Fluent on HPC Systems

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Key Words

- Fluent
- HPC Systems

Presentation Components

- Fluent Simulation Case study,
- Parallel Computing-101,
- Code Scaling & Speedup
- Fluent Extreme Scaling on NCSA “mega” HPC system
- Runnig Fluent Remotely on the Cluster

Parametric Study of Effect of Geometirc Configuration of Microjets in an Axisymmetric Dump Combustor Flow

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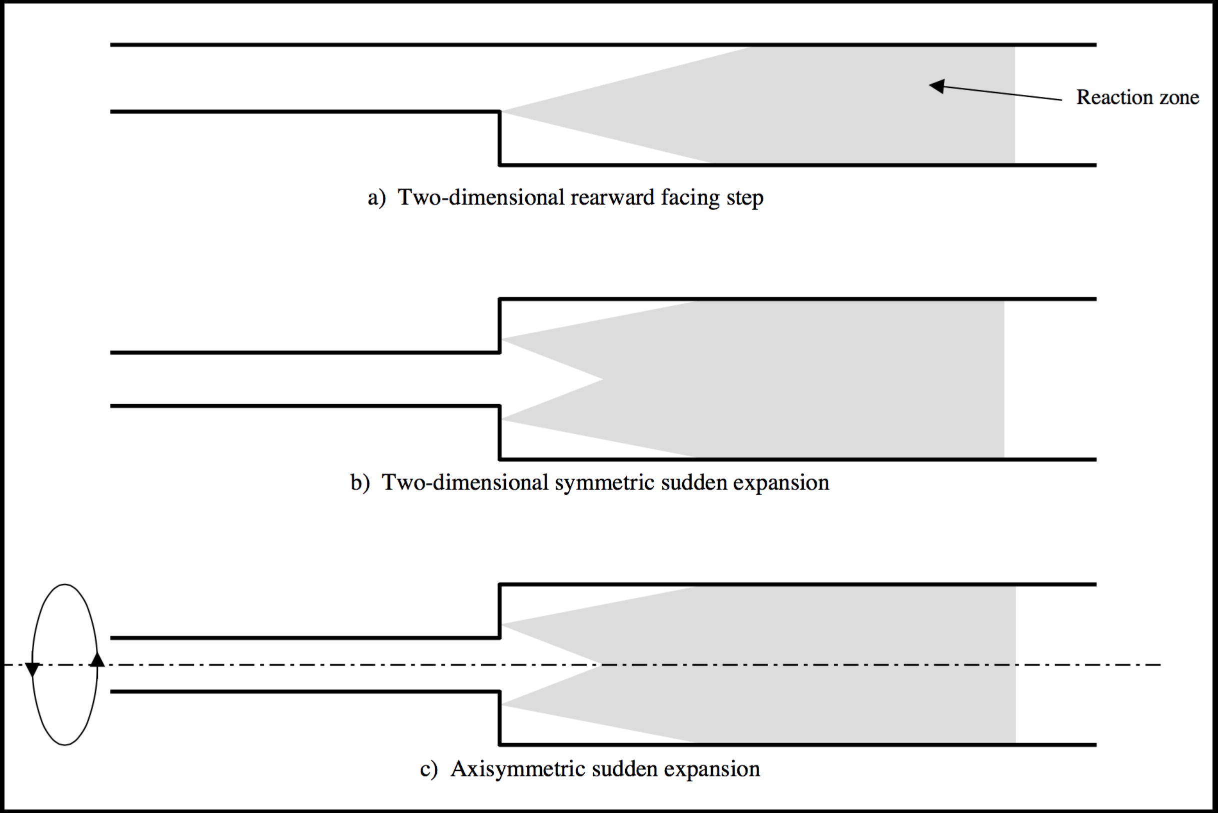
Agenda

- Introduction
- Objectives
- Configuration & Boundary Conditions
- Simulation Tools & Models
- Results
- Conclusions
- Questions

Introduction

- Main types of Dump Combustors:
  - Planar
  - Axi-Symmetric
- Applications of Microjets in Dump Combustors:
  - *Flameholdes in Ramjet Engines (better mixing and burning),*
  - *Reducing noise generated from high-speed jets including shock noise,*

