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Title: MCNP6 Parallel Performance Analysis: How to Efficiently Run MCNP6 in Parallel

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MCNP6 Parallel Performance Analysis: How to Efficiently Run MCNP6 in Parallel

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Introduction

To take advantage of multi-core computer architecture, MCNP6 provides two independent methods to run problems in parallel: task-based threading using OpenMP and distributed processing supported by the Message Passing Interface (MPI).

How to setup and run MCNP6 in parallel depends on several factors, including the computing hardware as well as the problem to be run. This presentation will discuss how MCNP6 runs in parallel, present the results of several sample problems with the goal of providing some insight on how to run MCNP in parallel effectively.

Comparison of Threading and MPI in MCNP6

	Threading	MPI
Ease of use	Integrated into MCNP	Requires additional software
Versatility	Limited to neutron, photon, and electron particles only -- No model physics	Works with all MCNP features
CPU utilization	All processes transport particles	Manager process only sends and collects data; it does no particle transport
Memory usage	Geometry and cross section data memory is shared	No memory shared
CPU overhead	Requires thread locks so that only one thread at a time can run certain sections of the code	Each process runs independently
Inter-process data transfer and collection	None – done internally	Manager broadcasts data to individual processes and collects the results when they are finished.
Number of parallel processes	Limited to one core	None -- can run across nodes of a cluster or computers on a network

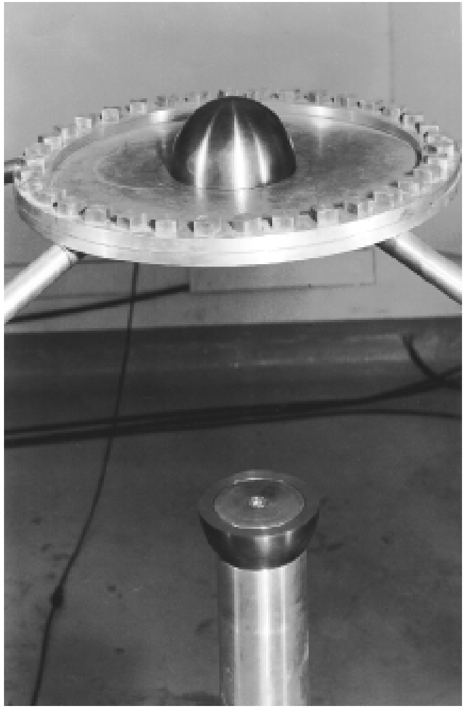
Except for UM preprocessing, only particle transport is run in parallel.

Sample Problem: Godiva

```
 Godiva   Solid Bare HEU sphere  HEU-MET-FAST-001
1          1        4.7984e-02         -1        imp:n=1
2          0                            1        imp:n=0

1          so       8.7407

prdmp j -1e6 j 1 1e9
sdef    cel=1     erg=d1    rad=d2    pos=0.0 0.0 0.0
sp1     -3
si2     0.0     8.7407
sp2     -21     2
totnu
c ------------- ENDF/B-VII ---------------
m1         92234.70c   4.9184e-04
           92235.70c   4.4994e-02
           92238.70c   2.4984e-03
c -----------------------------------------
print
kcode      10000   1.0   80    800
```



Run godiva

```
time mcnp6 i= godiva.inp
. . . . . . . . . . .
 source distribution written to file srctq
cycle=   800
      run terminated when     800 kcode cycles were
done.

 =====>     409.14 M histories/hr    (based on wall-
clock time in mcrun)

comment.
 comment. Average fission-source entropy for the last
half of cycles:
 comment.      H=  7.42E-01  with population std.dev.=
1.40E-03
 comment.
 comment.
 comment. Cycle   17 is the first cycle having fission-
source
```

```
 comment.   entropy within 1 std.dev. of the average
 comment.   entropy for the last half of cycles.
 comment.   At least this many cycles should be
discarded.
 comment. Source entropy convergence check passed.
 comment.

final k(col/abs/trk len) = 0.999574     std dev =
0.000217


 ctm =          1.17    nrn =          411408359
 dump     2 on file runtpf.h5    nps =      8001005    coll =
29312333
 mcrun  is done


real    1m12.282s
user    1m5.402s
sys     0m6.060s
```

