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Atelier "Codes de champs" – Computer laboratory class "Introduction to CFD-based fire models"

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Introduction

This document is provided in support of the computer laboratory class entitled "*Introduction to CFD-based fire models*" and taught as part of the CNRS School of Fire Science and Applications organized in Porticcio, Corsica (France) on May 30 – June 4, 2015.

Students in this class are invited to run simple test cases representative of the different topics found in fire modeling and using two leading fire modeling software: the Fire Dynamics Simulator (FDS) developed by the National Institute of Standards and Technology, USA, and FireFOAM developed by FM Global, USA. FDS and FireFOAM are both open-source software that can be downloaded from the following URLs:

- FDS: *https://code.google.com/p/fds-smv/*
- FireFOAM: *https://github.com/fireFoam-dev/fireFoam-2.2.x*

The FDS website contains detailed documentation and interested students are invited to consult these documents, starting with the FDS User Guide (McGrattan, K., McDermott, R., Weinschenk, C., Overholt, K., Hostikka, S., and Floyd, J., "*Fire Dynamics Simulator (Version 6) – User's Guide*," NIST Special Publication 1019, Sixth Ed., National Institute of Standards and Technology, Gaithersburg, MD, USA, 2014). Also, some of the test cases below are directly taken or inspired from the suite of FDS examples provided with the FDS release. These cases are described in the FDS Verification Guide (McGrattan, K., Hostikka, S., McDermott, R., Floyd, J., Weinschenk, C., and Overholt, K., "*Fire Dynamics Simulator (Version 6) – Volume 2: Verification*," NIST Special Publication 1018, Sixth Ed., National Institute of Standards and Technology, Gaithersburg, MD, USA, 2014). The version of FDS used during the preparation of this class is FDS Version 6.1.2.

The FireFOAM website does not contain a user guide yet. FireFOAM is being developed based on a general-purpose CFD software called OpenFOAM (*http://www.openfoam.org/*) and beginner users are invited to consult the OpenFOAM User Guide (see *http://www.openfoam.org/docs/*). The version of FDS used during the preparation of this class is FDS Version 2.2.x.

Access to the Deepthought2 linux cluster at the University of Maryland (UMD)

The FDS and FireFOAM fire models have been installed on the UMD Linux cluster called Deepthought2 (*https://www.glue.umd.edu/hpcc/dt2.html*). Access to Deepthought2 is provided to students of the CNRS School of Fire Science and Applications during the

duration of this course. Issues associated with the installation of FDS or FireFOAM will not be addressed as part of this course.

Students will find input files to run FDS and FireFOAM on available Deepthought2 accounts. Students are invited to run cases on Deepthought2 and move files between Deepthought2 and local computers using SSH. Local computers can be used to: (1) modify the input files; (2) post-process and visualize the simulation results. FDS results can be visualized using a graphics software package called Smokeview. FireFOAM results can be visualized using a graphics software package called ParaView. Smokeview and ParaView are freeware; both software have been installed on local computers.

Main features of the student access to Deepthought2:

- Use PuTTY (SSH client)
- URL of UMD linux cluster: *login.deepthought2.umd.edu*
- List of usernames and passwords:

fmc-sbd	avesuereaboq
fmc-sbe	iaplanthrubs
fmc-sbf	mysagildeser
fmc-sbg	npochawmishw
fmc-sbh	nuggitanumul
fmc-sbi	isgoshnabibc
fmc-sbj	hmarkopiahai
fmc-sbk	onkorrapeois
fmc-sbl	enaedadellha
fmc-sbm	cirahiedorac
fmc-sbn	kiessamisshr
fmc-sbo	wellehypecri
fmc-sbp	lesflerletot
fmc-sbq	poucisgralgo
fmc-sbr	eignichevolh
fmc-sbs	idynuchapihi
fmc-sbt	akemottsigob
fmc-sbu	tibiereaeafd

- Important notice: the Deepthought2 accounts will be disabled after the Computer Laboratory class on June 4, 2015.

Useful Linux commands

Deepthought2 uses a Linux operating system. Here is a list of useful commands that may be needed in order to work on the UMD cluster.

- "pwd": give pathname of current directory

- "cd [*directory name*]": change from current directory to *directory name*
- "ls –l": list files contained in current directory
- "cp [*filename1*] [*filename2*]: copy existing *filename1* to new file called *filename2*
- "mv [*filename1*] [*filename2*]: rename existing file called *filename1* to new file called *filename2*
- "rm [*filename*]": remove *filename*
- "more [*filename*]": list content of ASCII text file called *filename*
- "tail [*filename*]": list end of ASCII text file called *filename*
- "grep -in [*character string*] [*filename*]": find *character string* in *filename*

FDS cases

1) **Case 1: Radiation**

A simple radiation test case that serves to illustrate the importance of the discretization of angular space for an accurate solution of the radiative transfer equation.

