3ème École des Sciences des Incendies et Applications (ESIA)

Numerical Workshop (Fire Modeling)

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Introduction to FDS

- The purpose of this section is to
  - Take a first user approach to the Fire Dynamics Simulator (FDS) developed by NIST (*https://pages.nist.gov/fds-smv/*)
    - **Version 6.7.7**
  - Walk through the different steps involved in setting up and running FDS
    - McGrattan, K., Hostikka, S., Floyd, J., McDermott, R., Vanella, M., "*Fire Dynamics Simulator – User's Guide*," NIST Special Publication 1019, Sixth Ed., National Institute of Standards and Technology, Gaithersburg, MD, USA, 2021

Installation of FDS

- FDS version v6.7.7
- McGrattan, K., Hostikka, S., Floyd, J., McDermott, R., Vanella, M., "*Fire Dynamics Simulator – User's Guide*," NIST Special Publication 1019, Sixth Ed., National Institute of Standards and Technology, Gaithersburg, MD, USA, 2021
  - Chapter 2
- Web information
  - Windows: *https://www.youtube.com/watch?v=MXuuSBJAkLA* and *https://fdstutorial.com/how-to-run-a-fds-job-on-windows/*
  - Mac: *https://www.youtube.com/watch?v=ZzptCR1HBb4*
  - Linux: *https://www.youtube.com/watch?v=lpeqg2Bm6a0*
- Or install PyroSim

FDS code structure

- Code structure:
  - "fds *filename.fds*"

Input file:

- *filename.fds*

Output files:

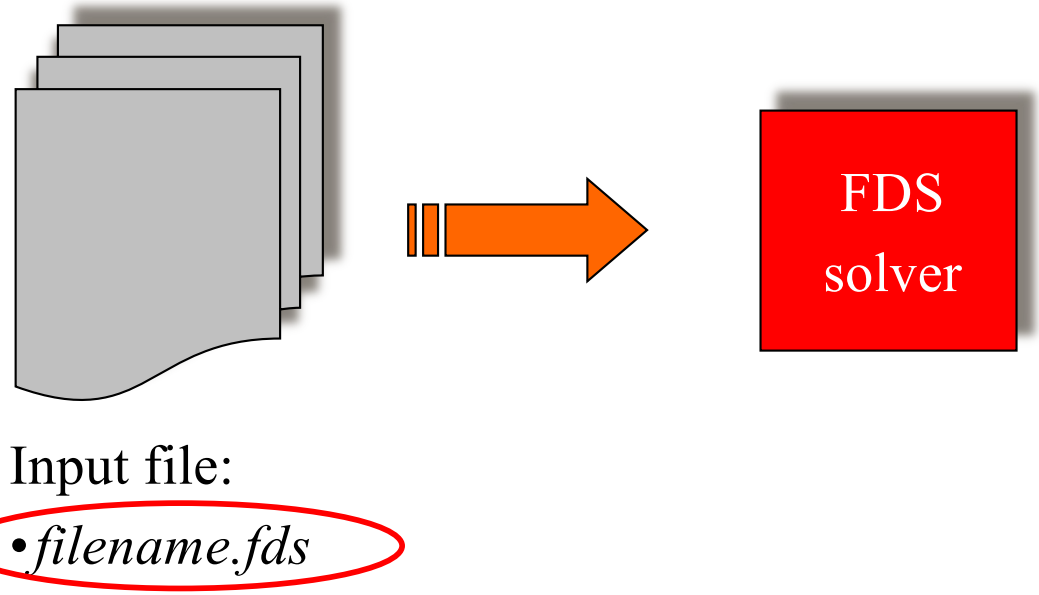
basic output file for monitoring progress
- *filename.out*

time history of global/local quantities
- *CHID_hrr.csv*
- *CHID_devc.csv*

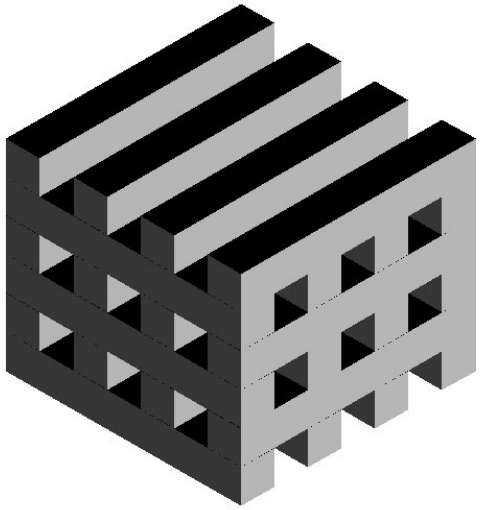
graphics files
- *CHID.xyz*
- *CHID_nnnn_nnn.q*

FDS code structure

- Code structure:
  - Pre-processing stage

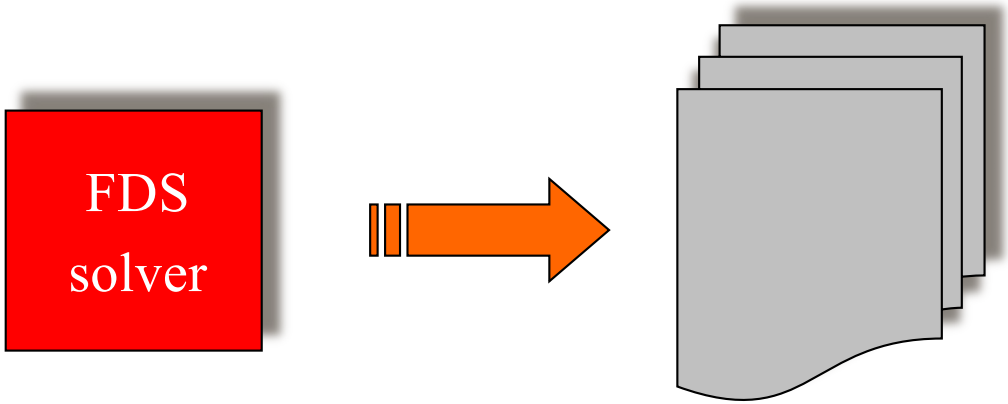


Pre-processor
(PyroSim, Solidworks,
AutoCAD, etc)



