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Title: Criticality Benchmark Calculations using PARTISN:
Comparisons using MENDF5 and MENDF6 Nuclear Data
Libraries

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***Criticality Benchmark Calculations using PARTISN:
Comparisons using MENDF5 and MENDF6
Nuclear Data Libraries***

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Criticality Benchmark Calculations using PARTISN: Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries

Ronald J. Ellis (ORNL), James J. Yugo (ORNL), Stephanie C. Frankle (LANL),
and Robert C. Little (LANL)

ABSTRACT

A project was undertaken to assess strengths and weaknesses in the MENDF5 and MENDF6 nuclear data libraries through the analysis of critical assembly benchmarks using the LANL discrete ordinates transport code PARTISN. As an initial analysis of the effects and anomalous results of some limitations in the MENDF libraries, this current work assesses differences in k_{eff} calculations between the PARTISN cases (with MENDF5 and MENDF6 nuclear data libraries) and MCNP cases (with ENDF/B-V and ENDF60 nuclear data libraries), and compares these results to the experimental data.

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Criticality Benchmark Calculations using PARTISN: Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries

Presentation Outline

- **Introduction**
- **Nuclear Data Libraries**
- **Comparisons of PARTISN results with MCNP calculations and with experiment**
- **Discussion and Observations**
- **Summary**

Criticality Benchmark Calculations using PARTISN: Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries

Introduction

- A suite of 86 criticality benchmark cases was developed at LANL to be suitable for the validation of nuclear data. (S.C. Frankle, LA-13594; 1999)
- The suite of criticality benchmark cases comprises one-, two-, and three-dimensional models of U.S. and Russian criticality experiments.
- The 86 cases are actually represented by 91 input files, as several benchmarks are modeled in two different ways.
- The benchmarks represent a wide range of neutron energy spectra, and can be categorized as fast, intermediate, and thermal systems.
- The benchmarks involved several types of fissile material, and a variety of reflector materials including Be, BeO, C, Al, Fe, Ni, W, Th, ^{233}U , natural uranium, as well as bare core and solution reactors.

***Criticality Benchmark Calculations using PARTISN:
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Libraries***

- **The critical benchmarks are sorted into five general groupings of cases: ^{233}U [Jezebel, Flattop, ORNL], intermediate enrichment ^{235}U (IEU) [Jemima], high enrichment ^{235}U (HEU) [Godiva, Bigten, Flattop, ORNL], ^{239}Pu [Jezebel, Flattop, Thor, PNL], and mixed metal fueled cores [Zebra].**
- **In developing the models, the ICSBEP (International Criticality Safety Benchmark Evaluation Project) criticality benchmark experimental data compendium was used for most cases, and CSEWG (Cross Section Evaluation Working Group) data were needed for several cases.**
- **the suite of critical assembly benchmarks was analyzed through PARTISN calculations (using MENDF5 and MENDF6 libraries), and also calculated using MCNP-4C with ENDF/B-V and ENDF60 (ENDF/B-VI Release 2) nuclear data libraries.**

*Criticality Benchmark Calculations using PARTISN:
Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries*

- **PARTISN is a discrete ordinates radiation transport simulation code developed from the DANTSYS code system.**
- **The PARTISN code provides neutron transport solutions on orthogonal meshes with adaptive mesh refinement (AMR) in one, two, and three dimensions.**
- **A multigroup energy treatment is used in conjunction with the SN angular approximation.**
- **The benchmark cases were run with PARTISN Release 1.38 using the MENDF5 and MENDF6 nuclear data libraries.**
 - **PARTISN Release 2.99 was used on a subset of cases**

*Criticality Benchmark Calculations using PARTISN:
Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries*

- **The MENDF5 and MENDF6 nuclear data libraries were prepared primarily from ENDF/B-V (up to the final release update in 1987) and ENDF/B-VI (up to release 3 in 1995) nuclear evaluation data, respectively, as multigroup, isotopic nuclear data libraries. (R.C. Little, Los Alamos National Laboratory memorandum, XTM:96-82(U) (1996).)**
- **The nuclear data in MENDF5 and MENDF6 is also augmented by LANL Group T-2 and LLNL evaluation data.**
- **MENDF5 has data for 99 nuclides and MENDF6 has data for 167 nuclides.**
- **The MENDF5 and MENDF6 libraries were produced using the code NJOY and applying the LANL Claw Weighting Function to collapse all the cross sections to 30 neutron energy groups.**

***Criticality Benchmark Calculations using PARTISN:
Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries***

- **The MENDF5 and MENDF6 libraries include prompt fission nuubar data only and will lead to a lower k_{eff} (by an amount $\sim \beta_{\text{eff}}$) than ENDF60 results (calculated with total nuubar).**
- **For fast spectrum cases, the MENDF criticality calculations should be good when consideration is given to the total versus prompt**
- **However, the MENDF nuclear data libraries were not designed to perform well for intermediate spectrum systems, and especially thermal spectrum systems.**
- **The MENDF libraries include very few thermal groups, no up-scatter data nor $S(\alpha, \beta)$ data, and no self-shielding effects were incorporated (infinitely-dilute).**
- **The lack of self-shielded cross sections leads to higher scattering cross sections for reflector materials such as iron thereby increasing k_{eff} as a function of reflector thickness.**

Comparisons of PARTISN results with MCNP calculations and with experiment

- Traditionally, the results for the 91 benchmark case models have been presented in 13 sets of cases, characterized by type of core and/or reflector material
- In the following section, an overview of interesting case results is presented
- Then, a number of the more interesting sets of results are shown
 - In the first example, the full ICSBEP and CSEWG case identifiers are used; in the subsequent examples, the more compact MCNP case names are used
 - The final documentation for the study presents the complete name and identifier information for each case

