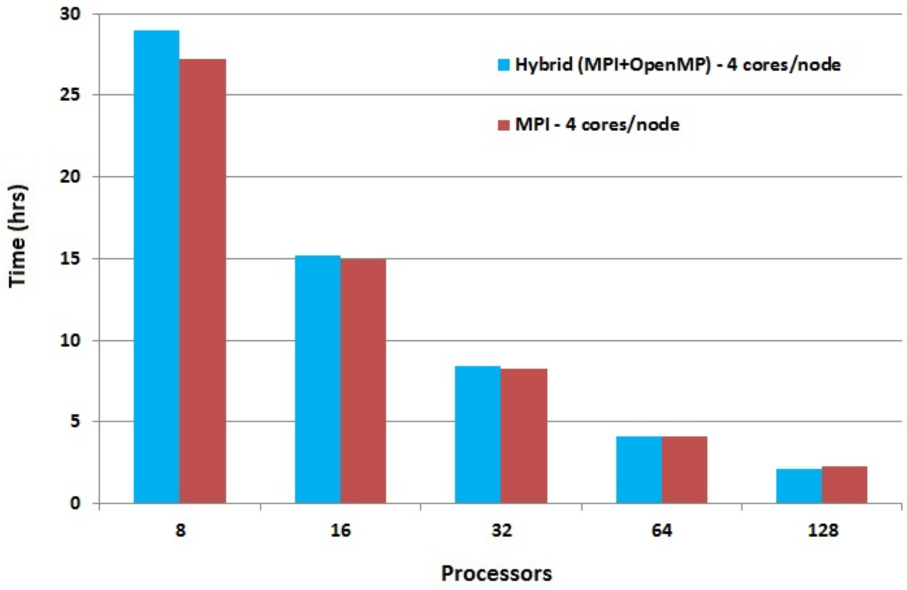

Development of OpenMP Parallelization for MFIX-DEM

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Motivation / Objectives

- **Motivation**
  - Different parallelization strategies are being considered on modern computer architectures that can lead to large performance gains of MFIX to allow calculations on more physically realistic systems.

- **Objectives**

  MPI parallelization for MFIX-DEM has been completed in the previous work at Virginia Tech group.

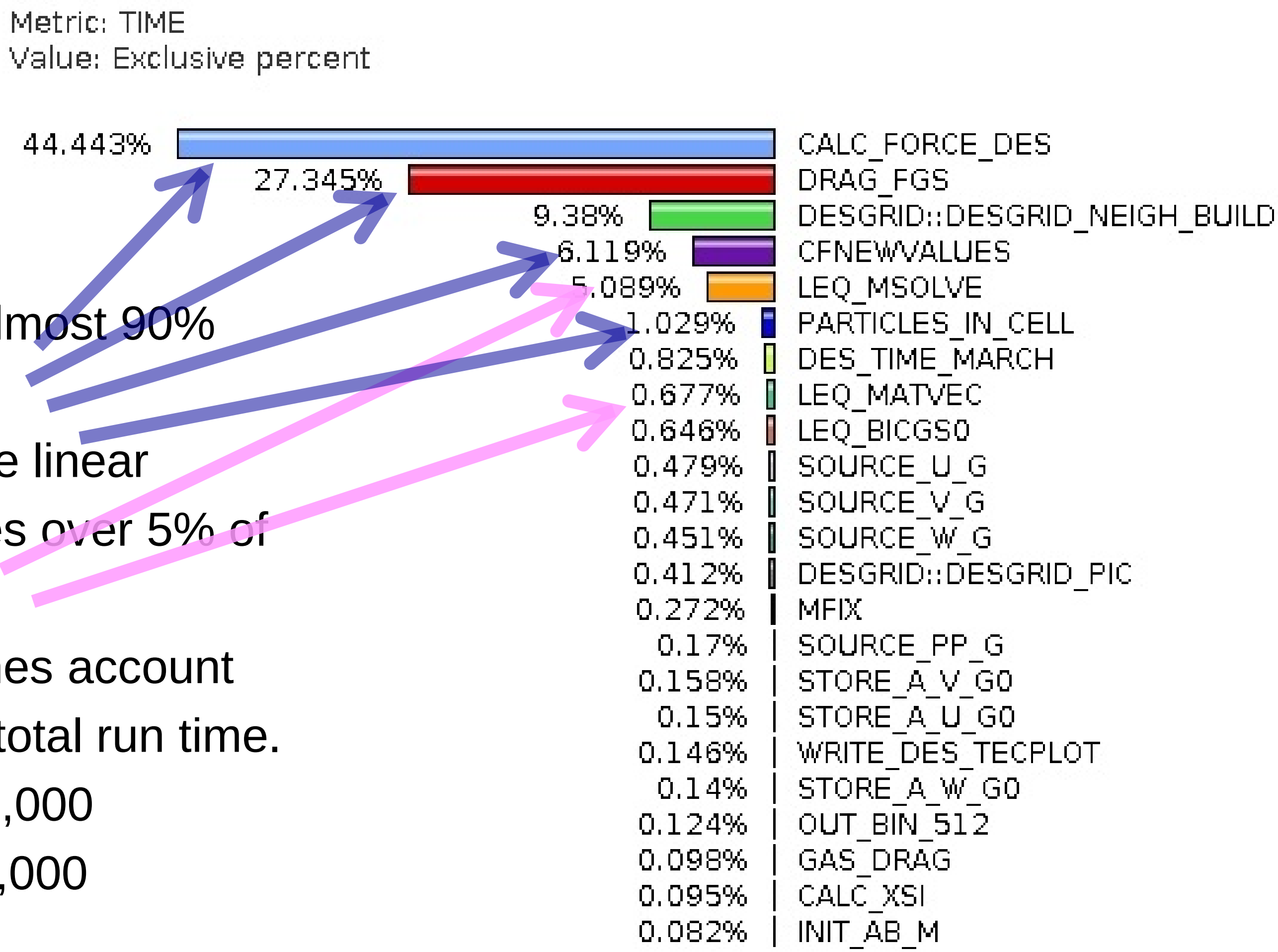
  - Enhance parallelization flexibility on multicore systems by OpenMP;
  - Improve scalability on multicore SMP cluster systems by Hybrid implementation of MPI+OpenMP;
  - Extend OpenMP instrumentation to co-processing (GPUs; Intel-MIC).

