EXPERT GROUP ON 3D RADIATION TRANSPORT BENCHMARKS

Benchmarking the Accuracy of Solution of 3-Dimensional Transport Codes and Methods over a Range in Parameter Space

17 April 2007
Monterey, California, USA
Expert Group on 3D Radiation Transport Benchmarks
Meeting on

Benchmarking the Accuracy of Solution of 3-Dimensional Transport Codes and Methods over a Range in Parameter Space

Embedded in the American Nuclear Society’s Mathematics & Computation Topical
6:00 pm on Tuesday, April 17, 2007
Los Angeles Room, Monterey Marriott Hotel, Monterey, California

Summary

6:00pm  Welcome and Introductions - Enrico Sartori, NEA/OECD

Enrico Sartori welcomed the 32 attendees (Annex I). He summarized the activities of the Expert Group starting with the Takeda Benchmark related to Control Rod Worth in six reactor configurations, whose results were published in 1990 when 3D transport calculations presented a serious computational challenge. The second exercise adopted by the Expert Group was the Kobayashi Benchmark involving three simple configurations with internal voids that were not characteristic of reactor cores. The third exercise, organized by Elmer Lewis, revisited the so-called C5G7 mini-core configuration and targeted the accuracy of the multiplication factor and the pin power distribution. The current Benchmark activity proposed by Yousry Azmy and endorsed by the Nuclear Science Committee of the OECD’s NEA is designed to test the performance of 3D transport methods and codes over a range in parameter space in a non-reactor configuration. As with previous benchmarks, the goal of this exercise is to identify required improvements in transport methods and codes. The Agenda was approved without modifications (Annex II).

6:15pm  Overview of the Benchmark Suite - Yousry Azmy, PSU

Azmy motivated the new Benchmark exercise by summarizing the three issues it is designed to address:

1. Permit more objective extrapolation/interpolation of the exercise’s result by covering a range in parameter space via a suite of 36 individual cases that the participants are invited to solve.
2. Verify that reported solutions are in the asymptotic regime, i.e. the numerical error decreases monotonically with model refinement, a necessary condition for enabling solution extrapolation to improve accuracy.
3. Report any deviations of selected code parameters from their default values, or options from their recommended settings, to help future users better utilize the advanced capabilities of transport codes to solve their most difficult problems.

Azmy then described the geometric setup of the suite of configurations and the parameter values defining the full set of cases included as well as the benchmark quantities to be reported. See the attached PowerPoint presentation for more detail.

The following questions were raised by the attendees during and following Azmy’s presentation:
1. **Where did cross sections like \( \sigma_T = 10 \) and \( c = 1.0 \) come from and what applications do they represent?**
   They are not necessarily physical in nature, they are intended only to cover a wide range in parameter space. Nevertheless, applications in radiative transfer might involve such a range of cross sections.

2. **How different is this suite of problems from Kobayashi’s 3-case Benchmark?**
   Here we cover a range in parameter space whereas in Kobayashi’s Benchmarks the three cases had fixed cross sections, and were specifically designed to investigate the effect of internal voids on the accuracy of the transport solution.

3. **Why do we need this Benchmark exercise instead of Barry Ganapol’s TIEL Benchmark?**
   This exercise is more responsive to the requirements/expectations of Verification & Validation activities related to 3D transport methods and codes. (TIEL: Analytical Benchmarks for Steady State Neutron Transport in Infinite Media - Source Series 1)

4. **What are the units of the quantities appearing in the Benchmark specification?**
   Generally they need only be consistent within a given code. Since typically macroscopic cross sections are provided in units of cm\(^{-1}\), then assume lengths are in units of cm and the source is in units of particles/cm\(^3\).sec.

5. **Is it really necessary to do 729 cases in this suite?**
   We only picked 3 values per model parameter. We cannot use fewer than 3 values if we expect to see a trend, and we wanted to test all model parameters, a total of 6 parameters. More importantly, with the shell script provided, running this many cases and collecting the required benchmark quantities should not be tedious. Nor should it be too computationally intensive because of the one-group specification and the vacuum boundary conditions that should provide rapid convergence of the inner iterations.

6. **To verify that the reported solutions are in the asymptotic regime, is it required to report 3 mesh refinements times 3 angular refinements?**
   No, it is typical in transport calculations that refining the spatial variable discretization must go hand in hand with refining the angular discretization. Hence, the participants need only provide results for 3 cases in which both variables are refined simultaneously.

