Title: Improved Verification and Validation Testing and Tools

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Improved Verification and Validation Testing and Tools

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Monte Carlo Codes Group (XCP-3)

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Overview

• Primary goal of software testing
  – The role of verification and validation

• Previously released V&V suites

• New Python-based framework

• Additional test suite(s)
Primary goal of software testing

- Test the code for *correctness*
- Correctness is defined with respect to some standard
  - Comparison to another code (version)
  - Comparison to (semi-)analytic results
  - Comparison to experiment measurements
Primary goal of software testing

- Test the code for correctness
- Correctness is defined with respect to some standard
  - Comparison to another code (version)
    Behavioral testing done for every code change during development
    Full end-to-end testing attempting to isolate behaviors / features
  - Comparison to (semi-)analytic results
    Ensuring the algorithms indeed solve the transport equation
    Simplified problems and mock data used to isolate code / algorithm implementation
  - Comparison to experiment measurements
    Ensuring the combination of algorithms and data compare well to nature / reality
    Applies only to application area being tested and compared

Current MCNP6 Testing Practices
Primary goal of software testing

- Test the code for correctness
- Correctness is defined with respect to some standard
  - Comparison to another code (version)
  - Comparison to (semi-)analytic results
  - Comparison to experiment measurements

Current MCNP6 Testing Practices

REGRESSION

VERIFICATION

VALIDATION
Role of Verification and Validation

• Verification
  – Where analytical and semi-analytical solutions to the transport equation may exist, we want to ensure that MCNP is solving the correct equations

• Validation
  – Combination of code (MCNP) and nuclear data (ENDF/NJOY/ACE) work together to produce results comparable to reality

• Full end-to-end tests exercising many separate features
  (input parsing, problem setup, nuclear data usage & collision physics, transport & random walk algorithm, tallying, dose/response functions, output, etc.)

• Long-standing reputation can be linked to extensive and robust V&V
Previously Released V&V Suites

MCNP6.2 Release
• Verification
  − k-effective (VERIFICATION\_KEFF)
  − 3-D fixed-source streaming (KOBUYASHI)
  − Variety of shielding problems (VERIFICATION\_SHLD\_SVDM)

• Validation
  − k-effective (VALIDATION\_CRITICALITY & VALIDATION\_CRIT\_EXPANDED)
  − 3-D fixed-source neutron and photon problems (VALIDATION\_SHIELDING)

Previous Releases
− High-energy physics (CEM \& LAQGSM)
Previously Released V&V Suites

Limitations in previously released V&V suites

- Mixture of Makefile, Perl, Windows .bat scripts used to execute problems (ALL)
  - Missing execution scripts entirely (CEM & LAQGSM)
- Problems cannot be run directly without preprocessing or suite-specific XSDIR files (CRITICALITY & CRIT_EXPANDED)
- Misleading suite not doing actual verification (SHLD_SVDM)
- Postprocessing results scripts inconsistent and/or missing (SHIELDING, CEM & LAQGSM)
- No job submission / cluster support (ALL)
- Plotting / visualization support missing, broken, or incomplete (ALL)
- Any sort of documentation requires manual intervention (ALL)
New Python-based Framework

- **Consistency** across suites
- **Extensible** to more suites and problem types
- **Automated** for all steps
  - Setup
  - Execute
  - Postprocess
  - Document
- Requires Python3
- Runs on Linux, Mac OS, & Windows

```
"general_info": {  
  "name": "GODIVA",  
  "icsbp_name": {  
    "material": "HEU",  
    "form": "MET",  
    "spectrum": "FAST",  
    "number": "001",  
    "case": ""  
  },  
  "description": "Bare HEU sphere"
},

"execution_info": {  
  "arguments": {  
    "i": "GODIVA",  
    "n": "GODIVA"
  },
  "outputs": {  
    "outp": "GODIVAo",  
    "mctal": "GODIVAm"
  },
  "inputs": {  
    "inp": "GODIVA"
  }
},

"experiment_data": {  
  "k-eff": {  
    "val": 1.0,  
    "std": 0.001
  }
}
```
New Python-based Framework

- Can be immediately used for any version of the code (input and data options must be considered)

- For developers
  - Can test code and data frequently
  - V&V reports are essential for a release