Follow the following steps:

- "cd": move to main directory of your account
- "cd FDS_6.1.2/RUN/Radiation": move to FDS/Radiation subdirectory
- *optional*: download the file called radiation_box_2000S.fds to your local computer; modify the file as needed; upload the new version of the file radiation_box_2000S.fds
- "sh run.job": submit the FDS simulation to the cluster
- "showq | grep -in [*account name*]": check start and follow progress of simulation job on cluster (account name is *account name*). Each simulation job is identified with a number called *jobID*
- "more slurm-[*jobID*].out" or "tail slurm-[*jobID*].out": check status of simulation job and when finished, check for possible errors
- "more radiation_box_2000S.out": check status of simulation job and when finished, check for possible errors; read number of angles actually used in the FDS simulation
- download the file called radiation_box_2000S_devc.csv; open the file with Excel and visualize/analyze the results.

File radiation_box_2000S.fds

```
1  &HEAD CHID='radiation_box_2000S', TITLE='Radiation heat transfer'/
2
3  &MESH XB=0.0,1.0,0.0,1.0,0.0,1.0, IJK=50,50,50 / Computational domain and CFD grid resolution
4
5  &MISC Y_CO2_INFTY=0., HUMIDITY=0. /
```

```
 6
 7  &RADI NUMBER_RADIATION_ANGLES = 2000
 8    TIME_STEP_INCREMENT    = 1
 9       ANGLE_INCREMENT           = 1 / Radiation parameters and RTE grid
resolution
10
11  &TIME T_END=1.0, DT = 0.1  /
12
13  &DUMP DT_DEVC = 0.1 /
14
15  &VENT XB=0.0,0.0,0.46,0.54,0.46,0.54,SURF_ID='HOT' / 8 cm x 8 cm radiant
source
16  &VENT MB='XMIN', SURF_ID='COLD' /
17  &VENT MB='XMAX', SURF_ID='COLD' /
18  &VENT MB='YMIN', SURF_ID='COLD' /
19  &VENT MB='YMAX', SURF_ID='COLD' /
20  &VENT MB='ZMIN', SURF_ID='COLD' /
21  &VENT MB='ZMAX', SURF_ID='COLD' /
22
23  &SURF ID = 'HOT',  TMP_FRONT  = 726.85
24              TAU_T      = 0.
25              EMISSIVITY = 1.0
26              HEAT_TRANSFER_COEFFICIENT = 0. /
27  &SURF ID = 'COLD', TMP_FRONT  =-272.15
28              TAU_T      = 0.
29              EMISSIVITY = 1.0
30              HEAT_TRANSFER_COEFFICIENT = 0. /
31
32  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.025,0.025
IOR=-1 /
33  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.075,0.075
IOR=-1 /
34  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.125,0.125
IOR=-1 /
35  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.175,0.175
IOR=-1 /
36  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.225,0.225
IOR=-1 /
37  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.275,0.275
IOR=-1 /
38  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.325,0.325
IOR=-1 /
39  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.375,0.375
IOR=-1 /
40  &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.425,0.425
IOR=-1 /
```

```
41 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.475,0.475
IOR=-1 /
42 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.525,0.525
IOR=-1 /
43 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.575,0.575
IOR=-1 /
44 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.625,0.625
IOR=-1 /
45 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.675,0.675
IOR=-1 /
46 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.725,0.725
IOR=-1 /
47 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.775,0.775
IOR=-1 /
48 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.825,0.825
IOR=-1 /
49 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.875,0.875
IOR=-1 /
50 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.925,0.925
IOR=-1 /
51 &DEVC QUANTITY = 'INCIDENT HEAT FLUX' XYZ = 1.0,0.975,0.975
IOR=-1 /
52
53 &TAIL /
```

File run.job

```
1 sbatch --reservation=class radiation_box_2000S.script
```

File radiation_box_2000S.script (account name fmc-sbc)

```
1 #!/bin/tcsh
2 #SBATCH --reservation=class
3 #SBATCH -t 00:15:00
4 #SBATCH --ntasks=1
5 #SBATCH --share
6
7 set WORKDIR=/homes/fmc-sbc/FDS_6.1.2/RUN/Radiation
8 cd $WORKDIR
9 pwd
10
11 mpirun -wdir $WORKDIR /homes/fmc-sbc/FDS_6.1.2/BIN/fds6_mpi
   radiation_box_2000S.fds
```

To-do list:

- change the number of radiation angles from 2000, to 1000, 500, 200, 100, 50; plot the incident heat flux (the irradiation) as a function of spatial location along the target surface

2) Case 2: Pyrolysis

A simple pyrolysis test case that serves to illustrate the importance of the spatial discretization used inside the solid phase for an accurate solution of the pyrolysis equations.