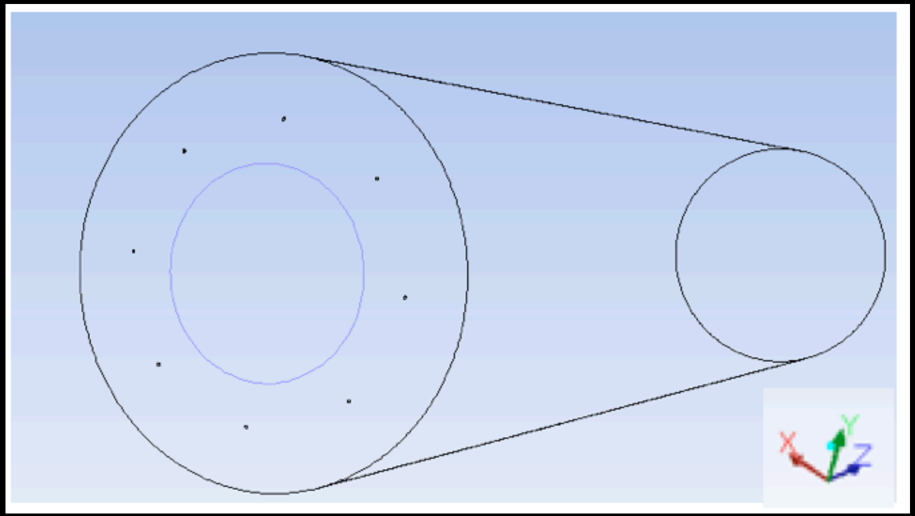


Objectives

- Part of an extensive numerical study on the effect of using microjets on the flow and energy fields in Dump Combustors:
    - Microjet Configuration:
        - ✓ Number of Microjets (None, 2, 4 & 8),
        - ✓ Microjets Diameter (dj),
        - ✓ Microjet Ring Arrangement (1 & 2),
    - Microjet Inlet Flow Parameters:
        - ✓ Injection Angle,
        - ✓ Injection Swirl Factor,
    - Turbulence Modeling:
        - ✓ RANS (modeling both large and small scale flow physics)
        - ✓ LES (resolving the large scales and modeling the small scales)

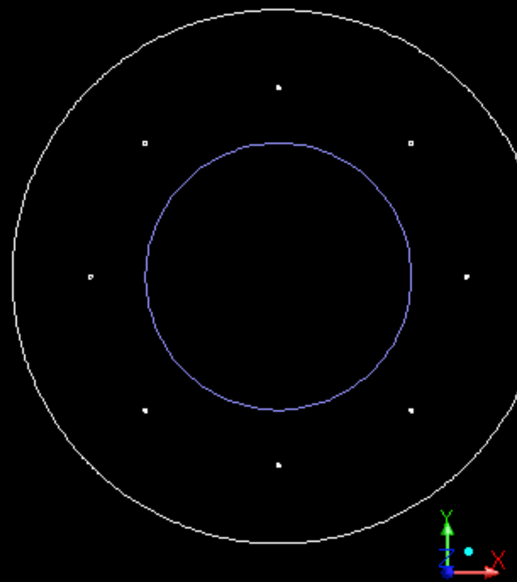
Configuration & Boundary Conditions

- ***<u>Axi-Symmetric Dump Combustor;</u>***
  - Radius (76mm, along x-y directions),
  - Length (762mm, along Z direction),
- ***<u>Main Inlet Flow;</u>***
  - Type: velocity Inlet,
  - Fluid: Premixed Propane "C_3H_8"-Air mixture, ER (0.65)
  - Velocity: Constant (22m/s),
  - Temp.: Constant (300K)
- ***<u>Walls:</u>*** Adiabatic
- ***<u>Outlet Type:</u>*** Pressure outlet



Configuration & Boundary Conditions

- ***<u>Microjets;</u>***
  - Diameter (dj=0.1mm),
  - Number (2, 4, & 8),
  - Rings:
    - ✓ One, midway along the step face, radius (rj=38mm),
    - ✓ Two, evenly allocated along the step face, radii (rj= 50.7mm & 63.3mm)
  - Inlet:
    - ✓ Type: Velocity inlet,
    - ✓ Fluid: Pure Air,
    - ✓ Velocity: Constant (91m/s),
    - ✓ Temp.: Constant (300K),
    - ✓ Jet MFR compared to MFR of Main Inlet: (0.13% for 2 jets)



Simulation Tools & Models

Tools:

- Mesher: Altair's Hypermesh
- Solver: Ansys-Fluent Commercial Code. V. 16.0

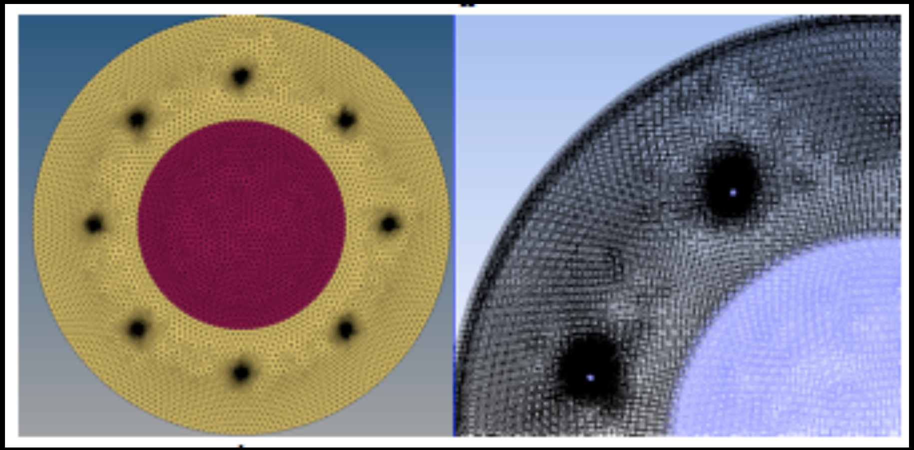
Models:

- Flow;
  - Incompressible,
  - Temperature-dependent density,
  - Mixing law for specific heat
- Turbulence;
  - Steady State RANS model,
  - Realizable (κ-ε),
  - Viscous heating, pressure gradient, and thermal effects enabled

