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Title: ANALYTICAL BENCHMARK TEST SET FOR CRITICALITY CODE VERIFICATION

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ANALYTICAL BENCHMARK TEST SET FOR CRITICALITY CODE VERIFICATION

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Abstract

A number of published numerical solutions to analytic eigenvalue (k_{eff}) and eigenfunction equations are summarized for the purpose of creating a criticality verification benchmark test set. The 75-problem test set allows the user to verify the correctness of a criticality code for infinite medium and simple geometries in one- and two-energy groups, one- and two-media, and both isotropic and linearly anisotropic neutron scattering. A three- and six-energy group infinite medium problem are also included in the test set. The problem specifications will produce both $k_{eff} = 1$ and the quoted k_{∞} to at least five decimal places. Additional uses of the test set for code verification are also discussed. Los Alamos report LA–13511 contains the details of all 75 test problems.

Introduction

This paper describes a set of benchmark problems with analytic eigenvalue (k_{eff}) and eigenfunction (flux) solutions to the neutron transport equation from peer-reviewed journal articles. The purpose of the test set is to verify that transport algorithms and codes can correctly calculate the analytic k_{eff} and fluxes to at least five decimal places. These test set problems from the literature include infinite medium, slab, cylindrical, and spherical geometries in one- and two-energy groups, one- and two-media, and both isotropic and linearly anisotropic scattering. A three-group infinite medium and a six-group variant k_∞ problem (unpublished) are also included in the test set.

Verification is defined as "the process of evaluating a system or component to determine whether the products of a given development phase satisfy the conditions imposed at the start of the phase[1] or as a "proof of correctness." **Confirmation (proof) of correctness** is "a formal technique used to prove mathematically that a computer program satisfies its specified requirements.[1] In contrast to verification, **validation** is defined as "the process of evaluating a system or component during or at the end of the development process to determine whether it satisfies specified requirements.[1] Thus, code verification checks that the intended calculations have been executed correctly, while code validation compares the calculated results with experimental data.

The objectives of the test set are to define and document a set of analytic benchmarks for verifying criticality codes. **Benchmark** is defined as "a standard against which measurement or comparisons can be made.[1] Available benchmarks for code verification do not focus on criticality problems.[2] Validation benchmarks from critical experiments do exist, but are not verification benchmarks.[3] An initial effort to compile a benchmark test set for criticality calculation verification was begun, but not completed.[4,5] The analytic benchmarks described here can be used to verify computed numerical solutions for k_{eff} and the associated flux with virtually no uncertainty in the numerical benchmark values.

Why These Solutions Serve as a Test Set

All critical dimensions, k_{eff}, and scalar neutron flux results quoted here are based on numerical computations using the analytic solutions to the k_{eff} eigenvalue (homogeneous) transport equation for "simple" problems. The analytic methods used include Case's singular eigenfunction,[6] F_N and S_N methods,[7,8] and Green's functions.[9] All of these test set problem specifications and results are from peer-reviewed journals, and have, in some cases, been solved numerically using more than one analytic solution. All calculated values for critical dimensions, k_{eff}, and the scalar neutron flux are believed to be accurate to at least five decimal places.

Scope of the Criticality Verification Test Set

The verification test set was chosen to represent a "wide" range of problems from the relatively small number of published solutions. These problems include simple geometries, few neutron energy groups, and simplified (isotropic and linearly anisotropic) scattering models. The problems use neutron cross sections that are reasonable representations of the materials described. These cross sections are **not** general purpose multi-group values. The cross sections are used because they are extracted from the literature results and are intended to be used only to verify algorithm performance and **not** to predict criticality experiments.

The basic geometries include an infinite medium, slab, cylinder, and sphere with one- and two-energy group representations of uniform homogeneous materials. The slab and cylinder geometries are one-dimensional; that is, each is finite in one dimension (thickness for slab and radius for the cylinders) and infinite elsewhere. The two-media problems surround each geometry with a specified thickness of reflector.