Follow the following steps:

- "cd": move to main directory of your account
- "cd FDS_6.1.2/RUN/Pyrolysis": move to FDS/Pyrolysis subdirectory
- *optional*: download the file called wood_pyrolysis_25_1.fds to your local computer; modify the file as needed; upload the new version of the file wood_pyrolysis_25_1.fds
- "sh run.job": submit the FDS simulation to the cluster
- "showq | grep -in [*account name*]": check start and follow progress of simulation job on cluster (account name is *account name*). Each simulation job is identified with a number called *jobID*
- "more slurm-[*jobID*].out" or "tail slurm-[*jobID*].out": check status of simulation job and when finished, check for possible errors
- "more wood_pyrolysis_25_1.out": check status of simulation job and when finished, check for possible errors; read grid resolution in solid phase actually used in the FDS simulation
- download the files called wood_pyrolysis_25_1_hrr.csv, wood_pyrolysis_25_1_devc.csv, wood_pyrolysis_25_1_prof_01.csv and wood_pyrolysis_25_1_prof_02.csv; open the files with Excel and visualize/analyze the results.

File wood_pyrolysis_25_1.fds

```
1  &HEAD CHID='wood_pyrolysis_25_1',TITLE='Fuel mass loss rate' /
2
3  &MESH IJK=4,4,4,XB=0.0,0.1,0.0,0.1,0.0,0.1 / Irrelevant here
4
5  &TIME TWFIN=7000., WALL_INCREMENT=1 /
6
7  &MISC SOLID_PHASE_ONLY=.TRUE., Y_O2_INFTY=0.01 / Solid phase calculation
8  &REAC FUEL='METHANE', CRITICAL_FLAME_TEMPERATURE=2000. / No combustion
9
10 &VENT MB='ZMIN', SURF_ID='WALL' /
11 &VENT MB='XMIN', SURF_ID='OPEN' /
```

```
&VENT MB='XMAX', SURF_ID='OPEN' /
&VENT MB='YMIN', SURF_ID='OPEN' /
&VENT MB='YMAX', SURF_ID='OPEN' /
&VENT MB='ZMAX', SURF_ID='OPEN' /

&SURF ID                    = 'WALL'
   MATL_ID                 = 'WOOD'
   THICKNESS               = 0.025
   BACKING                 = 'INSULATED'
   EXTERNAL_FLUX           = 25.
   RAMP_EF                 = 'External flux'
   HEAT_TRANSFER_COEFFICIENT = 10.
   STRETCH_FACTOR          = 1
   CELL_SIZE_FACTOR        = 1.0 / Wood sample and heat loading parameters
                             Solid grid resolution, Delta_xs ~ 270 microns

&RAMP ID = 'External flux', T=    0, F=1/
&RAMP ID = 'External flux', T=10000, F=1/

&MATL ID             = 'WOOD'
   EMISSIVITY       = 0.9
   CONDUCTIVITY     = 0.126
   DENSITY          = 663.
   SPECIFIC_HEAT    = 2.52
   N_REACTIONS      = 1
   A                = 5.25E+07
   E                = 1.256E+05
   SPEC_ID          = 'METHANE'
   MATL_ID          = 'CHAR'
   NU_SPEC          = 0.8
   NU_MATL          = 0.2
     HEAT_OF_REACTION = 0 / Source: Novozhilov et al., Fire Safety J. 27
(1996) 69-84

&MATL ID             = 'CHAR'
   EMISSIVITY       = 0.9
   CONDUCTIVITY     = 0.126
   DENSITY          = 133.
   SPECIFIC_HEAT    = 2.52 / Source: Novozhilov et al., Fire Safety J. 27 (1996)
69-84

&DUMP DT_DEVC=1, DT_HRR=1, DT_PROF = 50 /

&DEVC XYZ=0.02,0.02,0.0, QUANTITY='BURNING RATE',          IOR=+3,
ID='MLRPUA_1' /
```

```
54  &DEVC XYZ=0.05,0.05,0.0, QUANTITY='BURNING RATE',          IOR=+3,
ID='MLRPUA_2' /
55  &DEVC XYZ=0.08,0.08,0.0, QUANTITY='BURNING RATE',          IOR=+3,
ID='MLRPUA_3' /
56  &DEVC XYZ=0.05,0.05,0.0, QUANTITY='NET HEAT FLUX',         IOR=+3,
ID='QIN_2'   /
57  &DEVC  XYZ=0.05,0.05,0.0,  QUANTITY='RADIATIVE  HEAT  FLUX',
IOR=+3, ID='QRAD_2'   /
58  &DEVC  XYZ=0.05,0.05,0.0,  QUANTITY='CONVECTIVE  HEAT  FLUX',
IOR=+3, ID='QCON_2'   /
59  &DEVC  XYZ=0.05,0.05,0.0,  QUANTITY='INCIDENT  HEAT  FLUX',
IOR=+3, ID='QIN_2'   /
60  &DEVC  XYZ=0.05,0.05,0.0,  QUANTITY='WALL  TEMPERATURE'  ,
IOR=+3, ID='Temp_2'   /
61  &DEVC XYZ=0.05,0.05,0.0, QUANTITY='WALL THICKNESS' ,      IOR=+3,
ID='Delta_2'  /
62
63  &PROF XYZ=0.05,0.05,0.0, QUANTITY='TEMPERATURE',          IOR=+3,
ID='Temps_2'  /
64  &PROF XYZ=0.05,0.05,0.0, QUANTITY='DENSITY',              IOR=+3,
ID='rhos_2'   /
65
66  &TAIL /
```

