Validation of Nucldar Data using MC Codes

Using MC codes to valdiate codes & transport data

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Aims

The purpose of this work is to determine how different MC codes treat the nuclear data they use

1. Determine response of each MC code to nuclear data on the same geometry and data (ENDF/B-VIIR1)
2. Each code using the same data, i.e. the same ace file
3. Determine the reason for any discrepancy, return reason to evalator/data producer/code developer
4. I downloaded the data only 4 days ago...

Script

The system is setup to make our lives as easy as possible, breaking the system into three main parts

- `benchmark` - builds and runs input deck for each code
- `analysis` - creates a neutron spectra plot for each nuclide
- `build_report` - writes tex file containing each plot

Script - benchmark

- Script scans mcnp xsdir file and converts to other codes formats (Serpent/OpenMC)
- creates an input deck for each code for each nuclide
- submits each job to server
- wait.... for about 3 days

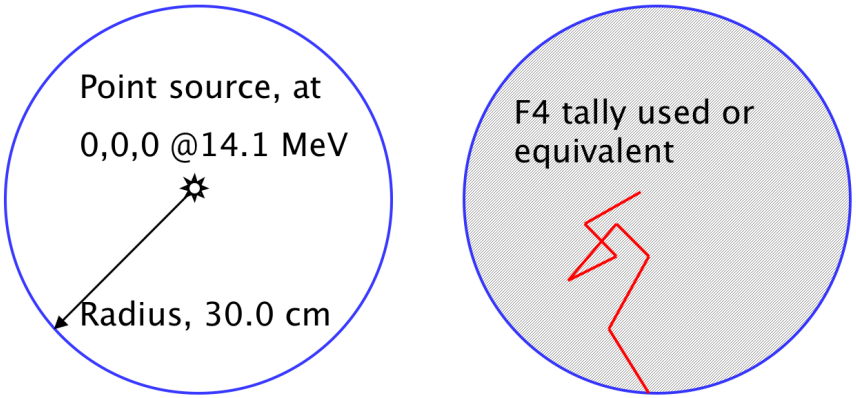
Script - analysis

- For each nuclides in the problem loops over the output data and produces spectra plots
- Produces meta-deta for each nuclide, like fraction of flux out of acceptable range
- Runs the R statistical analysis package to produce graphs

Script - build_report

- Builds LaTeXdocument containg full and zoomed plots
- Includes tables of total flux ratios and statistical errors

Geometry



Spectra binned in 616 TART format, the volume of the cell set to 1.0 cm^3 and the density is set to 1.0 g/cm^3

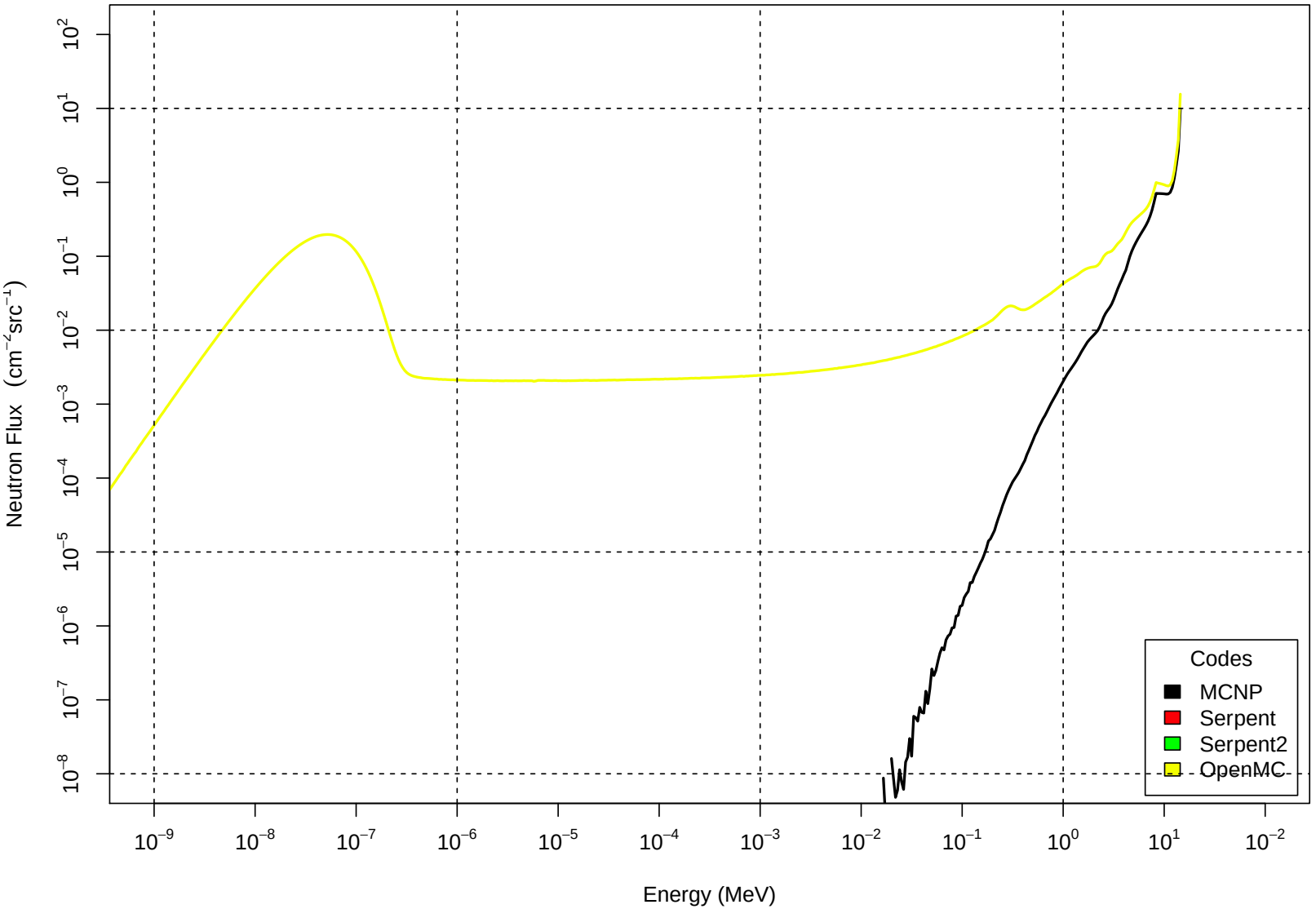
- Simulations ran for 100 Million histories
- Tracklength estimator in the sphere

- MCNP5 v1.6
- Serpent 1 & 2
- OpenMC
- No S(α,β)

Firstly

- I have no agenda, other than I want to see good agreement
- I am not claiming any one code is correct
- Unless I have good reason for doing so..