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The emphasis of the test set is on the fundamental eigenvalue, k_{eff}. All k_{eff} eigenvalues for finite fissile materials are unity to at least five decimal places. The k_{∞} values for a uniform homogeneous infinite medium are greater than unity. Few numerical eigenfunction solutions are published; consequently, mainly one-group and uniform homogeneous infinite medium fluxes are included in the test set results.

To assist in verification, each problem has a unique identifier. Since the test set includes bare and multi-media problems, there are two forms of the identifier. The first form is for a bare geometry:

Fissile Material – Energy Groups – Scattering – Geometry

The possible entries for each category are listed in Table I. The fissile materials and identifier consist of Pu-239 (PU), U-235 (U), highly enriched uranium-aluminum-water assembly (UAL), low enrichment uranium and D_2O reactor system (UD2O), and a highly enriched uranium research reactor (URR). The identifier may be followed by a letter to differentiate between different cross-section sets from nominally the same material. The table lists identifiers for the reflector material (if any), number of energy groups, scattering order, and geometry. The geometry is identified by the first two letters in the table. The exception is for the infinite slab lattice cell which uses ISLC. An example of the one material form of the identifier is:

U-2-0-SP

which is the identifier for a bare U-235 reactor (no reflector), 2 energy groups, isotropically scattering, in spherical geometry.

The second form of the identifier includes the reflecting material. The reflectors are usually H_2O with an exception of a three region Fe, Na, Fe reflector. Although many of the reflectors are identified as H_2O, the reflector cross sections are unique to each problem. Consequently, a letter may follow H2O indicating the H_2O cross section set used. The multi-media identifier form is:

Fissile Material - Reflecting Material (thickness) - Energy Groups - Scattering - Geometry

To separate multiple reflector thicknesses for the same fissile material, the thickness is given in parenthesis in the title in units of mean free paths (mfp). For example,

UD2O-H2O(10)-1-0-SL

is the identifier for a uranium and D_2O reactor with a H_2O reflector of 10 mean free path thickness, one-energy group, isotropically scattering, in slab geometry. An "IN" in parenthesis after the H2O means an <u>in</u>finite water reflector.

TABLE I: Nomenclature for Problem Identifiers

Fissile Material	Reflector Material	Energy Groups	Scattering Order	Geometry
PU	bare	1 group	0 – P_0 Isotropic	INfinite
U	H2O	2 groups	1 – P_1 Anisotropic	SLab
UD2O	Fe-Na	3 groups	2 – P_2 Anisotropic	CYlinder
UAL		6 groups		SPhere
URR				Infinite Slab Lattice Cell

Tables II, III, and IV summarize each of the 75 problems in the test set and give the page number in Los Alamos report LA–13511.[10] A mark in the "Flux" column appears if the associated normalized spatial neutron fluxes or energy group flux ratio are given. There are 43 problems in the one-energy group case; 30 problems assume isotropic scattering and 13 have anisotropic scattering. For the two-energy group problems, there are 30 problems subdivided into 26 isotropic scattering problems and 4 linearly anisotropic problems. Also included for an infinite medium are a three-group and a six-group (2 coupled sets of three groups) isotropic problem. The test set includes 24 infinite medium problems, 24 slabs, 9 one-energy group cylinders, 14 spheres, and 4 infinite slab lattice cells.

TABLE II: Overview and Page Location for One-Energy Group Problem Identifiers

Number	Problem Identifier	Flux	Page Number	Scattering
1	PUa-1-0-IN	x	16	Isotropic
2	PUa-1-0-SL		16	
3	PUa-H2O(1)-1-0-SL		17	
4	PUa-H2O(0.5)-1-0-SL		17	
5	PUb-1-0-IN	x	16	
6	PUb-1-0-SL	x	16	
7	PUb-1-0-CY	x	16	
8	PUb-1-0-SP	x	16	
9	PUb-H2O(1)-1-0-CY		17	
10	PUb-H2O(10)-1-0-CY		17	
11	Ua-1-0-IN	x	18	
12	Ua-1-0-SL	x	18	
13	Ua-1-0-CY		18	
14	Ua-1-0-SP	x	18	
15	Ub-1-0-IN	x	18	
16	Ub-H2O(1)-1-0-SP		19	
17	Uc-1-0-IN	x	18	
18	Uc-H2O(2)-1-0-SP		19	
19	Ud-1-0-IN	x	18	
20	Ud-H2O(3)-1-0-SP		19	
21	UD2O-1-0-IN	x	20	
22	UD2O-1-0-SL	x	20	
23	UD2O-1-0-CY		20	
24	UD2O-1-0-SP	x	20	

TABLE II (cont.)

