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:

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.

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 re-generate 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

---

**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

<table>
<thead>
<tr>
<th>Country</th>
<th>Name</th>
<th>Phone</th>
<th>Email</th>
<th>Address</th>
</tr>
</thead>
<tbody>
<tr>
<td>CANADA</td>
<td>HEBERT, Alain</td>
<td>Tel: +1 (514) 340 4471 ex.4519</td>
<td><a href="mailto:alain.hebert@polymtl.ca">alain.hebert@polymtl.ca</a></td>
<td>PO Box 6079, Station Centre-Ville Montreal, QUEBEC H3C 3A7</td>
</tr>
<tr>
<td></td>
<td>LE TELLIER, Romain</td>
<td>Tel:</td>
<td><a href="mailto:romain.le-rellier@polymtl.ca">romain.le-rellier@polymtl.ca</a></td>
<td>Po box 6079 Succursalle Centre ville H3C3A7 MONTREAL</td>
</tr>
<tr>
<td></td>
<td>MARLEAU, Guy</td>
<td>Tel: +1 514 340 4711 ext 4204</td>
<td><a href="mailto:guy.marleau@polymtl.ca">guy.marleau@polymtl.ca</a></td>
<td>Case Postale 6079 succ. Centre-Ville MONTREAL, QUEBEC H3C 3A7</td>
</tr>
<tr>
<td>FRANCE</td>
<td>AUSSOURD, Christian</td>
<td>Tel: +33 1 69 26 52 14</td>
<td><a href="mailto:christian.aussourd@cea.fr">christian.aussourd@cea.fr</a></td>
<td>B.P. 12 F-91680 BRUYERES-LE-CHATEL</td>
</tr>
<tr>
<td></td>
<td>ZMIJAREVIC, Igor</td>
<td>Tel: +33 1 69 08 84 75</td>
<td><a href="mailto:igor.zmijarevic@cea.fr">igor.zmijarevic@cea.fr</a></td>
<td>DEN/DM2S/SERMA Bat. 470 F-91191 GIF-SUR-YVETTE Cedex</td>
</tr>
<tr>
<td>GERMANY</td>
<td>BECKERT, Carsten</td>
<td>Tel:</td>
<td><a href="mailto:C.BECKERT@FZD.DE">C.BECKERT@FZD.DE</a></td>
<td>Postfach 51 01 19 D-01314 DRESDEN</td>
</tr>
<tr>
<td></td>
<td>LANGENBUCH, Siegfried</td>
<td>Tel: +49 89 3200 4424</td>
<td><a href="mailto:lab@grs.de">lab@grs.de</a></td>
<td>Postfach 13 28 D-85748 GARCHING</td>
</tr>
<tr>
<td></td>
<td>PAUTZ, Andreas</td>
<td>Tel: +49 9131 18 97580</td>
<td><a href="mailto:Andreas.Pautz@areva.com">Andreas.Pautz@areva.com</a></td>
<td>Bunsenstrasse 43 91058 Erlangen</td>
</tr>
<tr>
<td></td>
<td>ZWERMANN, Winfried</td>
<td>Tel: +49 89 32004 425</td>
<td><a href="mailto:Winfried.Zwermann@grs.de">Winfried.Zwermann@grs.de</a></td>
<td>D-85748 GARCHING</td>
</tr>
</tbody>
</table>
**KOREA (REPUBLIC OF)**

CHO, Nam Zin  
Tel: +82 (42) 869 3819  
Department of Nuclear and Quantum Engineering  
Fax: +82 (42) 869 3810 or 5859  
Korea Advanced Institute of Science and Technology  
Eml: nzcho@kaist.ac.kr  
373-1 Kusong-dong, Yusong-gu  
Daejeon 305-701

**SOUTH AFRICA**

TOMASEVIC, Djordje  
Chief Scientist  
Tel: +27 12 305 5536  
Fax: +27 12 305 5166  
Nuclear Energy Corporation of S. Africa Limited  
P.O. Box 582  
Pretoria, 0001