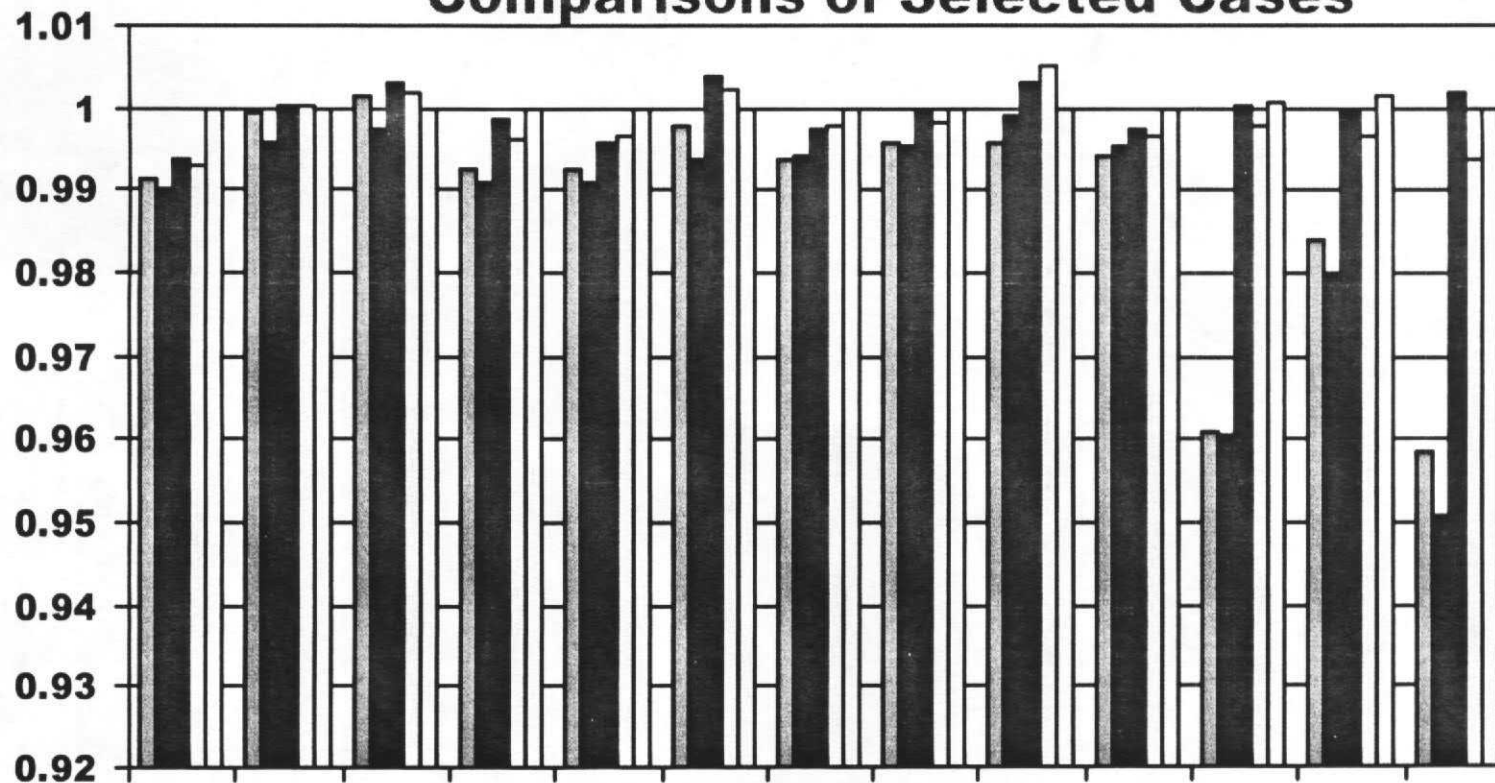
TABLE 1: Comparisons of k_{eff} from Representative Criticality Benchmark Cases

Benchmark Case Identifier	Case Description	Code and Nuclear Data Library				Experimental Benchmark
		PARTISN (MENDF5) k_{eff}	PARTISN (MENDF6) k_{eff}	MCNP (ENDF/B-V) $k_{eff} \pm 1\sigma$	MCNP (ENDF60) $k_{eff} \pm 1\sigma$	
U233-MET-FAST-001	Jezebel-23, Bare sph. U233	0.99151	0.99033	0.99366±0.00051	0.99289±0.00055	1.000±0.001
U233-MET-FAST-006	Flattop-23, Nat. U refl. U233 sph.	0.99946	0.99593	1.00011±0.00067	1.00011±0.00069	1.0000±0.0014
CSEWG F-24	Flattop-23, Nat. U refl. U233 sph. (gap)	1.00139	0.99749	1.00314±0.00070	1.00181±0.00065	1.000±0.001
HEU-MET-FAST-001	Godiva, Unrefl. HEU sphere	0.99274	0.99097	0.99856±0.00057	0.99615±0.00057	1.000±0.001
HEU-MET-FAST-001	Godiva, Unrefl. HEU sph., Nested	0.99273	0.99098	0.99598±0.00060	0.99680±0.00059	1.000±0.001
HEU-MET-FAST-028	Flattop-25, Nat. U Refl. HEU Sphere	0.99780	0.99383	1.00409±0.00064	1.00230±0.00062	1.0000±0.0030
PU-MET-FAST-001	Jezebel-Pu Bare Pu239 w/4.5% Pu240	0.99380	0.99430	0.99727±0.00054	0.99771±0.00056	1.000±0.002
PU-MET-FAST-002	Jezebel-Pu Bare sph. Pu239 w/ 20% Pu240	0.99565	0.99536	0.99944±0.00060	0.99811±0.00054	1.000±0.002
PU-MET-FAST-006	Flattop, Nat U Refl. Pu Sph.	1.00005	0.99898	1.00294±0.00074	1.00498±0.00069	1.0000±0.0030
MIX-MET-FAST-001	HEU refl. Pu sphere	0.99434	0.99415	0.99754±0.00058	0.99667±0.00057	1.0000±0.0016
U233-SOL-THERM-001 (2)	ORNL-6 unrefl. Sph. U nitrate w/B	0.96091	0.96073	1.00044±0.00040	0.99767±0.00038	1.0005±0.0033
HEU-SOL-THERM-032	ORNL-10 refl. Sph. U. nitrate w/B	0.98419	0.98017	0.99960±0.00026	0.99664±0.00024	1.0015±0.0026
PU-SOL-THERM-011 (18-1)	PNL-3 Bare Sph. 2 wt% Pu240	0.95833	0.95076	1.00202±0.00052	0.99365±0.00052	1.0000±0.0052