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6:30pm **Brief Tutorial on Benchrun Script - Kursat Bekar, PSU**

Bekar presented an overview of the shell script “benchrun” that executes all cases in the suite of benchmark problems. He described its modular structure and each module’s functionality: generating cross sections; generating the input files suitable for the target code; executing the target code; collecting the benchmark quantities from the code’s output; tabulation of the benchmark results, and error with respect to the reference solution, in ASCII and in PDF formats. These functions can be executed in their entirety, or if desired certain functions can be executed individually. For example a user might wish to regenerate the tabulated results only using previously generated solution files. Also, the script allows the user to run all cases in the benchmark suite, or execute a single case or group of cases, e.g. cases the user had trouble converging. Bekar also illustrated the changes a user must make to adapt the script to their target code, and showed several screen shots of how the various commands are executed by the “benchrun”. Next he showed a sample table output, and covered the naming convention for the input, output, and data files as encoded by “benchrun” for all the cases in the suite. See the attached PowerPoint presentation for more detail.

The following question was raised by the attendees following Bekar’s presentation:

1. **In what format does “benchrun” generate the cross sections file/library?**
   In the native format of the target code. The participant’s code must have a utility to prepare the cross sections file in a format suitable for its use, so the user will modify “benchrun” to execute that utility and generate the proper cross section library as s/he would in a straight (manual) run of your target code.
code. In other words, the script automates what the user would otherwise do by hand in the exact same sequence, with the exact same intermediate files.

7:00pm Overview of MCNP Reference Solutions - Forrest Brown, LANL

Brown described his approach to obtaining a high quality reference solution with MCNP to the suite of benchmark configurations. He stated that initial results are available but that comparisons with the results obtained by Bekar at PSU are desirable. Indications are that some cases will require increasing the number of histories. Brown also noted that for some of the difficult cases in the suite of problems variance reduction is necessary. While MCNP has the ability to parametrize configurations included in the suite, parametrizing the weight windows is a novel problem that he will tackle. See the attached PowerPoint presentation for more detail.

The following question was raised by the attendees following Brown’s presentation:
1. What uncertainties do you estimate in the final version of the reference solution?
   Different quantities computed in different configurations will have varying levels of uncertainties. It is too early to predict the outcome but every effort will be made to reduce uncertainties to a level that would make the error estimates for deterministic codes meaningful.

7:15pm Discussion - Attendees

Two open questions were brought to the floor by Azmy:
1. How should the large number of benchmark quantities computed in the benchmark be presented in digestible form?
   Azmy proposed using $L_1$, $L_2$, and $L_\infty$ norms of the computed quantities, but he would not discount alternative presentation methods. For example, the fraction of benchmark quantities that satisfy a certain criterion, e.g. in asymptotic regime or error smaller than $\varepsilon$, can be reported. Azmy asked for input from the participants on this topic before too long. If no further proposals are submitted by the community, the above-mentioned norms will be adopted.

2. How to deal with benchmark quantities that are 100 mean-free-paths (mfp) away from the source?
   The selection of the cross sections and height of the outer parallelepiped to cover two orders of magnitude created a situation in which for some configurations in the suite of benchmarks, a few individual benchmark quantities are comprised of particles that traverse 100 mfp from the source. Neither the Monte Carlo reference solution nor deterministic methods’ solution will predict such quantities accurately, in addition to the fact that they are of no practical interest. Azmy offered two options to deal with these quantities: to skip reporting and including in the comparison of all such quantities, or to reduce the value of 10 in the benchmark parameters to 5 implying a maximum of 25 mfp thickness for all computed quantities. Note that in the first option, not all cases in the benchmark suite that include a 100 mfp thickness in their entirety would be skipped, only the few quantities that involve transport of particles across 100 mfp would have been skipped. Upon discussion of the two options the attendees chose the second option.