Run godiva with 2 threads

```
time mcnp6 i= godiva.inp tasks 2
. . . . . . . . . . . .
 source distribution written to file srctq        cycle=
800
      run terminated when     800 kcode cycles were done.


 =====>      815.62 M histories/hr    (based on wall-clock
time in mcrun)


 comment.
 comment. Average fission-source entropy for the last
half of cycles:
 comment.      H=  7.42E-01  with population std.dev.=
1.40E-03
 comment.
 comment.
 comment. Cycle   17 is the first cycle having fission-
source
```

```
 comment.   entropy within 1 std.dev. of the average
 comment.   entropy for the last half of cycles.
 comment.   At least this many cycles should be
discarded.
 comment.
 comment. Source entropy convergence check passed.
 comment.

 final k(col/abs/trk len) = 0.999574     std dev =
0.000217


 ctm =          1.15   nrn =          411408359
 dump    2 on file runtpg.h5   nps =     8001005   coll =
29312333
 mcrun  is done


real    0m36.655s
user    1m8.906s
sys     0m3.052s
```

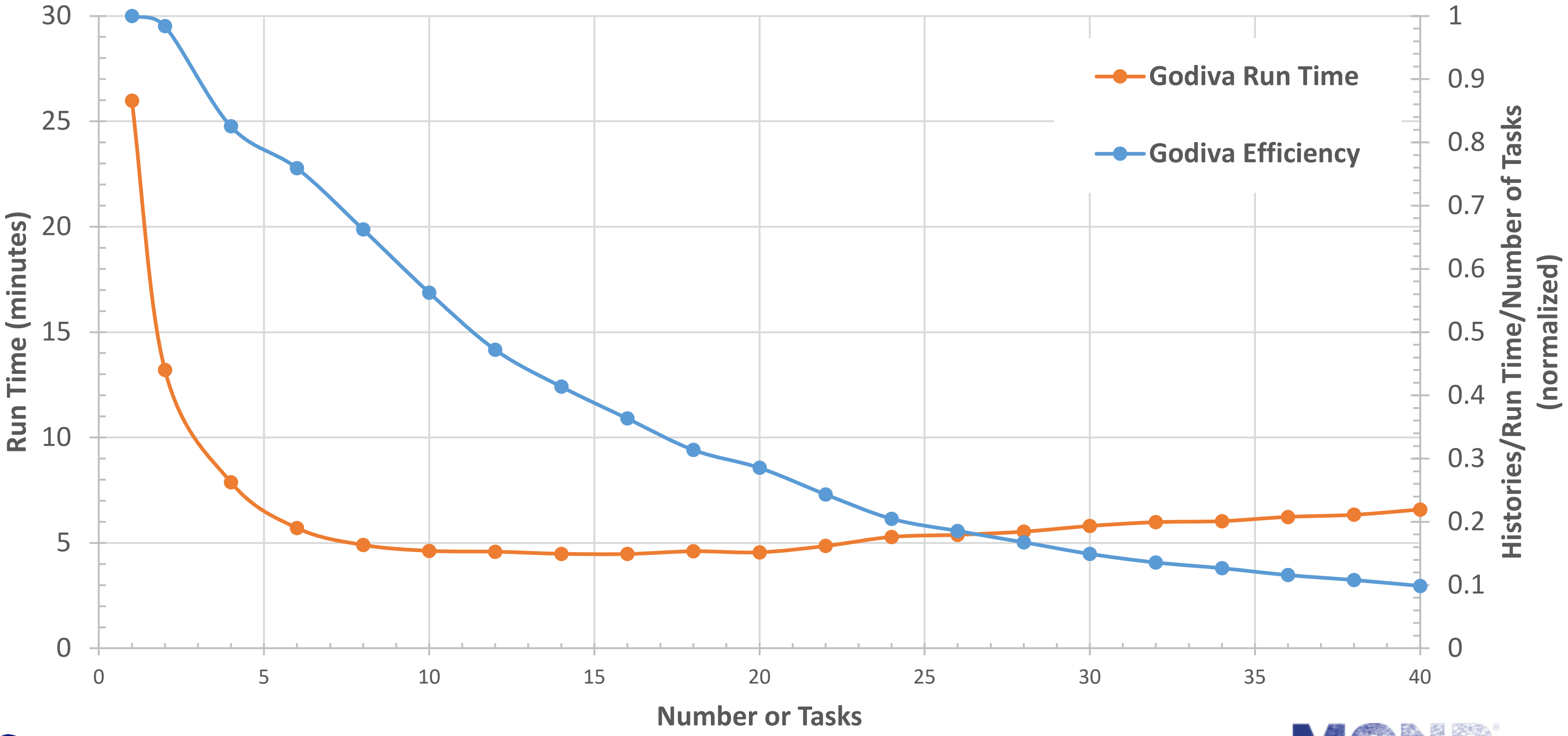
Godiva Timing Results for Different Numbers of Tasks