FDS code structure

- Code structure:
  - Post-processing stage



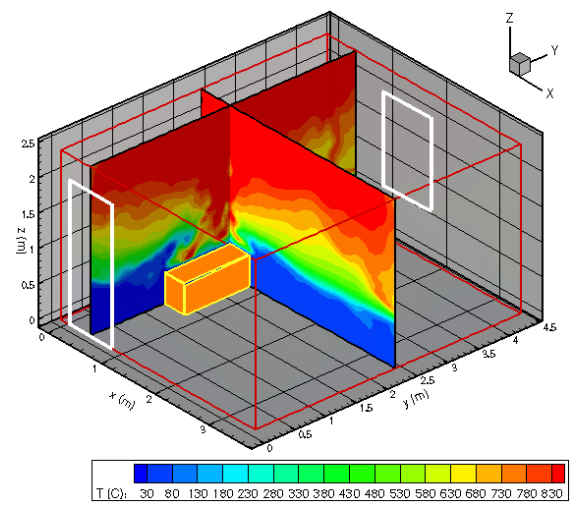
Output files:

basic output file for monitoring progress | • *filename.out*

time history of global quantities | • *CHID_hrr.csv*

graphics files { • *CHID.xyz* • *CHID_nnnn_nnn.q*

Post-processor
(Smokeview, Tecplot, etc)



FDS input data file

- Example *CompartmentFire1.fds*: specify FDS input parameters

```
This is a demonstration calculation. Properties are artificially manipulated and may not be
    realistic.

&HEAD CHID='CompartmentFire1', TITLE='Example room fire simulation'  /

&MESH IJK=52,66,24, XB=0.00, 5.20,-2.00, 4.60, 0.00, 2.40 /
//&MESH IJK=26,33,12, XB=0.00, 5.20,-2.00, 4.60, 0.00, 2.40 /

&TIME T_END=1000 /

*** Configuration: fire room and outside space *** Begin
&SURF ID            = 'WALL'
    DEFAULT         = .TRUE.
    RGB             = 200,200,200
    MATL_ID         = 'GYPSUM PLASTER'
    THICKNESS       = 0.012 /
(…)
```

FDS input data file

- Example *filename.fds*: specify FDS input parameters
  - **Fortran syntax:** input files organized as a list of records (formatted as Fortran namelist records); each record starts with the ampersand character &, followed by the name of the record (SURF ID), followed by a list of input parameters (separated by commas), and terminated by a slash /

```
&SURF ID='SIDE_WALL',
   MATL_ID='CONCRETE',
   THICKNESS    = 0.15 /
```

start of record

name of namelist group

end of record

FDS input data file

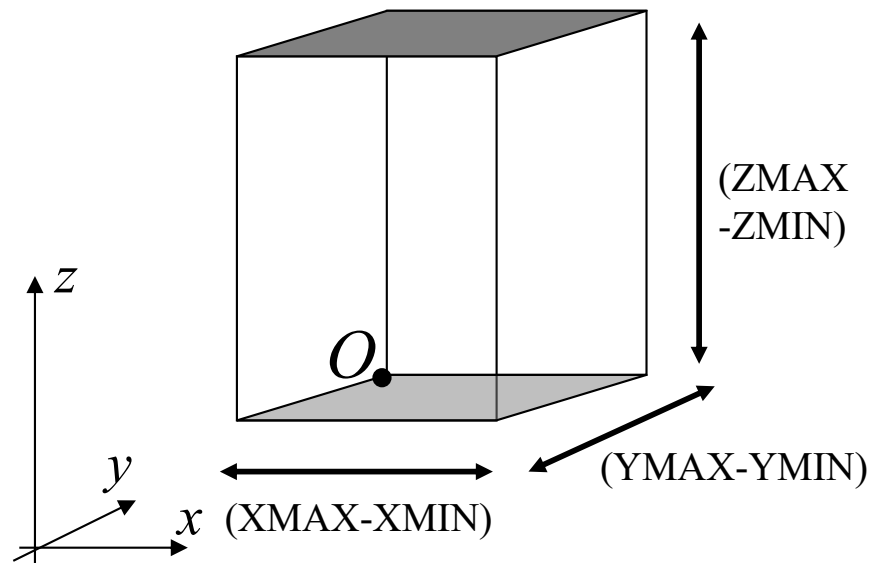
- HEAD namelist group: specify job name (CHID) and brief comment (TITLE)

&HEAD CHID='CompartmentFire1', TITLE='Example room fire simulation' /

- MESH namelist group: specify size of computational domain

&MESH IJK=52,66,24, XB=0.00, 5.20,-2.00, 4.60, 0.00, 2.40 /

- Rectangular-shaped domain
- Domain width = 5.2 m
- Domain depth = 6.6 m
- Domain height = 2.4 m



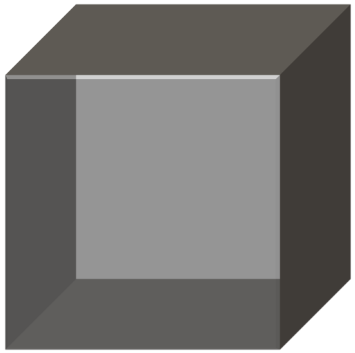
FDS input data file

- MESH namelist group: specify computational grid

&MESH IJK=52,66,24, XB=0.00, 5.20,-2.00, 4.60, 0.00, 2.40 /

- Uniform spatial resolution; grid cell geometry = cube

➡ $\Delta x = \Delta y = \Delta z = 0.1$ m.



FDS input data file

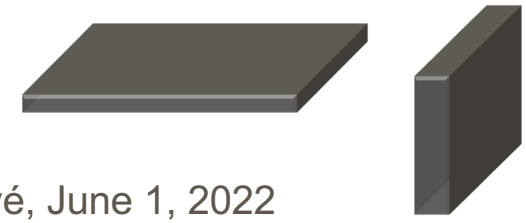
- MESH namelist group: specify computational grid

&MESH IJK=52,66,24, XB=0.00, 5.20,-2.00, 4.60, 0.00, 2.40 /

- Other choices are possible
- Non-uniform spatial resolution; grid cell geometry = rectangular parallelepiped

$\Delta x = \Delta y = 10\,\text{cm}$; $\Delta z = 5\,\text{cm}$

- **Caution:** keep aspect ratio close to unity



Not good choices! (except close to solid walls)

FDS input data file

- TIME namelist group: specify computational duration (T_END)

```
&TIME T_END=1000 /
```

FDS input data file

- SURF and MATL namelist groups: specify parameters of wall boundaries (thermal properties, wall thickness, *etc*)

```
&SURF ID = 'WALL'
    DEFAULT = .TRUE.
    RGB = 200,200,200
    MATL_ID = 'GYPSUM PLASTER'
    THICKNESS = 0.012 /
&MATL ID = 'GYPSUM PLASTER'
    FYI = 'Quintiere, Fire Behavior'
    CONDUCTIVITY = 0.48
    SPECIFIC_HEAT = 0.84
    DENSITY = 1440. /
```