Additional discussion points:
3. Barry Ganapol explained that this is a computational not a mathematical benchmark since the reference solution is not analytical.
   Correction was accepted by the organizers and the benchmark document will be revised accordingly.
4. **Why distribute the reference solution instead of holding a blind test of the participating codes?**

Three reasons motivated the organizers’ decision to distribute the reference solution: the first is that MCNP is publicly available and most participants are likely to check their solutions against it before reporting the results. Second, the “benchrun” script computes the error in the computed solutions against the provided reference solution, hence withholding the latter will require that collection of the reportable results must be done at a later time. Third, the organizers will have access to the reference solution and will also participate in the exercise with the TORT code; it seems fair that other participants have access to the same information as the organizers. Azmy described this situation to the attendees and then asked them to express their preference. A large majority preferred a blind test. Hence it was agreed that the reference solution will not be distributed to participants for six months during which time the exercise will be considered blind. After this period, every participant who submits a solution set will receive a copy of the reference solution that will allow him/her to compute and report the observed errors. The policy of permitting and accepting revised solutions will be determined in the future.

8:00pm Adjourn

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**DECISIONS & ACTION ITEMS**

1. The parameter set included in the benchmark document and also in the “benchrun” script will be revised to reflect the participants’ decision to limit the maximum transport thickness to 25 mfp. Also, the benchmark document will be revised to describe this as a computational benchmark.

2. The revised document and “benchrun” script will be re-issued.

3. Since the first phase of the benchmark will be blind, the reference solution will be removed from the distribution; the remaining distributed items are of sufficiently small size to be posted on the web site for downloading by participants: <http://www.nea.fr/html/science/eg3drtb/>.

4. After six months from the start date, the reference solution will be provided (on CD due to the large size) to any participant who submits a solution to the benchmark exercise.

5. The next meeting on this benchmark exercise will be held in conjunction with either the ANS Annual Meeting, Anaheim, California, in mid-June 2008, or PHYSOR 2008, Interlaken, Switzerland, in September 2008. If by December 2007, more than 5 submissions are received, a meeting in Anaheim will be scheduled with the expectation that more submissions will occur in the first half of 2008. Otherwise the organizers will strongly urge the participants to submit contributions by early summer to enable a meeting in Interlaken in early Autumn.
## Annex I

**First Meeting on 3D Transport Suite of Benchmarks, Monterey, 17.IV.07**

### List of Participants

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Annex II

Expert Group on 3D Radiation Transport Benchmarks
Nuclear Energy Agency Nuclear Science Committee (NEA-NSC)
of the
Organization for Economic Cooperation and Development (OECD)

First Organizational Meeting on
Benchmarking the Accuracy of Solution of 3-Dimensional Transport Codes
and Methods over a Range in Parameter Space

6-8 pm, Tuesday, April 17, 2007
San Diego Room, Monterey Marriott Hotel, Monterey, California

Agenda

6:00   Welcome and Introductions                           Enrico Sartori
6:15   Overview of the Benchmark Suite                    Yousry Azmy
6:30   Brief Tutorial on “benchrun” Script                Kursat Bekar
7:00   Overview of MCNP Reference Solutions               Forrest Brown
7:15   Discussion (Open Questions: + Presentation of Results; + 100mfp cases)
8:00   Conclusion
Benchmarking the Accuracy of Solution of 3-Dimensional Transport Codes and Methods over a Range in Parameter Space

Sponsored by the Nuclear Energy Agency Nuclear Science Committee of the Organization for Economic Cooperation & Development

Y. Y. Azmy
Department of Mechanical & Nuclear Engineering
The Pennsylvania State University

Introduction

- Third Benchmark exercise organized by the NEA’s Expert Group on 3-D Radiation Transport Benchmarks

- Mathematical Benchmarks:
  - Compare results to high-quality reference solution
  - Focus: solution method/algorithms
  - Geometric & nuclear (cross sections) data fixed & given

- In this exercise we examine three main issues
Issue 1. Suite of Benchmark

- Typical benchmark exercises:
  - Specify single configuration to be solved by participants
  - Hence conclusions specific to particular configuration
  - Deviations from benchmark configuration require subjective extrapolation of conclusions

- We propose entire suite of benchmark configurations:
  - Cover wide range in parameter space spanned by the problem geometry & nuclear data
  - Cover two orders of magnitude in each relevant parameter
  - Permit users to interpolate, or extrapolate, estimates of a given code's performance in a specific application