Simulation Tools & Models

<u>Models (Cont.):</u>

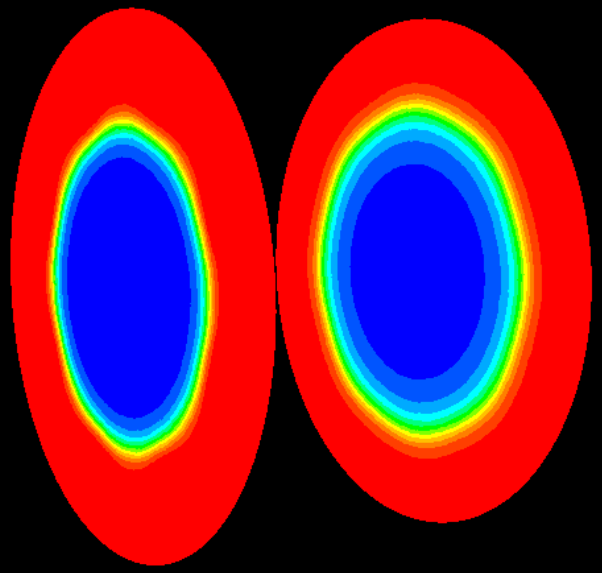
- Chemical Reaction;
  - 2-step “Propane-Air” reaction,
  - 6-volumetirc species,
  - Turbulence-chemistry interaction: Eddy dissipation model and inlet diffusion and diffusion energy source enabled
- Numerics:
  - Coupled solver,
  - Pressure-velocity formulation,
  - Second-order spatial discretization,
  - Pseudo-transient formulation for temporal discretization,
  - Mesh: Polyhedral unstructured elements.



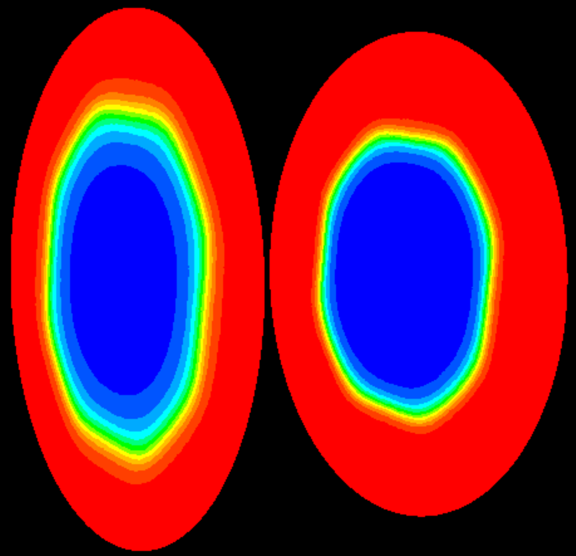
Results

Effect of Microjet:

- Microjets are adding a 3D effect to the flow for better mixing and burning.



One ring

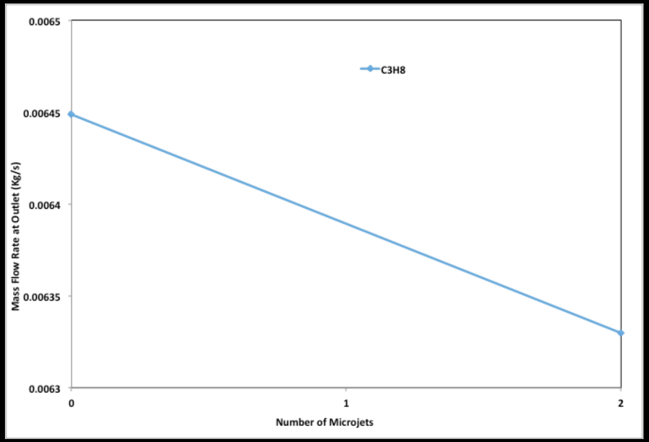


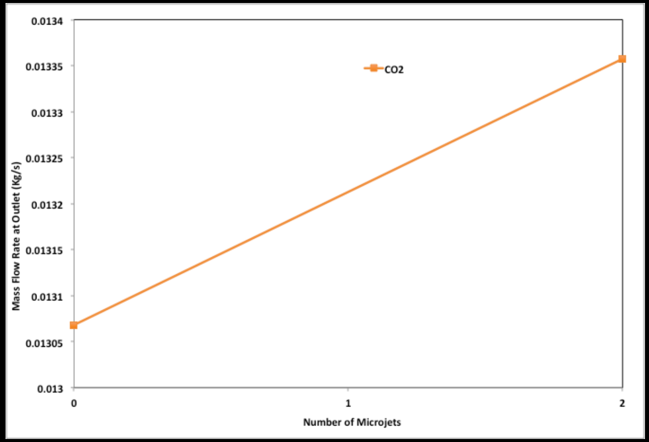
Two rings

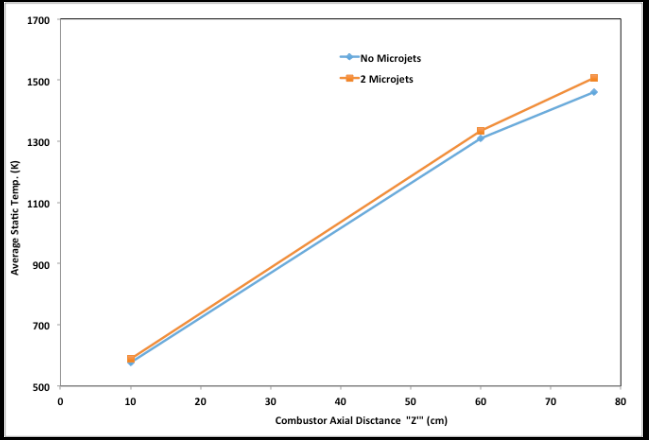
Results

Effect of Microjet:

- Microjets are promoting the combustion which is shown in:
  - Less urburnt fuel at combustor exit (1.8%),
  - Higher CO2 at combustor exit (2.2%),
  - Higher temperature throughout the length of the combustor (3.2%).



