File-Based One-Way BISON Coupling in VERA: Overview

Oak Ridge National Laboratory
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Setup

• We’ll start by copying files over to your home dir:
  
  ```
  cp -r /projects/vera-users-grp/training/session10 .
  ```

  ```
  cd session10
  ```

• And do a quick `ls -l` command:

```bash
drwxrwsr-x 2 stimshan vera-users-grp 52 Feb 6 11:10 bison_from_vera
drwxrwsr-x 2 stimshan vera-users-grp 52 Feb 6 11:11 bison_from_vera_1.5D
drwxrwsr-x 2 stimshan vera-users-grp 52 Feb 6 11:11 bison_from_vera_ifba
drwxrwsr-x 2 stimshan vera-users-grp 52 Feb 6 11:11 bison_from_vera_silicide
drwxrwsr-x 2 stimshan vera-users-grp 52 Feb 6 11:12 mpact
drwxrwsr-x 2 stimshan vera-users-grp 72 Feb 6 11:12 qtr_core
drwxrwsr-x 2 stimshan vera-users-grp 113 Feb 6 11:09 templates
drwxrwsr-x 2 stimshan vera-users-grp 52 Feb 6 11:12 temp_table
```
mpact run.pbs

- Open run.pbs:

```bash
# parse input
if $verain; then
    if [ -f $case.xml ]; then rm -f $case.xml; fi
    echo "=================================================="
    echo "  Parsing VERA input $case.inp"
    echo "=================================================="
    perl $parser $case.inp $case.xml
    ls -l $case.xml
    date
    echo
fi

# run MPACT
if $mpact; then
    if [ -f $case.xml ]; then
        #if [ -f *.res ]; then rm -f *.res; fi
        echo "=================================================="
        echo "  Running MPACT Job on $cores cores"
        echo "=================================================="
        mpirun -n $cores $exe $case.xml
        date
    fi
fi
```
Once you understand what it will do, run `qsub run.pbs`:
This will take about 10 minutes...we’ll come back
Outline

• BISON Within VERA
  – Tiamat, Tiamat-Inline, **Offline**
  – Fuel Temperature Tables
• Generating Standalone Inputs
• Executing BISON
• Post-Processing
  – Outputs Available
  – Running bison_post
  – VERAView
• Current Target Application (WBN1)
  – Cycle 1-3 Results
  – AP1000 Rod Ejection
  – Recent ATF Progress
Motivation

• MPACT/CTF have become more mature
  – More attention to additional physics (fuel performance, coolant chemistry, etc.)
• BISON
  – Developed by INL and built on the MOOSE framework
  – high-fidelity, finite element-based fuel performance simulations
  – swelling, densification, relocation, gap closure, clad creep, etc.
  – Used in several applications within CASL:
    • Tiamat (more tightly coupled simulations)
    • Fuel Temperature Tables for VERA-CS
• File-based one-way coupling reads the VERA output HDF5 and populates input files that BISON can process:
  – Normalized Axial Power Distribution
  – Rod Power History
  – Moderator Temperature Distribution or Clad Outer Surface Temperature
  – Links multicycle data up, following a rod throughout its history
Fuel Temperature Tables

• VERA currently uses pre-tabulated tables to provide more accurate fuel temperatures
  – Tables are based on the difference between the fuel temperature and the moderator temperature
  – \( \Delta T = aP + bP^2 \)

• Improvements have been made to the BISON tables:
  – Adopted a uniform LHR approach
  – Allows for higher burnups and powers

• Can generate tables using volume-averaged fuel temperature or effective fuel temperature
Example Table Results
Generating Standalone Inputs
VERA ASCII Input – General Overview

- We’ll cover more details of the VERA ASCII input in the examples, though most of you have some experience already:
  - STATE
    - boron
    - power
    - depletion steps
  - ASSEMBLY
  - INSERT
  - CONTROL
  - CORE

- Separate input files are necessary for each cycle and shuffle (more)
Generating Standalone Inputs
VERA ASCII Input – Shuffling Specification

