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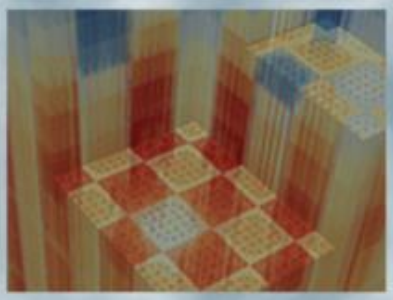

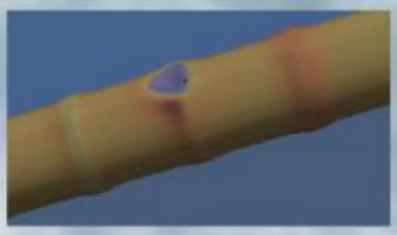

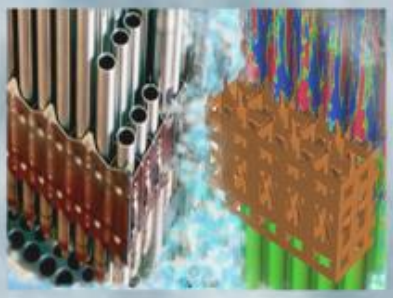

Consortium for Advanced Simulation of LWRs

MPACT User's Manual

Version 4.1

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11/1/2019

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Revision Log

Revision	Date	Affected Pages	Revision Description
0	7/24/2019	All	Initial Release
1	11/1/2019	18-70	Removed notation input tables for standard input
		2,3,8,17	added bibliography and citations, clarified requirements

Document pages that are:

Export Controlled:	None
IP/Proprietary/NDA Controlled:	None
Sensitive Controlled:	None
Unlimited:	All

MPACT User's Manual

Approvals:

Digitally signed by Brendan Kochunas
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11/11/2019

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11/12/2019

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Contents

1 Introduction **2**
1.1 Problem Reporting Methods . . . 2
1.2 Description of Training . . . 3
1.3 Computer System Vulnerabilities . . . 3
1.4 Mathematical and Numerical Models . . . 3
1.5 Functional Requirements . . . 3
1.6 Code Capabilities and Limitations . . . 4

2 Executing MPACT **5**
2.1 Serial Execution . . . 5
2.2 Parallel Execution . . . 5

3 Input and Output File Description **7**
3.1 VERA Common Input . . . 7
3.2 VERA Common Output . . . 7
3.3 VERA Sample Input Cases . . . 8
3.4 VERA Cross Section Library . . . 8

4 Using MPACT with the VERA Common Input **16**
4.1 MPACT Block . . . 16

Bibliography **18**

1. Introduction

The MPACT code is designed to perform high-fidelity light water reactor (LWR) analysis using whole-core pin-resolved neutron transport calculations on modern parallel-computing hardware. The code consists of several libraries which provide the functionality necessary to solve steady-state eigenvalue problems. Several transport capabilities are available within MPACT including both 2-D and 3-D Method of Characteristics (MOC). A three-dimensional whole core solution based on the 2D-1D solution method provides the capability for full core depletion calculations.

Specific features available in the current release of MPACT are:

- Support for Linux-based Operating Systems (32-bit and 64-bit)
- OpenMP parallelism for MOC sweeps
- Support for MPACT and AMPX working cross section library formats
- Steady-state eigenvalue calculations using power iteration
- Transient calculations
- 2-D and 3-D MOC transport solvers
- 2D-1D full core solution
- Depletion capability
- Generalized pressurized water reactor (PWR) geometry
- Export of computational and results mesh to VTK and VTU files
- Visualization via VisIt

The purpose of this document is to provide users with sufficient background to be able to utilize MPACT for PWR design and analysis applications. For a more detailed description of the methods or sofware design, the reader is directed to the theory and programmer's documentation.

This user document is divided into several chapters. After this introduction, an overview is provided regarding code execution capabilities and limitations in both serial and parallel environments. Finally, a detailed description of the user input is provided.

1.1 Problem Reporting Methods

For specific questions about the use of MPACT, the licensing of the code, or to report bugs users are encouraged to send an email to `caslsupport@ornl.gov`. When reporting bugs, users are requested to attach the problematic input

to the email and to provide information in the body of the email about the code version, machine, runtime environment and any other relevant details to permit debugging. The problem reporting methods are described in "VERA-QA-10: VERA Problem Reporting and Corrective Action".