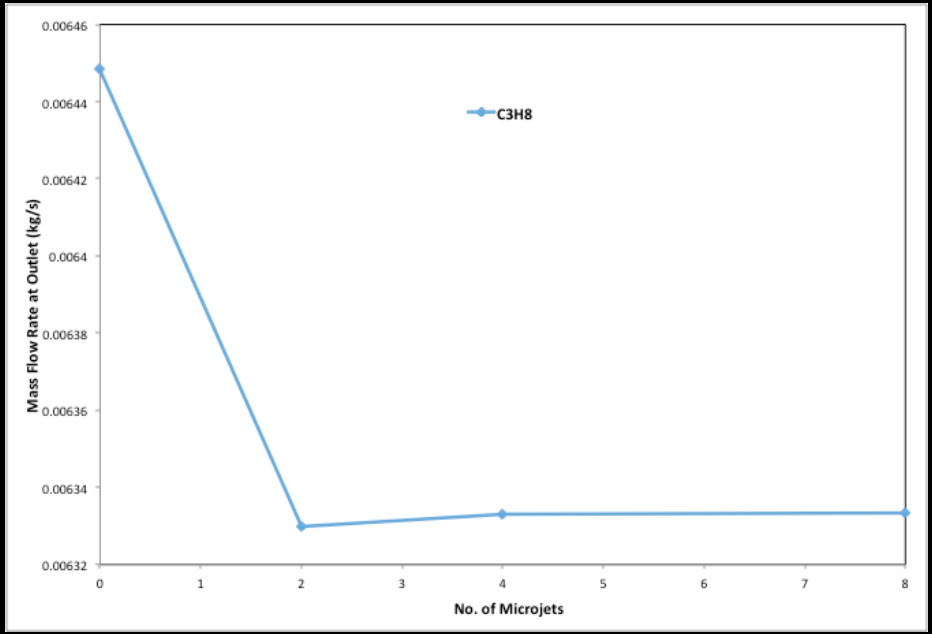




Results

Effect of number of Microjet:

- (Two) microjets showed lowest level of unburnt fuel leaving the combustor.

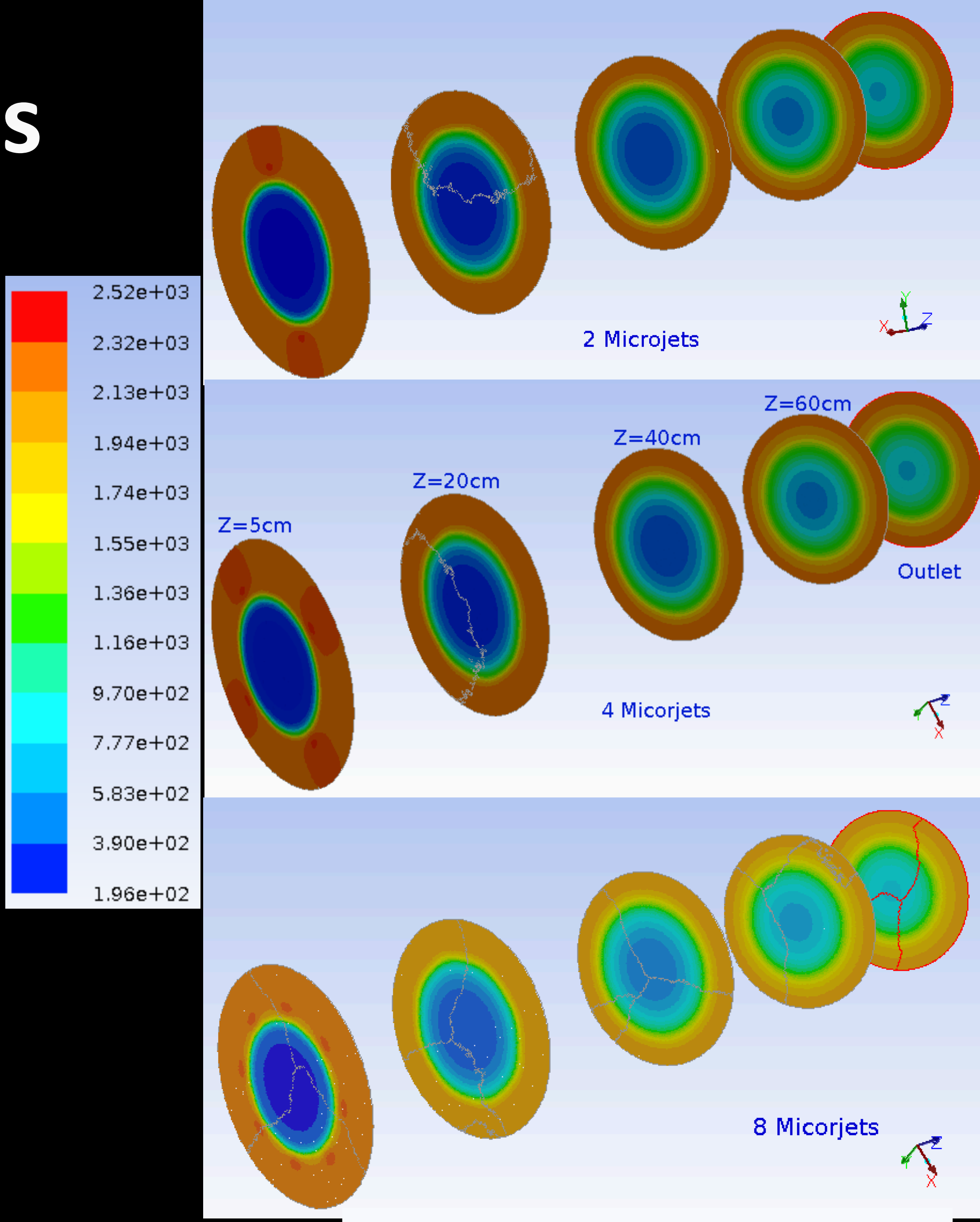


Results

Effect of Number of Microjet:

2, 4 & 8 Microjets

- Temperature Contours at different cross sections



Contours of Static Temperature (k)

Effect of Number of Rings:

One and two rings for 4 and 8 microjets

- Avg. Static Temp. (K) at different cross sections.

→ The (2) rings shows an increase in the avg. static temp downstream the combustor passing the mixing zone.

4 microjets	Z=10 cm	Z=40 cm	Z=60 cm	Outlet
One ring	596.8092	1030.8998	1328.49	1503.26
Two rings	594.19	1037.98	1335.26	1509.07

8 microjets	Z=10 cm	Z=40 cm	Z=60 cm	Outlet
One ring	607.5655	1025.9675	1321.9694	1496.5941
Two rings	583.47	1042.61	1337.21	1509.34

Effect of Number of Rings:

One and two rings for 4 and 8 microjets

- Mass fractions at outlets.

→ The (2) rings show better combustion as less unburnt fuel, more combustion product (CO2) and less oxygen at the combustor outlet.

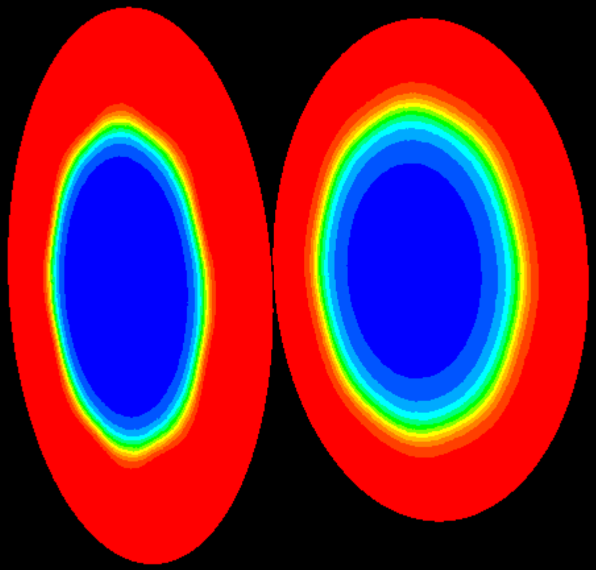
4 microjets	C_3H_8	O_2	CO_2
One ring	0.05671	0.05998	0.09628
Two rings	0.05653	0.05931	0.09683

8 microjets	C_3H_8	O_2	CO_2
One ring	0.05668	0.0609325	0.0955604
Two rings	0.05628	0.05945	0.0968

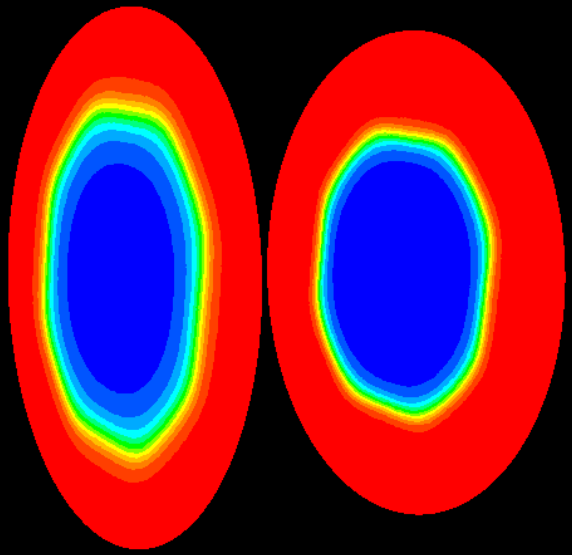
Effect of Number of Rings:

One and two rings for 4 and 8 microjets

- Contours of mass fraction of CO_2



One ring



Two rings

Conclusions

- Microjets are adding a 3D effect to the flow for better mixing and burning.
- Microjets are promoting the fuel burning which is shown in less urburnt fuel at combustor exit and higher temperature throughout the length of the combustor.
- Distributing the microjets over two rings enhanced the air-fuel mixing especially in the mixing zone downstream of the step base. It led to slight enhancement in Combustion presented in decrease in unburnt fuel, decrease in air and increase in combustion products at the combustor outlet.