Method

- Evaluate Initial OpenMP Performance
  - TAU (Tuning and Analysis Utilities) profiling along with PDT (Program Database Toolkit)
- Identify the major (time-consuming) routines
- Analyze the data structures on loop level in these routines
- Assign variables with different attributes, e.g. private or shared, for OpenMP implementation
- Set the intermediate variables as private to replace global variables to realize OpenMP parallelization if necessary.
- Modification Principle:
  - In compliance with the existing framework of MFIX

MFIX-DEM

Initial Performance Evaluation – Exclusive Time



☞ DEM solver takes almost 90% of the total time.

☞ Preconditioner of the linear equation solver takes over 5% of the total time

☞ The major subroutines account for over 95% of the total run time.

☞ Total Particles – 80,000
Total Cells – 18,000

Major Routines for OpenMP Parallelization

- Parallelize these major routines for OpenMP implementation
  - **In DEM solver**
    - Contact force computation
      - *calc_force_des.f*
    - Drag force computation
      - *drag_fgs.f*, including *calc_des_drag_gs* and *des_drag_gs*
    - Locating the particle in fluid cell (particles in cell)
      - *particles_in_cell and comp_mean_fields_interp*
  - **In Fluid solver**
    - Linear equation solver of Bi-Conjugate Gradients Stabilized method (BiCGSTAB)
      - *leq_msolve (line iterative preconditioners)*

Typical Problems for OpenMP Parallelization in MFIX-DEM

- In MFIX-DEM, there are two main kinds of do-loops, in which care needs to be taken with OpenMP parallelization
  - One kind of do-loops is over all fluid cells; the inner do-loop is over the particles in the corresponding cell and often using the neighbor cells quantities.
    - Note: the neighbor cells maybe spread across threads for OpenMP implementation
  - Another kind of do-loops is over all particles, in which fluid cell indices are used.
    - Note: the total number of particles is spread over threads and the particles locating to a fluid cell maybe spread across threads.