Number of Tasks		
1	=====>	409.14 M histories/hr
2	=====>	815.62 M histories/hr
4	=====>	1353.13 M histories/hr
8	=====>	2029.36 M histories/hr

Number of Tasks				
1	ctm =	1.17	nrn =	411408359
2	ctm =	1.15	nrn =	411408359
4	ctm =	1.36	nrn =	411408359
8	ctm =	1.79	nrn =	411408359

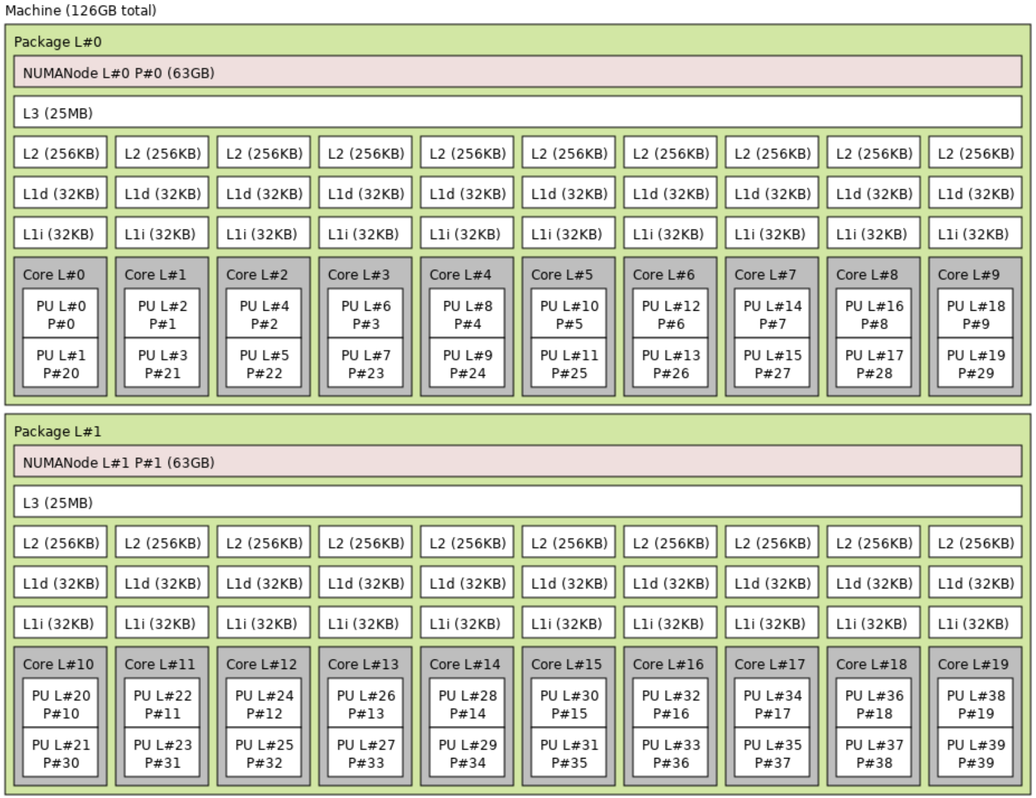
Number of Tasks		
1	real	1m12.282s
2	real	0m36.655s
4	real	0m22.637s
8	real	0m15.561s