Questions

Fluent Scaling

Scaling

- Code Architecture:
  - Serial “sequential” parts,
  - Parallelizable parts
- Code Scaling: running the same code on more cores and reducing the execution “wall-clock” time.
- Scaling Limitations:
  - The portion of the serial “sequential” part of the code,
  - Communication & I/O time,

Speedup

- Speed Up:

$$S = \frac{T_{old}}{T_{new}}$$

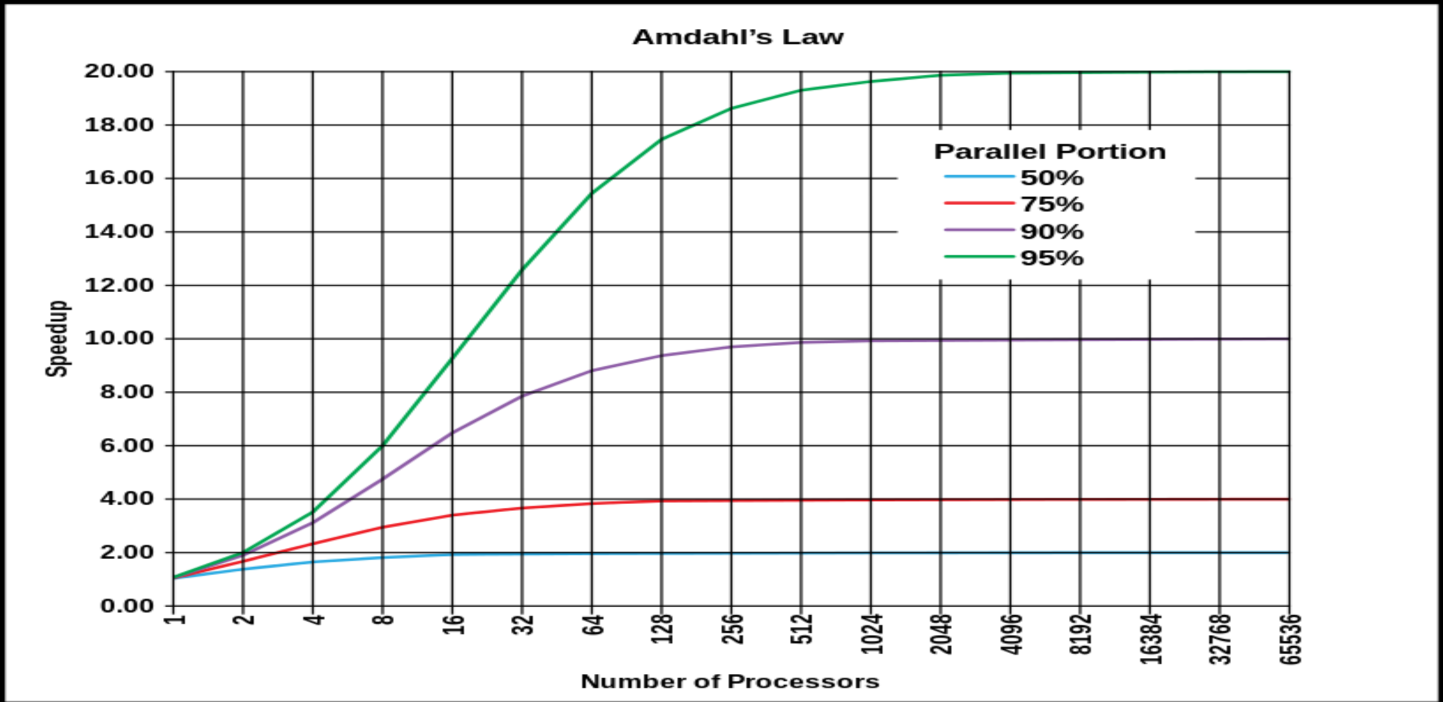
where:

- S is the resultant speedup.
- T_{old} is the old execution time, i.e., without the improvement.
- T_{new} is the new execution time, i.e., with the improvement.