**SWEDEN**

KOZLOWSKI, Tomasz  
KTH Nuclear Power Safety  
Tel: +46 8 553 788 22  
KTH (Royal Institute of Technology)  
Fax: +46 8 553 788 30  
Roslagstullsbacken 21  
10691 Stockholm

**UNITED KINGDOM**

COPESTAKE, Alan  
Rolls Royce Marine Power  
Tel: +44 1 332 667124  
P.O. Box 2000  
Fax: +44 1 332 622 939  
Derby DEZ1 7XX  
Eml: alan.copestake@rolls-royce.com

SMEDLEY-STEVENSON, Richard P.  
AWE(A) Aldermaston  
Tel: +44 1 18 9824173  
Building A70.2, Room 103  
Fax: +44 1 18 9824820  
Eml: rsmedley-stevenson@awe.co.uk

**UNITED STATES OF AMERICA**

AZMY, Yousry  
Dept. of Mechanical & Nuclear Engineering  
Tel: +1 (814) 865 0039  
The Pennsylvania State University  
Eml: yya3@psu.edu  
University Park, PA 16802

BEKAR, Kursat B.  
Department of Mechanical and Nuclear Engineering  
Tel: +1 814 865 8429  
The Pennsylvania State University  
Fax: +1 814 865 8499  
138 Reber Bldg  
University Park, PA 16802

BROWN, Forrest  
Los Alamos National Laboratory  
Tel: +1 505 667 7581  
MS F663, P.O. Box 1663  
Fax: +1 505 665 3046  
Los Alamos, NM 87545

DONOVA, Tim  
KAPL  
Tel:  
PO BOX 1072  
Fax:  
12301-1072 SCHENECTADY, NY  
Eml: donovat@kapl.gov

FIENO, Tom  
KAPL  
Tel:  
PO BOX 1072  
Fax:  
12301-1072 SCHENECTADY, NY  
Eml: fieneote@kapl.gov

GANAPOL, Barry D.  
University of Arizona  
Tel: +1 520 621 4728  
Dept. of Aerospace and Mechanical Engineering, Rm. 727, AME Bldg.  
Fax: +1 520 621 8191  
1130 N. Montain Ave  
Tucson, AZ 85711  
Eml: ganapol@cowboy.ame.arizona.edu
HAGHIGHAT, Alireza
Nuclear and Radiological Engineering
202 Nuclear Sciences Building
University of Florida
Gainesville, FL 32608
Tel: +1 352 392 1415
Fax: +1 352 392 3380
Eml: haghighat@ufl.edu

HURSIN, Mathieu
Dept. of Nuclear Engineering
University of California
BERKELEY, CA 94720
Tel: +1 865 574 6176
Fax: +1 8652414046
Eml: mhursin@ecn.purdue.edu

KIRK, Bernadette L.
Director
RSICC/ORNL
PO Box 2008
Bldg. 5700, MS 6171
Oak Ridge, TN 37831-6171
Tel: +1 865 574 6176
Fax: +1 8652414046
Eml: kirkbl@ornl.gov

LEWIS, Elmer E.
Northwestern University
Dept. of Mech. Eng.
Technological Institute
2145 Sheridan Road
Evanston, IL 60201
Tel: +1 847 491 3579
Fax: +1 847 491 3915
Eml: e-lewis@northwestern.edu

LEWIS, David W.
Idaho National Laboratory
PO Box 1625, MS 3860
IDAHO FALLS, ID 83415-3860
Tel: +1 208 526 7627
Fax: +1 208 526 2930
Eml: david.nigg@inl.gov

LEWIS, Michael A.
Argonne National Laboratory
Bldg 208
9700 South Cass Avenue
ARGONNE, IL 60439-4842
Tel: +1 630 252 4500
Fax: +1 630 252 4500
Eml: masmith@anl.gov

LEWIS, Glenn E.
Nuclear & Radiological Engineering
University of Florida
Gainesville, FL 32611
Tel: +1 352 392 1401
Fax: +1 352 392 3380
Eml: sjoden@ufl.edu