- For everyone else
  - Can add application-specific V&V suites
  - Can support SQA needs

```
Directory structure
```

```
vnvstats /
|- README.md
|- support /
  |- mcnpvnv.py (MCNP-specific V&V functionality)
  |- vnv /
    |- README.md (Generic V&V functionality)
    |- __init__.py
    |- benchcalc.py (Benchmark/experiment handling)
    |- commandline.py (Command line parser and execution)
    |- compare.py (Compare results from calculations/experiments)
    |- plotndoc.py (Tabulation of results, plotting and documentation)
    |- slurmin.py (Support SLURM submission and job execution)
    |- tests /
  |- validation /
    |- criticality /
      |- README.md (Drives criticality suite)
      |- VnV.py (Contains each benchmark model and description)
      |- experiments /
        |- shielding /
        |- lockwood /
        |- ...
    |- verification /
      |- keff /
      |- kobayashi /
      |- ...
```
New Python-based Framework

- List
  - Query test suite for available test problems

```python
python VnV.py list
```
New Python-based Framework

• Setup
  – Creates a calculation tree of benchmarks selected

    ```
    python VnV.py setup --calcdir_name testA
    ```

  – Example of calculation tree with only listed benchmarks

    ```
    python VnV.py setup --calcdir_name testB BIGTEN FLAT25 GODIVA
    ```
New Python-based Framework

• Execution
  - Runs all problems in existing calculation directory
    python VnV.py execute --calcdir_name testA

  - Builds command line from execution_info group

  - Option examples:
    --executable_name mcnp6
    --jobs 2 concurrent execution
    --ntrd 8 threads for each job
    --nmpi 4 ranks for each job

---

```
"general_info": {
  "name": "GODIVA",
  "icsbep_name": {
    "material": "HEU",
    "form": "MET",
    "spectrum": "FAST",
    "number": "001",
    "case": ""
  },
  "description": "Bare HEU sphere"
},

"execution_info": {
  "arguments": {
    "i": "GODIVA",
    "n": "GODIVA"
  },
  "outputs": {
    "outp": "GODIVAO"
  },
  "inputs": {
    "inp": "GODIVA"
  },
  "experiment_data": {
    "k-eff": {
      "val": 1.0,
      "std": 0.001
    }
  }
}
```
New Python-based Framework

• Execution Submission
  - Submits all problems in existing calculation directory via slurm/sbatch
    
    ```
    python VnV.py execute_slurm --calcdir_name testA
    ```

  - Option examples:
    --nodes 1  
    --time 120  
    --stride 8  
    --wait 

    --pre_cmd  
    --post_cmd  

  node allocation  
  time allocation in minutes  
  jobs per sbatch job submitted  
  wait for execution to complete before proceeding  

  commands to run before and/or after MCNP  
  execution within sbatch submission script
New Python-based Framework

- **Postprocessing**
  - Reads calculation output files and processes results into calculation description.json
    ```
python VnV.py postprocess \ 
    --calcdir_name testA
    ```
  - Adds calculation_data and calculation_info objects to JSON file
    - experiment_data and calculation_data directly comparable
  - All suites will likely postprocess MCNP results differently
  - Using MCNPTools wherever possible
New Python-based Framework

• Documentation
  - Retrieves experiment and simulation results from calculation description.json and prepares documentation
    ```python
    python VnV.py document \--calcdir_name testA
    ```
  - Results are tabulated into text and LaTeX form
  - Plots are generated into PNG outputs
  - Between LaTeX text, tables, and PNG plots, a V&V report is nearly done

