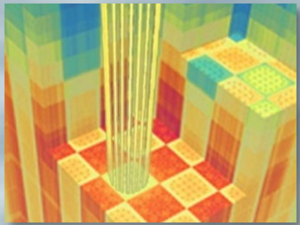
VERA Training: 3D Assemblies

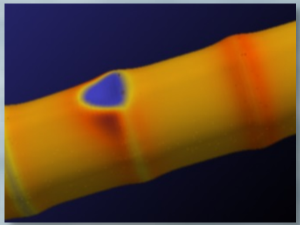
VERA Training – Core Simulator

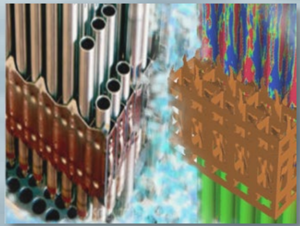
February 13, 2019

VERA Users Group Meeting

Oak Ridge National Laboratory







CASL
The Consortium for Advanced Simulation of LWRs
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Training Objectives

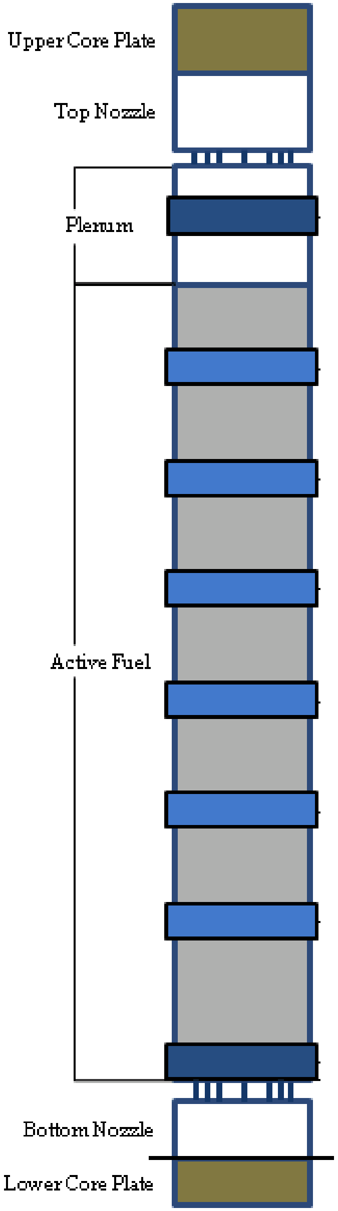
Learn how to:

- Set up 3D Problems
- Set axial mesh
- Add grids, nozzles, core plates, etc.
- Set number of cores
- Add T/H Feedback with CTF
- Run Multiple Statepoints

3D Assemblies

- Setting up 3D problems is very similar to 2D problems
- Instead of a single 2D lattice, you need to define multiple 2D lattices for each unique axial "slice" of the assembly
  - Fuel Region
  - Blankets (if present)
  - Plenum
  - End Plugs
  - Gap regions
- Add top/bottom core plates and nozzles
- Add grids

All axial elevations are relative to top of lower core plate



3D Assembly Elevations

```
[ASSEMBLY]
  cell 1     0.4096 0.418 0.475 / U31 he zirc4
  cell 3            0.561 0.602 / mod    zirc4      ! guide/instrument tube
  cell 4            0.418 0.475 /     he zirc4      ! plenum
  cell 5                  0.475 /        zirc4      ! end plug
  cell 6                  0.475 /        mod        ! empty

  lattice FUEL
       3
       1 1
       1 1 1
       3 1 1 3
       1 1 1 1 1
       1 1 1 1 1 3
       3 1 1 3 1 1 1
       1 1 1 1 1 1 1 1
       1 1 1 1 1 1 1 1 1

  lattice PLEN
       3
       4 4
       4 4 4
       3 4 4 3
       4 4 4 4 4
       4 4 4 4 4 3
       3 4 4 3 4 4 4
       4 4 4 4 4 4 4 4
       4 4 4 4 4 4 4 4 4
```

```
  lattice PLUG
       3
       5 5
       5 5 5
       3 5 5 3
       5 5 5 5 5
       5 5 5 5 5 3
       3 5 5 3 5 5 5
       5 5 5 5 5 5 5 5
       5 5 5 5 5 5 5 5 5

  lattice GAP
       3
       6 6
       6 6 6
       3 6 6 3
       6 6 6 6 6
       6 6 6 6 6 3
       3 6 6 3 6 6 6
       6 6 6 6 6 6 6 6
       6 6 6 6 6 6 6 6 6
```

```
  axial ASSY
              6.053
        GAP   10.281
        PLUG  11.951
        FUEL 377.711
        PLEN 393.711
        PLUG 395.381
        GAP  397.51
```