• Managed through the shuffle_label card in the STATE block

<table>
<thead>
<tr>
<th>Shuffle Label</th>
<th>3B-10</th>
<th>4G-2</th>
<th>4H-1</th>
<th>4A-11</th>
<th>4H-13</th>
<th>4M-2</th>
<th>3K-14</th>
</tr>
</thead>
<tbody>
<tr>
<td>L-1</td>
<td>P-6</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>B-12</td>
</tr>
<tr>
<td>K-2</td>
<td>+</td>
<td>+</td>
<td>F-14</td>
<td>+</td>
<td>N-4</td>
<td>+</td>
<td>J-4</td>
</tr>
<tr>
<td>R-7</td>
<td>+</td>
<td>R-9</td>
<td>L-10</td>
<td>+</td>
<td>A-5</td>
<td>H-14</td>
<td>J-1</td>
</tr>
<tr>
<td>3N-6</td>
<td>+</td>
<td>B-7</td>
<td>+</td>
<td>R-11</td>
<td>H-3</td>
<td>+</td>
<td>D-3</td>
</tr>
<tr>
<td>4A-6</td>
<td>+</td>
<td>C-8</td>
<td>+</td>
<td>C-14</td>
<td>+</td>
<td>E-1</td>
<td>P-7</td>
</tr>
<tr>
<td>4C-2</td>
<td>+</td>
<td>D-13</td>
<td>+</td>
<td>P-12</td>
<td>F-7</td>
<td>+</td>
<td>C-12</td>
</tr>
<tr>
<td>4P-11</td>
<td>+</td>
<td>K-9</td>
<td>M-13</td>
<td>+</td>
<td>M-7</td>
<td>E-15</td>
<td>N-13</td>
</tr>
<tr>
<td>4A-7</td>
<td>+</td>
<td>L-14</td>
<td>+</td>
<td>K-7</td>
<td>R-10</td>
<td>M-3</td>
<td>+</td>
</tr>
<tr>
<td>4N-10</td>
<td>+</td>
<td>K-3</td>
<td>B-13</td>
<td>E-14</td>
<td>H-15</td>
<td>+</td>
<td>M-14</td>
</tr>
<tr>
<td>3C-10</td>
<td>+</td>
<td>D-2</td>
<td>+</td>
<td>J-15</td>
<td>E-2</td>
<td>F-11</td>
<td>+</td>
</tr>
<tr>
<td>P-9</td>
<td>+</td>
<td>M-9</td>
<td>G-4</td>
<td>F-15</td>
<td>C-13</td>
<td>A-9</td>
<td>+</td>
</tr>
<tr>
<td>F-9</td>
<td>+</td>
<td>+</td>
<td>L-2</td>
<td>+</td>
<td>E-6</td>
<td>+</td>
<td>P-3</td>
</tr>
<tr>
<td>N-12</td>
<td>P-5</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>C-4</td>
</tr>
</tbody>
</table>

The Consortium for Advanced Simulation of LWs
A DOE Energy Innovation Hub
[BISON]
solve_type standalone
  fuel_pin_input_file_template = ../..//bison.template
  power_file = ../..//c1/depl/c1.h5 ../..//c2/depl/c2.h5 ../..//c3/depl/c3.h5
  cycle_xml = ../..//c1/depl/c1.xml ../..//c2/depl/c2.xml ../..//c3/depl/c3.xml
  shuffle_xml = ../..//c2/shuffle/c2.xml ../..//c3/shuffle/c3.xml
  only_cycle = 3
  mesh_type = smeared_pellet
  output_average_axial_values = true
  mesh_clad_bot_gap_height = 1.52e-3
  executioner_start_time = 0.0
  executioner_dtmin = 0.1
Generating Standalone Inputs
VERA ASCII Input – The BISON Block

- `solve_type <tiamat|tiamat-inline|standalone|temp_table>`
- `fuel_pin_input_file_template`
  - relative/absolute path to the BISON template file (covered later)
- `power_file`
  - location(s) of HDF5 output files from VERA-CS
- `cycle_xml`
  - location(s) of cycle depletion XML inputs files
  - Pulls geometry and fuel specification data for each rod
- `shuffle_xml`
  - location(s) of cycle depletion XML inputs files
  - Pulls shuffle maps between cycles
- `only_cycle`
  - tells preprocessor to only generate inputs for this cycle
- Other values feed into corresponding entries in the template file
Generating Standalone Inputs