Data-Sharing Attributes in OpenMP Program

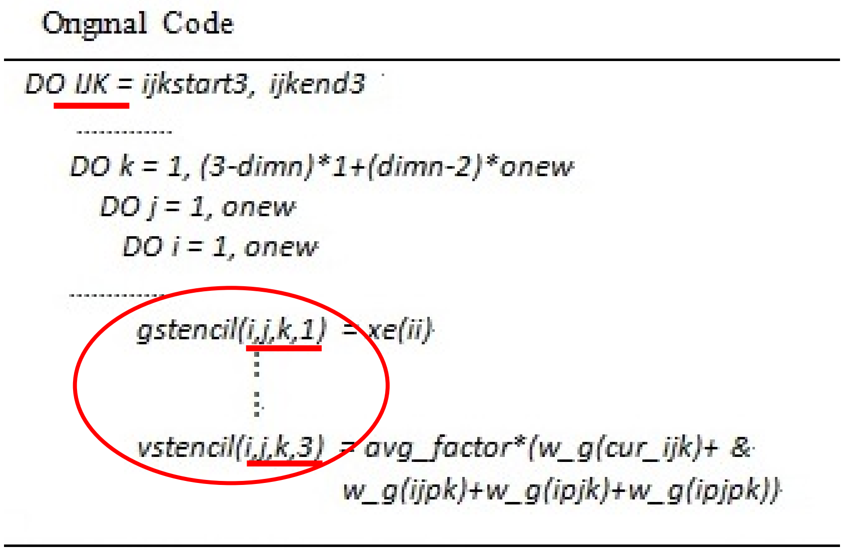
❑ *In an OpenMP program, there are two basic types*:

- SHARED
  - ✔ All threads can read and write the data simultaneously, unless protected through a specific OpenMP construct
  - ✔ All changes made are visible to all threads

- PRIVATE
  - ✔ Each thread has a copy of the data
  - ✔ No other thread can access this data
  - ✔ Changes only visible to the thread owning the data

A Typical OpenMP Example in MFIX-DEM

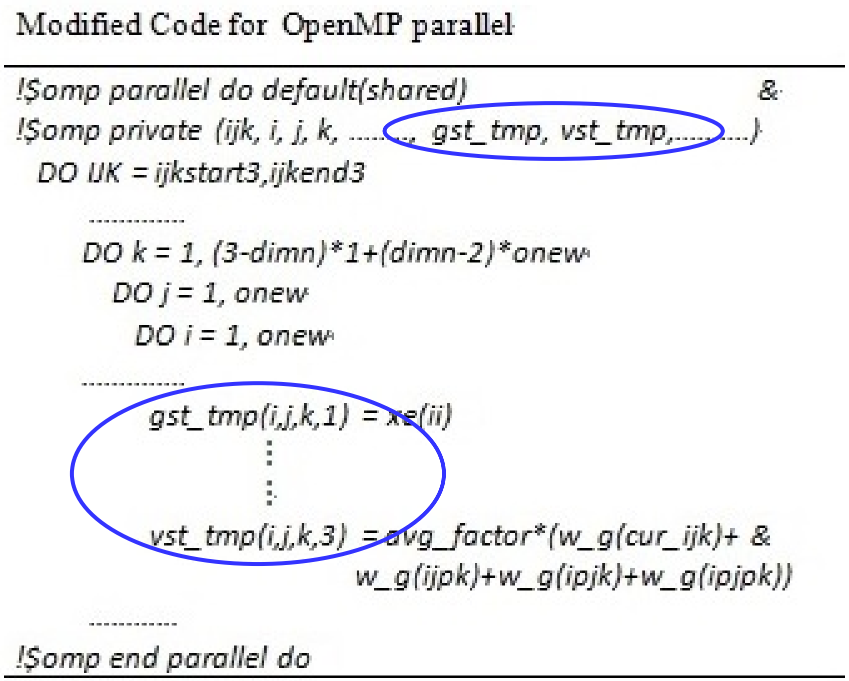
The following code fragments exist in every interpolating calculation in MFIX-DEM model



Ongnal Code

```
DO IJK = ijkstart3, ijkend3
  ...............
  DO k = 1, (3-dimn)*1+(dimn-2)*onew
    DO j = 1, onew
      DO i = 1, onew
  ...............
        gstencil(i,j,k,1)  = xe(ii)
                  :
                  :
        vstencil(i,j,k,3)  = avg_factor*(w_g(cur_ijk)+ &
                              w_g(ijpk)+w_g(ipjk)+w_g(ipjpk))
```

- The code index *IJK* loops over all fluid cells to calculate the fluid velocity interpolating at the particle location.
- For each fluid cell, the global variables *gstencil* and *vstencil* calculate the geometry and the velocity factors for interpolation.
- In the original code, because each fluid cell is visited sequentially, *gstencil* and *vstencil* will have unique values corresponding to that fluid cell before it goes to the next fluid cell.