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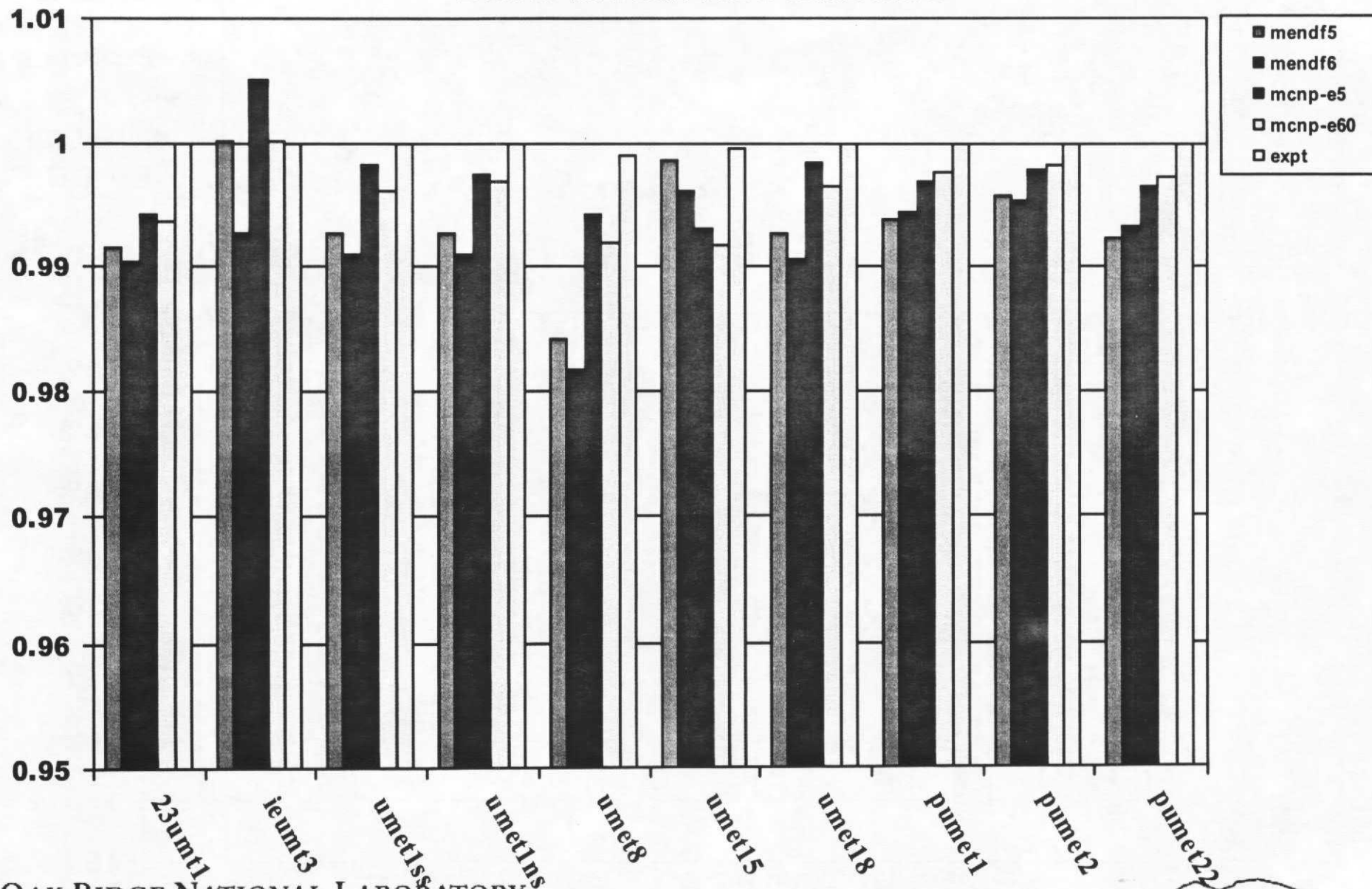
Criticality Benchmark Calculations: Comparisons of Selected Cases