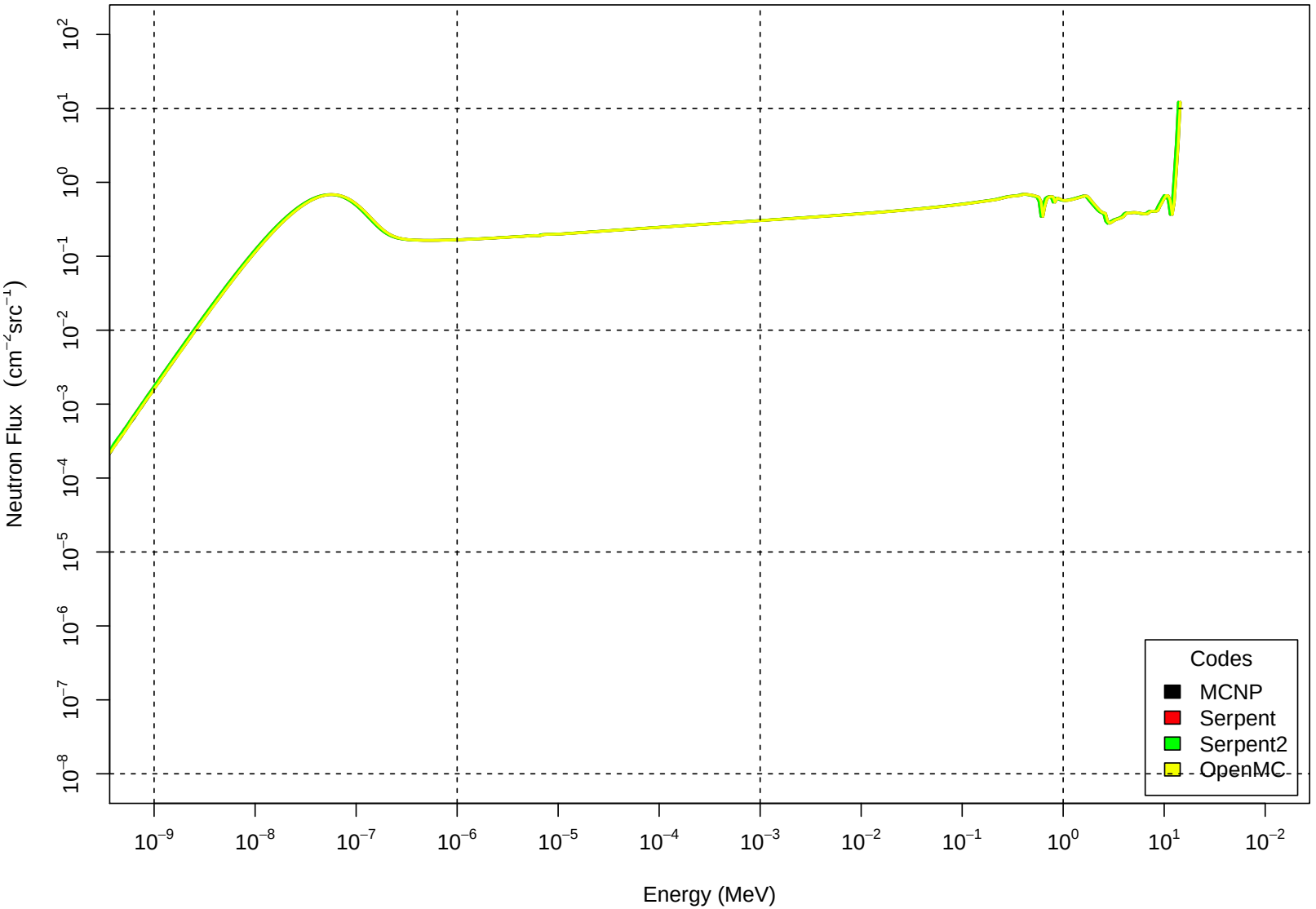
Wrong - ^{7}Be


Neutron Flux (cm^{-2}src^{-1})
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{-2}
Energy (MeV)
Codes
MCNP
Serpent
Serpent2
OpenMC

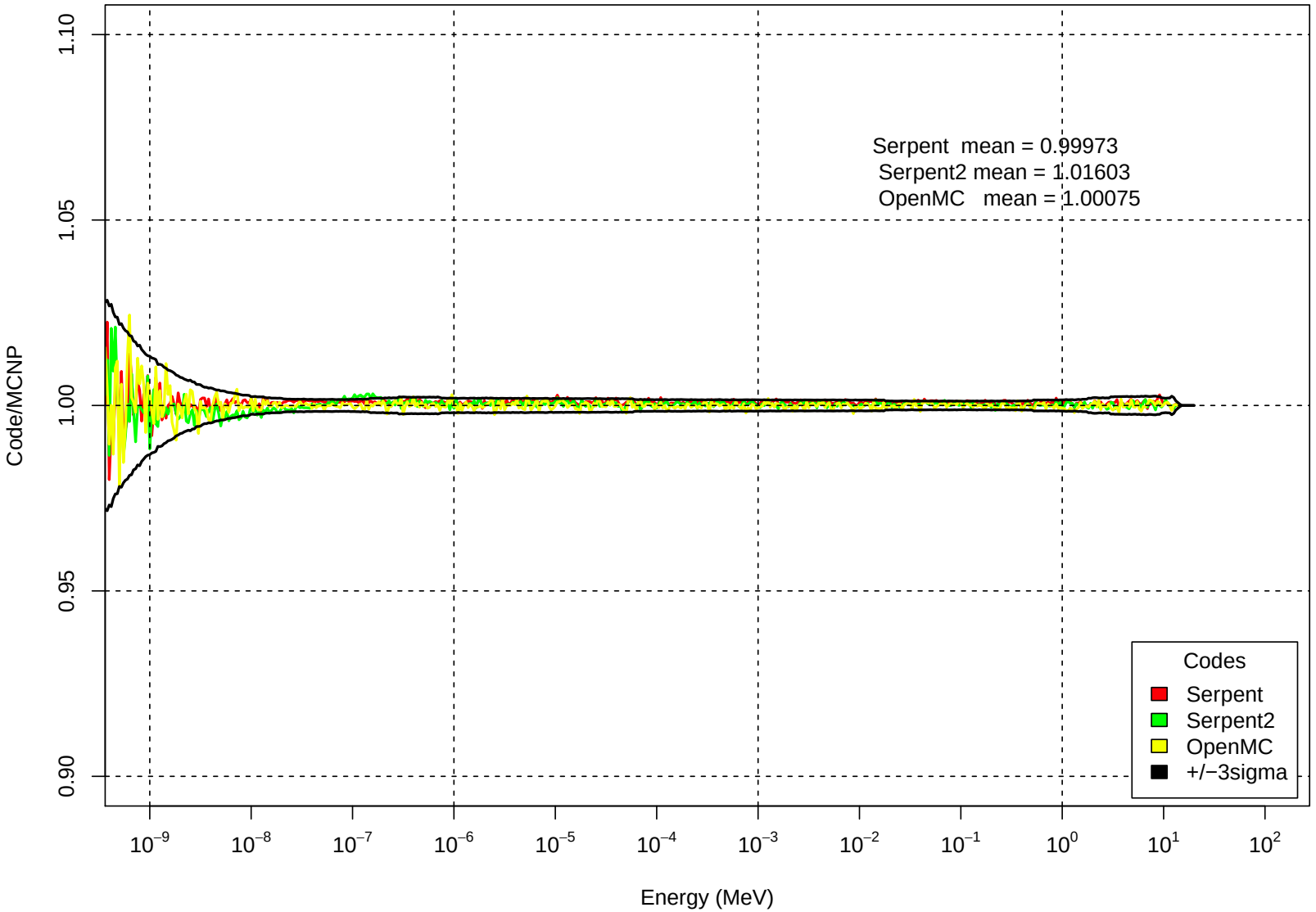
Wrong - ^{7}Be

- In this case, dah dah dah..... it looks like its MCNP
- Serpent 1 & 2 both failed to read the data
- ACE File Gen @293.6K for n-004_Be_007 (R. Arcilla, NNDC)
- MCNP - no warnings
- Serpent - `Warning: Nuclide is missing (n,gamma) channel`
- Also thinks the data are truncated at 8.1 MeV