Conductivity (W/m-K)
Specific heat (kJ/kg-K)
Mass density (kg/m3)

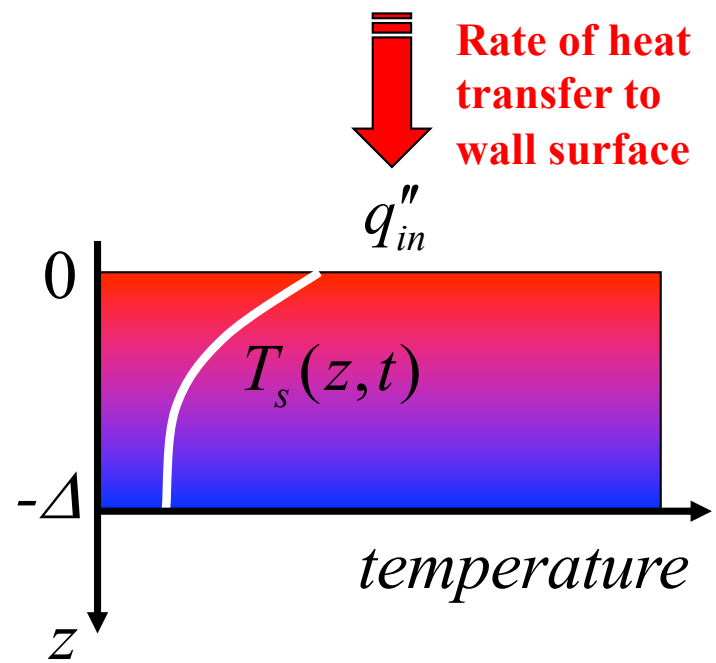
FDS input data file

- Treatment of: (1) ignition of solid flammable materials; (2) heat losses occurring at compartment solid walls
  - Heat conduction across compartment walls described by a local one-dimensional problem in the direction normal to the wall surface:
    - Heat equation

$$\rho_s c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial z}\left(k_s \frac{\partial T_s}{\partial z} \right)$$

    - Boundary condition (at gas-solid interface)

$$\underbrace{\dot{q}''_{in}(t)}_{\substack{\text{net heat flux} \\ \text{from gas phase} \\ \text{(radiation, convection)}}} = \underbrace{-k_s \frac{\partial T_s}{\partial z}(0,t)}_{\substack{\text{heat flux to wall interior} \\ \text{(conduction)}}}$$



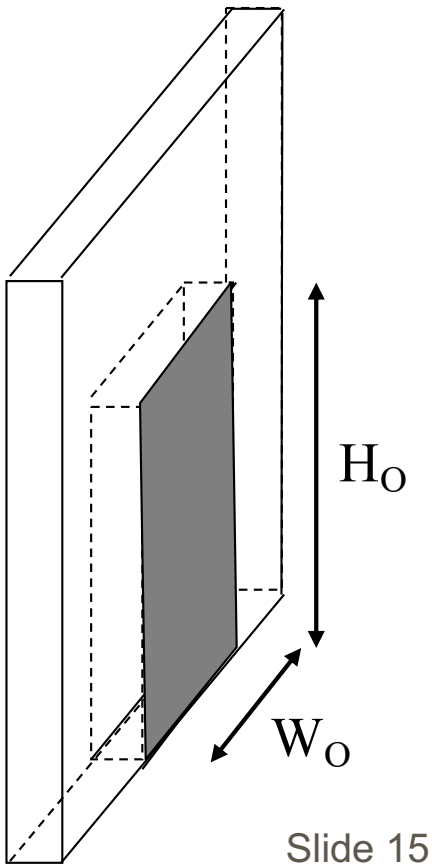
FDS input data file

- OBST namelist group: specify location/properties of 3D solid object (default surface boundary conditions)

&OBST XB= 0.00, 5.20,-0.10, 0.00, 0.00, 2.40 / Front wall

- HOLE namelist group: open vent across 3D solid object

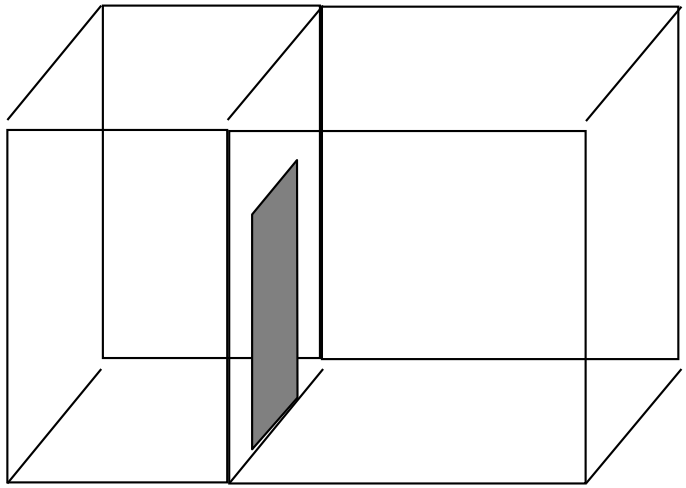
&HOLE XB= 4.00, 5.00,-0.11, 0.01, 0.00, 2.00 / Door



FDS input data file

- VENT namelist group: specify location/properties of 2D solid/gas surface (specify boundary conditions)

```
&VENT XB=0.00, 5.20,-2.00, 0.00, 0.00, 0.00, SURF_ID='INERT' /
&VENT XB=0.00, 0.00,-2.00, 0.00, 0.00, 2.40, SURF_ID='OPEN'  /
&VENT XB=5.20, 5.20,-2.00, 0.00, 0.00, 2.40, SURF_ID='OPEN'  /
&VENT XB=0.00, 5.20,-2.00,-2.00, 0.00, 2.40, SURF_ID='OPEN'  /
&VENT XB=0.00, 5.20,-2.00, 0.00, 2.40, 2.40, SURF_ID='OPEN'  /
```



FDS input data file

- REAC namelist group: specify parameters of combustion model

```
&REAC FUEL = 'POLYURETHANE'
    FYI = 'C_6.3 H_7.1 N O_2.1, NFPA Handbook, Babrauskas'
    SOOT_YIELD = 0.10
    N = 1.0
    C = 6.3
    H = 7.1
    O = 2.1 /
```