1.2 Description of Training

There is no required training, but for users running MPACT in a Unix/Linux environment, it is recommended to know how to work from the linux command line. When running in parallel with MPI[1], knowledge of parallelism is useful as well.

1.3 Computer System Vulnerabilities

Running MPACT on any machine is not known to expose the system to any security vulnerabilities at this time.

1.4 Mathematical and Numerical Models

There are many mathematical and numerical models and corresponding assumptions used in MPACT. For a thorough explanation, the user can review the details in the MPACT Theory Manual.

1.5 Functional Requirements

The high level requirements that are specified in the Software Requirements Document are listed below:

1. all current PWR fuel designs including:
   (a) UO2 Fuel
   (b) 14x14 to 17x17 designs from Westinghouse, B&W, and CE
   (c) 16x16 CE lattices with large water rods
   (d) annular fuel pellets
   (e) axial varying assembly enrichments (e.g. axial blankets)
   (f) 2D and 3D capabilities
   (g) single fuel pin calculations with square boundaries
2. all current PWR burnable absorbers including:
   (a) WABA inserts
   (b) Pyrex inserts
   (c) integral gadolinia absorber
   (d) integral erbia
   (e) IFBA
   (f) B4C rods
   (g) TPBAR absorbers

3. all current PWR movable control rods designs, including:
   (a) B4C absorbers
   (b) AIC absorbers
   (c) axially varying absorbers
4. all currently operating PWR core geometry, except cores with CE offset assemblies
   (a) baffles
   (b) pressure vessels
   (c) neutron pads
5. planned SMR core designs from NuScale
6. water moderator and water moderator with dissolved boron
7. isotopic depletion of fuel materials
8. steady-state and transient analysis
9. depletion in units of hours, GWD/MT, and EFPD
10. thermal expansion
11. variable axial mesh

1.6 Code Capabilities and Limitations

The current code capabilities are specified by the functional requirements and are listed above. Requirements not explicitly stated in this list are assumed to be limitations. Limitations in capability may be partial or full, where partial means a feature supporting another requirement may exist but is not fully tested or NQA-1 compliant.

2. Executing MPACT

Depending on how MPACT was configured, compiled, and installed, it may be executed in serial and/or parallel. The following sections outline the procedures for running the code in either serial or parallel. When run as a standalone analysis tool, MPACT is executed from the command line.

2.1 Serial Execution

The syntax for MPACT is shown below:

```
$> <path_to_MPACT>/mpact.exe [<input_file> [<output_file> [<log_file>]] | -help]
```

All command line arguments are optional. The meaning of each is described as:

- `-help` - Displays the help message. This message describes the command line arguments and their usage.
- <`input_file`> - The name of the input file to process. If no input file is listed, then MPACT tries to process the file `mpact.inp` in the present working directory. The <`input_file`> may include an absolute or relative path to the file. This file must exist and be readable prior to execution.
- <`output_file`> - The file to use for writing the default output. If no file is listed then a file with <casename>.out will be created in the present working directory. In general, if the output file does not exist it will be created, and if it already exists it will be replaced **without** warning. <`output_file`> may include an absolute or relative path. The directory pointed to by the path must exist prior to execution.
- <`log_file`> - The file to use for writing the execution log information. If no file is listed then a file with <casename>.log will be created in the present working directory. In general, if the log file does not exist, it will be created, and if it already exists it will be replaced **without** warning. <`log_file`> may include an absolute or relative path. The directory pointed to by the path must exist prior to execution.

2.2 Parallel Execution

MPACT may only be executed in parallel if a parallel build has been installed. MPACT uses two kinds of parallel models. The first is the shared memory model which is based on the OpenMP standard (`http://www.openmp.org`) and the other is a distributed memory model which is based on the MPI Standard. If the MPACT executable is built with MPI then it is executed differently than in serial, but otherwise the serial description in the previous section is correct. When executing MPACT with MPI the command has the following syntax:

```
$> <mpirun_cmd> [<mpi_options>] <mpact_exe> [<mpact_options>]
```

- <mpirun_cmd> - This is the command used to launch MPI executables. This command can vary because different machines may have different implementations of the MPI library installed. Therefore, it is suggested the user consult the documentation for their cluster or workstation for this command and its arguments. For most implementations of MPI (such as OpenMPI, `http://www.open-mpi.org/`) the <mpirun_cmd> command is `mpirun`.
- <mpirun_options> - These are command line arguments for <mpirun_cmd>. Again, the user should consult their machine's documentation for usage.
- <mpact_exe> - The name of the MPACT executable that is installed. Typically, one should include the full path to the executable since the parallel execution environment may not have the same PATH setting as the run time environment in which the <mpirun_cmd> was invoked.
- <mpact_options> - The command line arguments for MPACT. See the Serial Execution section of this chapter for a complete description.