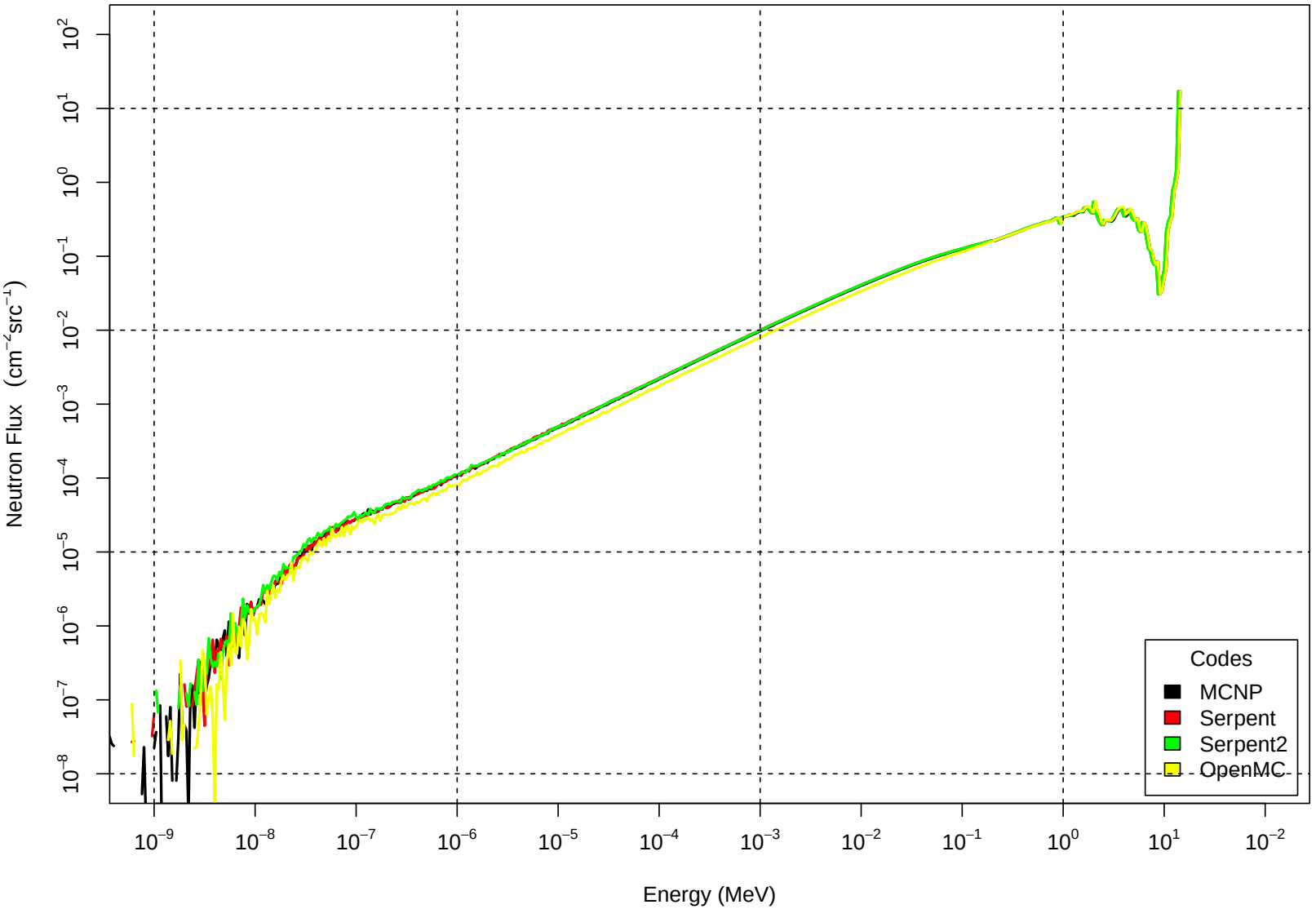
Right - ^{9}Be


Neutron Flux (cm^{-2}src^{-1})
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{-2}
Energy (MeV)
Codes
MCNP
Serpent
Serpent2
OpenMC