Converting to XML

- Once the VERA inputs have been constructed, they need to be converted to XML to prepare for execution
- Same procedure as was covered earlier using react2xml.pl:

  react2xml.pl vera.inp vera.xml
Generating Standalone Inputs

Running VERA-CS – Multicycle/Shuffling Procedure

• As mentioned before separate input files are necessary for each cycle depletion and shuffle between each cycle
  – This is standard for all VERA simulations
• Restart files are necessary
• Shuffles are executed based on the restart from the previous case with basically a null-depletion step to write a new restart file once shuffling is complete
• The next cycle starts from there this procedure repeats as necessary
Generating Standalone Inputs

Running XML2MOOSE – The BISON Templates

• Found in MOOSEExt/test/ (and training material)
  – bison_2D_sm.template
  – bison_2D_tm.template
  – bison_1.5D.template

• Contains all the blocks needed
  – Standard UO$_2$ Fuel
  – Smeared Pellet R-Z
  – Internal Mesh Generator (though external mesh can be provided)

• Many parameters are automatically populated by XML2MOOSE (#VERA_DEFINED)
  – Geometry
    • Pellet/Clad radii
    • Top/Bottom Gap heights
  – Material specifications
    • Fuel enrichment
    • Porosity
    • Clad density
  – IFBA rod identification
Generating Standalone Inputs

Running XML2MOOSE – The BISON Template

- Dozens of modifiable parameters (#VERA_MODIFIABLE)
  - Initial fill gas pressure (can be different for IFBA)
  - Mesh parameters (fuel/clad elements, more resolved burnup mesh)
  - Roughness coefficients
  - Iteration bounds
  - Execution/PETSc options

- Some blocks will be omitted based on solve_type
  - TIAMAT requires several blocks that standalone BISON does not and vice versa

- As it is the basis for the standalone runs, it highly suggested to be comfortable with the template

- There was recently added a 1.5D template to complement the 2D-RZ simulations in the default template
Generating Standalone Inputs

Running XML2MOOSE – Execution

• Running XML2MOOSE is straight-forward and similar to the other preprocessors
• Consider if we had vera.xml generated by react2xml.pl...

xml2moose -c vera

...would create the BISON input files necessary to complete the case.
• It copies the template file, modifying the parameters for each rod
• NOTE: this is more work than most preprocessors do, so please be patient
Generating Standalone Inputs

Running XML2MOOSE – File Naming Convention

• Since there are a large number of files being create, distinguishing the file names is a very important step
• We’ll start by dissecting an example:
  vera_C03_ASSYB097_P009_6.5.1.4.5.6.bison.i
• “vera” - the filename sent into XML2MOOSE
• “C03” – the rod’s history starts in cycle 3
• “ASSYB” – the name of the assembly in the VERA ASCII input
• “097” – the assembly index in the core (next slide)
• “P009” – the pin index (9) in the assembly (slide after that)
• “6.5.1.4.5.6” – the stack of cell indexes used to construct the rod
Generating Standalone Inputs

Running XML2MOOSE – File Naming Convention (Assembly Indexing)

- NOTE: this may check to a label-based index in the near future
Generating Standalone Inputs

Running XML2MOOSE – File Naming Convention (Pin Indexing)
Generating Standalone Inputs

Running XML2MOOSE – Imposed Transition Times

• Because convergence issues can be encountered if the system changes too quickly, some transition times are imposed as appropriate

• Each BISON simulation starts at cold zero power (CZP)

• A 3 hr period is used to go from CZP to hot zero power (HZP)
  – Includes pressure ramp and thermal feedback

• A 24 hr period is imposed to go from HZP to the first state point power in VERA-CS
  – With more explicit startup simulation the first power is very low, though

• A similar 24 hr period is used from the last statepoint power down to HZP at the end of the cycle

• Also used for step changes in power
Generating Standalone Inputs

Running XML2MOOSE – Regression Tests

- Currently 13 regression tests available:
  - bison_from_vera
  - bison_from_vera_1.5D
  - bison_from_vera_clad
  - bison_from_vera_fast_flux
  - bison_from_vera_ifba
  - bison_from_vera_multi
  - bison_from_vera_multi_qtr_onlyC3
  - bison_from_vera_multi_qtr_shuffle_mir
  - bison_from_vera_multi_qtr_shuffle_rot
  - bison_from_vera_multi_temp_table
  - bison_from_vera_tm
  - bison_from_vera_tm_fecral
  - bison_from_vera_tm_u3si2

- These capture nearly all of the currently supported use-cases
- When starting to use this capability, these would be a good starting point
Generating Standalone Inputs