Godiva Threading Performance

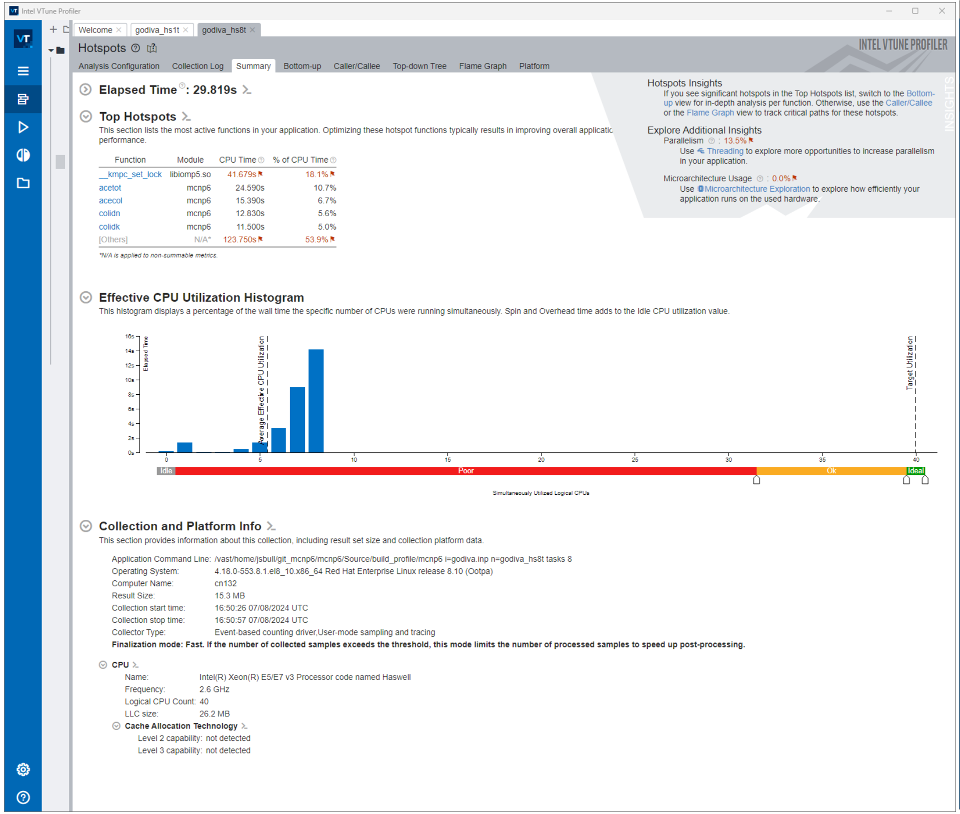


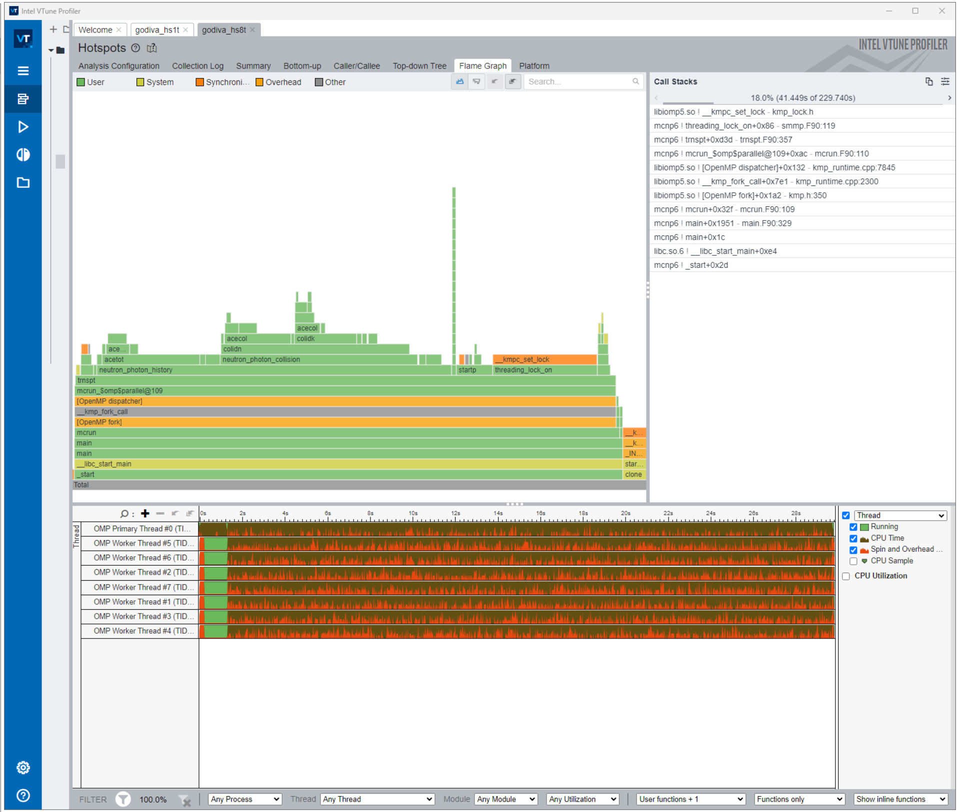
Computer Hardware Used For This Analysis