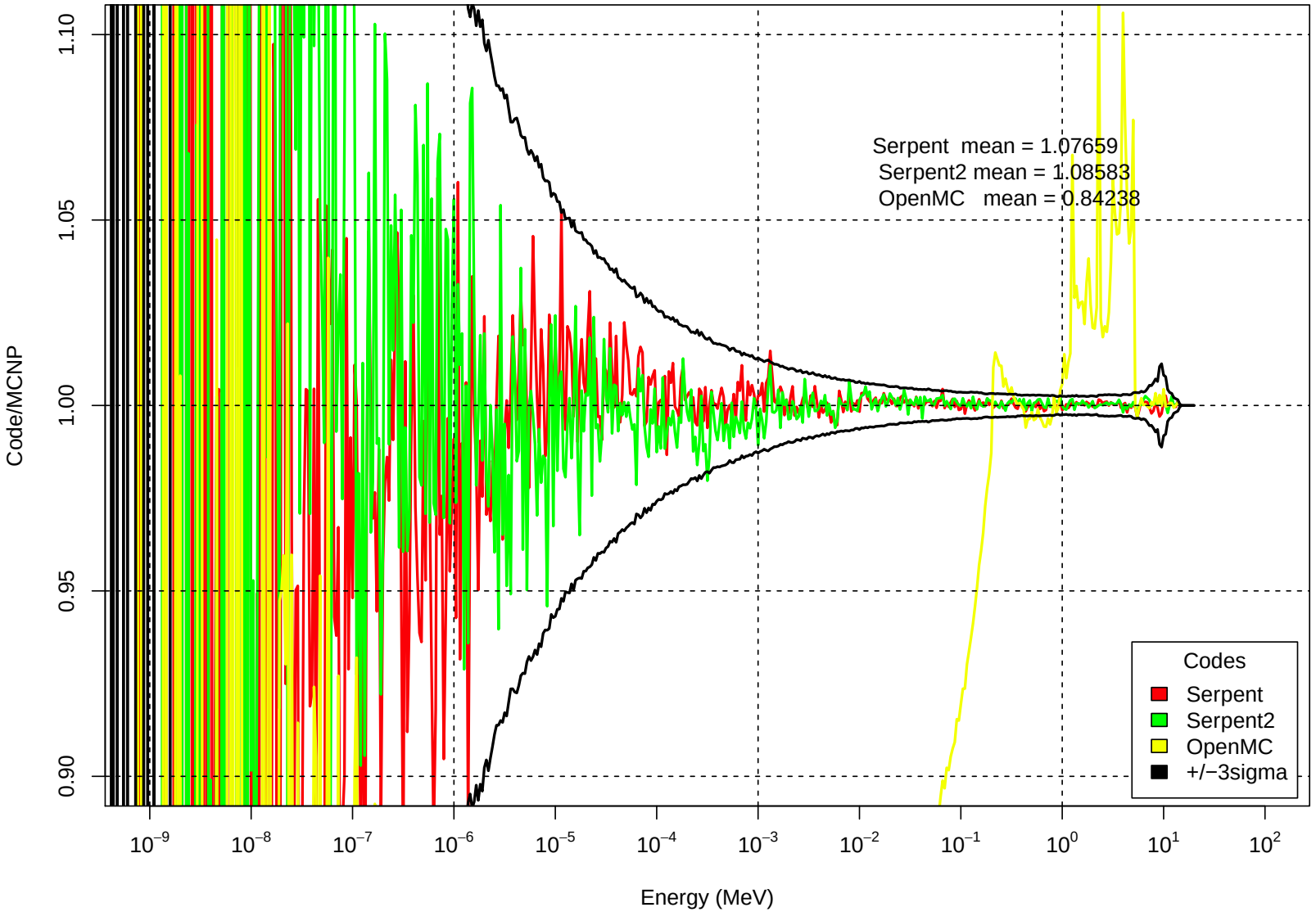
Right - ^{9}Be


Serpent mean = 0.99973
Serpent2 mean = 1.01603
OpenMC mean = 1.00075
Codes
Serpent
Serpent2
OpenMC
+/−3sigma
Code/MCNP
Energy (MeV)
1.10
1.05
1.00
0.95
0.90
10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2}

Right - ^{15}N


Neutron Flux (cm^{-2}src^{-1})
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{-2}
Energy (MeV)
Codes
MCNP
Serpent
Serpent2
OpenMC

Right - ^{15}N


Serpent mean = 1.07659
Serpent2 mean = 1.08583
OpenMC mean = 0.84238
Codes
Serpent
Serpent2
OpenMC
+/−3sigma
Code/MCNP
Energy (MeV)
0.90
0.95
1.00
1.05
1.10
10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2}

Wrong - ^{15}N

- OpenMC ??
- Seen previously with other development codes, issue with the anisotropy of inelastic scattering

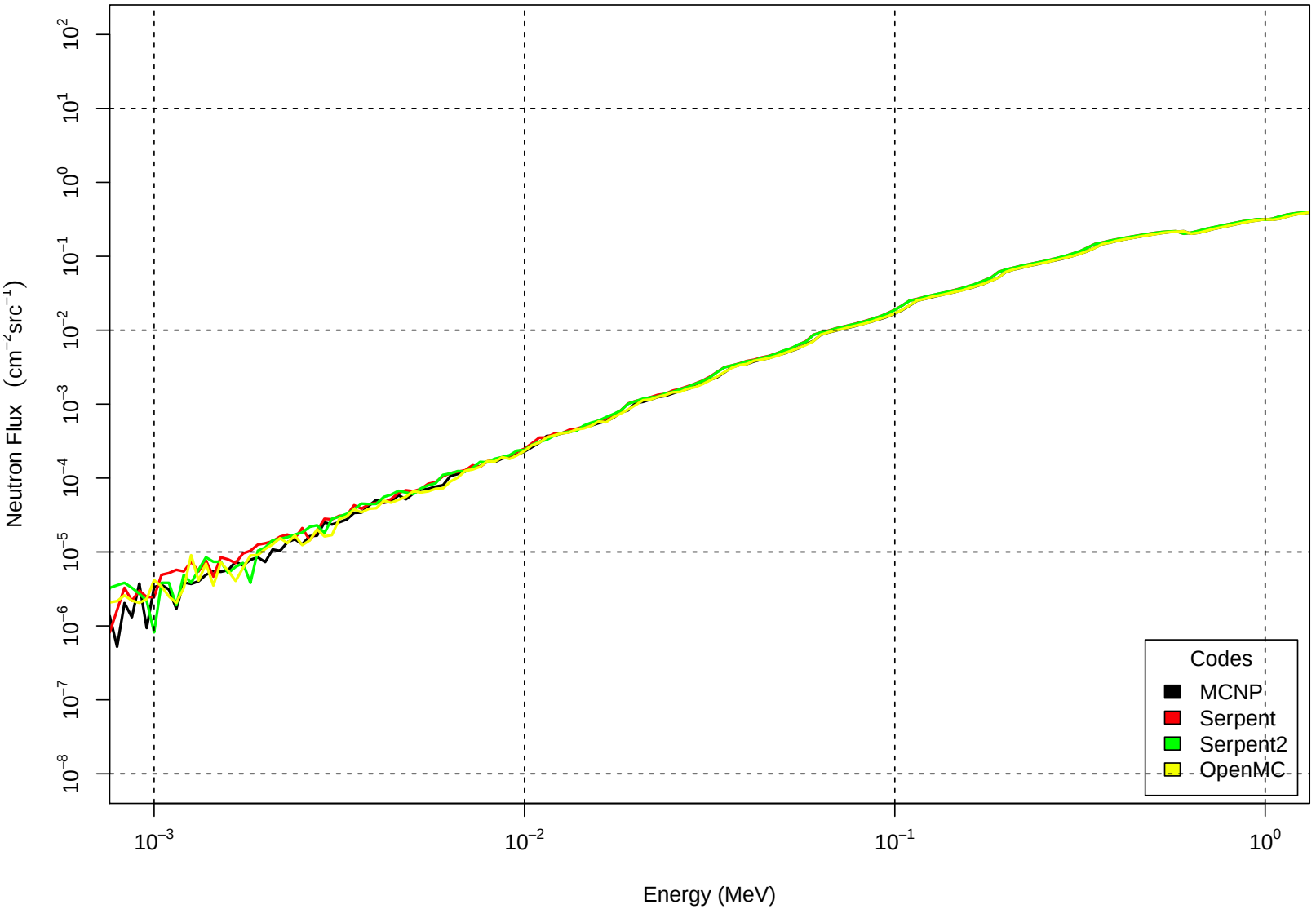
Wrong - ^{22}Na

- Serpent `Processing XS data:`
  `Isotope 11022.71c (Na-22)...`
  `Warning:  59 negative ures ptable values.`
- OpenMC `ERROR STOP`
  `WARNING: Negative value(s) found on probability table for nuclide 11022.71c`
  `ERROR: Too many rejections on evaporation spectrum.`
  `Batch:  1`
  `Generation:  0`
- MCNP ran to completion
- ENDF/B-VII.1: ACE File Gen @293.6K for n-011_Na_022 (R. Arcilla, NNDC) mat1122 04/20/12 probability tables used from 1.5000E-02 to 1.0000E-01 mev.