Issue 2. Asymptotic Regime

- Model refinement ≠ decreasing error: desirable not inevitable!
  - Asymptotic regime: error decreases monotonically with refinement
  - Outside asymptotic regime: fortuitous small error possible, followed by increased error with refinement
  - Generally, user does not know exact/reference solution ≠ erroneous extrapolation of solution away from exact value

- We propose solving benchmark on sequence of refined models:
  - A straightforward, albeit non-rigorous, verification that solutions are within asymptotic regime:
    - Solve the problem on sequence of refined models
    - Observe monotonic approach of solution to limit
  - Participants free to select:
    - Numerical method
    - Level of discretization of the angular and spatial variables
  - Required to verify that reported solutions are within the asymptotic regime
Issue 3. Defaults & Options

- Most production level transport codes possess many options & adjustable parameters
  - Designed to address broad variety of difficult problem configurations
  - Powerful tools in the hands of an expert user
  - Rare for a nuclear scientist with physics expertise to also possess sufficient expertise in a specific transport code
  - Hence many code developers set defaults, or provide recommended settings for non-expert users

- We propose stating any none-standard settings
  - Participants, presumably expert in their own codes, must report deviations from default/recommended settings
  - Will help future users understand available options in given transport code
  - Will aid selection of adjustable options/parameters when defaults fail

Description of Benchmark Problems

- Outer/inner parallelepiped
  - Index 1/2:
    - Square base, y-scaled
    - Vacuum BCs
    - Scattering ratios: c₁ & c₂

- Unit source:
Suite Specification

- **Suite constructed by independently varying 6 parameters**

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Reporting Requirements

- **For each run participants required to report:**
  - Three model refinement levels of angular & spatial variables
  - Any non-default settings of optional methods or adjustable parameters implemented in the employed code

- **For each benchmark configuration in suite participants must provide the following per benchmark quantity:**
  - Three values corresponding to three levels of model refinement
  - Relative error with respect to reference value, provided by organizers, for each level of model refinement
  - Indication of whether the solution is in the asymptotic regime
Benchmark Quantities

- Scalar flux averaged over:
  - Volume in parallelepiped 1 not in 2
  - Parallelepiped 2

- Net leakage out of 8 faces

- Scalar flux averaged over 13 subvolumes

Executing the Suite of Problems

- Suite of benchmark problems comprised of a total of $3^6 = 729$ cases

- Each case to be executed multiple times in order to verify asymptotic convergence

- Shell script (next presentation) provided to automate:
  - Execution of target code
  - Collection & tabulation of required benchmark quantities
  - Computation of error relative to supplied reference solution

- Two open questions to be discussed shortly
Present Status

- Early version of shell script distributed by NEA:
  - One revision since distribution

- Preliminary Reference solution obtained with MCNP
  - Poor statistics for some cases: optically thick configurations
  - Will verify with Forrest Brown's before finalizing Reference

- Suggestions/comments to: yya3@psu.edu

- Schedule:
  - Start: March 2007
  - Meeting: 2008
  - End: March 2009
Benchmarking the Accuracy of Solution of 3-Dimensional Transport Codes and Methods over a Range in Parameter Space

benchrun-1.1

Kursat B. Bekar

Department of Mechanical and Nuclear Engineering
The Pennsylvania State University
OVERVIEW

- designed to facilitate participation in the NEA Benchmark exercise
- designed for UNIX/LINUX platforms
- enabling
  1. execution of all cases
  2. execution of individual cases
  3. ranges of cases
- this script automates:
  1. Setup of input files (per case) for the target transport code.
  2. Execution of target transport code for all cases in the suite.
  3. Collection of benchmark quantities (per case) from output file(s).
  4. Tabulation of benchmark quantities for documentation or archiving.

April 17, 2007

Kumar H. Baker, Penn State University, USA

OVERVIEW

Input generation for the transport code:

```
INPUT GENERATION MOD.U.L.E.

generate input filename
  \rightarrow L_{\text{gamma}}, S1, c1 \text{ and } S2, c2

calculate boundary points
  \rightarrow L_{\text{gamma}}, S1, c1 \text{ and } S2, c2

generate material ID
  \rightarrow \text{input template, CODETMP, CODETMPDIR}

read and modify input template
  \rightarrow \text{Pre-processor code, PREP}

execute pre-processor
  \rightarrow \text{transport code input file}
```

April 17, 2007

Kumar H. Baker, Penn State University, USA
OVERVIEW

Execution of transport code:

CODE EXECUTION MODULE:

- generate input filename
- check input file(s)
- generate output filename
- execute transport code

OVERVIEW

Output processing (Collection of data):

OUTPUT PROCESSING MODULE:

- generate input filename
- calculate boundary points
- generate material ID
- execute post-processor code

April 17, 2007

Kumar R. Baker, Penn State University, USA
OVERVIEW

**Table generation (Presenting data):**

**TABLE GENERATION MODULE:**

- generate data filename
- read reference solution data (MCNPS)
- read data generated by post-processor
- calculate % error, create tables

L, gamma, S1, e1 and S2, e2
reference data path, RDPOOL
reference data files
data files
LaTeX, DUTILC

*table in PDF format*
*table, comma separated for MS-Excel*

April 17, 2007
Kumav B. Beker, Penn State University, USA

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**OPTION SUMMARY**

**Usage:** benchrun [ options ]

- `-h|--help`, writes option summary
- `-x|--xsec`, only generate cross-sections.
- `-i|--input`, only generate transport code inputs.
- `-p|--postprocess`, process transport code outputs.
- `-e|--execute`, execute transport code with previously generated inputs.
- `-t|--table`, tabulate results in LaTeX table format
  (requires LaTeX and DUTILC)

April 17, 2007
Kumav B. Beker, Penn State University, USA
OPTION SUMMARY

Usage: benchrun [ options ]

--single L gamma sigma1 c1 sigma2 c2

Perform calculation for a single case with L, gamma, sigma1, c1, sigma2 and c2 values.

--group [ L=LL gamma=GG s1=SS1 c1=C1 s2=SS2 c2=CC2 ]

Perform calculations for a given group of cases.

April 17, 2007
Karat E. Baker, Penn State University, USA

OPTION SUMMARY – user defined parameters

Usage: benchrun [ options ]

--code=[NAME] Name of the transport code executable
--codedir=[DIR] Directory where the transport code executable resides
--codetmp=[NAME] File name for the transport code input template
--codetmpdir=[DIR] Directory where the input template file resides
--post=[DIR/NAME] Full pathname for the post-processor of the transport code output
--prep=[DIR/NAME] Full pathname of the pre-processor of the transport code input
--rdpool=[DIR] Directory where the results of the reference MCNP5 calculation reside
How to use script:

User defined parameters:
These are defined by the user either in the script, via edits, or interactively on the command line executing script.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODEDIR</td>
<td>directory where the code executable resides</td>
</tr>
<tr>
<td>CODE</td>
<td>name of executable</td>
</tr>
<tr>
<td>CODETMPDIR</td>
<td>directory where the code input template resides</td>
</tr>
<tr>
<td>CODETMP</td>
<td>name of code input template</td>
</tr>
<tr>
<td>POSTP</td>
<td>post-processing code with its full path</td>
</tr>
<tr>
<td>PREP</td>
<td>pre-processing code with its full path</td>
</tr>
<tr>
<td>RDPOOL</td>
<td>directory where the reference MCNP results reside</td>
</tr>
</tbody>
</table>

April 17, 2007
Kurmit B. Deka, Penn State University, USA
How to use script: **individual cases**

```
/home/bhub/NEA-Benchmark$ /benchrun --single 0.1 0.1 0.1 0.5 0.1 0.5
Message: Code executable is found in the given directory
Message: code executable is ok. Continue check..
Message: code input template file is found in specified directory
Message: Code post-processor is found in specified directory
Message: Code pre-processor is found in specified directory
Message: Generating inputs for the cases given
Message: Input generation is successfully completed
```

April 17, 2007

Kunar B. Bhowmik, Penn State University, USA

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How to use script: **range of cases**

```
/home/bhub/NEA-Benchmark$ /benchrun --group 1=0.1 s1=0.1 c1=0.5 -1 -e
Message: Code executable is found in the given directory
Message: code executable is ok. Continue check..
Message: Code input template file is found in specified directory
Message: Code pre-processor is found in specified directory
Message: Generating inputs for the cases given
Message: Input generation is successfully completed
Message: Executing code for the cases given
```