3. Input and Output File Description

MPACT has two input processors: one for processing the common input that is used with CASL's VERA code suite and another for processing MPACT's native input format.

3.1 VERA Common Input

The VERA common input is an ASCII input file that is processed to create an XML-like (eXtensible Markup Language) input file. The reader is referred to the VERA Common Input User's Manual [2] for a complete description of input cards that can be specified to control functionality in MPACT. However, a brief description follows. A VERA input file describes the reactor model hierarchically. A primary feature of the core simulator is that a single input is used to drive all of the multiphysics codes. The benefits of this approach are that users only need to understand and be proficient with one input, and it also ensures that all codes are working from a single, common geometry description of the problem to reduce errors. The input is structured with several blocks, each having their own set of cards. This input is similar to how the MPACT native input is structured. The MPACT native input is not a NQA-1 compliant feature.

3.2 VERA Common Output

When a case successfully completes, it generates an HDF5 (Hierarchical Data Format) output file. This file is structured to list core and pin-wise data for each state run for the case. The type of data added to the output file depends on the physics being run for the case, and any output options associated with the code. Some sample output values include:

- keff
- pin_exposures
- pin_powers
- pin_fuel_temp

The file can be viewed graphically using the python code VERAView. For a full list of output values, the user can reference the VERAOut user manual.

3.3 VERA Sample Input Cases

Sample inputs, that are suggested in-use tests, to run with VERA can be found in the VERAIn repository, under the directory verain/Progression_Problems. Within this directory are cases that begin with a simple 2-D pin cell and grow in size and complexity to a full 3-D cycle depletion of a reactor with thermal hydraulic feedback. These cases require varying amounts of computation and memory to run. Problems in suites 1 and 2 can be easily run in serial on a laptop or personal computer.

3.4 VERA Cross Section Library

The current cross section library has 51 energy groups and 303 isotopes that can be used when constructing materials for inputs. The energy group bounds are the upper group limit and are:

Group	Upper Bound (eV)
1	2.00E+07
2	6.43E+06
3	4.30E+06
4	2.35E+06
5	1.36E+06
6	8.20E+05
7	4.92E+05
8	2.00E+05
9	7.30E+04
10	5.00E+04
11	2.00E+04
12	9.50E+03
13	2.25E+03
14	9.50E+02
15	3.05E+02
16	1.43E+02
17	7.60E+01
18	4.83E+01
19	3.00E+01
20	1.44E+01
21	1.19E+01
22	8.10E+00
23	7.15E+00
24	6.25E+00
25	5.40E+00
26	5.00E+00
27	4.70E+00
28	3.73E+00
29	2.47E+00
30	1.86E+00
31	1.45E+00
32	1.25E+00
33	1.18E+00
34	1.13E+00
35	1.08E+00

36	1.01E+00
37	9.75E-01
38	9.25E-01
39	7.50E-01
40	6.25E-01
41	5.00E-01
42	3.50E-01
43	2.75E-01
44	2.00E-01
45	1.50E-01
46	1.00E-01
47	8.00E-02
48	6.00E-02
49	4.00E-02
50	3.00E-02
51	1.00E-02

The list of isotopes, their descriptions and cross section set types are listed below. If an isotope is a fission product, it is listed as FP. If an isotope has any n,2n or n,3n data, a 2 or 3 will respectively appear in the column. It should be noted that the only isotope with resonance upscatter data is U-238.