File run.job

```
1   sbatch --reservation=class wood_pyrolysis_25_1.script
```

File wood_pyrolysis_25_1.script (account name fmc-sbc)

```
1   #!/bin/tcsh 1 #!/bin/tcsh
2   #SBATCH --reservation=class
3   #SBATCH -t 00:15:00
4   #SBATCH --ntasks=1
5   #SBATCH --share
6
7   set WORKDIR=/homes/fmc-sbc/FDS_6.1.2/RUN/Pyrolysis
8   cd $WORKDIR
9   pwd
10
11  mpirun  -wdir  $WORKDIR  /homes/fmc-sbc/FDS_6.1.2/BIN/fds6_mpi
wood_pyrolysis_25_1.fds
```

To-do list:

- change the discretization used in the solid phase, *i.e.* change the parameter CELL_SIZE_FACTOR from 1, to 0.75, 1.5, 3, 6 and 12; plot the fuel mass loss rate as a function of time

3) Case 3: Vortex

A simple vortex flow test case that serves to illustrate the importance of the spatial discretization used in the gas phase for an accurate solution of the flow equations.

Follow the following steps:

- "cd": move to main directory of your account
- "cd FDS_6.1.2/RUN/Vortex": move to FDS/Vortex subdirectory
- *optional*: download the file called vort_trans_5.fds to your local computer; modify the file as needed; upload the new version of the file vort_trans_5.fds
- "sh run.job": submit the FDS simulation to the cluster
- "showq | grep -in [*account name*]": check start and follow progress of simulation job on cluster (account name is *account name*). Each simulation job is identified with a number called *jobID*
- "more slurm-[*jobID*].out" or "tail slurm-[*jobID*].out": check status of simulation job and when finished, check for possible errors
- "more vort_trans_5.out": check status of simulation job and when finished, check for possible errors
- download the files called vort_trans_5_line.csv, vort_trans_5_0*.sf and vort_trans_5.smv; open the .csv file with Excel and visualize/analyze the results; open the .smv file using Smokeview.

File vort_trans_5.fds

```
1   &HEAD CHID = 'vort_trans_5', TITLE = 'Transported 2D Vortex' /
2
3   &MESH IJK = 50,1,50, XB = -0.05,0.05, -0.001,0.001, -0.05,0.05 /
4
5   &TIME T_END = 1.0 /
6
7   &MISC   DNS           = .TRUE.,
8       STRATIFICATION  = .FALSE.,
9       BAROCLINIC      = .FALSE.,
10      NOISE           = .FALSE.,
11      CFL_MAX         = 0.5,
12      GVEC(3)         = 0.0,
13      PROJECTION      = .TRUE.
14      OVERWRITE       = .FALSE. /
15
16  &CSVF UVWFILE = 'vort_trans_5_uvw.csv' /
17
```

```
18  &RADI RADIATION = .FALSE. /
19
20  &SPEC ID = 'AIR', VISCOSITY = 1.199266e-5, BACKGROUND = .TRUE. /
21
22  &VENT PBX = -0.05, SURF_ID = 'PERIODIC' /
23  &VENT PBX =  0.05, SURF_ID = 'PERIODIC' /
24  &VENT PBZ = -0.05, SURF_ID = 'PERIODIC' /
25  &VENT PBZ =  0.05, SURF_ID = 'PERIODIC' /
26
27  &DUMP DT_DEVC_LINE = 0.0 /
28  &SLCF PBY = 0.00, QUANTITY = 'PRESSURE',     CELL_CENTERED =
.TRUE. /
30  &SLCF PBY = 0.00, QUANTITY = 'VORTICITY Y' CELL_CENTERED =
.TRUE. /
31  &SLCF PBY = 0.00, QUANTITY = 'VELOCITY',   VECTOR = .TRUE. /
32
33  &DEVC ID = 'Vort_x', XB = -0.049,0.049, 0.0,0.0, 0.0,0.0, QUANTITY =
'VORTICITY Y',
34       POINTS = 50, TIME_AVERAGED = .FALSE. /
35
36  &DEVC ID = 'Vort_z', XB = 0.0,0.0, 0.0,0.0, -0.049,0.049, QUANTITY =
'VORTICITY Y',
37       POINTS = 50, TIME_AVERAGED = .FALSE. /
38
39  &TAIL /
```