NIGG, David W.
Idaho National Laboratory
2525 N. Fremont
P.O. Box 1625, MS 3860
IDAHO FALLS, ID 83415-3860
Tel: +1 208 526 7627
Fax: +1 208 526 2930
Eml: david.nigg@inl.gov

NIGG, David W.
Idaho National Laboratory
PO Box 1625, MS 3860
IDAHO FALLS, ID 83415-3860
Tel: +1 208 526 7627
Fax: +1 208 526 2930
Eml: david.nigg@inl.gov

Palmiotti, Giuseppe (Pino)
Reactor Analysis Division
Argonne National Laboratory
Bldg 208
9700 South Cass Avenue
ARGONNE, IL 60439-4842
Tel: +1 630 252 2858
Fax: +1 630 252 4500
Eml: GPalmiotti@anl.gov

Palmiotti, Giuseppe (Pino)
Reactor Analysis Division
Argonne National Laboratory
Bldg 208
9700 South Cass Avenue
ARGONNE, IL 60439-4842
Tel: +1 630 252 2858
Fax: +1 630 252 4500
Eml: GPalmiotti@anl.gov

ROSA, Massimiliano
Dept. of Mechanical & Nuclear Eng.
The Pennsylvania State University
229 Reber Bldg.
University Park, PA 16802
Tel: +1 814 865 8499
Fax: +1 814 865 8499
Eml: mzr127@psu.edu

SMITH, Micheal A.
Argonne National Laboratory
Bldg 208 Rm L102
9700 South Cass Ave
Argonne IL 60439
Tel: +1 630 252 3469
Fax: +1 630 252 3469
Eml: masmith@anl.gov

Sjoden, Glenn E.
Nuclear & Radiological Engineering
University of Florida
202 Nuclear Sciences Building
Gainesville, FL 32611
Tel: +1 352 392 1401
Fax: +1 352 392 3380
Eml: sjoden@ufl.edu

Yi, Ce
Nuclear and Radiological Engineering
202 Nuclear Sciences Building
University of Florida
Gainesville, FL 32608
Tel: +1 352 392 3380
Fax: +1 352 392 3380
Eml: yice@ufl.edu
International Organisations
SARTORI, Enrico
OECD/NEA Data Bank
Le Seine-Saint Germain
12 boulevard des Iles
F-92130 Issy-les-Moulineaux
France
Tel: +33 1 45 24 10 72 / 78
Fax: +33 1 45 24 11 10 / 28
Eml: sartori@nea.fr
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/algorithm
  - 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 $\Rightarrow$ decreasing error: desirable not inevitable!
  - Asymptotic regime: error decreases monotonically with refinement
  - Outside asymptotic regime: fortuitously small error possible, followed by increased error with refinement
  - Generally, user does not know exact reference solution $\Rightarrow$ 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 non-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, \( \mu \) scaled
  - Vacuum BCs
  - Scattering ratios: \( c_1 \) & \( c_2 \)

- Unit source:
Suite Specification

- Suite constructed by independently varying 6 parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>0.1 to 10.0</td>
</tr>
<tr>
<td>γ</td>
<td>0.1 to 0.9</td>
</tr>
<tr>
<td>σ₁</td>
<td>0.1 to 10.0</td>
</tr>
<tr>
<td>c₁</td>
<td>0.5 to 10.0</td>
</tr>
<tr>
<td>σ₂</td>
<td>0.1 to 10.0</td>
</tr>
<tr>
<td>c₂</td>
<td>0.5 to 10.0</td>
</tr>
</tbody>
</table>

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

---

OUTLINE

- Overview
- Option summary
- How to use script: Examples
- Naming Files
- How to modify script

April 17, 2007

Kursat B. Bekar, Penn State University, USA
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
Kurt C. Baker, Penn State University, USA
OVERVIEW

Execution of transport code:

**CODE EXECUTION MODULE:**

- **generate** input filename
  - $L_{\text{gamma}}, S1, c1$ and $S2, c2$
- **check input file(s)**
- **generate** output filename
  - $L_{\text{gamma}}, S1, c1$ and $S2, c2$
- **execute transport code**
  - transport code, CODE code path, CODEDR input file
  - transport code output(s)