Number	Problem Identifier	Flux	Page Number	Scattering
25	UD2O-H2O(1)-1-0-SL		20	
26	UD2O-H2O(10)-1-0-SL		20	
27	UD2O-H2O(1)-1-0-CY		20	
28	UD2O-H2O(10)-1-0-CY		20	
29	Ue-1-0-IN	x	21	
30	Ue-Fe-Na-1-0-SL	x	21	
31	PU-1-1-IN	x	22	Anisotropic
32	PUa-1-1-SL		22	
33	PUa-1-2-SL		22	
34	PUb-1-1-SL		22	
35	PUb-1-2-SL		22	
36	Ua-1-1-CY		23	
37	Ub-1-1-CY		23	
38	UD2Oa-1-1-IN		24	
39	UD2Oa-1-1-SP		24	
40	UD2Ob-1-1-IN		24	
41	UD2Ob-1-1-SP		24	
42	UD2Oc-1-1-IN		24	
43	UD2Oc-1-1-SP		24	

TABLE III: Overview and Page Location for Two-Energy Group Problem Identifiers

Number	Problem Identifier	Flux	Page Number	Scattering
44	PU-2-0-IN	x	27	Isotropic
45	PU-2-0-SL		27	
46	PU-2-0-SP		27	
47	U-2-0-IN	x	28	
48	U-2-0-SL		28	
49	U-2-0-SP		28	
50	UAL-2-0-IN	x	29	
51	UAL-2-0-SL		29	
52	UAL-2-0-SP		29	
53	URRa-2-0-IN	x	30	
54	URRa-2-0-SL	x	30	
55	URRa-2-0-SP		30	
56	URRb-2-0-IN	x	31	
57	URRc-2-0-IN	x	31	
58	URRb-H2Oa(1)-2-0-SL		31	
59	URRb-H2Oa(5)-2-0-SL		31	
60	URRb-H2Oa(IN)-2-0-SL		31	
61	URRc-H2Oa(IN)-2-0-SL		31	
62	URRd-2-0-IN	x	32	
63	URRd-H2Ob(1)-2-0-ISLC		32	

TABLE III (cont.)

Number	Problem Identifier	Flux	Page Number	Scattering
64	URRd-H2Ob(10)-2-0-ISLC		32	
65	URRd-H2Oc(1)-2-0-ISLC		32	
66	URRd-H2Oc(10)-2-0-ISLC		32	
67	UD2O-2-0-IN	x	33	
68	UD2O-2-0-SL		33	
69	UD2O-2-0-SP		33	
70	URRa-2-1-IN	x	34	Anisotropic
71	URRa-2-1-SL	x	34	
72	UD2O-1-1-IN	x	35	
73	UD2O-2-1-SL		35	

TABLE IV: Overview and Page Location for Three- and Six-Energy Group Problem Identifiers

Number	Problem Identifier	Flux	Page Number	Scattering
74	URR-3-0-IN	x	36	Isotropic
75	URR-6-0-IN	x	38	

Uses of the Criticality Verification Test Set

LA–13511 provides all necessary problem definitions and published critical dimensions, k_{eff}, and scalar neutron flux results to verify a criticality transport algorithm or code and associated numerics such as random number generation and round-off errors. All material cross sections provided are macroscopic, so the atom density used by the code should be unity. Not all of the analytic solutions from the references are used, however, because the number of problems in the test set becomes too large. LA–13511 contains the complete list of 45 references.