- Treatment of combustion
  - (Extended) global combustion equation

$$C_{6.3}H_{7.1}N_1O_{2.1} + (7.025 - 0.5\times y - 0.875\times z)(O_2 + \beta N_2) \longrightarrow (6.3 - y - 0.9\times z)CO_2 + (3.55 - 0.05\times z)\,H_2O + yCO + zC_{0.9}H_{0.1} + ((7.025 - 0.5\times y - 0.875\times z)\times\beta + 0.5)N_2$$

FDS input data file

- Treatment of combustion
  - (Extended) global combustion equation

$$C_{6.3}H_{7.1}N_1O_{2.1} + (7.025 - 0.5\times y - 0.875\times z)(O_2 + \beta N_2) \longrightarrow (6.3 - y - 0.9\times z)CO_2 + (3.55 - 0.05\times z)\,H_2O + yCO + zC_{0.9}H_{0.1} + ((7.025 - 0.5\times y - 0.875\times z)\times\beta + 0.5)N_2$$

$$\eta_{CO} = \frac{y\times M_{CO}}{M_{C_{6.3}H_{7.1}N_1O_{2.1}}}$$

$$\eta_{soot} = \frac{z\times M_{C_{0.9}H_{0.1}}}{M_{C_{6.3}H_{7.1}N_1O_{2.1}}}$$

FDS input data file

- Treatment of fuel pyrolysis occurring in flammable solid materials
  - OBST namelist group: specify location/properties of 3D solid object

```
*** First fuel package
&OBST XB= 1.40, 3.00, 3.80, 4.60, 0.40, 0.60, SURF_ID='UPHOLSTERY' /
Couch, seat cushions
&OBST XB= 1.20, 1.40, 3.80, 4.60, 0.00, 0.80, SURF_ID='UPHOLSTERY' /
Couch, armrest
&OBST XB= 3.00, 3.20, 3.80, 4.60, 0.00, 0.80, SURF_ID='UPHOLSTERY' /
Couch, armrest
&OBST XB= 1.40, 3.00, 4.40, 4.60, 0.60, 1.20, SURF_ID='UPHOLSTERY' /
Couch, back cushions
```

FDS input data file

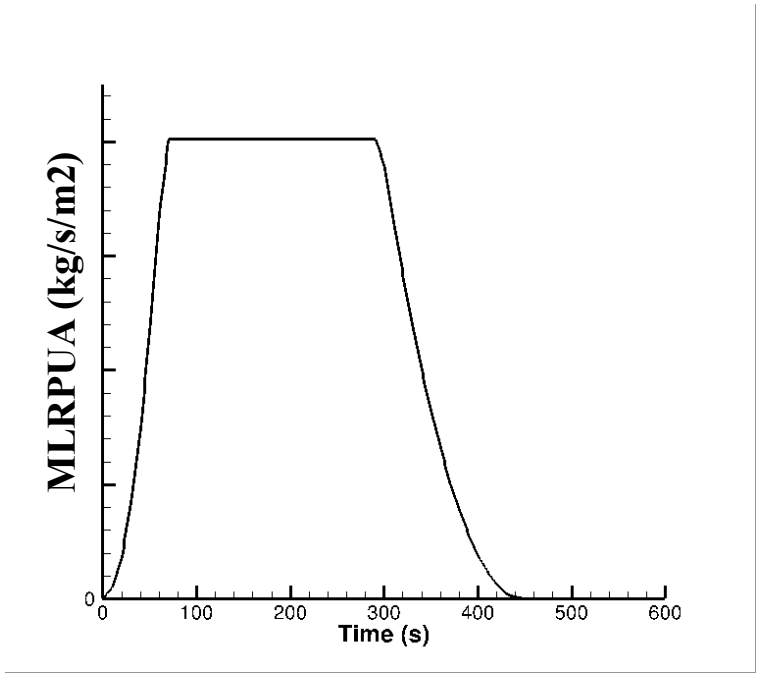
- Treatment of fuel pyrolysis occurring in flammable solid materials
  - SURF namelist group: specify surface boundary conditions (prescribed local fuel mass loss rate)

```
&SURF ID = 'UPHOLSTERY'
COLOR = 'MELON'
MATL_ID = 'FUEL1'
HRRPUA = 300.
RAMP_Q = 'HRR_FUEL1'
IGNITION_TEMPERATURE = 300.
HEAT_OF_VAPORIZATION = 500.
BACKING = 'INSULATED'
THICKNESS = 0.1 /
```

FDS input data file

- Treatment of fuel pyrolysis occurring in flammable solid materials
  - SURF namelist group: specify surface boundary conditions (prescribed local fuel mass loss rate)

```
&RAMP ID='HRR_FUEL1', T= 0.0,  F=0.000 /
&RAMP ID='HRR_FUEL1', T= 10.0, F=0.063 /
(…)
&RAMP ID='HRR_FUEL1', T= 40.0, F=1.000 /
&RAMP ID='HRR_FUEL1', T=203.0, F=1.000 /
&RAMP ID='HRR_FUEL1', T=210.0, F=0.703 /
(…)
&RAMP ID='HRR_FUEL1', T=244.0, F=0.000 /
&RAMP ID='HRR_FUEL1', T=600.0, F=0.000 /
```



FDS input data file

- Treatment of fuel pyrolysis occurring in flammable solid materials
  - MATL namelist group: specify thermal properties of material

```
 &MATL ID = 'FUEL1'
FYI = 'Properties do not correspond to a real material'
CONDUCTIVITY = 0.1
DENSITY = 500
SPECIFIC_HEAT = 1
EMISSIVITY = 0.85 /
```

FDS input data file

- Treatment of ignition
  - MATL namelist group: specify thermal properties of material

```
&SURF ID='BURNER', HRRPUA=1000., RAMP_Q='HRR_BURNER', COLOR='RED' /
&RAMP ID='HRR_BURNER', T= 0.0,   F=0.0  /
&RAMP ID='HRR_BURNER', T= 1.0,   F=1.0  /
&RAMP ID='HRR_BURNER', T= 180.0, F=1.0  /
&RAMP ID='HRR_BURNER', T= 181.0, F=0.0  /
&VENT XB= 2.40, 2.60, 3.40, 3.60, 0.00, 0.00, SURF_ID='BURNER' / Ignition source near couch
```

$$HRR = HRRPUA \times (0.2 \times 0.2) = 1000 \times (0.2 \times 0.2) = 40 \text{ kW}$$