April 17, 2007
Kumar D. Bekar, Penn State University, USA

OVERVIEW

Output processing (Collection of data):

**OUTPUT PROCESSING MODULE:**

- **generate** input filename
  - $L_{\text{gamma}}, S1, c1$ and $S2, c2$
- **output filename, data filename**
- **calculate** boundary points
  - $L_{\text{gamma}}$
- **generate** material ID
  - $S1, c1$ and $S2, c2$
- **execute** post-processor code
  - Post-processor code, POSTP output file(s)
  - data file

April 17, 2007
Kumar D. Bekar, Penn State University, USA
OVERVIEW

Table generation (Presenting data):

**TABLE GENERATION MODULE:**

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

**LaTeX, DVUTILS**

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

April 17, 2007

Kumar B. Baker, Penn State University, USA

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 DVutils)*
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
Kumar B. Baker, Penn State University, USA
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.

```
CODEDIR : directory where the code executable resides
CODE : name of executable
CODETMPDIR : directory where the code input template resides
CODETMP : name of code input template
POSTP : post-processing code with its full path
PREP : pre-processing code with its full path
RDPOOL : directory where the reference MCNP results reside
```

April 17, 2007
Kunar B. Beber, Penn State University, USA
10

How to use script: Input generation

```
kbb@kbbhome:/NEA-Benchmark$ ./benchrun -l
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
kbb@kbbhome:/NEA-Benchmark$
```
How to use script: individual cases

```
benchrun --single 0.1 0.1 0.1
```

How to use script: range of cases

```
benchrun --group 0.1 0.1 0.1 0.1 0.1
```

April 17, 2007
Krzysztof Sikora, Penn State University, USA
How to use script: command line parameter definition

```
/kbo@kbbhome/NEA-Benchmark$ ./benchrun --code=merp5 --codedir=./ -e
Message:
  Code executable is found in the given directory
Message:
  Code executable ok. Continue check..
Message:
  Executing code for the cases given

/kbo@kbbhome/NEA-Benchmark$ ./benchrun --code=merp5 --codedir=./ -t
Message:
  Reference data directory is found in the file system.
Message:
  Missing some file(s) for table generation. Skipping these case(s).
Message:
  Please check message file for further information
Message:
  Table generation is successfully completed for the given cases
```

April 17, 2007  Khorst B. Behrens, Penn State University, USA  14
Benchmarks for Accuracy of Solutions of 3-Dimensional Transport Codes and Methods over a Range in Parameter Space

**benchrun-1.1**

How to use script: Sample file

Results of your transport code, CODE, and the percentage error between the result of your code and the Benchmark calculations (MENDS) for L=10.0

<table>
<thead>
<tr>
<th>File</th>
<th>Method</th>
<th>Code</th>
<th>Value</th>
<th>Error</th>
<th>&quot;b&quot; Value</th>
<th>&quot;b&quot; Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-a</td>
<td>F</td>
<td>1.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.23</td>
<td>0.03</td>
</tr>
<tr>
<td>1-b</td>
<td>F</td>
<td>1.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.23</td>
<td>0.03</td>
</tr>
<tr>
<td>1-c</td>
<td>F</td>
<td>1.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.23</td>
<td>0.03</td>
</tr>
<tr>
<td>1-d</td>
<td>F</td>
<td>1.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.23</td>
<td>0.03</td>
</tr>
<tr>
<td>2-a</td>
<td>F</td>
<td>1.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.23</td>
<td>0.03</td>
</tr>
<tr>
<td>2-b</td>
<td>F</td>
<td>1.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.23</td>
<td>0.03</td>
</tr>
<tr>
<td>2-c</td>
<td>F</td>
<td>1.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.23</td>
<td>0.03</td>
</tr>
<tr>
<td>2-d</td>
<td>F</td>
<td>1.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.23</td>
<td>0.03</td>
</tr>
</tbody>
</table>