Modified Code for OpenMP parallel

```
!$omp parallel do default(shared)                                  &
!$omp private (ijk, i, j, k, ......., gst_tmp, vst_tmp,............)
  DO IJK = ijkstart3,ijkend3
    ...............
    DO k = 1, (3-dimn)*1+(dimn-2)*onew
      DO j = 1, onew
        DO i = 1, onew
    ...............
          gst_tmp(i,j,k,1)  = xe(ii)
                    :
                    :
          vst_tmp(i,j,k,3)  = avg_factor*(w_g(cur_ijk)+ &
                               w_g(ijpk)+w_g(ipjk)+w_g(ipjpk))
    ..............
!$omp end parallel do
```

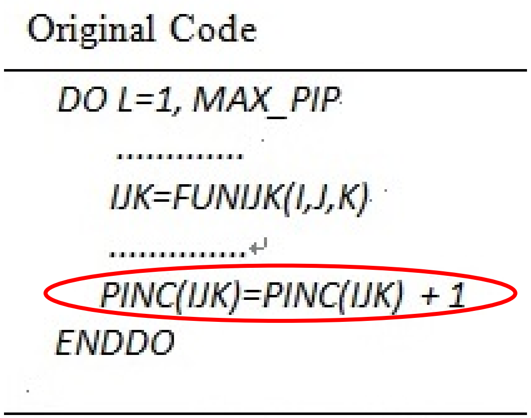
- In an OpenMP parallel do loop, *gstencil* and *vstencil* are global and shared between threads, and do not have an *IJK* dimension.
- The arrays *gstencil* and *vstencil* should be set as private to avoid a race condition by defining private arrays *gst_tmp* and *vst_tmp* for OpenMP parallel.

Another Typical Problem with OpenMP in MFIX-DEM

- Reduction Operations
  - When a variable has been declared as SHARED because all threads need to modify its value, it is necessary to ensure that only one thread at a time is writing/updating the memory location of the considered variable, otherwise unpredictable results will occur.
  - By using the clause REDUCTION it is possible to solve this problem, since only one thread at a time is allowed to update the value, ensuring that the final result will be the correct one.

Another Typical OpenMP Example in MFIX-DEM

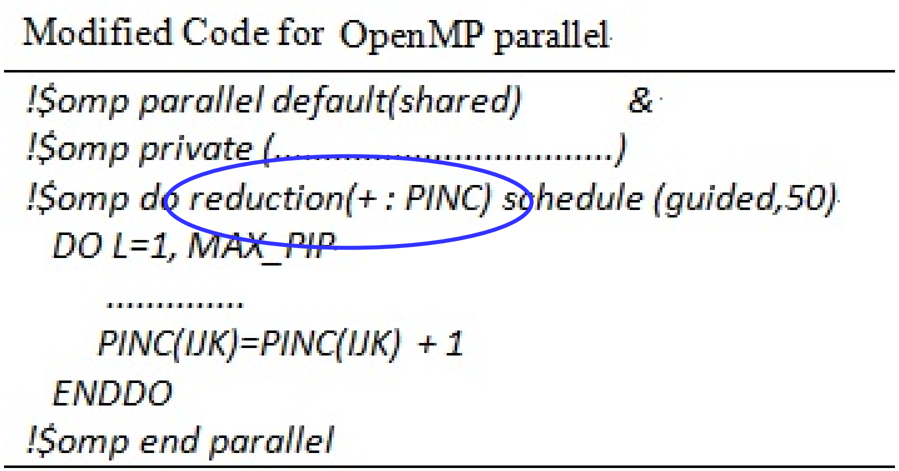
The following code fragments from the subroutine *particles_in_cell* to bin particles in fluid cells.



Original Code

```
DO L=1, MAX_PIP
     .............
     IJK=FUNIJK(I,J,K)
     ..............
    PINC(IJK)=PINC(IJK) + 1
ENDDO
```

- The code loops over all particles and bins particles in fluid cells based on particles(i, j, k) indices.
- *PINC(IJK)* is a global array to store the number of particles in a fluid cell.
- In the sequential code, each particle is visited sequentially and binned in the corresponding fluid cell to increment the value of *PINC(IJK)*.