FDS input data file

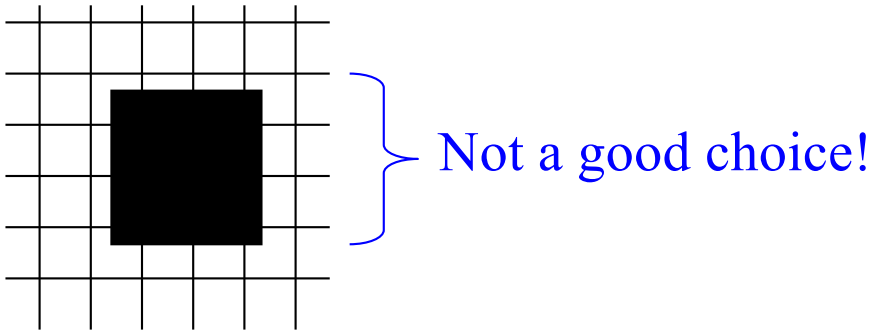
- Coordinates of volumes/surfaces and grid resolution

  $\Delta x = \Delta y = \Delta z = 0.1$ m.

  - Grid lines are distributed every 10 cm from the boundaries of the computational domain
  - Spatial coordinates of vents and obstructions need to match grid line locations

&OBST XB= 1.40, 3.00, 3.80, 4.60, 0.40, 0.60, SURF_ID='UPHOLSTERY' /

  - **Caution:** match object boundaries with grid lines



FDS input data file

- Diagnostics
  - SLCF: generate animation/graphic files readable in Smokeview for a simulated QUANTITY evaluated in a plane surface

```
*** Gas phase
&SLCF PBX=2.50, QUANTITY='HRRPUV' /
&SLCF PBX=2.50, QUANTITY='TEMPERATURE' /
&SLCF PBX=2.50, QUANTITY='VELOCITY', VECTOR=T /
&SLCF PBX=2.50, QUANTITY='VOLUME FRACTION', SPEC_ID='OXYGEN' /
```

FDS input data file

- Diagnostics
  - DEVC: generate .csv file readable in Excel for a simulated QUANTITY measured at a point, or integrated across a surface or a volume

```
*** Gas phase
&DEVC XB= 4.00, 5.00, 0.00, 0.00, 0.00, 2.00, QUANTITY='MASS FLOW',
ID='MFR' / Integrated diagnostics
&DEVC XB= 4.00, 5.00, 0.00, 0.00, 0.00, 2.00, QUANTITY='MASS FLOW +',
ID='MFRp' / (Door)
&DEVC XB= 4.00, 5.00, 0.00, 0.00, 0.00, 2.00, QUANTITY='MASS FLOW -',
ID='MFRm' /
```

$$\dot{m}_{net} = \dot{m}_{in} - \dot{m}_{out}$$

$$\dot{m}_{in} = \dot{m}''_{in} \times A_{door}$$

$$\dot{m}_{out} = \dot{m}''_{out} \times A_{door}$$

FDS input data file

- Diagnostics
  - DEVC: generate .csv file readable in Excel for a simulated QUANTITY measured at a point, or integrated across a surface or a volume

```
*** Solid phase
&DEVC ID='QIN', XYZ = 2.6,2.3,0.0, IOR = +3, QUANTITY = 'TOTAL HEAT FLUX' / Local diagnostics
&DEVC ID='QRAD', XYZ = 2.6,2.3,0.0, IOR = +3, QUANTITY = 'RADIATIVE HEAT FLUX' / (Floor)
&DEVC ID='QCONV', XYZ = 2.6,2.3,0.0, IOR = +3, QUANTITY = 'CONVECTIVE HEAT FLUX' /
&DEVC ID='G', XYZ = 2.6,2.3,0.0, IOR = +3, QUANTITY = 'INCIDENT HEAT FLUX' /
&DEVC ID='Twall', XYZ = 2.6,2.3,0.0, IOR = +3, QUANTITY = 'WALL TEMPERATURE' /
```

$$\dot{q}''_{net} = \dot{q}''_{rad} + \dot{q}''_{conv}$$
$$= \left(\epsilon_{surf} G - \epsilon_{surf} \sigma T_{surf}^4\right) + h\left(T_g - T_{surf}\right)$$

FDS input data file

- Diagnostics
  - DEVC: generate .csv file readable in Excel for a simulated QUANTITY measured at a point, or integrated across a surface or a volume

*** Solid phase
&DEVC ID='MLRPUA', XYZ = 2.6,2.3,0.0, IOR = +3, QUANTITY = 'BURNING RATE' /
&DEVC XB=0.00,5.20,0.00,4.60,0.00,0.00, QUANTITY='BURNING RATE', SPATIAL_STATISTIC='SURFACE INTEGRAL', ID='MLR-carpet' / Integrated diagnostics

$$\dot{m}_f''$$

$$\dot{m}_f = \dot{m}_f'' \times A_{surface}$$

FDS input data file

- Diagnostics
  - BNDF: generate animation/graphic files readable in Smokeview for a simulated QUANTITY evaluated on all solid surfaces

```
*** Solid phase
&BNDF QUANTITY='GAUGE HEAT FLUX'  /
&BNDF QUANTITY='WALL TEMPERATURE' /
&BNDF QUANTITY='BURNING RATE'     /
```

FDS output files

- *filename.out*: basic output file used for checking correct reading of input variables and for monitoring progress of ongoing calculation; MUST BE READ!

Fire Dynamics Simulator

Current Date : May 26, 2022 12:13:19
Revision : **FDS6.7.7-0-gfe0d4ef38-release**
Revision Date : Thu Nov 18 17:10:22 2021 -0500
Compiler : Intel ifort 2021.4.0
Compilation Date : Nov 19, 2021 08:14:42

MPI Enabled; Number of MPI Processes: 1
OpenMP Enabled; Number of OpenMP Threads: 4

MPI version: 3.1
MPI library version: Open MPI v4.1.0, package: Open MPI gforney@bevo.el.nist.gov Distribution, ident: 4.1.0, repo rev: v4.1.0, Dec 18, 2020