Wrong - ^{23}Na

- OpenMC `ERROR: Too many rejections on evaporation spectrum.`
  `Batch: 1`
  `Generation: 0`
- MCNP, and the Serpents ran to completion

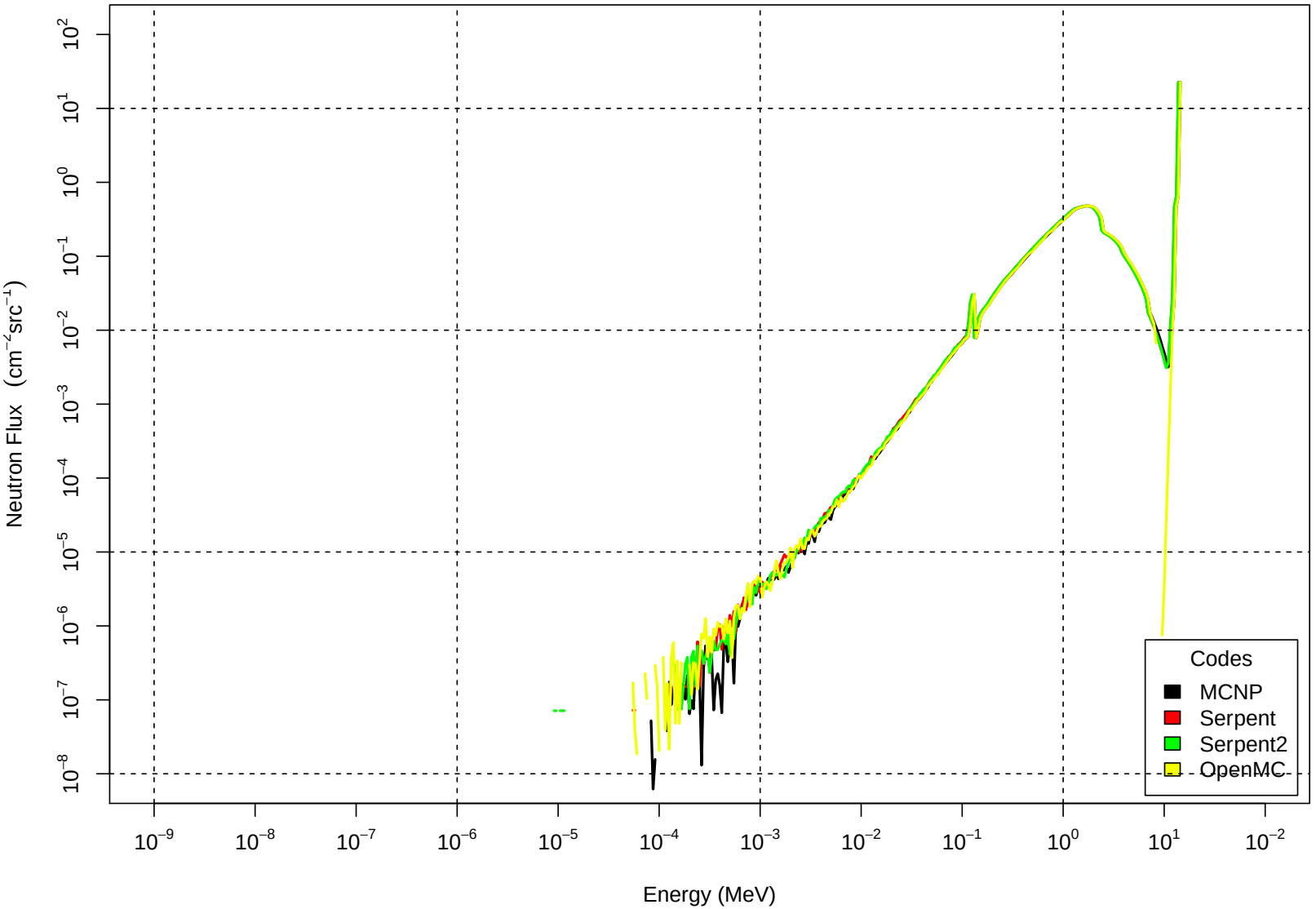
Weird - ^{36}S


Neutron Flux (cm^{-2}src^{-1})
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-3}
10^{-2}
10^{-1}
10^{0}
Energy (MeV)
Codes
MCNP
Serpent
Serpent2
OpenMC