assembly name

lattice names

Elevations

3D Core Plates and Nozzles

```
[CORE]
  size   1              ! one assembly
  rated  17.67 0.6823   ! MW, Mlbs/hr
  apitch 21.5
  height 406.337        ! Distance between core plates

  core_shape
    1

  assm_map
    ASSY

  lower_plate ss  5.0 0.5   ! mat, thickness, vol frac
  upper_plate ss  7.6 0.5

  bc_rad reflecting         ! No reflecting BC on top and
bottom
```

Need correct rated power for an assembly, and correct core height

Core plates apply to all assemblies, so they are in CORE block

```
[ASSEMBLY]

  lower_nozzle  ss 6.053 6250.0  ! mat, height, mass (g)
  upper_nozzle  ss 8.827 6250.0  ! mat, height, mass (g)
```

Different assemblies can have different nozzle descriptions

Nozzles and core plates are modeled as “smeared” materials, the material is smeared with coolant

3D Assembly Grids

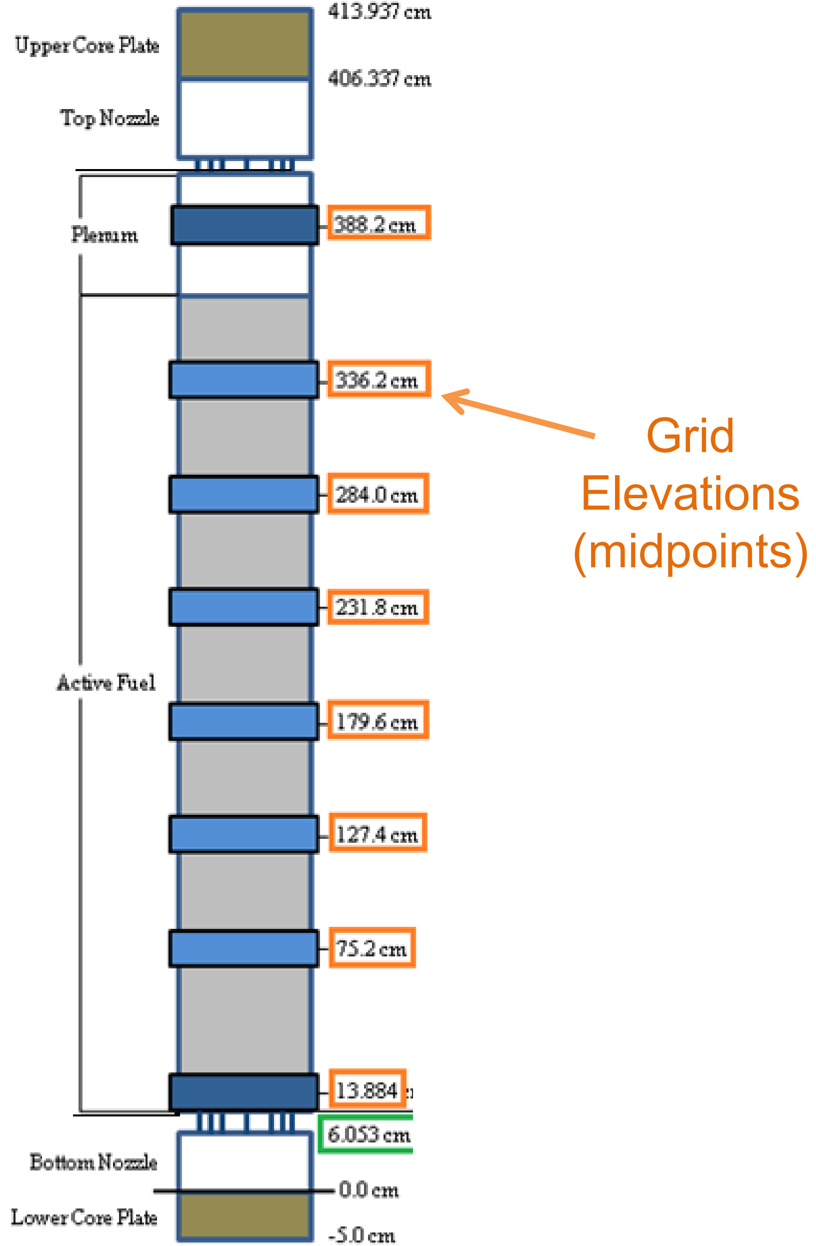
Define grid types
(usually inconel and zirc)
and grid midpoints

```
[ASSEMBLY]

! Grid types: name, mass (g), height (cm),

  grid END inc    3.866 1017
  grid MID zirc4  3.810 875

  grid_axial
      END  13.884
      MID  75.2
      MID 127.4
      MID 179.6
      MID 231.8
      MID 284.0
      MID 336.2
      END 388.2
```