- Linux RedHat 8.10
- Intel Xeon(R) CPU E5-2600 v3, Haswell
  - 2 sockets
  - 10 cores/socket
  - Hyperthreading on
    - 20 logical CPUs/socket
  - 2 NUMA nodes, one per socket



Intel Vtune Profiler



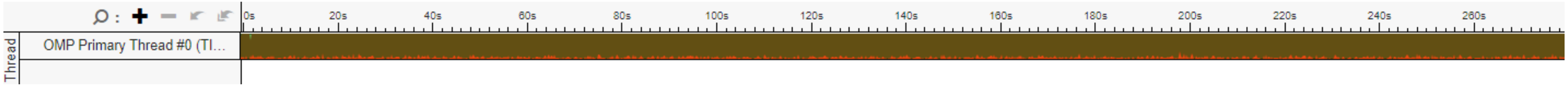


Godiva CPU Cycle Breakdown

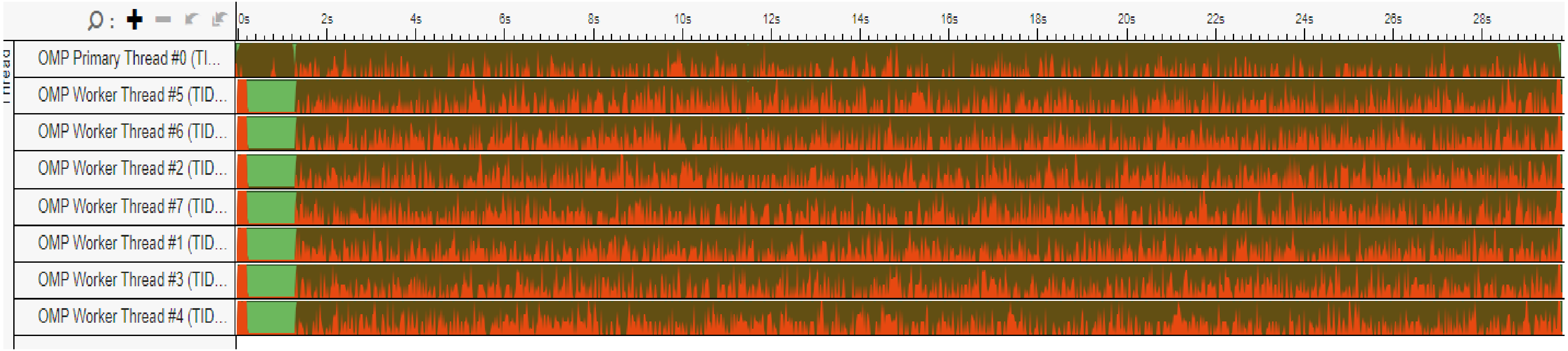
Top-level CPU Time (seconds)	Number of Tasks		
	1	8	40
Total CPU Time	278	230	2,693
Time spent executing MCNP	261	161	268
Time threads are locked	2	24	774
Time spent managing the threads (overhead)	14	44	1,650
Effective CPU utilization	1.0	5.4	3.5
Elapsed Time	280	30	77

How is MCNP Using CPU Cycles

1 task



8 tasks



Running MCNP Idle Spin and overhead

How is MCNP Using CPU Cycles – 40 Tasks

Running MCNP Idle Spin and overhead

What's Causing the Spin and Overhead Time?