File run.job

```
1   sbatch --reservation=class vort_trans_5.script
```

File vort_trans_5.script (account name fmc-sbc)

```
1   #!/bin/tcsh 1 #!/bin/tcsh
2   #SBATCH --reservation=class
3   #SBATCH -t 02:00:00
4   #SBATCH --ntasks=1
5   #SBATCH --share
6
7   set WORKDIR=/homes/fmc-sbc/FDS_6.1.2/RUN/Vortex
8   cd $WORKDIR
9   pwd
10
11  mpirun -wdir $WORKDIR /homes/fmc-sbc/FDS_6.1.2/BIN/fds6_mpi
vort_trans_5.fds
```

To-do list:

- use the MATLAB pre-processor vort_trans.m and change the discretization used in the gas phase, *i.e.* change values of I and K in the parameter IJK from 50 to 20, 100 and 200; use the MATLAB post-processor vort_trans_plot.m and plot the vorticity along the centerline $y = 0$ at time $t = 1$ second

4) Case 4: Spread

A simple vertical wall flame test case that serves to illustrate the flame spread capabilities as well as the parallel computing capabilities of FDS.

Follow the following steps:

- "cd": move to main directory of your account
- "cd FDS_6.1.2/RUN/Spread": move to FDS/Spread subdirectory
- *optional*: download the file called spread_10cm.fds to your local computer; modify the file as needed; upload the new version of the file spread_10cm.fds
- "sh run.job": submit the FDS simulation to the cluster
- "showq | grep -in [*account name*]": check start and follow progress of simulation job on cluster (account name is *account name*). Each simulation job is identified with a number called *jobID*
- "more slurm-[*jobID*].out" or "tail slurm-[*jobID*].out": check status of simulation job and when finished, check for possible errors
- "more spread_10cm.out": check status of simulation job and when finished, check for possible errors
- download the files called spread_10cm_hrr.csv, spread_10cm_devc.csv, spread_10cm.smv and the files with .xyz, .q, .bf, .s3d and .sz extensions; open the .csv file with Excel and visualize/analyze the results; open the .smv file using Smokeview.