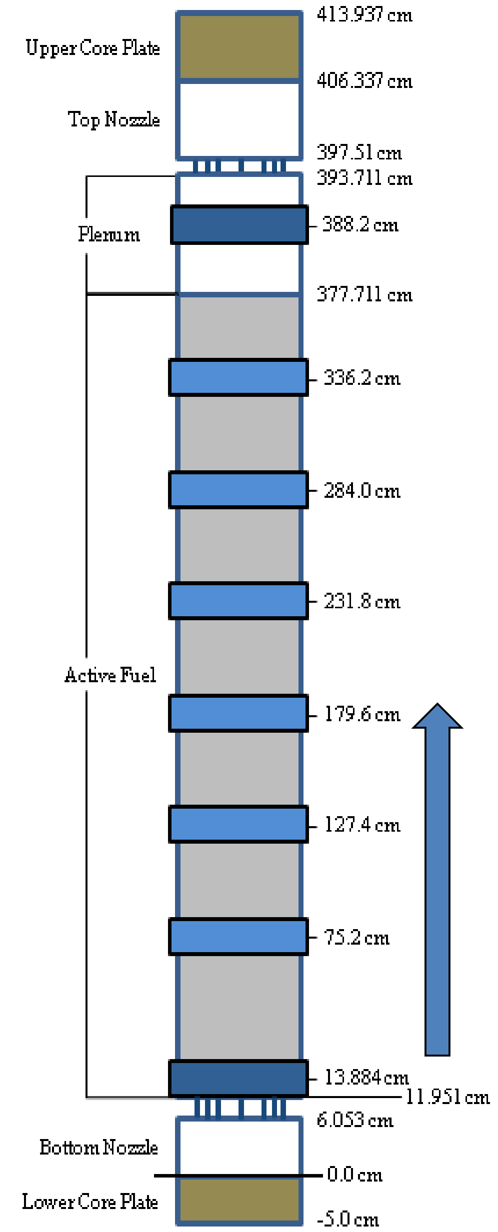


* Note format of grid card changed in 3.7

3D Mesh

- The axial edit bounds set the mesh for both the axial edits and T/H coupling
- All user-specified axial boundaries in the assembly descriptions, and the grid boundaries must be included (tedious)
- The code adds planes automatically above and below the core plates.
- Typical mesh sizes range from 3-4" between spacer grids and fuel boundaries
- Meshes should also be added at burnable poison boundaries, if possible
- Thin regions (less than a few cm's) should be avoided

```
[EDITS]
  axial_edit_bounds
      11.951
      15.817
      24.028
      32.239
      40.45
      48.662
      56.873
      65.084
      73.295
      77.105
      85.17
      93.235
      101.3
      109.365
      117.43
      125.495
      129.305
      137.37
      145.435
      153.5
      161.565
      169.63
      177.695
      181.505
      189.57
      197.635
      205.7
      213.765
      221.83
      229.895
      233.705
      241.77
      249.835
      257.9
      265.965
      274.03
      282.095
      285.905
      293.97
      302.035
      310.1
      318.165
      326.23
      334.295
      338.105
      346.0262
      353.9474
      361.8686
      369.7898
      377.711
```



Parallel Decomposition

- Domain decomposition can be used to split problem up into axial and radial parallel regions
- Total number of CPU cores
  = axial regions x radial regions
- Radial decomposition will be described in full-core section
- Axial decomposition is done by plane
- With N planes, **you can assign from 1 to N CPU cores to problem**