1 task

Function	CPU Time (s)	% of CPU Time
acetot	30	10.80%
uname	25	9.10%
acecol	24	8.80%
getrusage	22	7.90%
colidn	17	6.10%
[Others]	159	57.30%

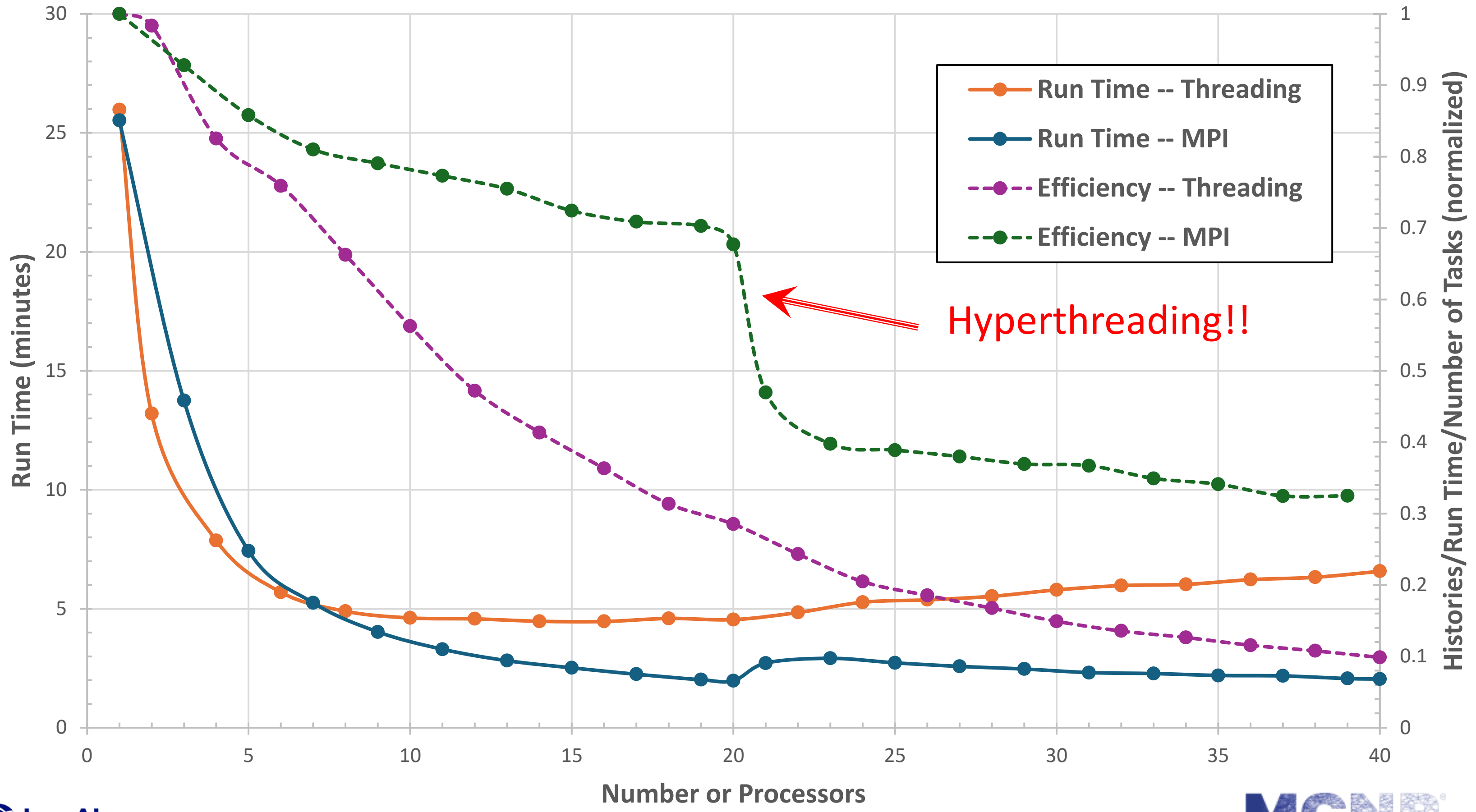
40 tasks

Function	CPU Time (s)	% of CPU Time
__kmpc_set_lock	2,291	85.10%
__kmp_fork_barrier	100	3.70%
acetot	35	1.30%
acecol	27	1.00%
colidn	22	0.80%
[Others]	217	8.10%

```
if( sources_need_locks )  call threading_lock_on(THREADING_LOCK_SOURCE)
if( kbp>0 .or. history_thread%kdb<0 ) then
  exit HISTORY_LOOP
```

For criticality problems, source particles are processed one thread at a time.