Job TITLE : Example room fire simulation
Job ID string : CompartmentFire1

Grid Dimensions, Mesh 1

• • •

FDS output files

- *CHID_hrr.csv*: time history of useful global quantities

s	kW	kW	kW	kW	kW	kW	kW	kW	kW	kg/s	kg/s	kg/s
Time	HRR	Q_RADI	Q_CONV	Q_COND	Q_DIFF	Q_PRES	Q_PART	Q_ENTH	Q_TOTAL	MLR_AIR	MLR_POLYURETHANE	MLR_PRODUCTS
0.00E+00	0.00E+00	-5.44E-04	-1.20E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-5.44E-04	0.00E+00	0.00E+00	0.00E+00
1.01E+00	1.78E+01	-7.76E+00	1.58E-01	-1.09E-01	3.12E-03	0.00E+00	0.00E+00	8.28E+00	1.00E+01	0.00E+00	1.15E-03	0.00E+00
2.00E+00	4.12E+01	-1.24E+01	4.70E-01	-6.46E-01	6.75E-03	0.00E+00	0.00E+00	2.85E+01	2.87E+01	0.00E+00	2.10E-03	0.00E+00
3.01E+00	4.02E+01	-1.24E+01	4.65E-01	-7.55E-01	7.05E-03	0.00E+00	0.00E+00	2.75E+01	2.75E+01	0.00E+00	2.10E-03	0.00E+00
4.00E+00	4.00E+01	-1.23E+01	4.48E-01	-1.14E+00	7.03E-03	0.00E+00	0.00E+00	2.70E+01	2.70E+01	0.00E+00	2.10E-03	0.00E+00
5.02E+00	3.98E+01	-1.24E+01	4.62E-01	-1.70E+00	7.02E-03	0.00E+00	0.00E+00	2.61E+01	2.61E+01	0.00E+00	2.10E-03	0.00E+00
6.02E+00	3.93E+01	-1.25E+01	4.15E-01	-2.17E+00	6.80E-03	0.00E+00	0.00E+00	2.51E+01	2.51E+01	0.00E+00	2.10E-03	0.00E+00
7.01E+00	4.04E+01	-1.27E+01	4.31E-01	-2.63E+00	6.92E-03	0.00E+00	0.00E+00	2.54E+01	2.55E+01	0.00E+00	2.10E-03	0.00E+00
8.01E+00	3.98E+01	-1.27E+01	4.08E-01	-2.98E+00	6.64E-03	0.00E+00	0.00E+00	2.45E+01	2.45E+01	0.00E+00	2.10E-03	0.00E+00
9.01E+00	4.01E+01	-1.23E+01	4.21E-01	-3.16E+00	6.69E-03	0.00E+00	0.00E+00	2.51E+01	2.51E+01	0.00E+00	2.10E-03	0.00E+00
1.00E+01	3.99E+01	-1.28E+01	4.08E-01	-3.49E+00	6.32E-03	0.00E+00	0.00E+00	2.41E+01	2.40E+01	0.00E+00	2.10E-03	0.00E+00
1.10E+01	4.01E+01	-1.27E+01	3.98E-01	-3.98E+00	5.91E-03	0.00E+00	0.00E+00	2.38E+01	2.39E+01	0.00E+00	2.11E-03	0.00E+00
1.20E+01	4.05E+01	-1.28E+01	4.12E-01	-4.12E+00	5.50E-03	0.00E+00	0.00E+00	2.40E+01	2.40E+01	0.00E+00	2.11E-03	0.00E+00
1.30E+01	3.93E+01	-1.27E+01	3.79E-01	-4.37E+00	5.05E-03	0.00E+00	0.00E+00	2.26E+01	2.26E+01	0.00E+00	2.11E-03	0.00E+00
1.40E+01	4.02E+01	-1.28E+01	3.99E-01	-4.41E+00	4.57E-03	0.00E+00	0.00E+00	2.34E+01	2.34E+01	0.00E+00	2.11E-03	0.00E+00
1.50E+01	4.01E+01	-1.30E+01	3.89E-01	-4.44E+00	3.78E-03	0.00E+00	0.00E+00	2.31E+01	2.31E+01	0.00E+00	2.11E-03	0.00E+00
1.60E+01	4.01E+01	-1.27E+01	3.80E-01	-4.41E+00	3.18E-03	0.00E+00	0.00E+00	2.33E+01	2.34E+01	0.00E+00	2.12E-03	0.00E+00
1.70E+01	4.06E+01	-1.33E+01	3.66E-01	-4.51E+00	2.63E-03	0.00E+00	0.00E+00	2.32E+01	2.32E+01	0.00E+00	2.12E-03	0.00E+00
1.80E+01	4.02E+01	-1.31E+01	3.68E-01	-4.51E+00	2.02E-03	0.00E+00	0.00E+00	2.29E+01	2.29E+01	0.00E+00	2.12E-03	0.00E+00
1.90E+01	4.00E+01	-1.30E+01	3.90E-01	-4.42E+00	1.19E-03	0.00E+00	0.00E+00	2.31E+01	2.30E+01	0.00E+00	2.12E-03	0.00E+00
2.00E+01	4.05E+01	-1.34E+01	7.37E-03	-4.57E+00	-1.16E-04	0.00E+00	0.00E+00	2.25E+01	2.25E+01	0.00E+00	2.13E-03	0.00E+00
2.10E+01	4.09E+01	-1.34E+01	-1.34E+00	-4.55E+00	-1.44E-03	0.00E+00	0.00E+00	2.16E+01	2.16E+01	0.00E+00	2.13E-03	0.00E+00