Modified Code for OpenMP parallel

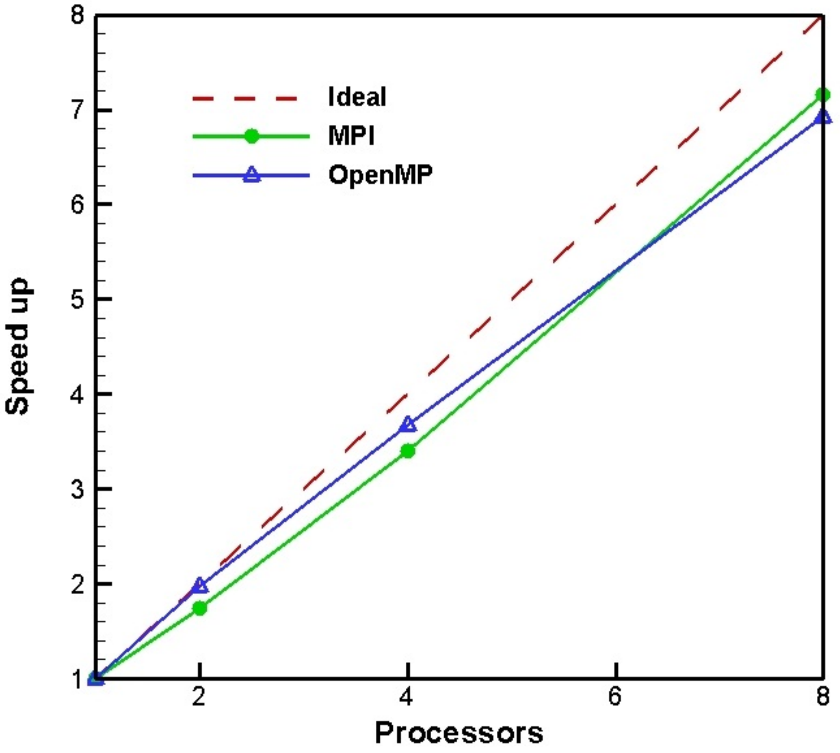
```
!$omp parallel default(shared)         &
!$omp private (................................)
!$omp do reduction(+ : PINC) schedule (guided,50)
  DO L=1, MAX_PIP

       .............
      PINC(IJK)=PINC(IJK) + 1
  ENDDO
!$omp end parallel
```

- In OpenMP implementation, the total number of particles is distributed over threads and particles belonging to a fluid cell maybe spread across threads.
- Care needs to be taken when updating shared variable *PINC*.
- With the REDUCTION clause, the OpenMP compiler generates code such that a race condition is avoided.

Scaling Analysis of OpenMP for MFIX-DEM After modifying major routines

- The 3D fluidized bed with 80,000 particles and 18,000 cells was simulated.
- A workstation:
  - ✓ Running Red Hat Enterprise Linux release 5.3
  - ✓ One node with two Intel Xeon 2.27GHz quad-core processors with a total memory of 24GB.
- Intel Compiler 13.1.
- OpenMP implementing on 2, 4 and 8 threads.

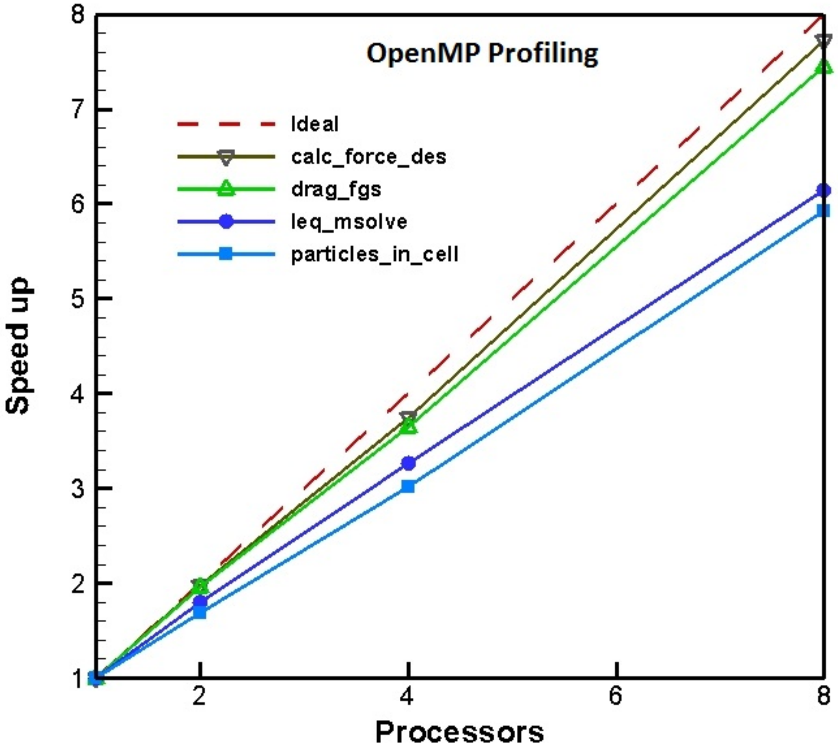


- Performance evaluation for full simulation with a speed up of 7x on 8 threads and an efficiency of 87% after modified for OpenMP parallel.