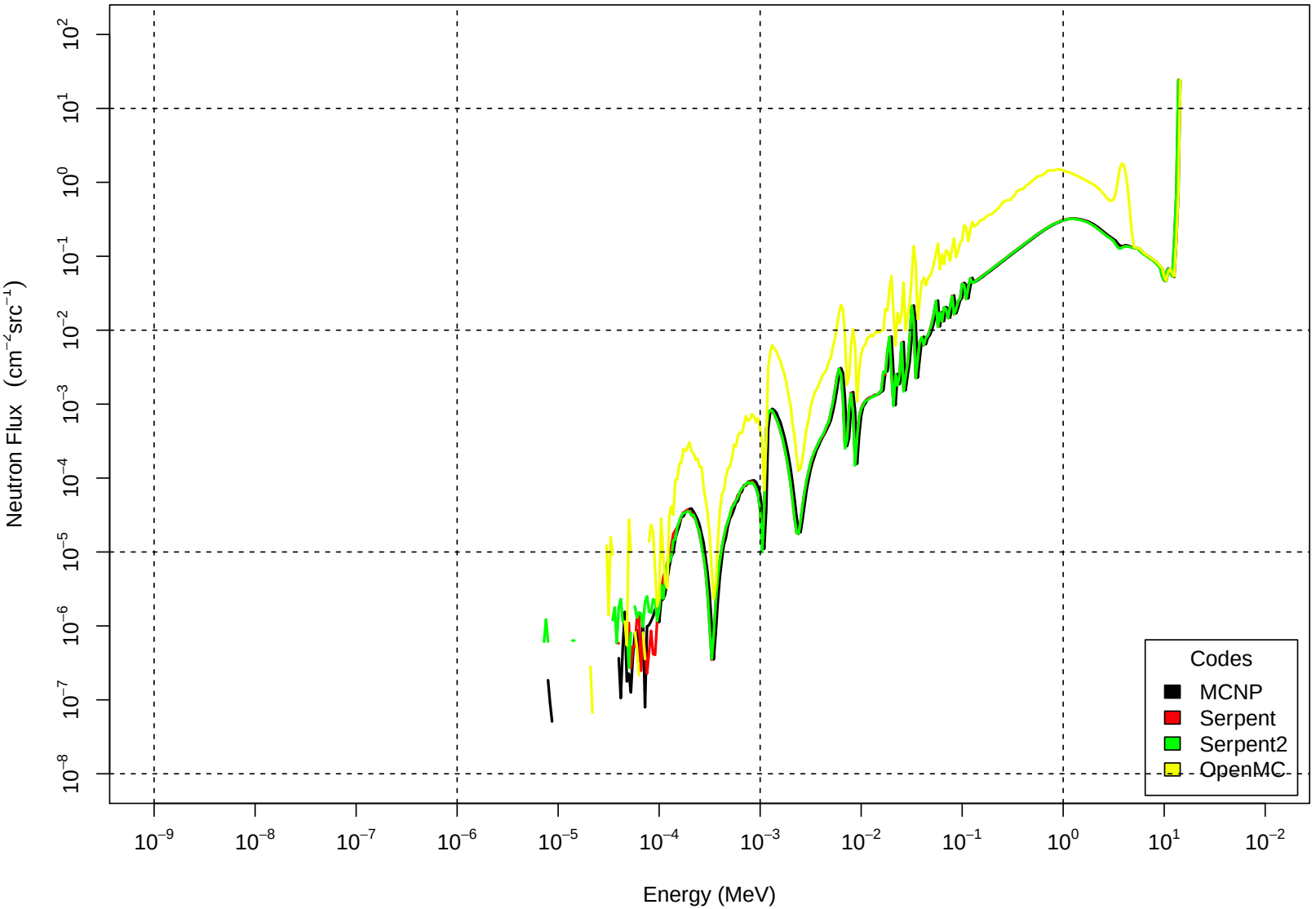
Wrong - ^{36}Ar

- Negative Ures again

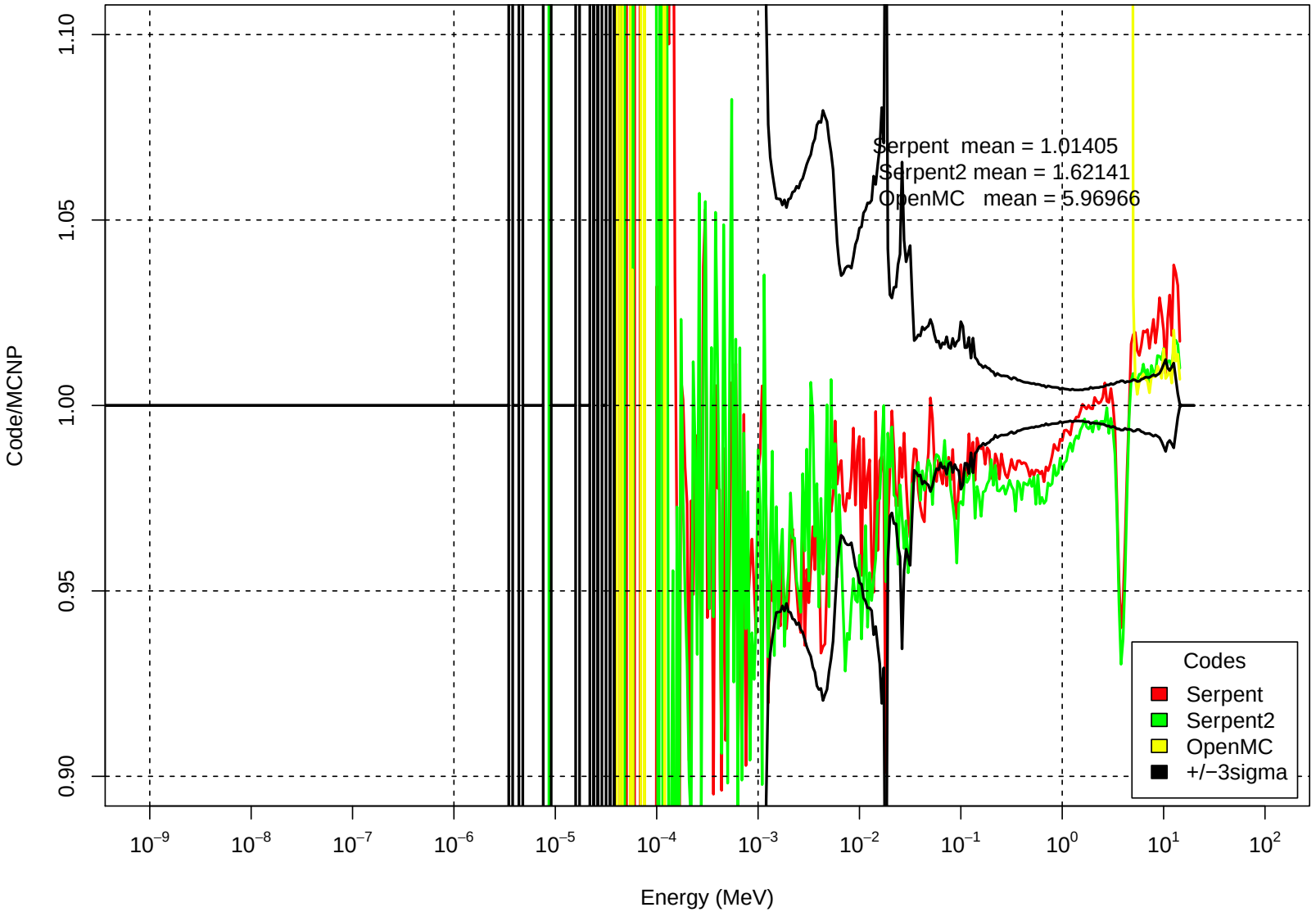
Weird - ^{38}Ar


Neutron Flux (cm^{-2}src^{-1})
Energy (MeV)
Codes
MCNP
Serpent
Serpent2
OpenMC

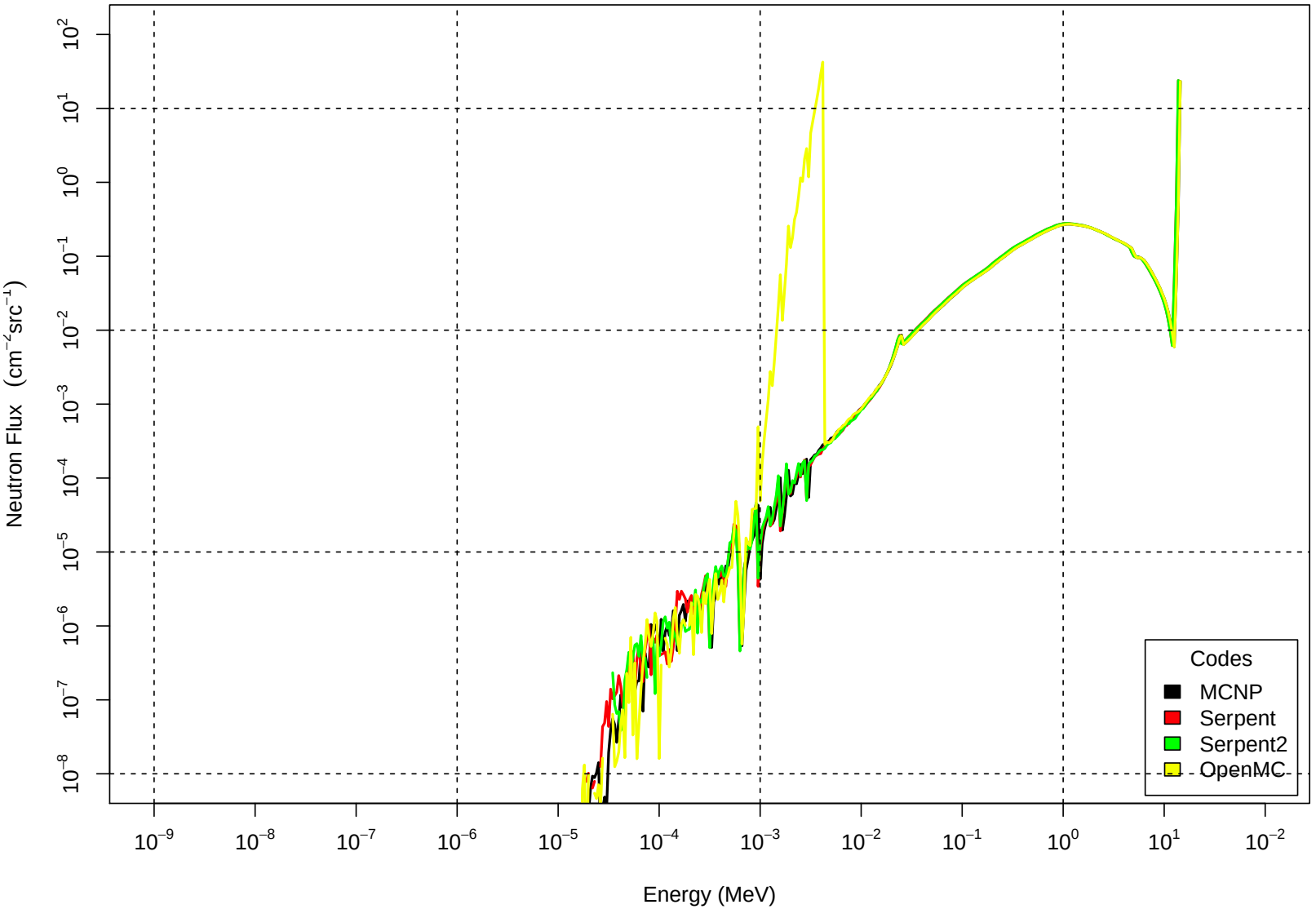
Weird - ^{55}Mn


Neutron Flux (cm^{-2}src^{-1})
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{-2}
Energy (MeV)
Codes
MCNP
Serpent
Serpent2
OpenMC