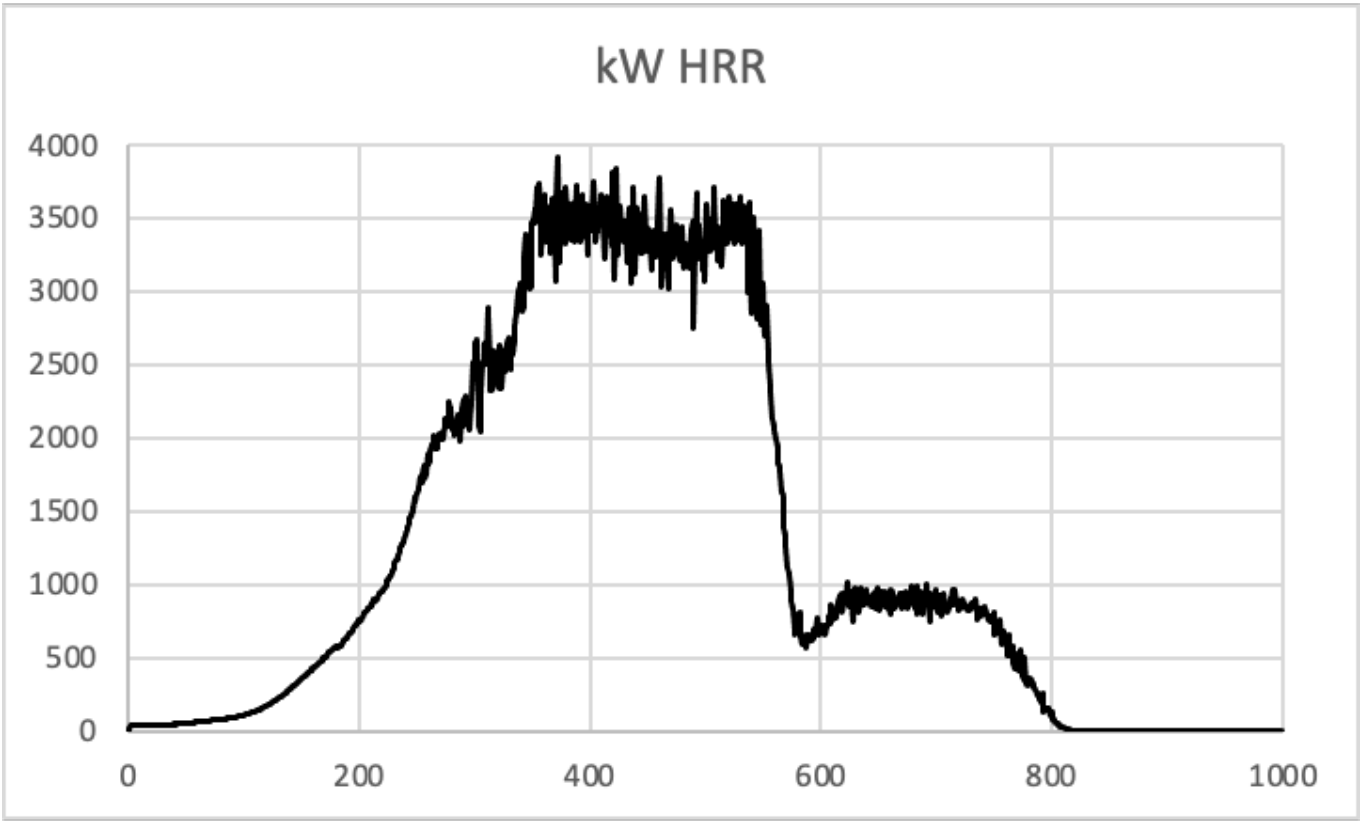
1st column time **2nd column HRR** **next-to-last column Fuel MLR**

FDS output files

- *CHID_nnnn_nnn.sf*: graphics SLCF files
- *CHID_nnnn_nnn.bf*: graphics BNDF files

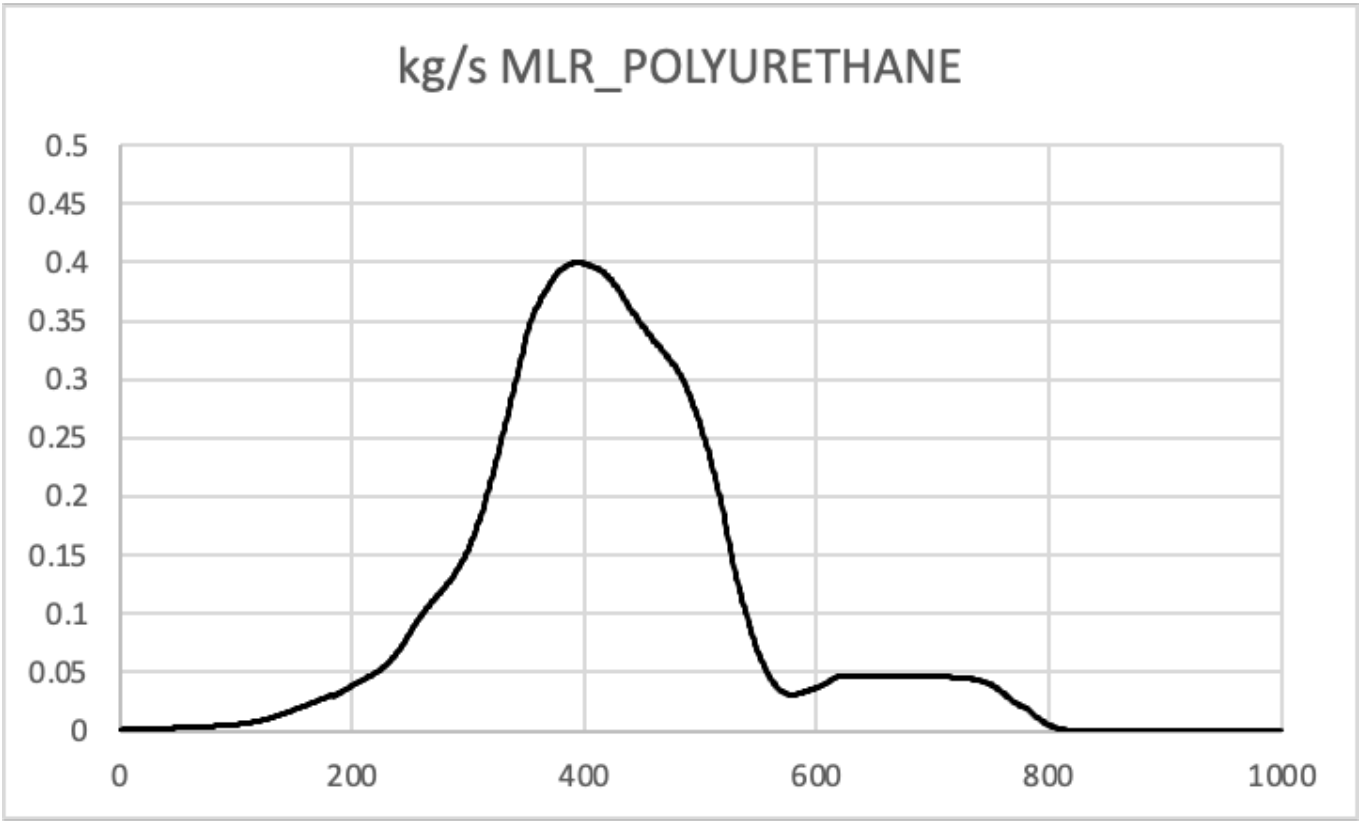
FDS example

- *CompartmentFire1_hrr.csv*
  - HRR ($0 \leq t \leq 1000$ s)