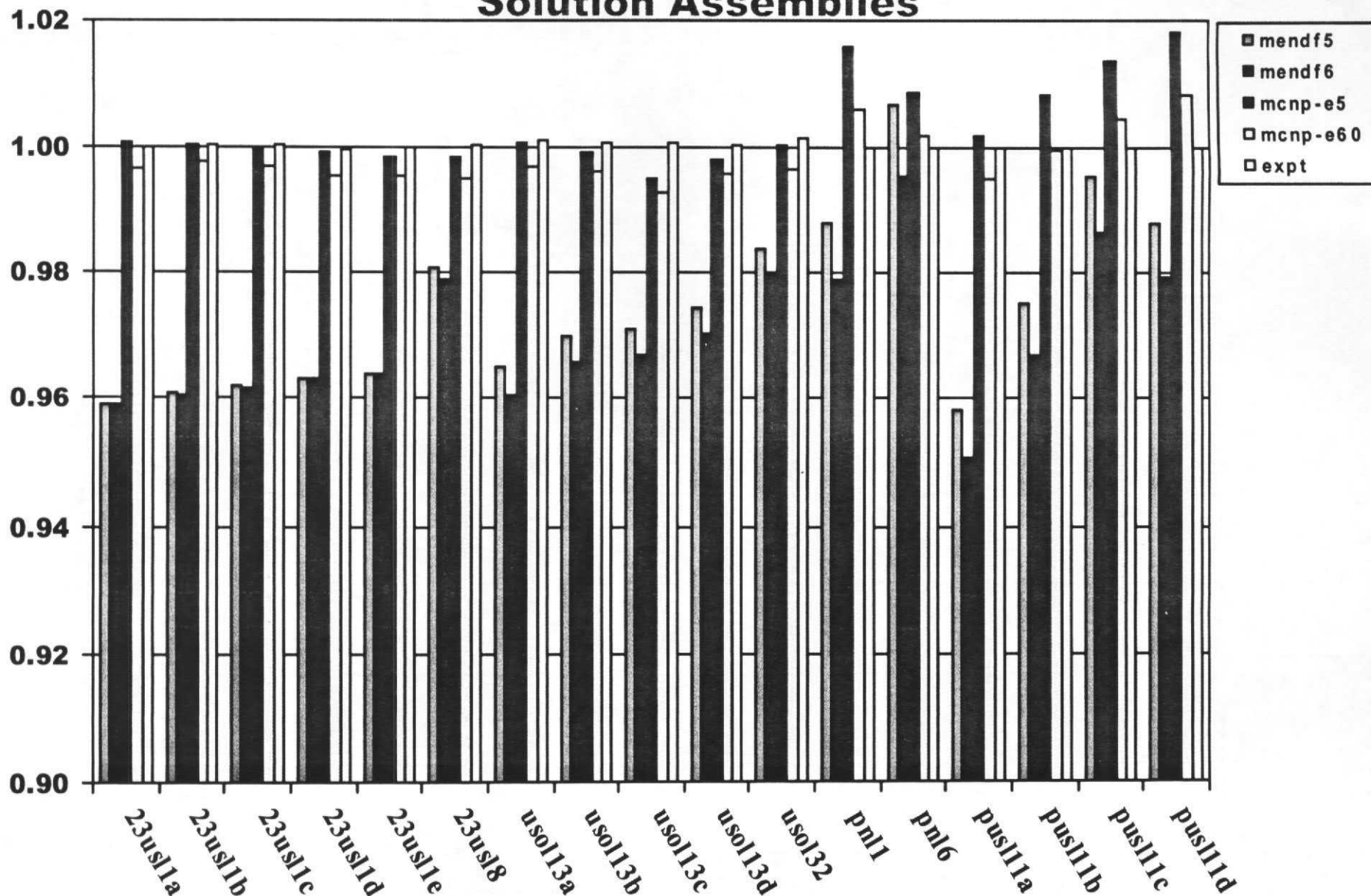
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Criticality Benchmark Calculations: Bare Metal Assemblies



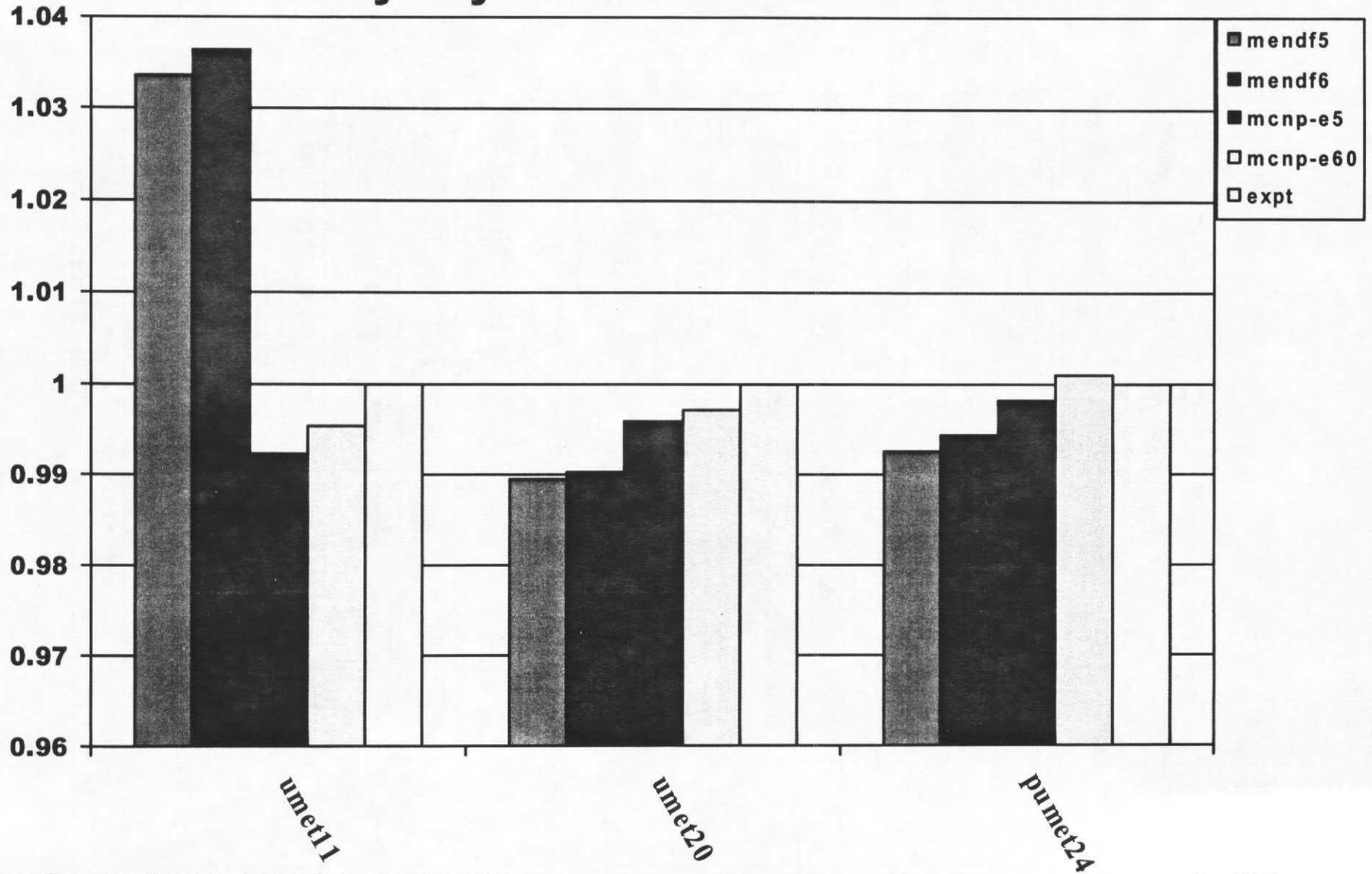
Criticality Benchmark Calculations: Solution Assemblies