Godiva Threading and MPI Performance



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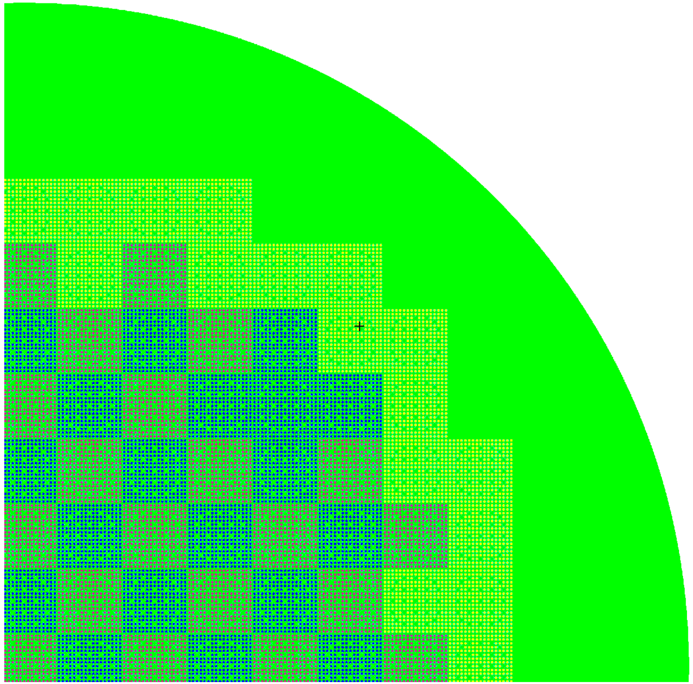
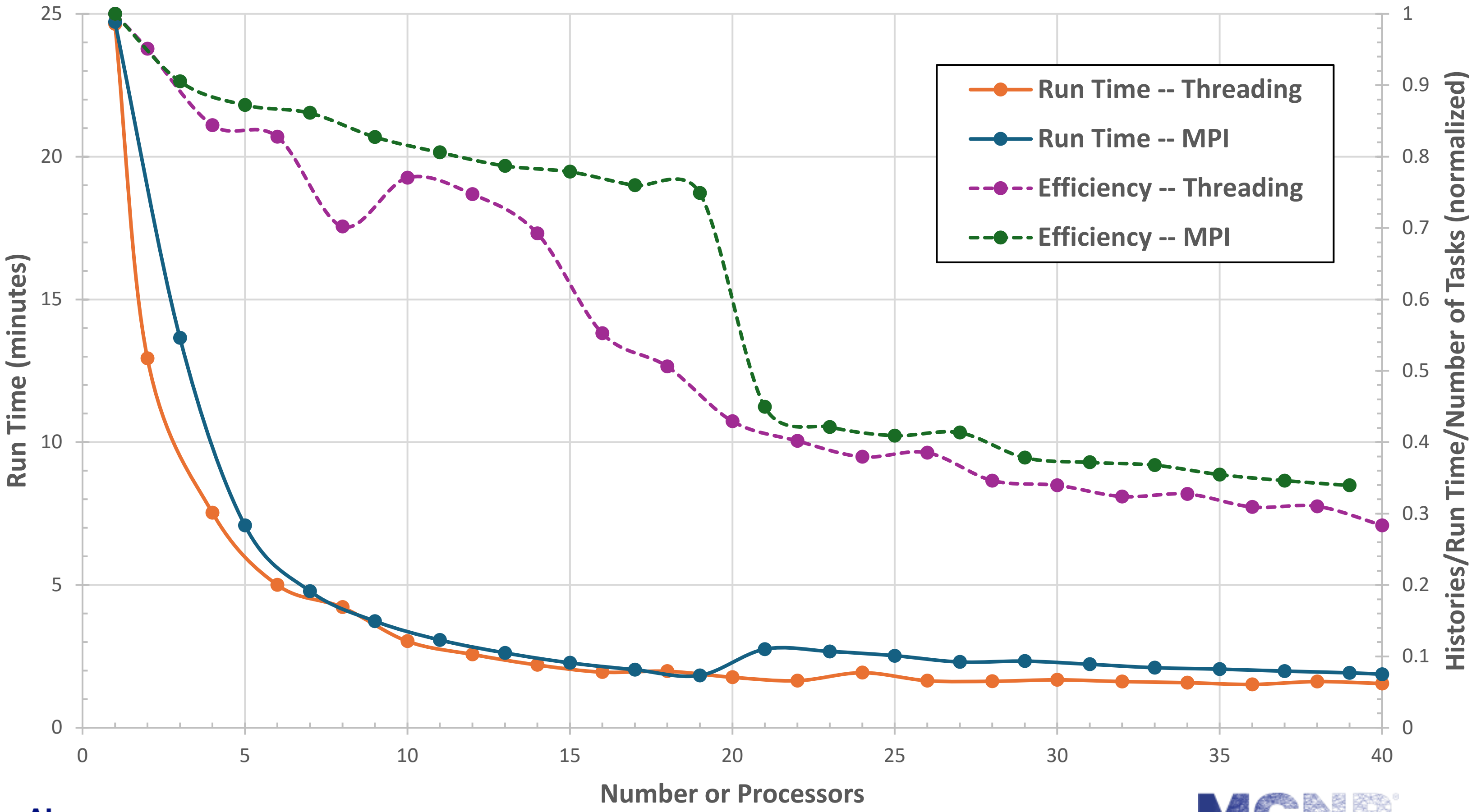
Sample Problem 2: PWR initial core, 2D model, 17x17 bundles

```
pwr2d-whole - PWR initial core, 2D model, 17x17 bundles
c  2.1%, 2.6%, and 3.1% enrichment for assemblies
c  Taken from "Whole Core Calculations of Power Reactors
c  by Use of Monte Carlo Method" by Nakagawa and Mori,
c  J. Nuc. Sci. and Tech., 30(7), 692-701 (1993)
c
1  1  6.60783e-2    -1          u=1    $ UO2 2.1%
2  5  4.310700e-2    1   -2     u=1    $ Zr
3  4  6.622400e-2    2          u=1    $ H2O
c
4  2  6.60798e-2    -1          u=2    $ UO2 2.6%
5  5  4.310700e-2    1   -2     u=2    $ Zr
6  4  6.622400e-2    2          u=2    $ H2O
c
7  3  6.60913e-2    -1          u=3    $ UO2 3.1%
8  5  4.310700e-2    1   -2     u=3    $ Zr
9  4  6.622400e-2    2          u=3    $ H2O
c
10  4  6.622400e-2   -3         u=4    $ H2O
11  5  4.310700e-2    3   -4    u=4    $ Zr
12  4  6.622400e-2    4         u=4    $ H2O
c
c ----- lattice of fuel/water, 2.1% enrichment
13  0       -5     lat=1        u=5   fill=  -8:8  -8:8 0:0
            1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
            1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
            1 1 1 1 1 4 1 1 4 1 1 4 1 1 1 1 1
            1 1 1 4 1 1 1 1 1 1 1 1 1 4 1 1 1
 ................
```

