00   1.00  -2.00   1.00   0.00   |-45.00| =  6.00
 0.00   0.00   0.00   0.00   0.00   1.00  -2.00   1.00   |-37.33| =  7.00
 0.00   0.00   0.00   0.00   0.00   0.00   1.00  -2.00   |-22.67| =  8.00
```

1. Matrix A is 8-by-8: N=8
2. Matrix B is 8-by-1: NRHS=1

   The number of right hand sides, i.e., the number of columns of B.
3. The leading dimension of A, simply, LDA=N
4. The leading dimension of B, simply, LDB=N
5. IPIV: integer array of dimension(N) for pivoting
6. INFO = 0 if successful

PDGESV of Scalapack

PDGESV(N, NRHS, A, IA, JA, DESCA, IPIV, B, IB, JB, DESCB, INFO)

```
-2.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   |-13.33| =  1.00
 1.00  -2.00   1.00   0.00   0.00   0.00   0.00   0.00   |-25.67| =  2.00
 0.00   1.00  -2.00   1.00   0.00   0.00   0.00   0.00   |-36.00| =  3.00
 0.00   0.00   1.00  -2.00   1.00   0.00   0.00   0.00   |-43.33| =  4.00
 0.00   0.00   0.00   1.00  -2.00   1.00   0.00   0.00   |-46.67| =  5.00
 0.00   0.00   0.00   0.00   1.00  -2.00   1.00   0.00   |-45.00| =  6.00
 0.00   0.00   0.00   0.00   0.00   1.00  -2.00   1.00   |-37.33| =  7.00
 0.00   0.00   0.00   0.00   0.00   0.00   1.00  -2.00   |-22.67| =  8.00
```

1. IA=JA=IB=JB=1, first row and column indexes of A and B
2. DESCA and DESCB: integer array descriptor of dimension (9) for the distributed matrix A.

Look at the code with explanation.

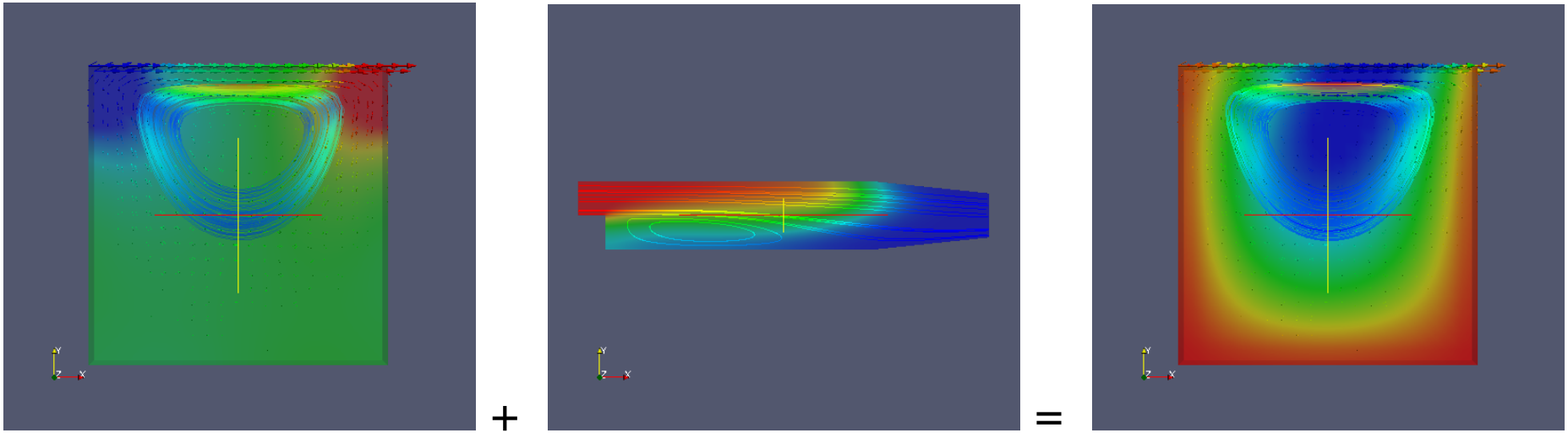
icoFoam (U) $\rightarrow$ scalarTransportFoam (T)

1. Solve Navier-Stokes' equation of incompressible flow for $\boldsymbol{V}(\boldsymbol{r}, t)$:

$$\rho\left(\frac{\partial \boldsymbol{V}}{\partial t} + \boldsymbol{V}\cdot\nabla\boldsymbol{V}\right) = -\nabla p + \mu\nabla^2\boldsymbol{V}$$

2. Solve heat equation for T using steady-state $\boldsymbol{U} = \boldsymbol{V}(\boldsymbol{r}, t\rightarrow\infty)$:

$$\frac{\partial T}{\partial t} + \nabla\cdot(\boldsymbol{U}T) - \nabla^2\left(D_T T\right) = 0$$



1. Case = cavity, icoFoam
2. Case = pitzDaily, scalarTransportFoam
3. Case = cavity-heat (new), scalarTransportFoam using U from icoFoam

Parallel OpenFOAM revisited

- Results
  1. serial run (81.fractal) took 71 seconds.
     speed up = 71/71 = 1.00
  2. parallel (np=4) run (82.fractal) took 84/4 = 21 seconds.
     speed up = 71/21 = 3.38
  3. parallel (np=8) run (85.fractal) took 129/8 = 16.125 seconds.
     speed up = 71/16.125 = 4.40
- Comments
  1. The low speed up with large number of processors is due to the small system size with the simple geometry.
  2. MPI calls within cores of the same node is faster than inter-node communication.
  3. p, U, and gmesh files are located for your test in /opt/cee619s13/class14/
  4. For parallel runs, decomposePar and reconstructPar should be used before and after icoFoam in parallel mode, respectively.

Dependent qsub

```
[mpiuser@fractal qsub-dependent]$ qsub first.pbs
91.fractal
[mpiuser@fractal qsub-dependent]$ qsub -W depend=afterok:91.fractal second.pbs
92.fractal
[mpiuser@fractal qsub-dependent]$ qstat
Job id                    Name             User            Time Use S Queue
------------------------- ---------------- --------------- -------- - -----
91.fractal                 PBS-firstJob     mpiuser          00:00:00 R batch
92.fractal                 PBS-secondJob    mpiuser                 0 H batch
[mpiuser@fractal qsub-dependent]$ qstat
Job id                    Name             User            Time Use S Queue
------------------------- ---------------- --------------- -------- - -----
91.fractal                 PBS-firstJob     mpiuser          00:00:00 C batch
92.fractal                 PBS-secondJob    mpiuser          00:00:00 C batch
```

- “91.fractal” is the job number of the first job.
- See files: first.pbs, second.pbs, and depJobSub.sh.