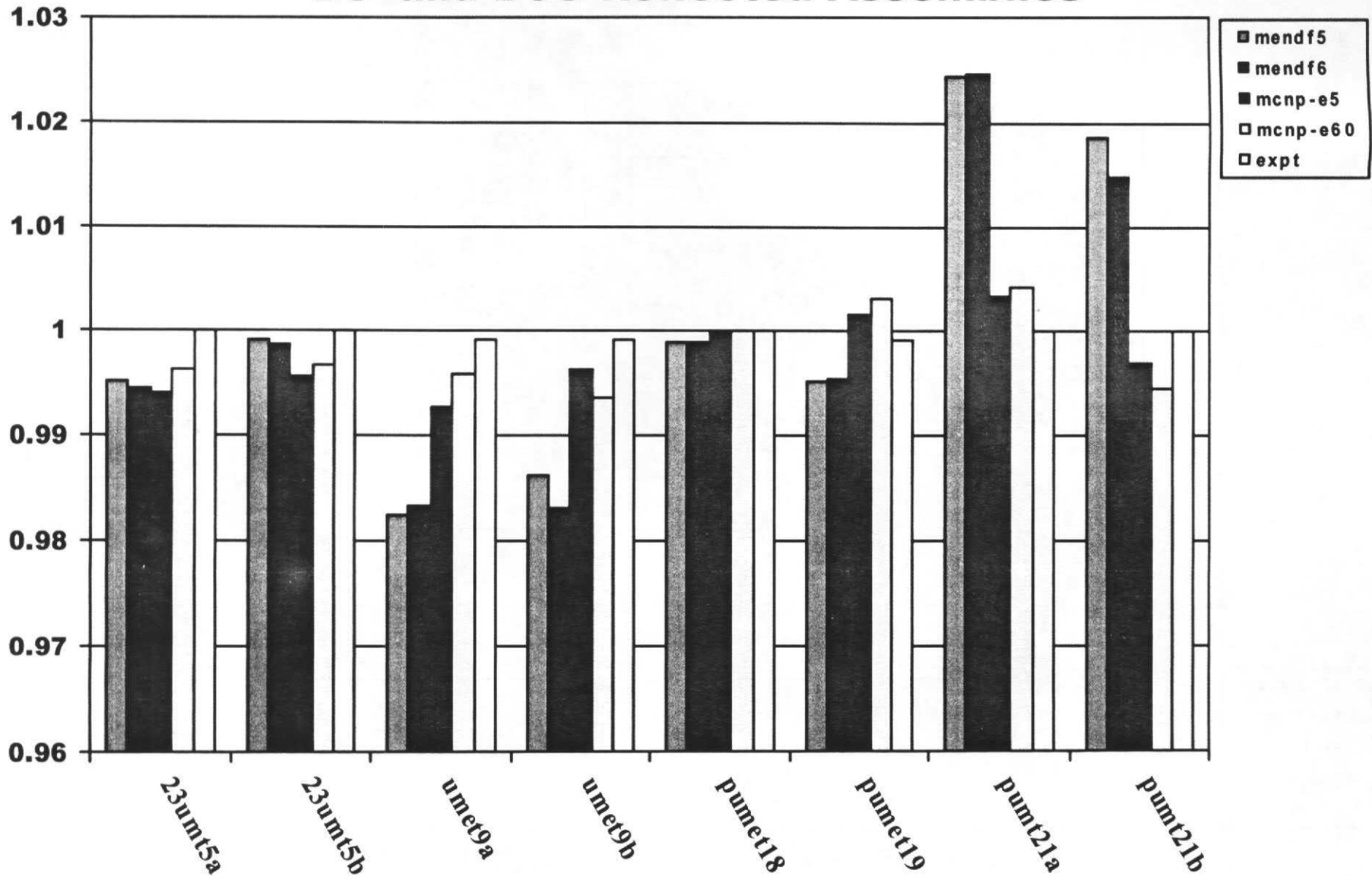
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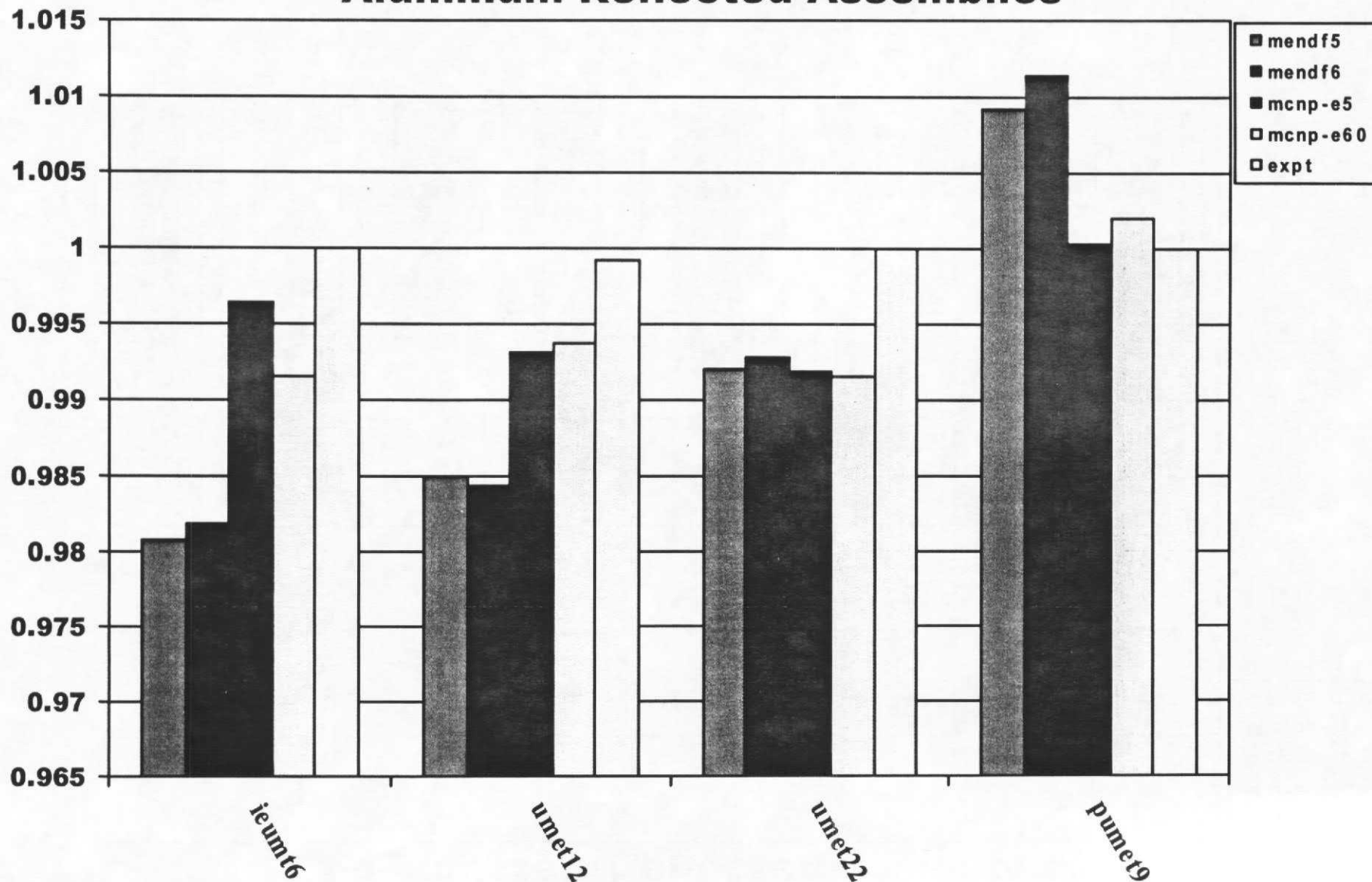
Criticality Benchmark Calculations: Polyethylene-Reflected Assemblies