April 17, 2007

Kumar B. Bhat, Penn State University, USA

---

Benchmarks for Accuracy of Solutions of 3-Dimensional Transport Codes and Methods over a Range in Parameter Space

**benchrun-1.1**

Naming Files

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Prefix</th>
<th>Extension</th>
</tr>
</thead>
<tbody>
<tr>
<td>L, gamma</td>
<td>.o</td>
<td>.o output file</td>
</tr>
<tr>
<td>S1, c1, S2, c2</td>
<td>.i</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. Bhat, Penn State University, USA
How to Modify Script

Modules:

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

---

How to Modify Script

Modules a, b, and c have the following general structure:

```plaintext
loop 1 in L
  loop gamma in Gamma
    loop signal1 in Signal1
      loop c1 in C1
        loop signal2 in Signal2
          loop c2 in C2
            -> generate some data for the case
            -> generate input file name
            BEGIN:MODIFICATION
              # screen(import_generation, execution, or post_processing)
              #
              END:MODIFICATION
            END:MODIFICATION
          end loop signal2
        end loop c1
      end loop signal1
    end loop C1
  end loop Gamma
end loop L
```
How to Modify Script

Sample modification for execute_cases module:

```c
loop i in L
  loop j in L
    if (j > i) 
      generate_input_filename
      # code knows input file names for this case so the value of variable Signame
      # code's output file name should be
      outname = echo $Signame
      outname = outname":"F ""("print 51" a")""
      outname = outname":"F ""("print 51" n")""
      
      # we defined execution with command line args
      $CODE_DIR.$CODE_exec=./$Signame.$ext=../$SIDE_DIR.$ext1 >> $CODE.log
      
      #
      
      inv outp $outname, via meshual $Signame; run exe
      
      # END MODIFICATION
      
      exit
    
    end loop j
  end loop i
end loop
```

April 17, 2007

Kurtis B. Bieder, Penn State University, USA
Sample modification for generate_inputs module:

```c
...#BEGIN MODIFICATION
# variable "insname" is automatically generated by the function
# generate_input.Elname. Please redirect or copy your input file
# to insname (other parts of this script only know insname or input file)
# benchrun accepts as input calculated parameters in the pre-processor code
# as command line arguments
#
# its arguments are:
# 1) insname, name of the MCNP input file
# 2) #1D, # of the first material
# 3) #2D, # of the second material
# 4) CODETMPD1, location of the input template
# 5) CODEMT, name of the input template
# 6) n vecor, n elements
# 7) y vector, m elements
# 8) z vector, p elements
#
# Use same structure for your input generator
# Otherwise, following command should be modified:
#
# Source: insname S1D1 S1D2 CODEMTPD1 CODEMT $[m[*]]$ $[y[*]]$ $[z[*]]$
#END MODIFICATION
```

and parameter loops (6 loops)

April 17, 2007

Kurt B. Becker, Penn State University, USA

22

---

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

```
username : USERNAME (optional)
date : DATE of post-processing (optional)
work : WORKING DIRECTARY (optional)
suffix : OUTPUT_FILENAME (optional)
```

Parameters:

```
L : L value of this case
Omega : GAMMA value of this case
Sigma1 : Sigma1 value of this case
c1 : c1 value of this case
Sigma2 : Sigma2 value of this case
c2 : C2 value of this case
```

```
RESULTS
```

<table>
<thead>
<tr>
<th>Item</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.a</td>
<td>a.nxxxEnExx (E1.2.5)</td>
</tr>
<tr>
<td>1.b</td>
<td>b.nxxxEnExx</td>
</tr>
<tr>
<td>2.a</td>
<td>a.nxxxEnExx</td>
</tr>
<tr>
<td>3.m</td>
<td>m.nxxxEnExx</td>
</tr>
</tbody>
</table>