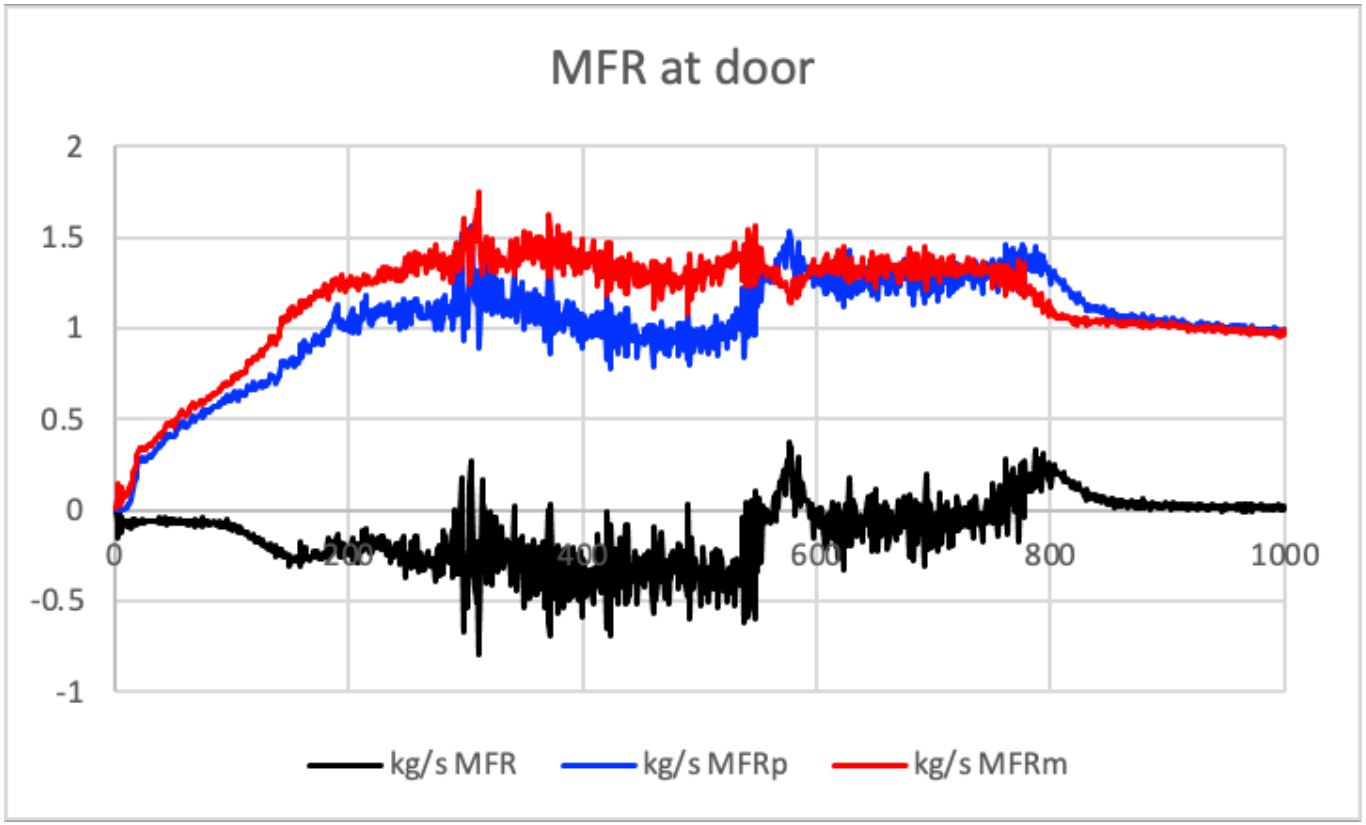
FDS example

- *CompartmentFire1_hrr.csv*
  - MLR ($0 \leq t \leq 1000$ s)



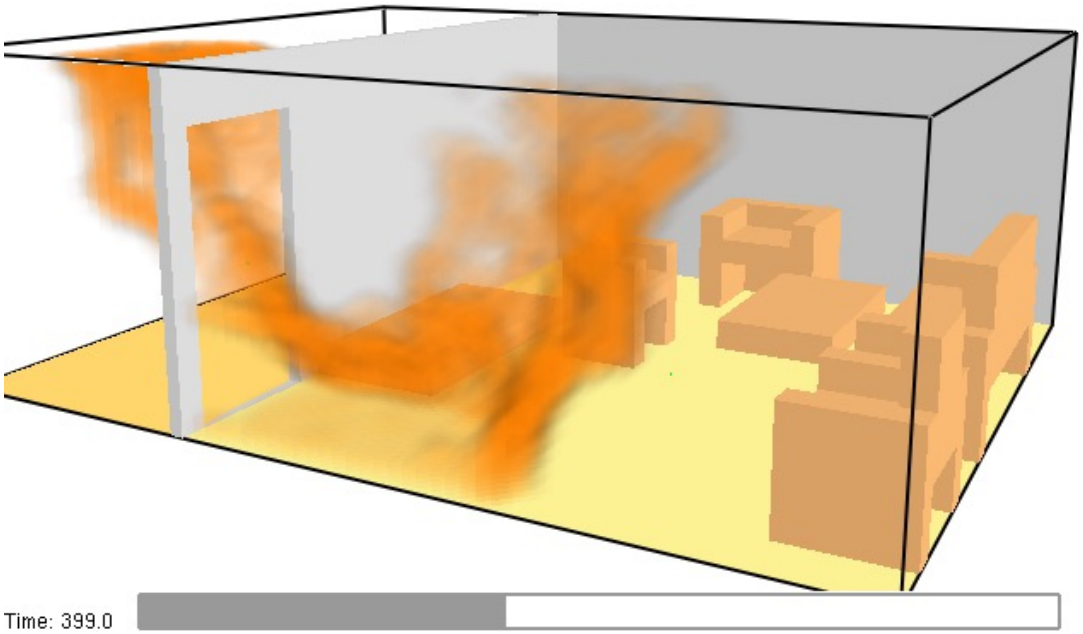
FDS example

- *CompartmentFire1_devc.csv*
  - Vent mass flow rates ($0 \leq t \leq 1000$ s)



FDS example

- *CompartmentFire1.smv*
  - Flame visualization (t = 399 s)



Summary

- The overall code structure and basic input/output files of FDS have been reviewed
  - There is no pre-processor provided with FDS and the users are generally expected to edit the input files manually or to use a separate software (*PyroSim*)
  - *Smokeview* is available to the users. Other graphics packages may also be used for post-processing tasks
- **To-do list**
  - Install FDS on your own computer or make sure that you have access to a computer that runs FDS
  - Download *CompartmentFire1.fds* from http://gdrfeux.univ-lorraine.fr/ecole2022/, then run FDS
  - Check results with *Excel* and *Smokeview*