File spread_10cm.fds

```
1  &HEAD CHID='spread_10cm', TITLE='Flame spread' /
2
3  //&MESH IJK=10,20,20,XB=0.0,1.0,0.0,2.0,0.0,2.0 / Computational domain and CFD resolution
4  &MESH IJK=10,10,10,XB=0.0,1.0,0.0,1.0,0.0,1.0 / MESH 1
5  &MESH IJK=10,10,10,XB=0.0,1.0,1.0,2.0,0.0,1.0 / MESH 2
6  &MESH IJK=10,10,10,XB=0.0,1.0,0.0,1.0,1.0,2.0 / MESH 3
7  &MESH IJK=10,10,10,XB=0.0,1.0,1.0,2.0,1.0,2.0 / MESH 4
8
9  &PRES VELOCITY_TOLERANCE=0.01, MAX_PRESSURE_ITERATIONS=100 /
10
11 &MISC SUPPRESSION=.FALSE. /
12
13 &TIME T_END=1800. /
```

```
14
15  &REAC FUEL='PROPANE', SOOT_YIELD=0.01 /
16
17  &RADI RADIATIVE_FRACTION = 0.4 /
18
19  &VENT XB= 0.0,0.0,0.5,1.5,0.5,1.5, SURF_ID='SHEET' /
20
21  &SURF ID                  = 'SHEET'
22     COLOR                = 'GRAY'
23     MATL_ID              = 'HDPE'
24     THICKNESS            = 0.025
25     BACKING              = 'INSULATED'
26     CELL_SIZE_FACTOR     = 0.5 / HDPE plate
27                                 Solid grid resolution, Delta_xs ~ 150 microns
28
29  &MATL ID                  = 'HDPE'
30     EMISSIVITY           = 0.92
31     ABSORPTION_COEFFICIENT = 1300.
32     CONDUCTIVITY         = 0.29
33     DENSITY              = 860.
34     SPECIFIC_HEAT        = 3.5
35     N_REACTIONS          = 1
36     A                    = 4.8E+22
37     E                    = 3.49E+05
38     SPEC_ID              = 'PROPANE'
39     NU_SPEC              = 1.
40     NU_MATL              = 0.
41     HEAT_OF_REACTION     = 920.
42     HEAT_OF_COMBUSTION       = 40000. / Source: FDS Validation Guide
(Section 14.1.2)
43
44  &SURF ID = 'FIRE', TMP_FRONT=1000., COLOR='RED'       / Hot surface for
ignition
45  &OBST XB = 0.1,0.2,0.5,1.5,0.5,0.6, SURF_ID = 'FIRE' / Ignitor
46
47  &VENT XB = 0.0,0.0,0.0,2.0,0.0,2.0, SURF_ID = 'INERT' / West
48  &VENT XB = 1.0,1.0,0.0,2.0,0.0,2.0, SURF_ID = 'OPEN'  / East
49  &VENT XB = 0.0,1.0,0.0,0.0,0.0,2.0, SURF_ID = 'OPEN'  / Front
50  &VENT XB = 0.0,1.0,2.0,2.0,0.0,2.0, SURF_ID = 'OPEN'  / Rear
51  &VENT XB = 0.0,1.0,0.0,2.0,0.0,0.0, SURF_ID = 'INERT' / South
52  &VENT XB = 0.0,1.0,0.0,2.0,2.0,2.0, SURF_ID = 'OPEN'  / North
53
54  &DUMP DT_PL3D=600., DT_DEVC=1.0, DT_HRR=1.0,
55     WRITE_XYZ=.TRUE.,
56     PLOT3D_QUANTITY(1)='TEMPERATURE',
57     PLOT3D_QUANTITY(2)='U-VELOCITY',
```

```
   58      PLOT3D_QUANTITY(3)='V-VELOCITY',
   59      PLOT3D_QUANTITY(4)='W-VELOCITY',
   60      PLOT3D_QUANTITY(5)='HRRPUV' /
   61
   62  &DEVC  XYZ=  0.0,1.00,0.51,  QUANTITY='NET  HEAT  FLUX',  IOR=+1,
ID='QIN1'  /
   63  &DEVC  XYZ=  0.0,1.00,1.00,  QUANTITY='NET  HEAT  FLUX',  IOR=+1,
ID='QIN2'  /
   64  &DEVC  XYZ=  0.0,0.51,1.00,  QUANTITY='NET  HEAT  FLUX',  IOR=+1,
ID='QIN3a' /
   65  &DEVC  XYZ=  0.0,1.49,1.00,  QUANTITY='NET  HEAT  FLUX',  IOR=+1,
ID='QIN3b' /
   66  &DEVC  XYZ=  0.0,1.00,1.49,  QUANTITY='NET  HEAT  FLUX',  IOR=+1,
ID='QIN4'  /
   67
   68  &DEVC XYZ= 0.0,1.00,0.51, QUANTITY='WALL TEMPERATURE', IOR=+1,
ID='TEMP1'  /
   69  &DEVC XYZ= 0.0,1.00,1.00, QUANTITY='WALL TEMPERATURE', IOR=+1,
ID='TEMP2'  /
   70  &DEVC XYZ= 0.0,0.51,1.00, QUANTITY='WALL TEMPERATURE', IOR=+1,
ID='TEMP3a' /
   71  &DEVC XYZ= 0.0,1.49,1.00, QUANTITY='WALL TEMPERATURE', IOR=+1,
ID='TEMP3b' /
   72  &DEVC XYZ= 0.0,1.00,1.49, QUANTITY='WALL TEMPERATURE', IOR=+1,
ID='TEMP4'  /
   73
   74  &DEVC  XYZ=  0.0,1.00,0.51,  QUANTITY='BURNING_RATE',  IOR=+1,
ID='MLR1'  /
   75  &DEVC  XYZ=  0.0,1.00,1.00,  QUANTITY='BURNING_RATE',  IOR=+1,
ID='MLR2'  /
   76  &DEVC  XYZ=  0.0,0.51,1.00,  QUANTITY='BURNING_RATE',  IOR=+1,
ID='MLR3a' /
   77  &DEVC  XYZ=  0.0,1.49,1.00,  QUANTITY='BURNING_RATE',  IOR=+1,
ID='MLR3b' /
   78  &DEVC  XYZ=  0.0,1.00,1.49,  QUANTITY='BURNING_RATE',  IOR=+1,
ID='MLR4'  /
   79
   80  &DEVC    XB=    0.0,0.0,0.5,1.0,0.5,1.0,    QUANTITY='BURNING_RATE',
IOR=+1,
   81                  STATISTICS='SURFACE INTEGRAL',
   82                  ID='MLR_total_a'  /
   83
   84  &DEVC    XB=    0.0,0.0,1.0,1.5,0.5,1.0,    QUANTITY='BURNING_RATE',
IOR=+1,
   85                  STATISTICS='SURFACE INTEGRAL',
   86                  ID='MLR_total_b'  /
```

```
 87
 88 &DEVC     XB=     0.0,0.0,0.5,1.0,1.0,1.5,     QUANTITY='BURNING_RATE',
IOR=+1,
 89                      STATISTICS='SURFACE INTEGRAL',
 90                      ID='MLR_total_c'  /
 91
 92 &DEVC     XB=     0.0,0.0,1.0,1.5,1.0,1.5,     QUANTITY='BURNING_RATE',
IOR=+1,
 93                      STATISTICS='SURFACE INTEGRAL',
 94                      ID='MLR_total_d'  /
 95
 96 &DEVC   XB=   0.0,0.0,0.5,1.0,0.5,1.0,   QUANTITY='SURFACE   DENSITY',
IOR=+1,
 97                      STATISTICS='SURFACE INTEGRAL',
 98                      ID='ML_total_a'  /
 99
100 &DEVC   XB=   0.0,0.0,1.0,1.5,0.5,1.0,   QUANTITY='SURFACE   DENSITY',
IOR=+1,
101                      STATISTICS='SURFACE INTEGRAL',
102                      ID='ML_total_b'  /
103
104 &DEVC   XB=   0.0,0.0,0.5,1.0,1.0,1.5,   QUANTITY='SURFACE   DENSITY',
IOR=+1,
105                      STATISTICS='SURFACE INTEGRAL',
106                      ID='ML_total_c'  /
107
108 &DEVC   XB=   0.0,0.0,1.0,1.5,1.0,1.5,   QUANTITY='SURFACE   DENSITY',
IOR=+1,
109                      STATISTICS='SURFACE INTEGRAL',
110                      ID='ML_total_d'  /
111
112 &BNDF QUANTITY='NET HEAT FLUX'    /
113 &BNDF QUANTITY='WALL TEMPERATURE' /
114 &BNDF QUANTITY='BURNING_RATE'     /
115
116 &TAIL/
```