April 17, 2007

Kurt B. Becker, Penn State University, USA

23
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</td>
<td>value (%error)</td>
<td>value (%error)</td>
<td>value (%error)</td>
</tr>
<tr>
<td>1.a</td>
<td>xxxxxxxxxx xxx.xxx</td>
<td>xxxxxxxxxx xxx.xxx</td>
<td>xxxxxxxxxx xxx.xxx</td>
</tr>
<tr>
<td>1.b</td>
<td>xxxxxxxxxx xxx.xxx</td>
<td>xxxxxxxxxx xxx.xxx</td>
<td>xxxxxxxxxx xxx.xxx</td>
</tr>
<tr>
<td>2.a</td>
<td>xxxxxxxxxx xxx.xxx</td>
<td>xxxxxxxxxx xxx.xxx</td>
<td>xxxxxxxxxx xxx.xxx</td>
</tr>
<tr>
<td>3.m</td>
<td>xxxxxxxxxx xxx.xxx</td>
<td>xxxxxxxxxx xxx.xxx</td>
<td>xxxxxxxxxx xxx.xxx</td>
</tr>
</tbody>
</table>

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

```
home/kbhome/NEA-Benchmarks $ ./benchrun --help
script of NEA Benchmark, version 1.1

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.
   -o --execute Execute transport code with previously generated input
              files.
   -t --table  Tabulate results in latex table format (requires latex
              and dvitex)
   -h --help   What you're reading
   --single L gamma signal c1 signal2 c2

   perform calculation for a single case with L, gamma, signal,
   c1, signal and c2 values.
```

April 17, 2007  Kavita B. Baker, Penn State University, USA  26

How to use script: Code execution

```
/home/kbhome/NEA-Benchmarks $ ./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  Kavita B. Baker, Penn State University, USA  27
Howto use script: Output processing

```
!NEA-Benchmarks$ ./benchrun -p
Message: code post-processor is found in specified directory
Message: Post-processing all outputs for the cases given
```

---

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

---

Howto use script: individual cases

```
!NEA-Benchmarks$ ./benchrun --single 0.1 0.2 0.3
Error: Wrong entry in command line. Option --single should be followed by six numeric entries.

!NEA-Benchmarks$ ./benchrun --single 0.1 0.1 0.5 0.1 9999
Error: Wrong entry in command line. Please check values for E, gamma, sigma, c1, sigma, c2 after option --single. Some entries are out of range defined in benchmark problem.
```

---

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

How to use script: command line parameter definition
Benchrun-1.1

How to use script: command line parameter definition

April 17, 2007

Kurtis B. Bailer, Penn State University, USA
Benchmarking the Accuracy of Solution of 3-Dimensional Transport Codes and Methods over a Range in Parameter Space

benchrun-1.1

How to use script: command line parameter definition

```bash
kbo@kbohome:/NEA-Benchmark$ ./benchrun --input=/path/W00GDIR -d
Error: Reference data directory is not found in the file system. Please check and enter the location of reference data correctly.

kbo@kbohome:/NEA-Benchmark$ ./benchrun --input=/path/W00GDIR/WRING -d
Error: Code input template file is found in specified directory

kbo@kbohome:/NEA-Benchmark$ ./benchrun --preprocessor=WRING_DIR/WRING -d
Error: Code pre-processor is not found in the file system. Please check and enter the pre-processor file name and its location correctly.
```

April 17, 2007
Kurmit B. Debbar, Penn State University, USA

---

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

benchrun-1.1

How to use script: Sample data file

```plaintext
# Sample data file

<table>
<thead>
<tr>
<th>Item</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.a</td>
<td>2.7111e+09</td>
</tr>
<tr>
<td>1.b</td>
<td>2.2327e+09</td>
</tr>
<tr>
<td>2.a</td>
<td>8.3199e+08</td>
</tr>
<tr>
<td>2.b</td>
<td>3.9800e+03</td>
</tr>
<tr>
<td>2.c</td>
<td>-4.4209e-01</td>
</tr>
<tr>
<td>2.e</td>
<td>4.2780e-02</td>
</tr>
<tr>
<td>2.f</td>
<td>6.7760e-03</td>
</tr>
</tbody>
</table>
```

April 17, 2007
Kurmit B. Debbar, Penn State University, USA
OECD/NEA Parameter Study Benchmark
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