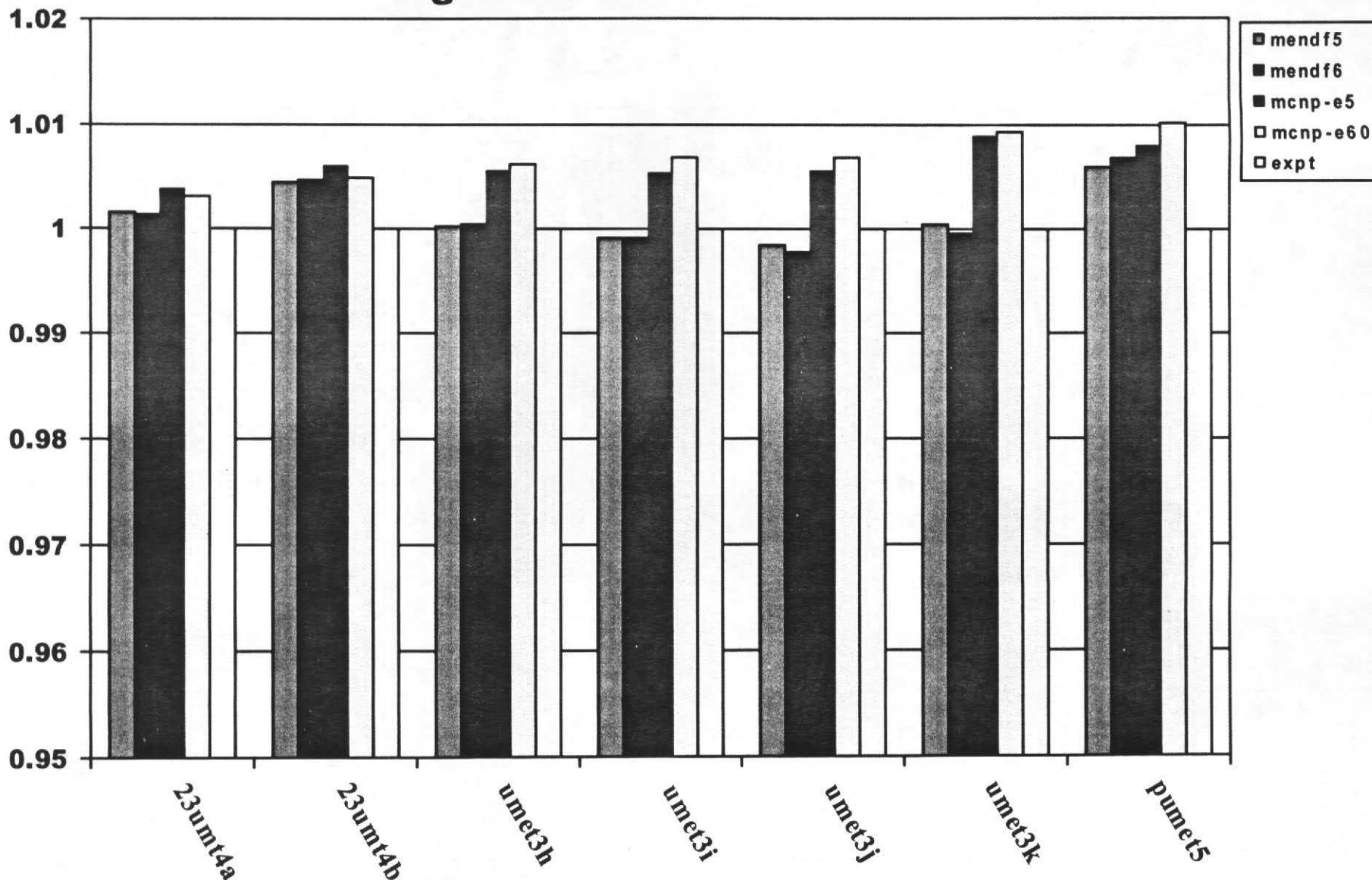
Criticality Benchmark Calculations: Be- and BeO-Reflected Assemblies