Scaling Analysis of OpenMP

– Major Routines

- Performance evaluation for major routines after modification with OpenMP directives. The speed up is as below:
  - calc_force_des.f:
    - 7.7x on 8 threads
  - drag_fgs.f
    - 7.4x on 8 threads
  - leq_msolve
    - 6.2x on 8 threads
  - particles_in_cell.f
    - 5.9x on 8 threads



☞ The 3D bubbling fluidized bed case with 80,000 particles was simulated.

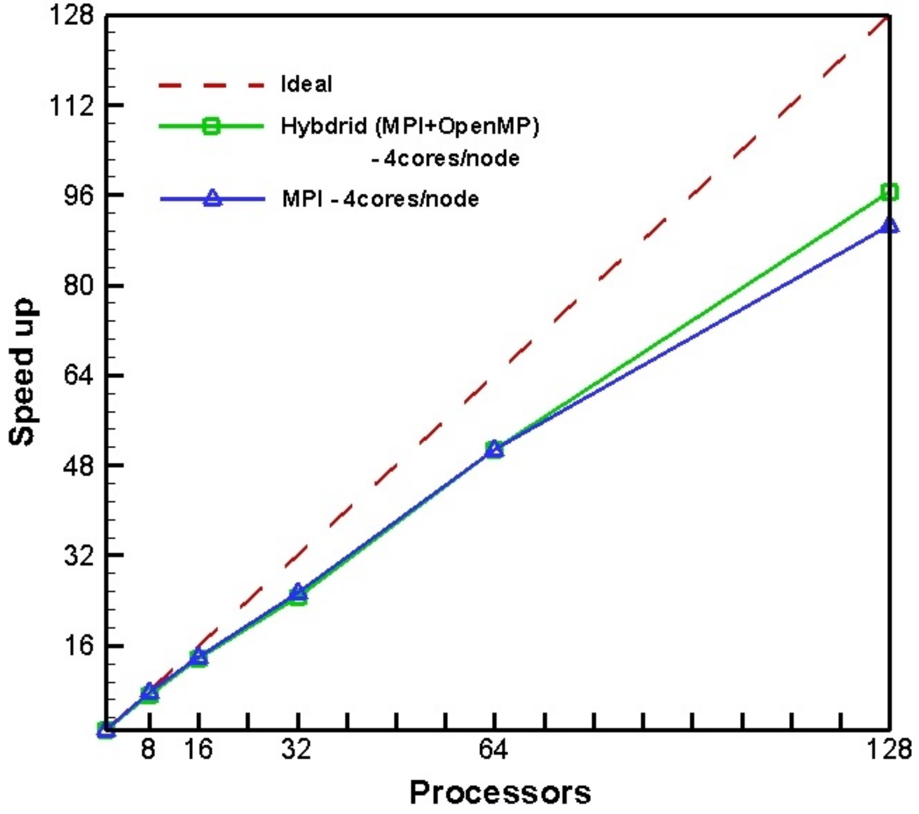
Large System – Hybrid MPI+OpenMP

- Total Particles – 1.28 million; Total cells – 409,600
- Hybrid parallelism of MPI+OpenMP implementation up to 128 processors
- SMP cluster:
  - 204 nodes Total
  - 2x Intel Xeon E5645 2.4GHz
  - 12 Cores per node
  - 24 GB Shared Memory per node
  - QDR Infiniband interconnect
- Intel Compiler 13.1
- Domain decomposition only in x and z directions for MPI
- Total physical simulation time is 0.5 seconds

Parameter	Value
Total Particles	1.28 million
Diameter	4 mm
Density	2700 kg/m^3
Coef. of restitution Particle, Wall	0.95, 0.95
Friction coefficient Particle, Wall	0.3, .03
Spring constant Particle, Wall	2400, 2400 N/m
Dimension Grid size	64×100×64 cm 64×100×64
Superficial Velocity	2.0 m/s
Time Step (Fluid, Solid)	5.0e^{-5} s, 8.6e^{-6} s
Number of processors	8,16,32,64,128

Scaling Analysis of hybrid MPI+OpenMP for large DEM system

- The hybrid calculation gives a speedup of 96x versus 89x for standalone MPI on 128 cores.
- As the number of MPI processes increases, the overhead of communicating ghost particles between MPI processes also increases.