Axial Mesh

- Note that it is not always obvious how many axial planes are in the problem due to the automatic treatment of the top and bottom planes (above and below active fuel)
- Often you have to run the problem once, then look at the edits.

```
============== Axial Mesh Data ==============
 =============================================
 AutoMesh Method          =          NONFUEL
 Minimum Axial Mesh       =  2.0000000000000
 Maximum Axial Mesh       =  20.000000000000
 Number of Axial Meshes =       58
 Mesh regions, starting from the bottom:
       Mesh Region       Mesh Thickness          Lower Height       Upper Height
             1          5.0000000000000         0.0000000000000         5.0000000000000
             2          6.0530000000000         5.0000000000000         11.053000000000
             3          5.8980000000000         11.053000000000         16.951000000000
             4          3.8660000000000         16.951000000000         20.817000000000
             5          8.2110000000000         20.817000000000         29.028000000000
             6          8.2110000000000         29.028000000000         37.239000000000
             7          8.2110000000000         37.239000000000         45.450000000000
           ……
            49          7.9212000000000         351.02620000000         358.94740000000
            50          7.9212000000000         358.94740000000         366.86860000000
            51          7.9212000000000         366.86860000000         374.78980000000
            52          7.9212000000000         374.78980000000         382.71100000000
            53          8.5560000000000         382.71100000000         391.26700000000
            54          3.8660000000000         391.26700000000         395.13300000000
            55          3.5780000000000         395.13300000000         398.71100000000
            56          3.7990000000000         398.71100000000         402.51000000000
            57          8.8270000000000         402.51000000000         411.33700000000
            58          7.6000000000000         411.33700000000         418.93700000000
```

58 axial planes in problem 3a

Load Balance

- To get the best performance, you should try to balance the computational load as evenly as possible
- Set the problem up so each core has same “load”, i.e. same number of axial planes
- For fastest run-time, use one plane per core
- For less CPU usage, use two or three planes per core
- Example – 58 axial planes
  - With 58 cores, there is one plane per core
  - With 29 cores, there is two planes per core
  - Using something in between (like 35) will not be any faster because some cores will have 1 plane and some cores will have 2 planes.
  - Run-time is dictated by the “slowest” core.

Setting Number of Nodes with PBS

- Computer nodes have multiple cores
- You can only request jobs with integer multiples of "nodes"
  - Lemhi has 40 cores/node (ppn – processors per node)
  - Other computers might have 12 or 24 or 32
- To find number of "nodes", divide total number of cores needed by cores/node, then round up
- For example, if you need 58 cores
  - 58/32=1.8125, so request 2 nodes
  - `#PBS -l nodes=2:ppn=32`
- You may run with more nodes and less cores/node if you need more memory (rarely needed)
- This is now automated, but you should be aware

Run Script automatically calculates correct number of nodes

Set Number of Cores

- Set number of cores in MPACT input

```
[MPACT]
  num_space 58  ! Axial decomposition
```

- Run script will calculate number of processors, create PBS run script (.pbs file), and submit it

Class Exercise 5: Run 3D Problem

- The 3D sample problem is "3a.inp"

```
cp $VERAHOME/share/VERAIn/Progression_Problems/3a.inp .
```

- The 3D Problems take longer to run, so you should use more cores and space decomposition than the 2D problem
- If possible, a good solution is to run one axial plane per core (or two planes per core)
- The sample input has 58 cores, but this can be changed

Copy Sample Input and Run

3D Questions for Discussion

- How do you add IFBA to 3D Problems?
  - You may need different axial zones for IFBA and/or blankets
- How do you add WABA to 3D Problems?
  - Need to add different axial zones in the INSERT block for WABA and/or blankets
  - Make sure the elevations in the INSERT block match the ASSEMBLY block
  - Add WABA axial boundaries to EDIT regions
- How do you deplete in 3D?
  - Same way as 2D

3D Assembly Output

```
*****************************************************************************
****************************** STATE_0001 ***********************************
*****************************************************************************

     State Summary
     -----------------------
     Core Exposure           0.00 MWD/MTHM
     Relative Power          0.00 %
     Thermal Power           0.00 MWt
     Relative Flow         100.00 %
     Absolute Flow          21.49 kg/s
     Inlet Temperature     326.85 C
     Boron Conc.          1300.00 ppm
     k-eff                   1.17586
```

Runs in about 0:45 min on 58 cores,
1:15 min on 29 cores
2:17 min on 16 cores
3D Visualization will be covered in later sections