The verification test set problems can be used in several ways. The user can choose to simply calculate the problems and compare forward and adjoint k_{eff} and neutron flux results with the benchmark solutions. However, there are several more verification processes that could be included. For example, in Monte Carlo codes, two forms of cross-section representation can be examined: multi-group and pointwise representation of multi-group data. In multi-group problems, an alternative verification procedure is to switch the energy groups when up-scattering is allowed in the code. To examine the alpha eigenvalue or time-dependent neutron decay or growth, the capture and total cross sections can be modified by α/v to represent subcritical and supercritical systems.

Another part of code verification is testing different representations of the same geometry (e.g., reflecting boundaries and lattices). An example is an infinite one-dimensional slab (finite in one dimension and infinite in the other two dimensions), which could be modeled as a three-dimensional cube with four reflective boundaries. Other geometry options can be tested by constructing several smaller cubes inside of the three-dimensional representation of a one-dimensional critical slab. The infinite medium problem can be represented by using large geometric boundaries, reflecting boundaries, or infinite lattices of finite shapes. Infinite medium problems can be used to verify constant scalar and angular flux in each energy group as well as scalar flux ratios for more than one energy group. Three-dimensional geometric representations of optically small objects can also be tested for k_∞ in infinite medium problems.[11] Purely absorbing one-group infinite medium problems can provide faster code verification since scattering does not alter the infinite medium k_∞.

Different calculation capabilities of a code should be tested using these problems. For Monte Carlo codes, different variance reduction methods such as analog or implicit capture and geometric splitting or Russian roulette can be verified. Cycle-to-cycle correlations in the estimated k_{eff} standard deviation must be taken into account to form valid k_{eff} confidence intervals. Statistically independent runs can be made and analyzed if necessary. The magnitude of any negative bias in k_{eff}, which is a function of the number of neutron histories per fission generation, also needs to be considered and made smaller than 0.00001.[12]

Deterministic codes can assess convergence characteristics and correctness of k_{eff} and the flux as a function of space and angle representation. Various characteristics of discrete ordinates numerics can also be checked such as the effects of eigenvalue search algorithms, angular redistribution terms in curvilinear geometries, ray effects, and various alternative geometric descriptions.

One-Group Example for Isotropic Cross Sections for U-235

TABLE V: One-Group Macroscopic Cross Sections (cm^{-1}) for U-235 (c = 1.30)

Material	ν	Σ_f	Σ_c	Σ_s	Σ_t	c
U-235 (a)	2.70	0.065280	0.013056	0.248064	0.32640	1.30

Using the cross sections for U-235 (a) in Table V, k_∞ = 2.25 (problem 11) with a constant angular and scalar flux everywhere. The critical dimension, r_c, and spatial flux ratios are given in Tables VI and VII for U-235 (a). The references are the same for both tables.

TABLE VI: Critical Dimensions, r_c, for One-Group Bare U-235 (c = 1.30)

Problem	Identifier	Geometry	r_c (mfp)	r_c (cm)	Reference
12	Ua-1-0-SL	Slab	0.93772556	2.872934	13
13	Ua-1-0-CY	Cylinder	1.72500292	5.284935	14,15
14	Ua-1-0-SP	Sphere	2.4248249802	7.428998	13

TABLE VII: Normalized Scalar Fluxes for One-Group Bare U-235 (c = 1.30)

Problem	Identifier	Geometry	r/r_c = 0.25	r/r_c = 0.5	r/r_c = 0.75	r/r_c = 1.0
12	Ua-1-0-SL	Slab	0.9669506	0.8686259	0.7055218	0.4461912
14	Ua-1-0-SP	Sphere	0.93244907	0.74553332	0.48095413	0.17177706

Summary

We have described a 75 problem verification test set with precise results for the critical dimensions, k_{eff} eigenvalue, and some eigenfunction (scalar neutron flux) results for infinite, slab, cylindrical, and spherical geometries for one- and two-energy group, multiple-media, and both isotropic and linearly anisotropic scattering. All test set problems specifications are from peer reviewed journals, and have, in many cases, been solved numerically by more than one analytic method. These calculated values for k_{eff} and the scalar neutron flux are believed to be accurate to at least five decimal places. Criticality codes can be verified using these analytic benchmark test problems.

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