Identifier	Description	Type	FP/Burnable	n,2n/n,3n
1001	H-1	full	-	-
1002	H-2	full	-	2
1003	T-3	abso	-	-
1006	H-1 in CH2	full	-	-
1040	H-1 in ZrH	full	-	-
2003	HE-3	abso	-	-
2004	HE-4	full	-	-
3006	LI-6	full	-	-
3007	LI-7	full	-	2
4009	BE-9	full	-	2
5000	B-NAT	full	-	-
5010	B-10	full	Burnable	-
5011	B-11	full	Burnable	-
6000	C-NAT	full	-	-
6001	C-GRAPH	full	-	-
7014	N-14	full	-	2
8001	O-16 in UO2	full	-	-
8016	O-16	full	-	-
9019	F-19	full	-	-
11023	NA-23	full	-	-
12000	MG-NAT	full	-	-
13027	AL-27	full	-	-
14000	SI-NAT	full	-	-
15031	P-31	full	-	-
16000	S-NAT	full	-	-
17000	CL-NAT	full	-	-
19000	K-NAT	full	-	-
20000	CA-NAT	full	-	-
22000	TI-NAT	full	-	-

23000	V-NAT	full	-	-
24000	CR-NAT	full	-	2
24050	CR-50	full	-	-
24052	CR-52	full	-	-
24053	CR-53	full	-	-
24054	CR-54	full	-	-
25055	MN-55	full	-	2
26000	FE-NAT	full	-	2
26054	FE-54	full	-	-
26056	FE-56	full	-	-
26057	FE-57	full	-	-
26058	FE-58	full	-	-
27059	CO-59	full	-	2
28000	NI-NAT	full	-	2
28058	NI-58	full	-	-
28060	NI-60	full	-	-
28061	NI-61	full	-	-
28062	NI-62	full	-	-
28064	NI-64	full	-	-
29063	CU-63	full	-	-
29065	CU-65	full	-	-
35581	BR-81	abso	FP	-
36582	KR-82	abso	FP	2
36583	KR-83	abso	FP	3
36584	KR-84	abso	FP	2
36585	KR-85	abso	FP	-
36586	KR-86	abso	FP	3
38589	SR-89	abso	FP	-
38590	SR-90	abso	FP	-
39589	Y-89	abso	FP	2
39590	Y-90	abso	FP	-
39591	Y-91	abso	FP	-
40000	ZR-NAT	full	-	2
40001	ZR-ZrH2	full	-	2
40090	ZR-90	full	-	-
40091	ZR-91	reso	Burnable	-
40092	ZR-92	full	-	-
40094	ZR-94	full	-	-
40096	ZR-96	reso	Burnable	-
40591	ZR-91	abso	FP	2
40593	ZR-93	abso	FP	-
40595	ZR-95	abso	FP	-
40596	ZR-96	abso	FP	2
41093	NB-93	full	-	-
41595	NB-95	abso	FP	-
42000	MO-NAT	full	-	3
42095	MO-95	abso	-	-
42595	MO-95	reso	FP	-
42596	MO-96	abso	FP	-
42597	MO-97	abso	FP	-
42598	MO-98	abso	FP	-

42599	MO-99	abso	FP	-
42600	MO-100	abso	FP	-
43599	TC-99	reso	FP	2
44600	RU-100	abso	FP	-
44601	RU-101	full	FP	-
44602	RU-102	abso	FP	-
44603	RU-103	abso	FP	-
44604	RU-104	abso	FP	-
44605	RU-105	abso	FP	-
44606	RU-106	abso	FP	-
45001	RH in homogenized detector	full	-	-
45002	RH in virtual detector	full	-	-
45103	RH-103	reso	Burnable	-
45603	RH-103	full	FP	2
45605	RH-105	full	FP	-
46604	PD-104	abso	FP	-
46605	PD-105	full	FP	-
46606	PD-106	abso	FP	-
46607	PD-107	full	FP	-
46608	PD-108	reso	FP	-
47107	AG-107	reso	-	3
47109	AG-109	reso	-	3
47609	AG-109	full	FP	3
47611	AG-111	abso	FP	-
47710	AG-110M	abso	FP	-
48000	CD-NAT	full	-	-
48110	CD-110	full	-	-
48111	CD-111	full	-	-
48112	CD-112	full	-	-
48113	CD-113	full	-	2
48114	CD-114	full	-	-
48610	CD-110	abso	FP	-
48611	CD-111	abso	FP	-
48613	CD-113	abso	FP	2
49000	IN-NAT	full	-	-
49113	IN-113	reso	-	-
49115	IN-115	reso	-	-
49615	IN-115	full	FP	-
50000	SN-NAT	full	-	-
50112	SN-112	full	-	-
50114	SN-114	full	-	-
50115	SN-115	full	-	-
50116	SN-116	full	-	-
50117	SN-117	full	-	-
50118	SN-118	full	-	-
50119	SN-119	full	-	-
50120	SN-120	full	-	-
50122	SN-122	full	-	-
50124	SN-124	full	-	-
50125	SN-125	abso	-	-
51000	SB-NAT	full	-	-