April 17, 2007

Kunar B. Bhowmik, Penn State University, USA
How to use script: command line parameter definition

```
/home/kbb/NEA-Benchmark$ ./benchrun --code=mep5 --codadir=/c0
Message: Code executable is found in the given directory
Message: Code executable is ok. Continue check.
Message: Executing code for the cases given
```

April 17, 2007
Kuran B. Bekar, Penn State University, USA

How to use script: table generation

```
/home/kbb/NEA-Benchmark$ ./benchrun --rdpool=./rdpool -t
Message: Reference data directory is found in the file system.
Warning: Missing some file(s) for table generation. Skipping these case(s).
Please check message file for further information
Message: Table generation is successfully completed for the given cases
```

April 17, 2007
Kuran B. Bekar, Penn State University, USA
How to use script: Sample table

Results of your transport code, CODE, and the % error between the result of your code and the Reference solution (MCNP5) for L=1.0

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>% Error</th>
<th>Reference</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>1.075</td>
<td>1.0%</td>
<td>1.081</td>
<td>0.9%</td>
</tr>
<tr>
<td>1b</td>
<td>1.073</td>
<td>1.0%</td>
<td>1.080</td>
<td>0.9%</td>
</tr>
<tr>
<td>2a</td>
<td>1.073</td>
<td>1.0%</td>
<td>1.081</td>
<td>0.9%</td>
</tr>
<tr>
<td>2b</td>
<td>1.073</td>
<td>1.0%</td>
<td>1.081</td>
<td>0.9%</td>
</tr>
<tr>
<td>3a</td>
<td>1.073</td>
<td>1.0%</td>
<td>1.081</td>
<td>0.9%</td>
</tr>
</tbody>
</table>

April 17, 2007
Kumar B. Bokan, Penn State University, USA

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Naming Files

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Prefix</th>
<th>Extension</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>gamma</td>
<td>.c (output file)</td>
</tr>
<tr>
<td></td>
<td>S1</td>
<td>.i (input file)</td>
</tr>
<tr>
<td></td>
<td>.data</td>
<td>.data file</td>
</tr>
</tbody>
</table>

Files for the case L=10.0, gamma=0.5, S1=10.0, c1=0.5, S2=0.1, c2=0.5

April 17, 2007
Kumar B. Bokan, Penn State University, USA
How to Modify Script

Modules:

a) generate_inputs
b) execute_cases
c) postp_cases
d) generate_XS
e) make_tables
f) merging_data_files

---

April 17, 2007
Kurt B. Baker, Penn State University, USA
How to Modify Script

Sample modification for execute_cases module:

```plaintext
loop l in L
  loop gamma in Gamma
    loop c in C1
      loop x in C2
        loop y in C2
          loop z in C2
            generate_input_filename
            # code knows input file name for this case as the value of variable Gamma
            # code's output file name should be outname echo Gamma
            $(printf $1".o")
          # $tufunname echo $tufunname
            -F"" -I"" $(printf $1 "")
            # $MCRF execute with command line args:
            $CODEDIR/$CODE log="" Variables echo $MCRF_2 $MCRF_1 >> $CODE log
            =
            =
            =
            =
          # END MODIFICATION
        end loop z
      end loop y
    end loop x
  end loop gamma
end loop l
```

How to Modify Script

Interface block between input generator and pre-processor code
Interface block between output processor and post-processing code

```plaintext
* imname : input file name
* ID1 : ID/name of the first material
* ID2 : ID/name of the second material
* CODETMPDIR : directory where input template file resides (INPUT GENERATOR)
* CODETMP : input template filename (INPUT GENERATOR)
* x vector : 7 elements
* y vector : 7 elements
* z vector : 7 elements
```
Sample modification for generate_inputs module:

```plaintext
preprocessor loops (5 loops)

```

```
BEGIN MODIFICATION
# variable "inpName" is automatically generated by the function
# generate_input_filename. Please redirect or copy your input file
# or inpName (other parts of this script only know inpName as input file)
# benchmark script places calculated parameters in the pre-processor code
# as command line arguments
#
# m arguments are:
# 1) inpName, name of the MCNP input file
# 2) E1, all of the first material
# 3) E2, all of the second material
# 4) CODETMPDIR, location of the input template
# 5) CODETMP, name of the input template
# 6) n vector, 7 elements
# 7) y vector, 7 elements
# 8) z vector, 7 elements
#
# Use same structure for your input generator.
# Otherwise, following command should be modified
#
# SREP Simulation SID1 SID2 CODETMPDIR SCODETMPS "$[n[*]]" "$[y[*]]" "$[z[*]]"
#-END MODIFICATION
```

end parameter loops (4 loops)