- Amdahl's Law: Ex:
  - 5% serial
  - 95% Parallelizable

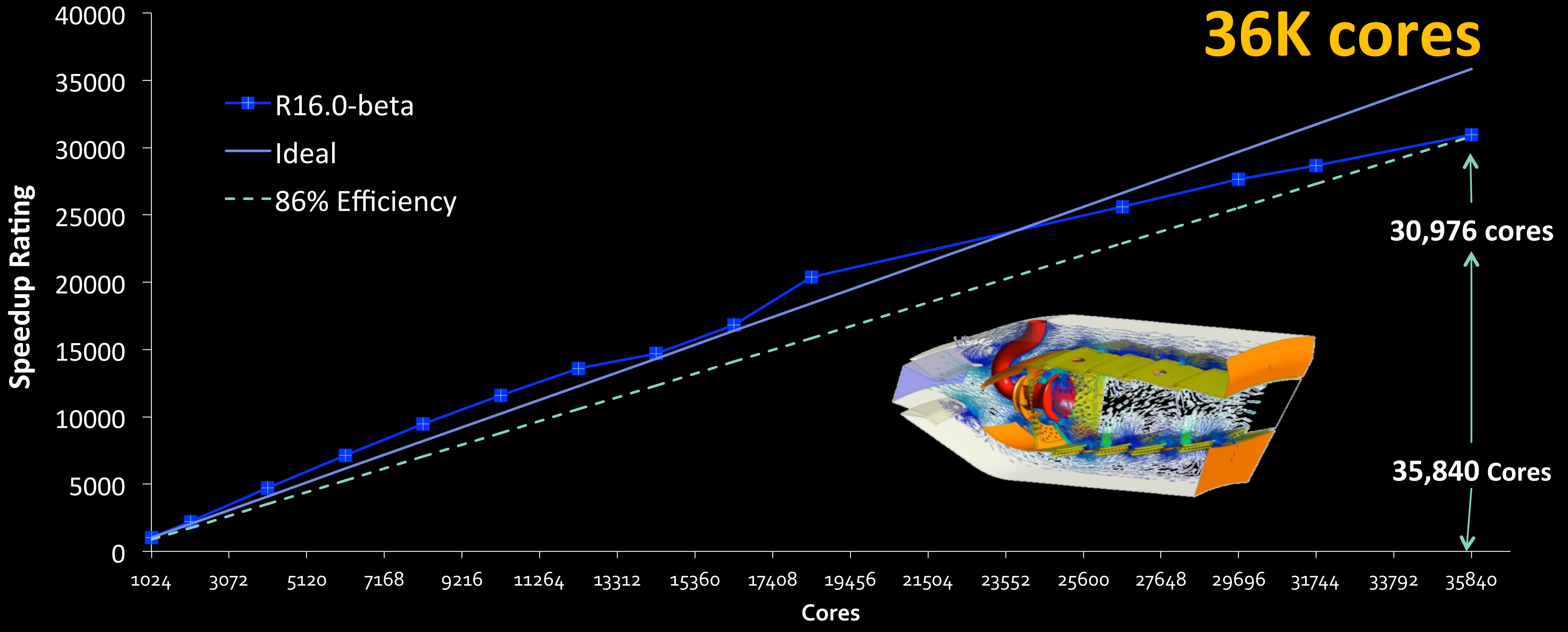
  →Min. Time=5/100

  →Max Speedup= 1/(5/100) = 20



Ansys-Fluent ver. 16.0 “beta”

Blue Waters *(Cray CLE6) “Ansys Gas Turbine Combustor, 830M Cells, Oct. 2014*



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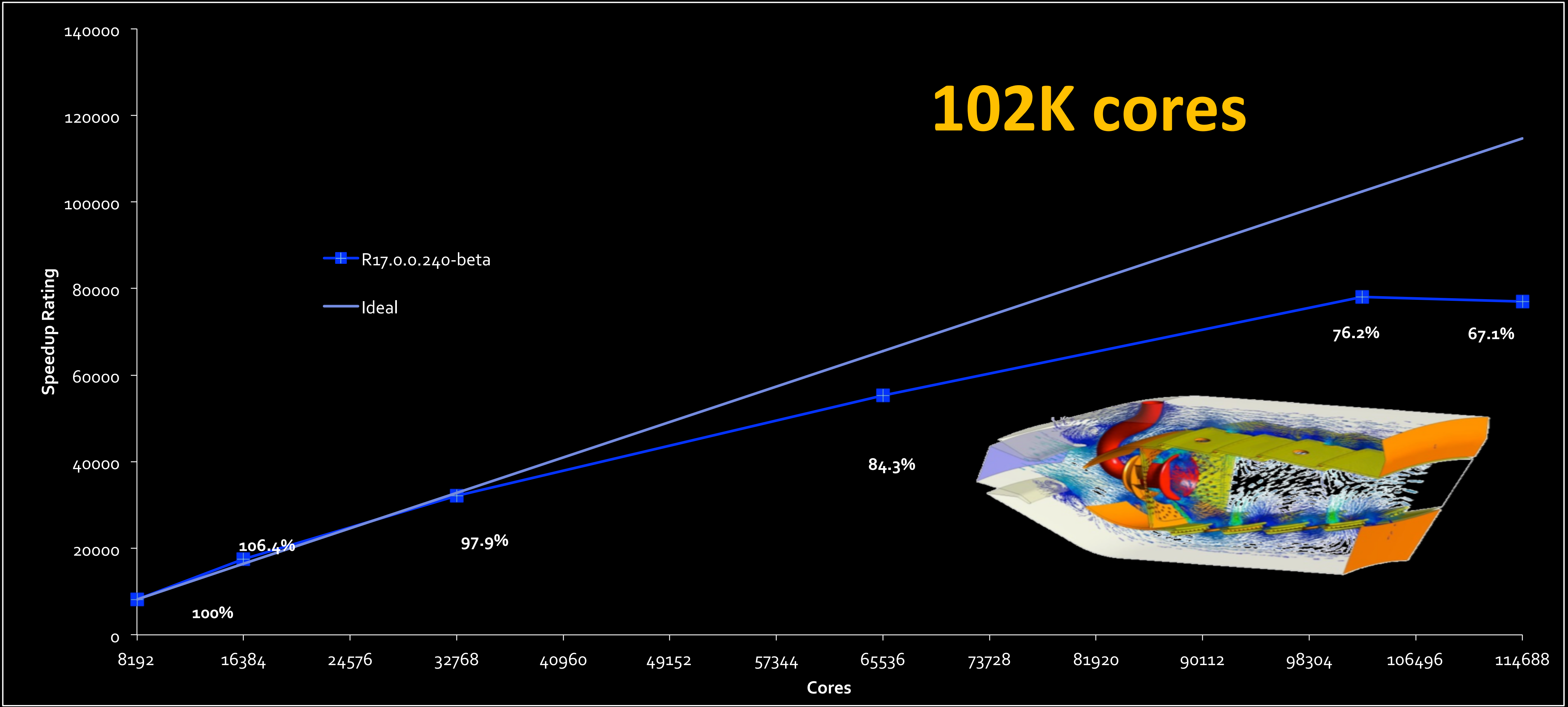
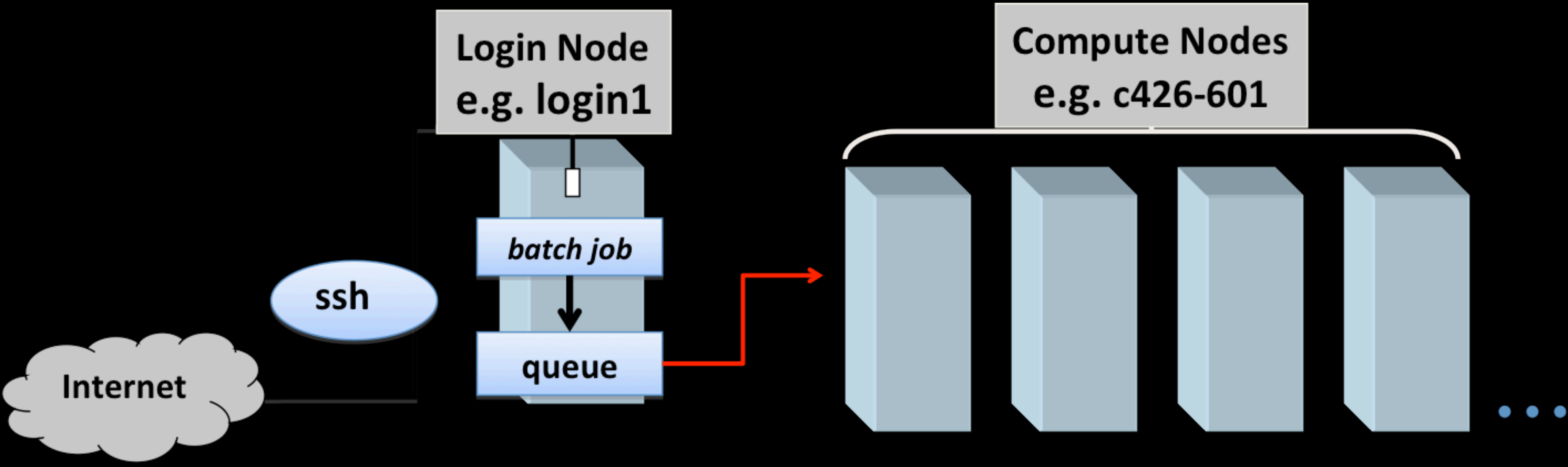