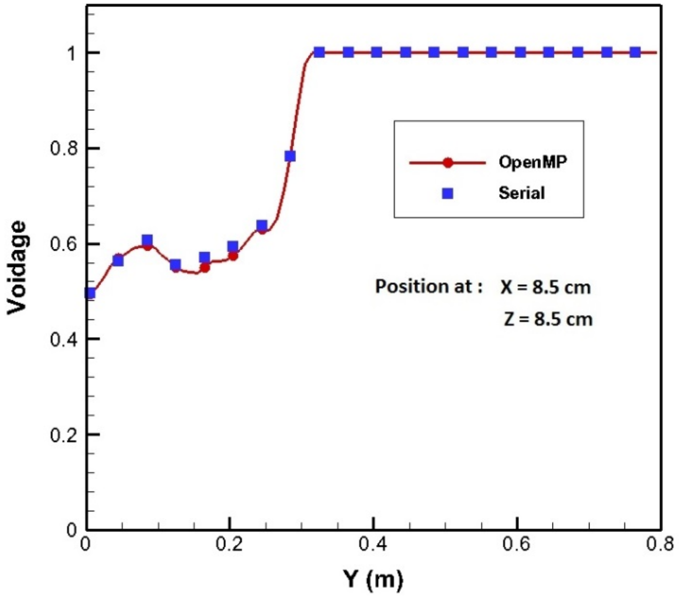
Total Particles – 1.28 million;
Total cells – 409,600

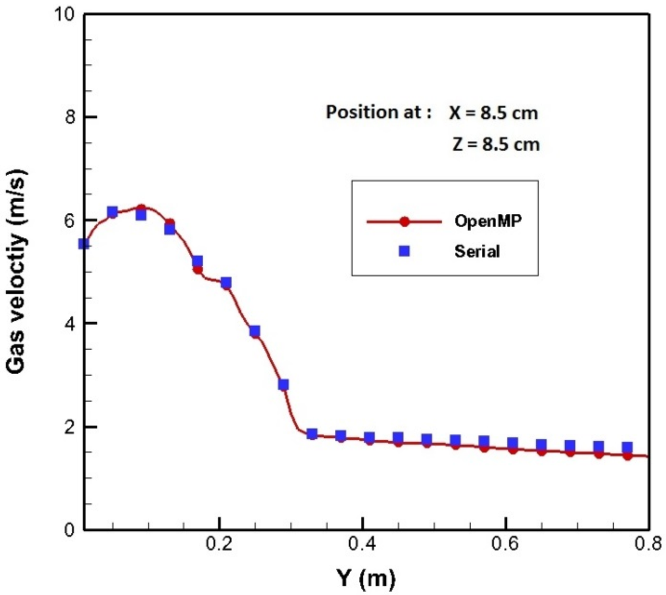
Validation

Ascertain the parallelization does not change in the physics.

- The 3D fluidized bed with 80,000 particles of 4mm diameter was simulated for this validation.
- The simulation was carried out for a total of 5 seconds.
- The time averaged profiles were obtained from 2.0-5.0 seconds.
- Results of time-averaged void fractions and gas velocity (V_g) were compared at the location x=8.5cm and z=8.5cm for serial and OpenMP (4 threads) implementation.

- *The validation shows that the parallel simulation does not alter the accuracy of the solution.*





Summary

- The parallel DEM solver for OpenMP implementation were developed for MFIX. Performance analysis was carried out to identify the time-consuming routines.
- After instrumentation with OpenMP directives, performance analysis shows an efficiency of 87% on 8 threads for a 3D MFIX-DEM bubbling fluidized bed with 80,000 particles.
- Hybrid parallelism (MPI + OpenMP) performance was evaluated for a large scale system of 1.28 million particles in a 3D bubbling fluidized bed on a large SMP cluster. The scaling analysis shows good scalability for MFIX-DEM up to 128 processors (10,000 particles/processors) with an efficiency of 75%.
- The validation of MFIX-DEM shows that the parallel simulation does not alter the accuracy of the solution.

Future Work

- **FY13 –**
  - Further scaling analysis for large scale DEM system by hybrid (MPI+OpenMP) parallel programming on large processor counts
  - Investigate MPPIC model with OpenMP directives
- **FW – Extend to co-processing architectures (GPUs, Intel-MIC)**