---

### HEU Calculation Benchmark Results

<table>
<thead>
<tr>
<th></th>
<th>Exp. k-eff</th>
<th>Exp. unc.</th>
<th>Calc. k-eff</th>
<th>Calc. unc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZEUS2</td>
<td>0.9997</td>
<td>0.0008</td>
<td>0.997547</td>
<td>0.000704</td>
</tr>
<tr>
<td>UH3C6</td>
<td>1.0000</td>
<td>0.0047</td>
<td>0.995685</td>
<td>0.000771</td>
</tr>
<tr>
<td>FLAT25</td>
<td>1.0000</td>
<td>0.0030</td>
<td>1.003410</td>
<td>0.000610</td>
</tr>
<tr>
<td>TT2C11</td>
<td>1.0000</td>
<td>0.0038</td>
<td>1.000900</td>
<td>0.000754</td>
</tr>
<tr>
<td>GODIVA</td>
<td>1.0000</td>
<td>0.0010</td>
<td>0.998775</td>
<td>0.000624</td>
</tr>
<tr>
<td>GODIVR</td>
<td>0.9985</td>
<td>0.0011</td>
<td>0.998897</td>
<td>0.000729</td>
</tr>
<tr>
<td>ORNL10</td>
<td>1.0015</td>
<td>0.0026</td>
<td>1.000050</td>
<td>0.000357</td>
</tr>
</tbody>
</table>

---

### IEU Calculation Benchmark Results

<table>
<thead>
<tr>
<th></th>
<th>Exp. k-eff</th>
<th>Exp. unc.</th>
<th>Calc. k-eff</th>
<th>Calc. unc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>BIGTEN</td>
<td>0.9948</td>
<td>0.0013</td>
<td>0.99523</td>
<td>0.000474</td>
</tr>
<tr>
<td>ICT2C3</td>
<td>1.0017</td>
<td>0.0044</td>
<td>1.00352</td>
<td>0.000711</td>
</tr>
<tr>
<td>IMF03</td>
<td>1.0000</td>
<td>0.0017</td>
<td>1.00186</td>
<td>0.000637</td>
</tr>
<tr>
<td>IMF04</td>
<td>1.0000</td>
<td>0.0030</td>
<td>1.00818</td>
<td>0.000647</td>
</tr>
</tbody>
</table>

...
New Python-based Framework

• Nominal workflow
  - Setup, execute, postprocess, and document a suite of test problems

```
python VnV.py setup \   
  --calcdir_name MCNP63_VV

python VnV.py execute \  
  --calcdir_name MCNP63_VV

python VnV.py postprocess \ 
  --calcdir_name MCNP63_VV

python VnV.py document \  
  --calcdir_name MCNP63_VV
```

Note: this is under active development and some changes may occur before official release
Additional Test Suite(s)

- Beyond the actual MCNP input files, two ingredients are required to create a new suite:
  - `description.json` files, each benchmark (easy)
    - `execution_info`: maps to MCNP command line options/arguments and input/output files
    - `experiment_data`: benchmark results used to compare to calculation results
  - `VnV.py` script, each suite (medium/hard)
    - `list`: same for all test suites
    - `setup`: same for all test suites (except where additional options are wanted, see bonus slide)
    - `execute`: same for all test suites
    - `execute_slurm`: same for all test suites
    - `postprocess`: unique to every test suite
    - `document`: unique to every test suite

This is likely where the most time is spent getting each suite setup.
Additional Test Suite(s)

- Finished incorporating Lockwood validation test suite
  - Electron transport energy deposition
    - Condensed history algorithm
    - Single event electrons
  - Several materials
  - 334 separate MCNP inputs
  - Reasonably computationally expensive
    (need cluster / high performance computing)

- Resurrecting LAQGSM and CEM validation test suites
  - No Makefile or other scripts to execute code and/or postprocess results
  - Gaining experience through old tests, documentation and trail of bread crumbs…
Summary

• All MCNP team supported V&V test suites are now developed in a separate repository from the MCNP source code within a Python-based framework
  - Python tools and scripts
  - Benchmark inputs and description JSON files
• This entire framework will be distributed with the upcoming MCNP6.3 release
• Most V&V test suites distributed with MCNP6.2 will be distributed in new framework
• New V&V test suites are done or being worked on for the MCNP6.3 release
• Looking forward to feedback and potential contributions
Questions?

Contact: mrising@lanl.gov
Suite specific command line options

• Easy to add command line options in VnV.py scripts for each individual suite

```python
command_args["setup"].add_argument(
    "--data",
    type=str,
    choices=["endf66", "endf70", "endf71", "endf80"],
    default="endf71",
    help="Data library to use, default endf71",
)
```

• Criticality and Rossi-alpha suites have `--data` option for setup step:

```bash
python VnV.py setup --calcdir_name test_endf71 --data endf71
python VnV.py setup --calcdir_name test_endf80 --data endf80
```

• Separate calculation tree for each `--data` option selected