51121	SB-121	full	-	-
51123	SB-123	full	-	-
51124	SB-124	full	-	-
51125	SB-125	full	-	-
51621	SB-121	abso	FP	-
51625	SB-125	abso	FP	-
51627	SB-127	abso	FP	-
52632	TE-132	abso	FP	-
52727	TE-127M	abso	FP	-
52729	TE-129M	abso	FP	-
53627	I-127	abso	FP	3
53629	I-129	abso	FP	-
53631	I-131	abso	FP	-
53635	I-135	abso	FP	-
54628	XE-128	abso	FP	3
54630	XE-130	abso	FP	3
54631	XE-131	reso	FP	3
54632	XE-132	abso	FP	3
54633	XE-133	abso	FP	-
54634	XE-134	full	FP	3
54635	XE-135	full	FP	-
54636	XE-136	abso	FP	3
54735	XE-135M	full	FP	-
55633	CS-133	reso	FP	2
55634	CS-134	abso	FP	-
55635	CS-135	abso	FP	-
55636	CS-136	abso	FP	-
55637	CS-137	abso	FP	-
56634	BA-134	abso	FP	-
56637	BA-137	abso	FP	-
56640	BA-140	abso	FP	-
57639	LA-139	abso	FP	-
57640	LA-140	abso	FP	-
58640	CE-140	abso	FP	-
58641	CE-141	abso	FP	-
58642	CE-142	abso	FP	-
58643	CE-143	abso	FP	-
58644	CE-144	abso	FP	-
59641	PR-141	abso	FP	3
59643	PR-143	abso	FP	-
60642	ND-142	abso	FP	-
60643	ND-143	full	FP	3
60644	ND-144	abso	FP	-
60645	ND-145	full	FP	3
60646	ND-146	abso	FP	3
60647	ND-147	abso	FP	-
60648	ND-148	abso	FP	3
60650	ND-150	abso	FP	3
61647	PM-147	full	FP	3
61648	PM-148	abso	FP	-
61649	PM-149	abso	FP	-

61651	PM-151	abso	FP	-
61748	PM-148M	full	FP	-
62152	SM-152	reso	-	3
62153	SM-153	full	Burnable	-
62647	SM-147	full	FP	3
62648	SM-148	abso	FP	-
62649	SM-149	full	FP	3
62650	SM-150	full	FP	2
62651	SM-151	full	FP	3
62652	SM-152	full	FP	3
62653	SM-153	abso	FP	-
62654	SM-154	abso	FP	-
63151	EU-151	reso	-	3
63152	EU-152	reso	Burnable	3
63153	EU-153	reso	-	3
63154	EU-154	reso	Burnable	3
63155	EU-155	reso	Burnable	3
63156	EU-156	full	Burnable	-
63157	EU-157	full	Burnable	-
63651	EU-151	abso	FP	3
63653	EU-153	full	FP	3
63654	EU-154	full	FP	3
63655	EU-155	full	FP	3
63656	EU-156	abso	FP	-
63657	EU-157	abso	FP	-
64152	GD-152	full	-	2
64154	GD-154	full	-	2
64155	GD-155	reso	-	2
64156	GD-156	reso	-	2
64157	GD-157	reso	-	2
64158	GD-158	reso	-	2
64160	GD-160	full	-	2
64654	GD-154	abso	FP	2
64655	GD-155	full	FP	2
64656	GD-156	full	FP	2
64657	GD-157	full	FP	2
64658	GD-158	full	FP	2
64660	GD-160	abso	FP	2
65159	TB-159	abso	-	-
65160	TB-160	abso	Burnable	-
65161	TB-161	abso	Burnable	-
65659	TB-159	abso	FP	-
65660	TB-160	abso	FP	-
65661	TB-161	abso	FP	-
66160	DY-160	reso	-	-
66161	DY-161	reso	-	-
66162	DY-162	reso	-	-
66163	DY-163	reso	-	-
66164	DY-164	reso	-	3
66660	DY-160	abso	FP	-
66661	DY-161	abso	FP	-