File run.job

```
1  sbatch --reservation=class spread_10cm.script
```

File spread_10cm.script (account name fmc-sbc)

```
1  #!/bin/tcsh 1 #!/bin/tcsh
2  #SBATCH --reservation=class
3  #SBATCH -t 01:00:00
```

```
4  #SBATCH --ntasks=4
5  #SBATCH --share
6
7  set WORKDIR=/homes/fmc-sbc/FDS_6.1.2/RUN/Spread
8  cd $WORKDIR
9  pwd
10
11 mpirun -wdir $WORKDIR /homes/fmc-sbc/FDS_6.1.2/BIN/fds6_mpi spread_10cm.fds
```

To-do list:

- try to change the spatial discretization used in the gas phase, *i.e*. change values of I, J and K in the parameter IJK from 10 to 20

FireFOAM cases

5) Case 1: Radiation

A simple radiation test case that serves to illustrate the importance of the discretization of angular space for an accurate solution of the radiative transfer equation.

Follow the following steps:

- "cd": move to main directory of your account
- "cd /homes/fmc-sbc/OpenFOAM/case-2.2.x/radiation" (account name fmc-sbc): move to OpenFOAM/radiation subdirectory
- "Allclean": clean directory
- "Allrun": prepare input files
- *optional*: "cd"; "cd /homes/fmc-sbc/OpenFOAM/case-2.2.x/radiation/constant"; download the file called radiationProperties to your local computer; modify the file as needed; upload the new version of the file radiationProperties
- "decomposePar": prepare parallel run
- "sbatch pf3D.script": submit the FireFOAM simulation to the cluster
- "showq | grep -in [*account name*]": check start and follow progress of simulation job on cluster (account name is *account name*). Each simulation job is identified with a number called *jobID*
- "more slurm-[*jobID*].out" or "tail slurm-[*jobID*].out": check status of simulation job and when finished, check for possible errors
- "more log.0": check status of simulation job and when finished, check for possible errors
- "reconstructPar": merge separate output files from each processor into common output files
- "sample": create file called Qcenterline_G_Qin_Qr.xy in postProcessing/sets/0.1
- download the file called Qcenterline_G_Qin_Qr.xy and plot the incident heat flux (the irradiation – 5th column in the ASCII file) as a function of spatial location along the target surface (3rd column)

File pf3D.script (account name fmc-sbc)

```
1  #!/bin/csh
2  #-------------------------------------------------
3  # Example SLURM job script to run MPI applications
4  #-------------------------------------------------
5
6  #SBATCH -N 1              # Total number of nodes requested (20 cores/node)
7  #SBATCH --ntasks=8        # Total number of mpi tasks requested
8  #SBATCH -t 01:00:00       # Run time (hh:mm:ss)
9  #SBATCH --share
10
11 #SBATCH --reservation=class
12
13 # Launch the MPI executable named "fireFOAM"
14 mpirun -np 8 fireFoam -parallel > log.0
```

To-do list:

- change the number of radiation angles by modifying the values of nPhi and nTheta specified in the file radiationProperties (OpenFOAM/case-2.2.x/radiation/constant directory); the total number of radiation angles is (4 x nPhi x nTheta); change from 64 to 256, 1024 and 4096.

6) Case 2: Pyrolysis

A simple pyrolysis test case that serves to illustrate the importance of the spatial discretization used inside the solid phase for an accurate solution of the pyrolysis equations.