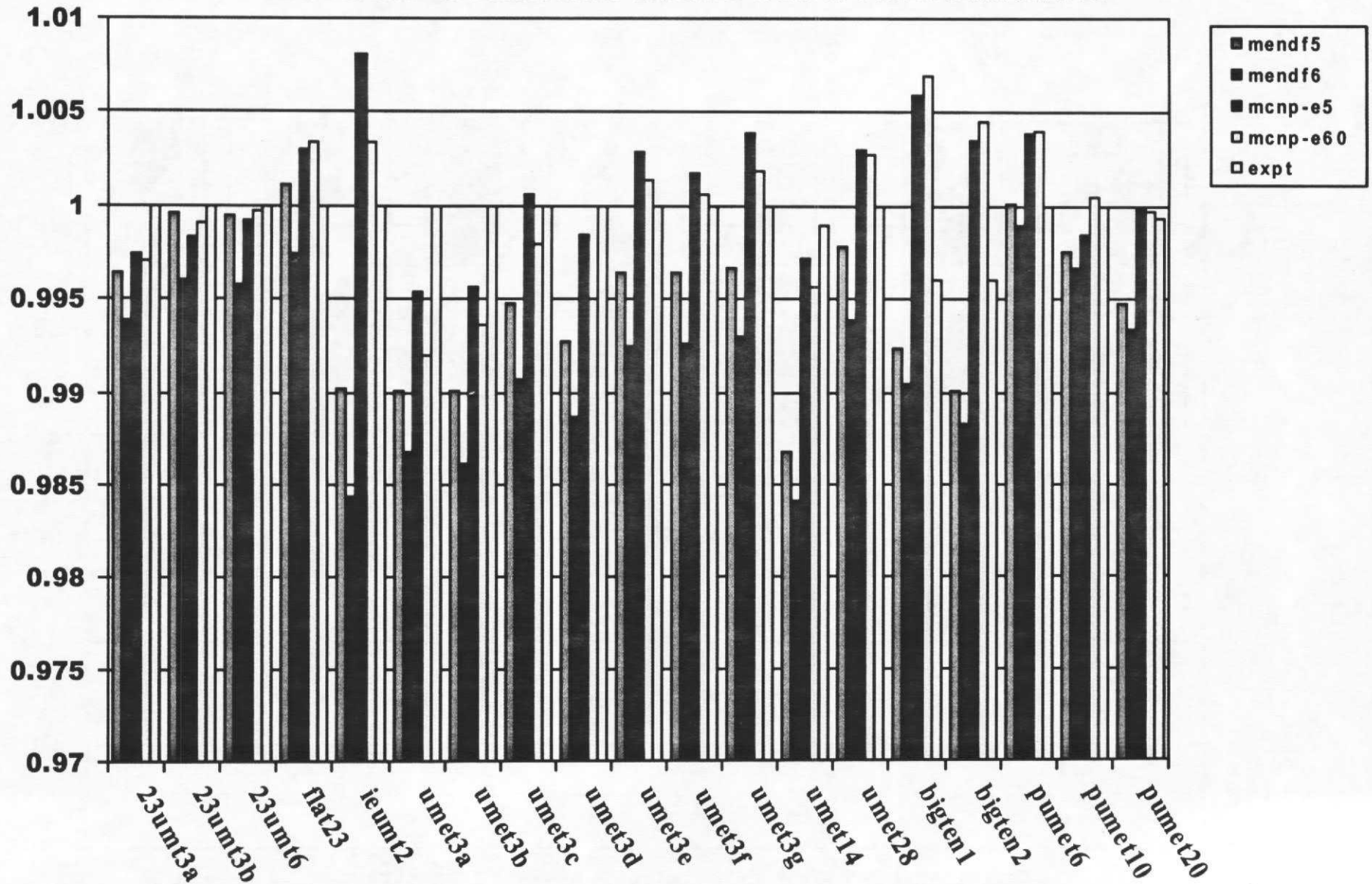
Criticality Benchmark Calculations: Aluminum-Reflected Assemblies