April 17, 2007
Kurt B. Belak, Penn State University, USA

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Benchmarking the Accuracy of Solution of 3-Dimensional Transport Codes and Methods over a Range in Parameter Space

benchrun-1.1

Data file structure for table generation
(output of post-processor code)

```
username : USERNAME (optional)
data : DATE of post-processing (optional)
pwd : WORKING DIRECTORY (optional)
input file name : INPUTNAME_input filename (optional)

Parameters:
L : L value of this case
Gamma : GAMMA value of this case
Signal1 : SIGNAL1 value of this case
c1 : c1 value of this case
Signal2 : SIGNAL2 value of this case
c2 : c2 value of this case

RESULTS
Item Value

1 a lxxxxxx Ext Hom(E12.5)
1 b txxxxxx Ext

2 a lxxxxxx Ext
3 m nxxxxxx Ext
```

April 17, 2007
Kurt B. Belak, Penn State University, USA
**Table structure**

<table>
<thead>
<tr>
<th>item</th>
<th>gamma=0.1</th>
<th>gamma=0.5</th>
<th>gamma=0.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>value (%) error</td>
<td>value (%) error</td>
<td>value (%) error</td>
<td></td>
</tr>
<tr>
<td>1.a</td>
<td>x.xxxxxxEnx xxx.xx</td>
<td>x.xxxxxxEnx xxx.xx</td>
<td>x.xxxxxxEnx xxx.xx</td>
</tr>
<tr>
<td>1.b</td>
<td>x.xxxxxxEnx xxx.xx</td>
<td>x.xxxxxxEnx xxx.xx</td>
<td>x.xxxxxxEnx xxx.xx</td>
</tr>
<tr>
<td>2.a</td>
<td>x.xxxxxxEnx xxx.xx</td>
<td>x.xxxxxxEnx xxx.xx</td>
<td>x.xxxxxxEnx xxx.xx</td>
</tr>
<tr>
<td>3.a</td>
<td>x.xxxxxxEnx xxx.xx</td>
<td>x.xxxxxxEnx xxx.xx</td>
<td>x.xxxxxxEnx xxx.xx</td>
</tr>
</tbody>
</table>

(formats: E12.5 and F6.2)
**How to use script: Option list, help page**

```
Usage: benchrun [options]

-a | --all     Run all cases, script generates all inputs and cross-sections, then executes and post-processes all cases.
-x | --xsec    Only generate cross-sections.
-i | --input    Only generate transport code inputs.
-p | --postprocess    Process transport code outputs.
-e | --execute    Execute transport code with previously generated inputs.
-t | --table    Tabulate results in LaTeX table format (requires LaTeX and DVITools).
-h | --help     What you're reading
--single L gamma sigma1 c1 sigma2 c2
Perform calculation for a single case with L, gamma, sigma1, c1, sigma2 and c2 values.
```

April 17, 2007
Kurt R. Baker, Penn State University, USA

**How to use script: Code execution**

```
Usage: benchrun [-e]

Message:
Code executable is found in the given directory

Message:
Code executable is ok. Continue check.

Message:
Executing code for the cases given
```

April 17, 2007
Kurt R. Baker, Penn State University, USA
How to use script: Output processing

```
# code post-processor is found in specified directory
Message: Post-processing all outputs for the cases given
```

How to use script: Individual cases

```
# Wrong entry in command line. Option --single should be followed by six numeric entries.
```

```
# Wrong entry in command line. Please check values for L,gamma,sigma1,sigma2,c2 after option --single. Some entries are out of range defined in benchmark problem.
```

April 17, 2007
Kyuhan B. Baker, Penn State University, USA
**How to use script: range of cases**

```
$ runtest8/benchmarks /benchmark --group L-6:1 a1=0.1 a5=0.1 -i
```

Options:
- `-i` : Run test 1
- `-l` : Run test 2
- `-c` : Run test 3
- `-r` : Run test 4