Follow the following steps:

- "cd": move to main directory of your account
- "cd /homes/fmc-sbc/OpenFOAM/case-2.2.x/pyrolysis" (account name fmc-sbc): move to OpenFOAM/radiation subdirectory
- "./Allclean": clean directory
- "./Allrun": prepare input files
- *optional*: "cd"; "cd /homes/fmc-sbc/OpenFOAM/case-2.2.x/pyrolysis/system"; download the file called extrudeToRegionMeshDict to your local computer; modify the file as needed; upload the new version of the file extrudeToRegionMeshDict
- *optional*: "cd"; "cd /homes/fmc-sbc/OpenFOAM/case-2.2.x/pyrolysis/0/panelRegion"; download the file called T to your local computer; modify the file as needed; upload the new version of the file T
- "sbatch pf3D.script": submit the FireFOAM simulation to the cluster

- "showq | grep -in [*account name*]": check start and follow progress of simulation job on cluster (account name is *account name*). Each simulation job is identified with a number called *jobID*
- "more slurm-[*jobID*].out" or "tail slurm-[*jobID*].out": check status of simulation job and when finished, check for possible errors
- "more log.0": check status of simulation job and when finished, check for possible errors
- download the file called faceSource.dat in postProcessing/panelRegion/patchPanelSolid/0 and plot the fuel mass loss rate (the 3rd column divided by the 2nd columnin the ASCII file) as a function of time (1st column)

File pf3D.script (account name fmc-sbc)

```
1  #!/bin/csh
2  #-------------------------------------------------
3  # Example SLURM job script to run MPI applications
4  #-------------------------------------------------
5
6  #SBATCH -N 1              # Total number of nodes requested (20 cores/node)
7  #SBATCH --ntasks=1        # Total number of mpi tasks requested
8  #SBATCH -t 01:00:00       # Run time (hh:mm:ss)
9  #SBATCH --share
10
11 #SBATCH --reservation=class
12
13 # Launch the MPI executable named "fireFOAM"
14 mpirun -np 1 fireFoam > log.0
```

To-do list:

- change the discretization used in the solid phase by modifying the value of nLayers specified in the file called extrudeToRegionMeshDict (/homes/fmc-sbc/OpenFOAM/case-2.2.x/pyrolysis/system); the resolution is uniform and equal to (thickness/ nLayers); plot the fuel mass loss rate as a function of time
- change the value of the irradiation by modifying the value of QrIncident specified in the file called T (/homes/fmc-sbc/OpenFOAM/case-2.2.x/pyrolysis/0/panelRegion); change from 25000 to 100000; plot the fuel mass loss rate as a function of time

7) Case 3: Vortex

A simple vortex flow test case that serves to illustrate the importance of the spatial discretization used in the gas phase for an accurate solution of the flow equations.

Follow the following steps:

- "cd": move to main directory of your account
- "cd OpenFOAM/case-2.2.x/singleVortex": move to OpenFOAM/Vortex subdirectory
- "Allclean": clean directory
- "Allrun": prepare input files
- *optional*: "cd"; "cd /homes/fmc-sbc/OpenFOAM/case-2.2.x/singleVortex/constant/polyMesh"; download the file called blockMeshDict to your local computer; modify the file as needed; upload the new version of the file blockMeshDict
- "decomposePar": prepare parallel run
- "sbatch pf3D.script": submit the FireFOAM simulation to the cluster
- "showq | grep -in [*account name*]": check start and follow progress of simulation job on cluster (account name is *account name*). Each simulation job is identified with a number called *jobID*
- "more slurm-[*jobID*].out" or "tail slurm-[*jobID*].out": check status of simulation job and when finished, check for possible errors
- "more log.0": check status of simulation job and when finished, check for possible errors
- "reconstructPar": merge separate output files from each processor into common output files
- "vorticity": add vorticity to output files
- download the entire singleVortex directory:
  - "cd /homes/fmc-sbc/OpenFOAM/case-2.2.x"
  - "tar -cvf singleVortex.tar singleVortex": creates archive file called singleVortex.tar
  - and on local computer: "scp -r fmc-sbc@login.deepthought2.umd.edu:/homes/fmc-sbc/OpenFOAM/case-2.2.x/singleVortex.tar ." (account name fmc-sbc)
- open "1.foam" with ParaView and visualize/analyze the results; save the vorticity profile along the centerline $y = 0$ at time $t = 1$ second

File pf3D.script (account name fmc-sbc)

```
1  #!/bin/csh
2  #--------------------------------------------------
3  # Example SLURM job script to run MPI applications
4  #--------------------------------------------------
5
6  #SBATCH -N 1              # Total number of nodes requested (20 cores/node)
7  #SBATCH --ntasks=4        # Total number of mpi tasks requested
8  #SBATCH -t 01:00:00       # Run time (hh:mm:ss)
9  #SBATCH --share
10
11 #SBATCH --reservation=class
```

```
12
13  # Launch the MPI executable named "fireFOAM"
14  ## mpirun -np 1 fireFoam > log.0
15  mpirun -np 4 fireFoam -parallel > log.0
```

To-do list:

- change the spatial discretization used in the gas phase by modifying the statement “hex (0 1 2 3 4 5 6 7) (50 50 1) simpleGrading (1 1 1)” in the file blockMeshDict (OpenFOAM/case-2.2.x/singleVortex/constant/polyMesh directory); change 50 to 20, 100 and 200.