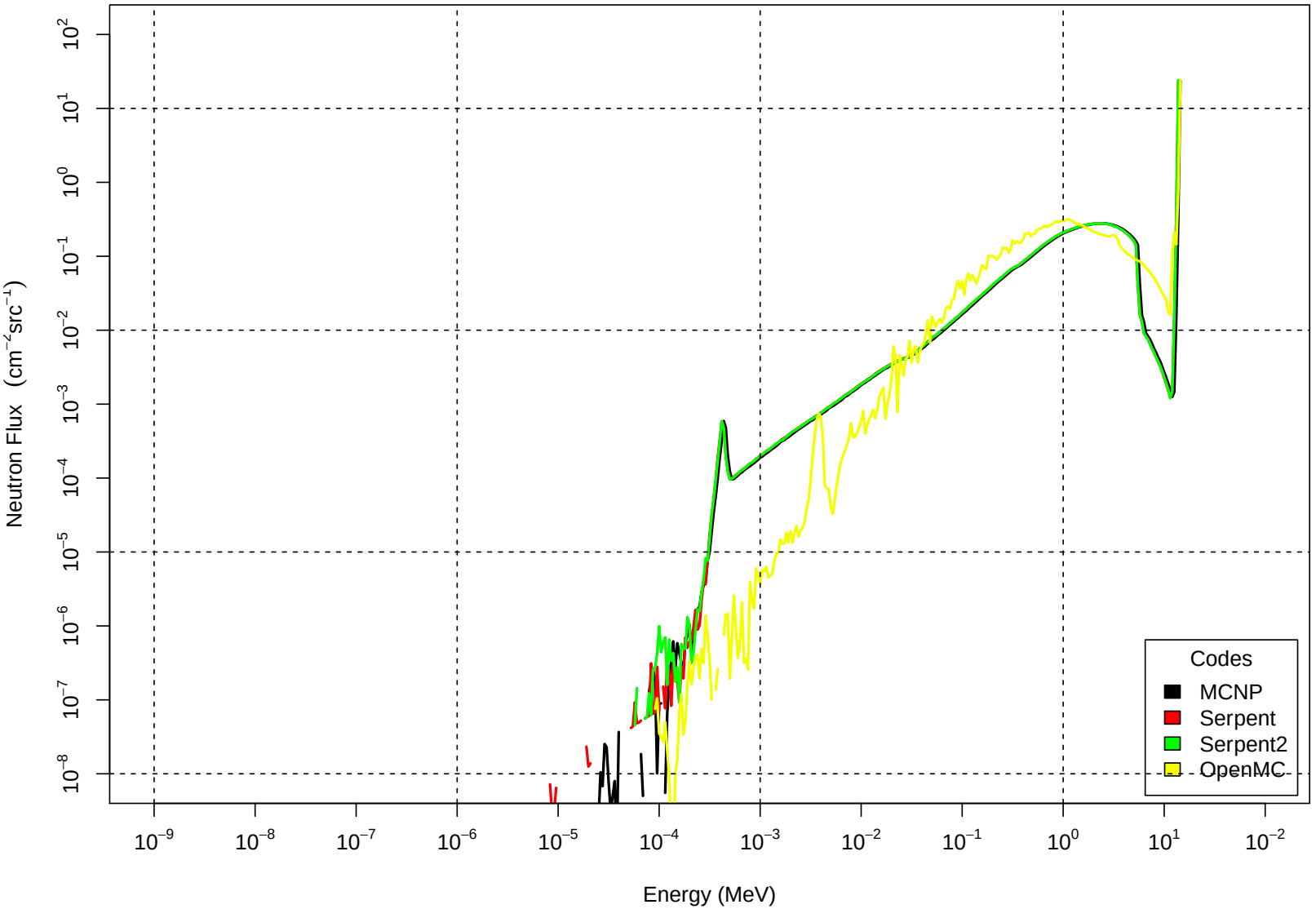
Weird - ^{55}Mn


Serpent mean = 1.01405
Serpent2 mean = 1.62141
OpenMC mean = 5.96966
Codes
Serpent
Serpent2
OpenMC
+/−3sigma
Code/MCNP
Energy (MeV)
1.10
1.05
1.00
0.95
0.90
10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2}