66662	DY-162	abso	FP	-
66663	DY-163	abso	FP	-
66664	DY-164	abso	FP	3
67165	HO-165	abso	-	3
67665	HO-165	abso	FP	3
68162	ER-162	full	-	-
68164	ER-164	full	-	-
68166	ER-166	reso	-	-
68167	ER-167	reso	-	-
68168	ER-168	full	-	-
68170	ER-170	full	-	-
71176	LU-176	full	-	-
72174	HF-174	full	-	2
72176	HF-176	reso	-	2
72177	HF-177	reso	-	2
72178	HF-178	reso	-	2
72179	HF-179	reso	-	2
72180	HF-180	reso	-	2
73181	TA-181	full	-	3
73182	TA-182	full	-	3
74000	W-NAT	full	-	3
74182	W-182	reso	-	2
74183	W-183	reso	-	2
74184	W-184	reso	-	2
74186	W-186	reso	-	2
77191	IR-191	abso	-	-
77193	IR-193	abso	-	-
79197	AU-197	full	-	-
82206	PB-206	full	-	-
82207	PB-207	full	-	-
82208	PB-208	full	-	-
83209	BI-209	full	-	3
90230	TH-230	full	-	3
90232	TH-232	reso	-	3
91231	PA-231	full	-	3
91232	PA-232	abso	Burnable	-
91233	PA-233	full	-	3
91234	PA-234	abso	Burnable	-
92232	U-232	full	-	3
92233	U-233	reso	-	3
92234	U-234	full	-	3
92235	U-235	reso	-	3
92236	U-236	reso	-	3
92237	U-237	full	-	3
92238	U-238	reso	-	3
93237	NP-237	full	-	3
93238	NP-238	full	-	-
93239	NP-239	full	-	3
94236	PU-236	full	-	3
94238	PU-238	reso	-	3
94239	PU-239	reso	-	3

94240	PU-240	reso	-	3
94241	PU-241	reso	-	3
94242	PU-242	reso	-	3
95241	AM-241	reso	-	3
95242	AM-242	full	-	-
95243	AM-243	full	-	3
95342	AM-242M	full	-	3
96242	CM-242	full	-	3
96243	CM-243	full	-	3
96244	CM-244	full	-	3
96245	CM-245	full	-	3
96246	CM-246	full	-	3
96247	CM-247	full	-	3
96248	CM-248	full	-	3
97249	BK-249	full	-	3
98249	CF-249	full	-	3
98250	CF-250	full	-	3
98251	CF-251	full	-	3
98252	CF-252	full	-	3

4. Using MPACT with the VERA Common Input

4.1 MPACT Block

The `MPACT` block in the VERA Common input is used to define all of the MPACT specific parameters needed. The inputs are broken up into various sections and groupings that apply to the same part of the code. The list of these sections are:

- Base Inputs
- 2D/1D Inputs
- CMFD Inputs
- Iteration Control Inputs
- Meshing Inputs
- Quadrature Set Inputs
- XS Library Inputs
- Parallel Environment Inputs
- Depletion Inputs
- Thermal-Hydraulic Inputs
- Transient Inputs

For a full list of the MPACT block input cards and their descriptions, please see the VERA Common Input User Manual [2].

When running the code, the user can expect to encounter errors describing improper input. They range in degrees of severity. An EXCEPTION_INFORMATION is simply an extra message the user may find useful. An EXCEPTION-_WARNING lets the user know that the code may have expected input, but did not find it and is using a default value instead. An EXCEPTION_ERROR informs the user of an input problem that must be resolved before the calculation can continue. The error message should be explanatory and inform the user of the necessary corrective action. The following list is not exhaustive, but here are some examples of different types of messages that are printed:

- #### EXCEPTION_INFORMATION #### XMLProc::SetupOptionPL - SCATT_METH_REFL parameter not present. Value from SCATT_METH will be used.

- #### EXCEPTION_WARNING #### Incorrect input to XMLProc::ScanState - boron is missing, using default value of 0 ppm!
- #### EXCEPTION_ERROR #### Incorrect input to XMLProc::ScanState - bank_labels and bank_pos are not the same dimensions!

Bibliography

[1] Open-mpi. https://www.open-mpi.org/.

[2] E. Walker. Vera common input user manual. Technical report, Oak Ridge National Lab, 2019.