Running Fluent in Batch Job

Submitting the job remotely on the cluster



Submitting Jobs- “Interactive”

- Getting an access to the compute nodes, transferring the windows enrionments, launching the code through the Graphics Users Intergace “GUI”.
- Running in “interactive” mode is not recommended for production jobs (slower performance), but rather for debugging and visualization only.

Launching command: **qsub -I**

For windows display: **qsub -I -X**

e.g. requesting 2 nodes with 40 cores total for 30 minutes (“normal” queue) with all environment variables exported:

qsub -I -V -l walltime=00:30:00,nodes=2:ppn=20

e.g. requesting 2 nodes with 64 cores total (AMD nodes) for 60 minutes:

qsub -I -V -l walltime=00:60:00,nodes=2:ppn=32 -q amd

Submitting Jobs – "Script"

#PBS -l walltime=2:00:00	– sets maximum wall clock time (hh:mm:ss)
#PBS -l nodes=32:ppn=20	– sets number of core (CPU's) and nodes
#PBS -q normal	– sets queue priority
#PBS -N 3disc-comp-impli	– sets batch job name (default = name of script file)
#PBS -A hye	– specifying the project "psn" (aka: "project code")
#PBS -o 3disc-comp-impli.out	– sets output file
#PBS -e 3disc-comp-impli.err	– sets error file

Submitting Jobs - Script

module load cfd/Ansys-16.0

– load the ANSYS 16.0 module

cd /scratch/users/user_name/xxx/xxxxx/

– cd to the "Work Directory". *Make sure all needed files are in this directory including any UDF's, If any.*

rm -f pnodes
cat $PBS_NODEFILE | sort > pnodes
set ncpus=`cat pnodes | wc -l`

– *Creating a "pnodes" file which lists all processors available for.*

fluent 3d –t40 -g -pib -cnf=pnodes -ssh -i 3disc-comp-impli.in >& 3disc-comp-impli.output

– Launching (3d) version of Fluent. This job uses 40 cores, (-g) suppresses the GUI, (-pib) to use InfiniBand interconnect fabric, (-cnf=pnodes) to list all processors available for spawning, (-ssh) to use ssh protocol between nodes, (-i) to read an input file (XXX.in), (>&) to print out a copy of all the activities in (XXX.output) file.

Submitting Jobs – Journal file

```
rc fluent.cas.gz
rd fluent.dat.gz
solve
dti 20 30

/
parallel/timer/usage
/
/
/
exit
```

– read the case file
– read the data file
– solve
– specify the time step and iterations

– print time usage

Submitting Jobs - Script

- Command to submit your batch script use **qsub [script name]**
- To check the status of ALL your submitted jobs: **qstat -u [your login]**
- Use **cdjob [jobID number]** to check files on batch working dir (while job is still running)

Job Monitoring

Monitoring status of job submission:

```
[ataha@iforge Fine]$ qsub 3disc_trim_fine.script
This job will be charged to account: aed
1297691.ifsched
[ataha@iforge Fine]$ qstat 1297691
Job ID                    Name             User            Time Use S Queue
------------------------- ---------------- --------------- -------- - -----
1297691.ifsched            ...Bench2013-40P ataha                  0 Q normal
[ataha@iforge Fine]$ 
```

qstat [jobID] can be used to check the status of this specific job.

showq command can be used to check the status of all jobs submitted.

Monitoring results can be done by checking the **.output** file in the submission directory

After batch job is finished, copy the file back to your local machine using FTP or other tools and post process the results.

Questions