Executing BISON

- One of the more interesting parts of the process
- A quarter core has roughly 15,000 rods
  - ~15,000 BISON inputs that need to be executed
- Some issues with running them all together using MultiApps
  - Limited Output (bug being investigated)
  - Convergence issues
- Most success has been obtained dividing into small batch jobs
  - Usually several hundred jobs of ~24 rods on Falcon
- However, not all systems support this approach
  - Active jobs limitations (Titan/Eos)
  - Restrictions on the number of mpirun/aprun calls per job
  - May pursue Multiapps in the future
Generating Standalone Inputs

*Post-Processing – Outputs Available*

- BISON outputs a CSV and an EXODUS file
- CSV
  - Typically Max/Min/Avg quantities of interest
    - Max/Min/Avg Fuel/Clad Temperature
    - Max/Min Clad Hoop Stress
    - Min. Gap Thickness
    - Rod Power, Burnup, Internal Pressure
- EXODUS
  - More finely resolved data (such as axial distributions)
  - Current post-processor is leveraging the SEACAS package to read these files
  - Limited to:
    - Fuel-Clad Gap Thickness
    - Max Centerline and Average Fuel Temperature
    - Max Clad Hoop Stress
Generating Standalone Inputs
Post-Processing – Running bison_post

- A postprocessor (bison_post) has been developed that reads appropriate data from the CSV file and consolidates that data onto the HDF5 file produced by VERA-CS
- With all output CSV files in the same directory, bison_post can be run just like XML2MOOSE

```
bison_post -c vera
```

- The HDF5 file can then be visualized with VERAView
Generating Standalone Inputs

*Post-Processing – Running bison_post*

- `cumulative_damage_index`
- `average_clad_temperature`
- `bison_burnup`
- `maximum_clad_hoop_stress`
- `minimum_clad_hoop_stress`
- `maximum_fuel_centerline_temperature`
- `minimum_gap_distance`
- `he_prod`
- `maximum_clad_temperature`
- `minimum_clad_temperature`
- `plenum_pressure`
- `plenum_temperature`
- `average_fuel_temperature`
- `rod_input_power`
- `rod_output_power`
Generating Standalone Inputs

Post-Processing – VERAView

radial_maximum_fuel_centerline_temperature: exposure 0.1207
User’s Manual

• All of the information covered here can also be found in the user’s manual
  – CASL-U-2016-1099-001

• Located in MOOSEExt/doc

• …and the CASL website
  – Previous version already available: https://info.ornl.gov/sites/publications/Files/Pub62883.pdf
Current Target Application – WBN1

Cycle 1 – Max Centerline Fuel Temp (K)
Current Target Application – WBN1

Cycle 1 – Min Gap Thickness (μm)
Current Target Application – WBN1
Cycle 1 – Max Clad Hoop Stress (MPa)
Current Target Application – WBN1

Cycle 2 – Max Centerline Fuel Temp (K)
Current Target Application – WBN1

Cycle 2 – Min Gap Thickness (μm)
Current Target Application – WBN1
Cycle 2 – Max Clad Hoop Stress (MPa)
Current Target Application – WBN1
Cycle 3 – Max Centerline Fuel Temp (K)
Current Target Application – WBN1

Cycle 3 – Min Gap Thickness (μm)
Current Target Application – WBN1

Cycle 3 – Max Clad Hoop Stress (MPa)
AP1000 Rod Ejection

• A lot of effort in CASL has focused on steady-state depletion validation and verification of VERA
• Some recent development focused on reactivity insertion accidents (RIA) such as with rod ejections
• Westinghouse has produced MPACT/CTF simulations of demonstration rod ejection cases (HFP/HZP)
• Left some open questions of important fuel performance parameters
• A one-way coupling of MPACT/CTF to Bison has previously been developed for depletion analyses
• Extended in this work for transient applications to support the RIA simulations in CASL
# AP1000® Core Layout