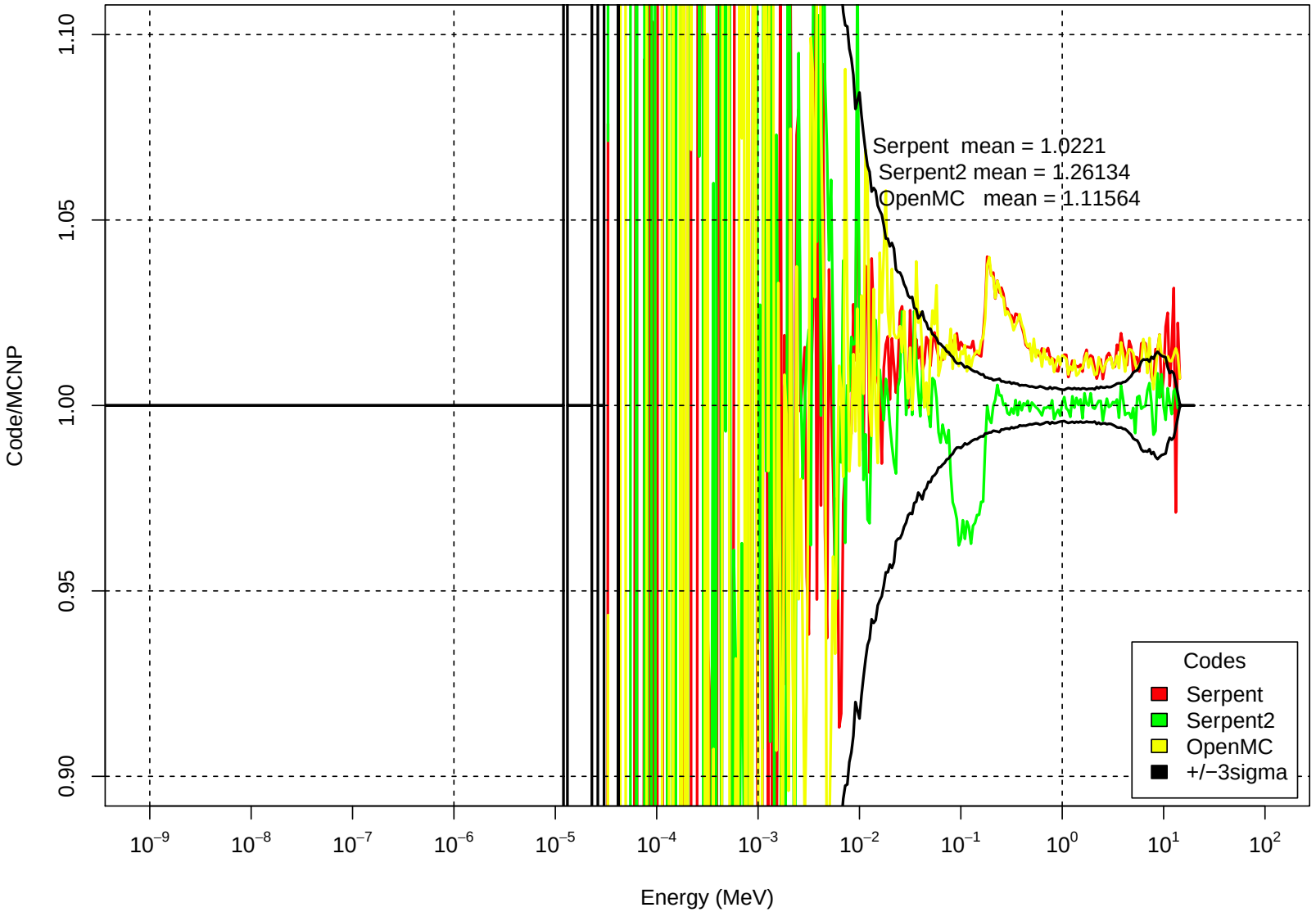
Weird - ^{58}Co


Neutron Flux (cm^{-2}src^{-1})
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{-2}
Energy (MeV)
Codes
MCNP
Serpent
Serpent2
OpenMC

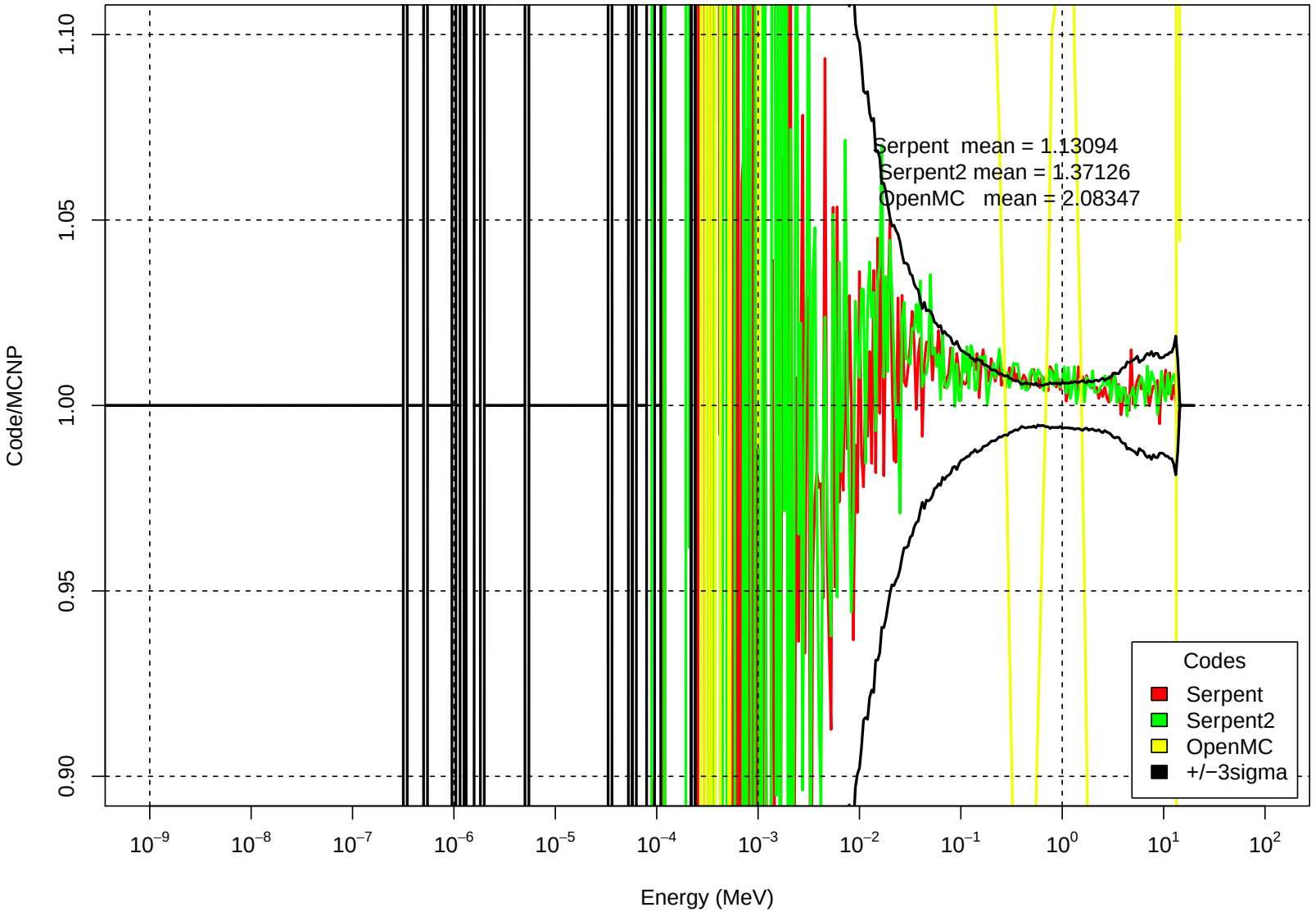
Weirder - ^{59}Co



Wrong - ^{74}As


Serpent mean = 1.0221
Serpent2 mean = 1.26134
OpenMC mean = 1.11564
Codes
Serpent
Serpent2
OpenMC
+/−3sigma
Code/MCNP
Energy (MeV)
1.10
1.05
1.00
0.95
0.90
10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2}

Poor - ^{149}Pm


Code/MCNP
1.10
1.05
1.00
0.95
0.90
Serpent mean = 1.13094
Serpent2 mean = 1.37126
OpenMC mean = 2.08347
Codes
Serpent
Serpent2
OpenMC
+/−3sigma
10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2}
Energy (MeV)

Explainable - ^{154}Eu

Poor Misc

- ^{44,46,48}Ca - OpenMC overestimate
- Sc,Ti,V,Cr,Fe - Agreement within appropriate range
- ^{59}Ni made OpenMC Segfault, others were ok
- If nuclide not mentioned its ok

Conclusions

- Total fluxes agree well and if had been used without spectra the differences would not have been noticed
- Most nuclides agree well, however several results were suspect
- Several bizarre misinterpretations of the data, ^{15}N

Extensions to this work

- Would like to be able to process my own data with NJOY
- Would like to be able to convert my NJOY processed data to Partisn format
- Would like to add PARTISN to the mix
- Would like to add Geant4 and Phits

Any questions?