Errors:
- Incorrect entry in command line. Option --group should be followed by at least one of the following six keywords:
  - L
  - gamma
  - a1
  - a5
  - c1
  - c5

```
$ runtest8/benchmarks /benchmark --group L-6:1 a1=0.1 a5=0.1 -l
```

Errors:
- Incorrect entry in command line. Please check values for L, gamma, a1, a5, c1, c5 after option --group. Some entries are out of range defined in benchmark problem.

```
$ runtest8/benchmarks /benchmark --group L-6:1 a1=0.1 --wrong-option
```

Errors:
- Unrecognized option in command line: --wrong-option

```
$ runtest8/benchmarks /benchmark
```

Errors:
- No option found in command line. Use: --group L-6:1 a1=0.1

---

**How to use script: command line parameter definition**

```
$ runtest8/benchmarks /benchmark --prepro=lambda -i
```

Message:
- Code input template file is found in specified directory.

Message:
- Code pre-processor is found in specified directory.

Message:
- Generating inputs for the cases given.

---

April 17, 2007

Kunzel B. Ebel, Penn State University, USA
How to use script: command line parameter definition

```
./benchrun --post=/path/to/postprocessor -p
```

Message:
Code post-processor is found in specified directory

```
./benchrun --post=/path/to/postprocessor -p
```

Message:
Post-processing all outputs for the cases given

April 17, 2007
Kurt R. Baines, Penn State University, USA

How to use script: command line parameter definition

```
./benchrun --codotmp=naa.tmp --codotmpdir=lib0
```

Error:
Given code input template location/directory, WRONGDIR is not found in the file system. Please check and enter code input template path correctly.

```
./benchrun --codotmp=naa.tmp --codotmpdir=lib0
```

Error:
Code input template file, WRONG2_FILE, is not found in the specified path. Please check and enter code input template and its location correctly.

```
./benchrun
```

April 17, 2007
Kurt R. Baines, Penn State University, USA
How to use script: command line parameter definition

```bash
kbb@kbbhome:/NEA-Benchmark$ ./benchrun --rpool=/WAGNDIR -c error
Reference data directory is not found in the file system.
Please check and enter the location of reference data correctly.

kbb@kbbhome:/NEA-Benchmark$ ./benchrun --prem=WAGNDIR/WRENC -1 error
Cone input template file is found in specified directory

Error:
Code pre-processor is not found in the file system.
Please check and enter the pre-processor file name and its location correctly.
```

How to use script: Sample data file

```
```

April 17, 2007
Kursat. B. Bekar, Penn State University, USA
OECD/NEA Parameter Study Benchmark
MCNP5 Reference Solutions

**CELL DESCRIPTIONS**

- CELL 1
  - 10 ZO XZ XO XZ XO XZ
  - 10 ZO XZ XO XZ

**PARAMETERS**

- **CELL 1**: L = 0.1, 1.0, 10.0
- **CELL 2**: L = 0.1, 1.0, 10.0
- **CELL 3**: L = 0.1, 1.0, 10.0
- **CELL 4**: L = 0.1, 1.0, 10.0
- **CELL 5**: L = 0.1, 1.0, 10.0
- **CELL 6**: L = 0.1, 1.0, 10.0
- **CELL 7**: L = 0.1, 1.0, 10.0
- **CELL 8**: L = 0.1, 1.0, 10.0
- **CELL 9**: L = 0.1, 1.0, 10.0
- **CELL 10**: L = 0.1, 1.0, 10.0

**MATERIALS**

- **MATERI1**: C1 = (1.0, -C1)
- **MATERI2**: C2 = (1.0, -C2)

**SURFACE DESCRIPTIONS**

- **SURFACE 1**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 2**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 3**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 4**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 5**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 6**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 7**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 8**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 9**: 1 2 3 4 5 6 7 8 9 10
- **SURFACE 10**: 1 2 3 4 5 6 7 8 9 10

**SOURCES**

- **SOURCE 1**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 2**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 3**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 4**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 5**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 6**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 7**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 8**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 9**: 1 2 3 4 5 6 7 8 9 10
- **SOURCE 10**: 1 2 3 4 5 6 7 8 9 10
MCNP5 Reference Solutions

- Reference solutions generated by both Kursat Bekar & Forrest Brown
  - Initial results
  - Need more histories

- In progress
  - Need to compare results
  - Need to add variance reduction
    - Novel problem: parameterize weight windows