Thermal-Hydraulic Feedback

- Next step is to add T/H feedback by Coupling to CTF
- Need to define realistic conditions so flow remains subcooled
  - core power
  - inlet temperature
  - coolant flowrate
  - core pressure
- Turn on "feedback"
- Need to generate a CTF input deck

```
[STATE]
  power    100.0   ! %
  flow     100.0   ! %
  tinlet   565 F
  pressure 2250    ! psia
  feedback on


[CORE]
  rated   17.67 0.6823    ! MW, Mlbs/hr
```

Generate CTF Input Deck

- CTF needs a separate input deck that is automatically generated from the XML file
- The CTF pre-processor is run with the command:

```
xml2ctf --xmlfile=p6.xml
```

- In the sample script, the CTF pre-processor is automatically called when "feedback" is turned on
- Run script will automatically do this, but you will notice some "deck.*" files in your run directory
- One drawback – you cannot run more than one coupled problems in the same directory at the same time

Run Script will automatically generate CTF input files

Parallel CTF

- CTF parallel decomposition is only on the assembly or quarter-assembly level (1 or 4 or 9 cores per assembly)
- CTF cannot be split into different axial planes.
- When running CTF in parallel, the preprocessor will create many CTF input decks
  - One input deck for each assembly named "deck.N.n.inp", where "N" is the total number of assemblies and "n" is the specific assembly number.
  - One master input deck "deck.master.inp"
  - (yes, it clutters up your directory)

```
[COBRATF]
  parallel 1   ! Parallel on
```

CTF cannot be run in parallel for single assembly problems

Class Exercise 6: Run Coupled Job (p6)

- Create subdirectory and copy sample problem

```
mkdir run_p6
cd run_p6
```

- Copy sample file from training directory

```
cp $VERAHOME/share/VERAIn/Progression_Problems/p6.inp .
```

- Run Job

```
verarun p6
```

- Wait….
- Check queue

```
qstat
```

Copy Input file and Submit

3D Coupled Problem Output

```
******************************************************************************
*************************** STATE_0001 ***********************************
******************************************************************************

    State Summary
    -----------------------
    Core Exposure            0.00 MWD/MTHM
    Relative Power         100.00 %
    Thermal Power            4.42 MWt
    Relative Flow          100.00 %
    Absolute Flow           21.49 kg/s
    Inlet Temperature      291.85 C
    Boron Conc.           1300.00 ppm
    k-eff                    1.16483
```

Runs in about 5:43 min on 58 cores

(Longer run-times due to CTF not being parallel)

Submit other jobs if time permits…

- Submit IFBA or WABA jobs
- Submit 3D depletion jobs

Multiple Statepoints

- You can run multiple statepoints in a single job by specifying different [STATE] blocks
- Variables "carry-over" from previous state

```
[STATE]
  power     100.0    ! %
  flow      100.0    ! %
  tfuel     556 F
  tinlet    556 F
  boron     975      ! ppm
[STATE]
  tinlet    564 F    ! ITC ARO
  tfuel     564 F
[STATE]
  rodbank D 0
  boron     902      ! ppm
  tinlet    556.0
  tfuel     556
[STATE]
  tinlet    564
  tfuel     564      ! ITC Bank D inserted
```

Multiple Statepoints (2)

- For compact input, you can also use semicolons to separate variables

```
[STATE]  power  48.7;  deplete EFPD   6.43
[STATE]  power  98.7;  deplete EFPD  24.54
[STATE]  power  62.8;  deplete EFPD  31.07
[STATE]  power  99.8;  deplete EFPD  36.13
[STATE]  power 100.0;  deplete EFPD  51.86
[STATE]  power  93.8;  deplete EFPD  79.07
[STATE]  power  99.6;  deplete EFPD 110.64
[STATE]  power  98.9;  deplete EFPD 137.00
[STATE]  power  35.5;  deplete EFPD 137.50
[STATE]  power  35.5;  deplete EFPD 138.58
[STATE]  power  80.0;  deplete EFPD 144.18
[STATE]  power  99.7;  deplete EFPD 155.65
[STATE]  power  99.3;  deplete EFPD 180.05
[STATE]  power  99.9;  deplete EFPD 208.66
[STATE]  power  99.5;  deplete EFPD 235.09
[STATE]  power  99.9;  deplete EFPD 265.81
[STATE]  power  99.8;  deplete EFPD 295.96
[STATE]  power   0.1;  deplete EFPD 304.00
```

Questions?

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