<table>
<thead>
<tr>
<th>Reg. #</th>
<th>Percent of Core</th>
<th>$^{235}$U AVG BLKT</th>
<th>$^{235}$U BLKT</th>
<th>IFBA Rods</th>
<th>WABA Rods</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10%</td>
<td>0.740</td>
<td>Absent</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>31%</td>
<td>1.580</td>
<td>Absent</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>18%</td>
<td>3.200</td>
<td>1.580</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>23%</td>
<td>3.776</td>
<td>3.200</td>
<td>68</td>
<td>$8L^a+4S^b$</td>
</tr>
<tr>
<td>5A</td>
<td>5%</td>
<td>4.376</td>
<td>3.200</td>
<td>88</td>
<td>$4I^c$</td>
</tr>
<tr>
<td>5B</td>
<td>3%</td>
<td>4.376</td>
<td>3.200</td>
<td>124</td>
<td>0</td>
</tr>
<tr>
<td>5C</td>
<td>10%</td>
<td>4.376</td>
<td>3.200</td>
<td>124</td>
<td>$8I^c$</td>
</tr>
</tbody>
</table>

$a$ L = Long  
$b$ S = Short  
$c$ I = Intermediate

---

![Diagram of AP1000® Core Layout]

- **FA w/ Ejected Rod**
- **Ejected Rod**
AP1000 Core Layout
VERA Rod Ejection Simulation

- Depleted to the end of the cycle (~18.5 GWd/MT)
- Fully inserted AO rod ejected (for an extreme case)
- HFP conditions specified during the depletion phase
VERA Rod Ejection Simulation

<table>
<thead>
<tr>
<th>Time Period</th>
<th>Time Step Size</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0–0.1</td>
<td>0.005</td>
<td>Rod ejection</td>
</tr>
<tr>
<td>0.1–1.2</td>
<td>0.010</td>
<td>No rod movement</td>
</tr>
<tr>
<td>1.2–2.0</td>
<td>0.025</td>
<td>Reactor trip</td>
</tr>
<tr>
<td>2.0–3.7</td>
<td>0.100</td>
<td>Reactor trip continues</td>
</tr>
<tr>
<td>3.7–5.0</td>
<td>0.100</td>
<td>No rod movement</td>
</tr>
</tbody>
</table>

- Power during transient phase is calculated
Max Power Rod Selection

- Normalized pin power distribution from peak timestep:
Results (Total Depletion)
Results (Total Depletion)
Results (Transient Phase)
Results (Transient Phase)
ATF Concepts

- While there are many concepts currently being explored, this work focused on what was available in Bison
  - Uranium silicide ($U_3Si_2$) fuel
  - FeCrAl cladding
- Several others have been in development for a while (SiC/SiC cladding) but not mature yet
- Others still are in the earlier stages of development (doped fuel and coated cladding)
- As other concepts become available in Bison, the tools used here can easily be extended to incorporate them
Single Rod Comparisons

• Assessing the results from three different configurations
  – Standard UO$_2$/ZIRLO rod
  – UO$_2$ with FeCrAl
  – U$_3$Si$_2$ with ZIRLO

• Used a representative three cycle power history for a rod from Watts Bar Cycles 1-3

• Corresponding dimensions:

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Fuel</th>
<th>Clad</th>
<th>Clad Width [cm]</th>
<th>Gap Width [um]</th>
<th>Pellet Radius [cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard</td>
<td>UO$_2$</td>
<td>ZIRLO</td>
<td>0.057</td>
<td>84</td>
<td>0.4096</td>
</tr>
<tr>
<td>FeCrAl</td>
<td>UO$_2$</td>
<td>FeCrAl</td>
<td>0.035</td>
<td>84</td>
<td>0.4316</td>
</tr>
<tr>
<td>U$_3$Si$_2$</td>
<td>U$_3$Si$_2$</td>
<td>ZIRLO</td>
<td>0.057</td>
<td>84</td>
<td>0.4096</td>
</tr>
</tbody>
</table>

• Though FeCrAl is targeted towards BWR designs, it was used simply for comparison here and to exercise the capability
Single Rod Comparisons

Minimum Gap Width

- Standard
- FeCrAl
- U3Si2

Distance [μm]

Time [days]

Power [kW]
Single Rod Comparisons

NOTE: during outage, the system pressure drops to atmospheric.
Single Rod Comparisons

Maximum Fuel Centerline Temperature

Temperature [K]

Time [days]

Standard
FeCrAl
U3Si2
U₃Si₂ Lead Test Assembly in WB, Cycle 1

- One assembly (D-12) was replaced with U₃Si₂ fuel (4.2% enriched)
LTA, Pin Powers (Normalized)
LTA, Centerline Fuel Temperature (K)
Next We’ll Look at Some Examples…

Questions?