Criticality Benchmark Calculations: Tungsten-Reflected Assemblies



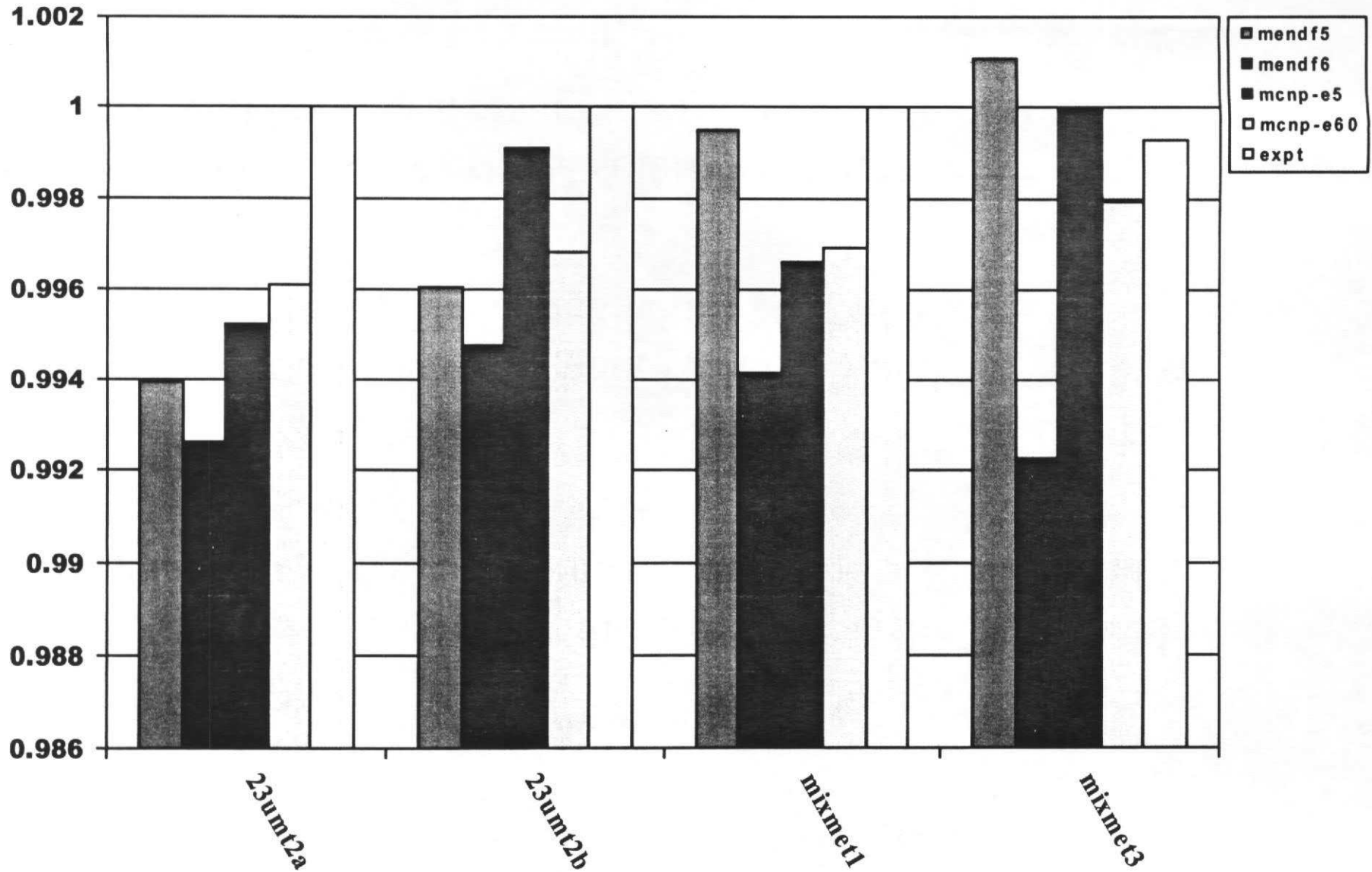
Criticality Benchmark Calculations: Normal Uranium-Reflected Assemblies



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Criticality Benchmark Calculations: HEU-Reflected Assemblies



*Criticality Benchmark Calculations using PARTISN:
Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries*

Observations

- The results for fast spectrum cases such as the bare metal benchmarks are modeled quite well with PARTISN and the MENDF nuclear data libraries
- k_{eff} is generally lower for both PARTISN and MCNP using ENDF/B-VI based data than with ENDF/B-V.
- The benchmarks of critical solution reactors show considerable low values for k_{eff} for most of the PARTISN (MENDF) calculations compared to the experimental data.

*Criticality Benchmark Calculations using PARTISN:
Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries*

Observations

- The PARTISN results are generally lower than the experimental k_{eff} values because MENDF5 and MENDF6 nuclear data only contain prompt fission nuabar data.
- As one measure of this effect, comparisons may be made to MCNP results (with ENDF/B-V and ENDF60 data) using both the prompt fission nuabar, and the total nuabar options.
- For the benchmarks cases of the bare metal assemblies:

<u>Δk_{eff} (MCNP – PARTISN)</u>	Prompt fission nuabar, only	Total nuabar
Avg Δk_{eff} (MENDF5 & ENDF/B-V)	-0.00092 ± 0.00037	0.00371 ± 0.00035
Avg Δk_{eff} (MENDF6 & ENDF60)	-0.00075 ± 0.00035	0.00470 ± 0.00036

**Criticality Benchmark Calculations using PARTISN:
Comparisons using MENDF5 and MENDF6 Nuclear Data
Libraries**

SUMMARY

- **A full k_{eff} analysis was performed with PARTISN for all 91 benchmark case models in the LANL Suite of Criticality Benchmarks**
- **The study offers a comparison between the k_{eff} results from PARTISN (using MENDF5 and MENDF6 nuclear data libraries), the Monte-Carlo code MCNP4C (using ENDF/B-V and ENDF60 nuclear data libraries) and the experimental benchmark critical data.**
- **The strengths and weaknesses of the MENDF5 and MENDF6 nuclear data libraries are discussed**