Publications

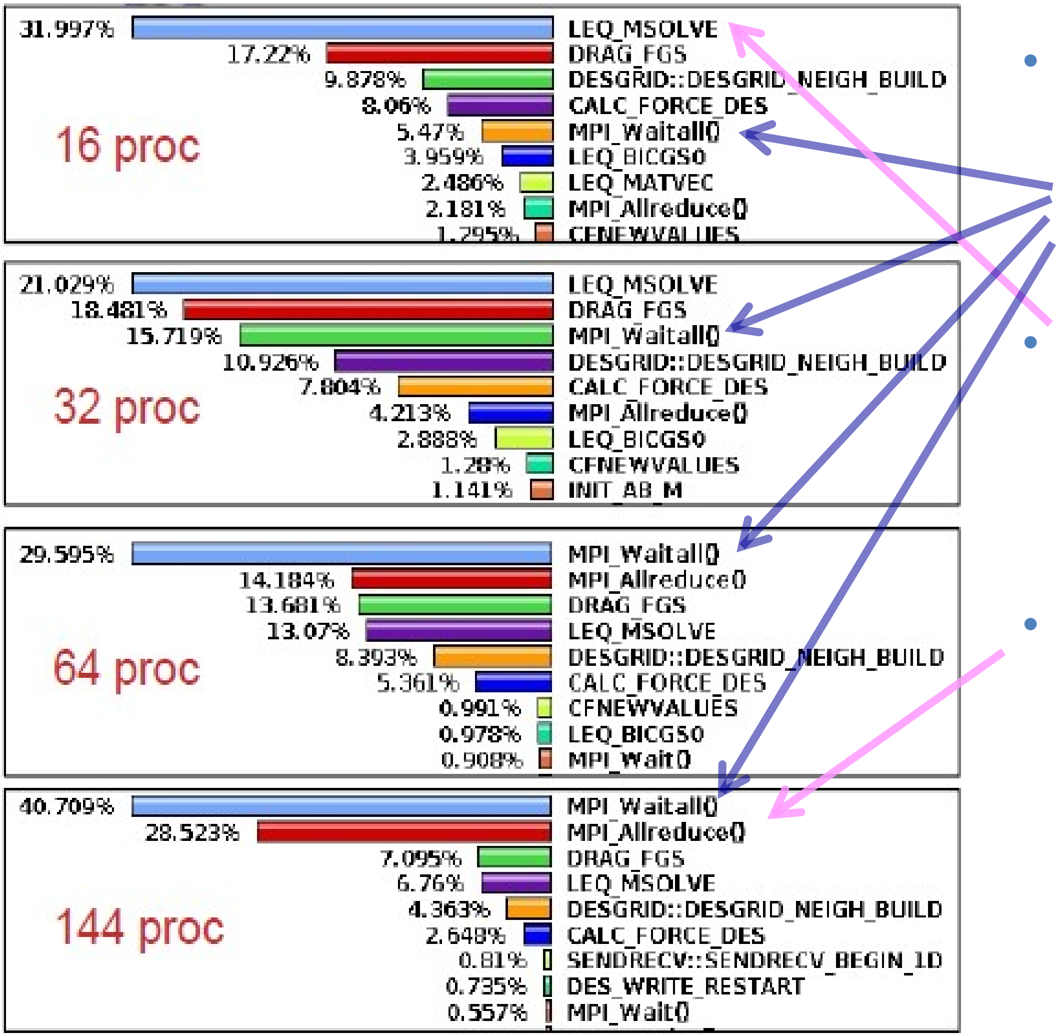
- [1] Handan Liu, Danesh Tafti and Tingwen Li. Hybrid Parallelism in MFIX CFD-DEM using OpenMP. Powder Technology. Under review.
- [2] Handan Liu, Danesh Tafti. Summary Report for MFIX Acceleration. Dec. 2012. Project Title: MFIX acceleration (number: 683.232.001).
- [3] Handan Liu, Danesh Tafti. Summary Report for MFIX Acceleration on New Code. March 2013. Project Title: MFIX acceleration (number: 683.232.001).
- [4] Handan Liu, Danesh Tafti. Summary Report for MFIX Acceleration on MPPIC. August 2013. Project Title: MFIX acceleration (number: 683.232.001).
- [5] Pradeep G., Danesh Tafti. Development of parallel DEM for the open source code MFIX. Powder Technology, 235 (2013) 33-41.
- [6] Amit Amritkar, Danesh Tafti, Rui Liu, Rick Kufrin, Barbara Chapman. OpenMP parallelism for fluid and fluid-particulate systems. Parallel Computing, 38 (2012) 501-517.

Thank You !

Questions?

Supplement

Scaling Analysis – Exclusive Time



- As number of processors increases time required for MPI communication increases
- For 16 processors hydrodynamic solver takes most of the time
- For 144 processors interface exchange takes 40% and MPI collective communication takes 28% of total time

Pradeep Gopalakrishnan, Danesh Tafti, Parallelization of Discrete Element Method, ORD 2.672.232.001.000 Merit Review, April 26, 2011