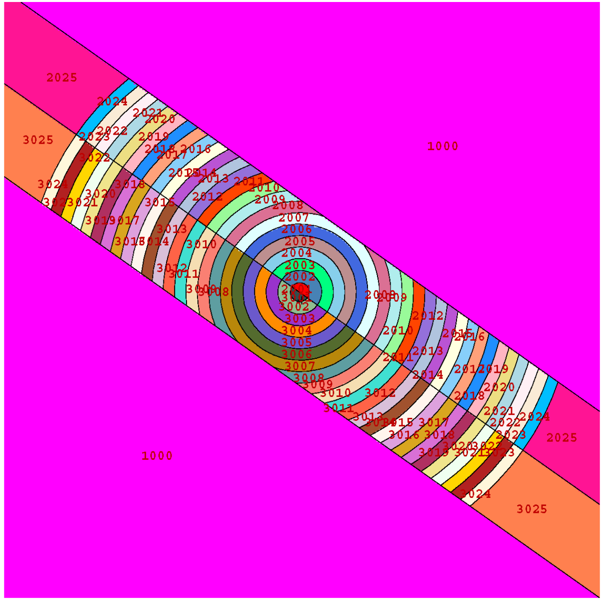


PWR Initial Core Threading and MPI Performance



Sample Problem 3: Fixed Source with 7.5 Million Tally Bins

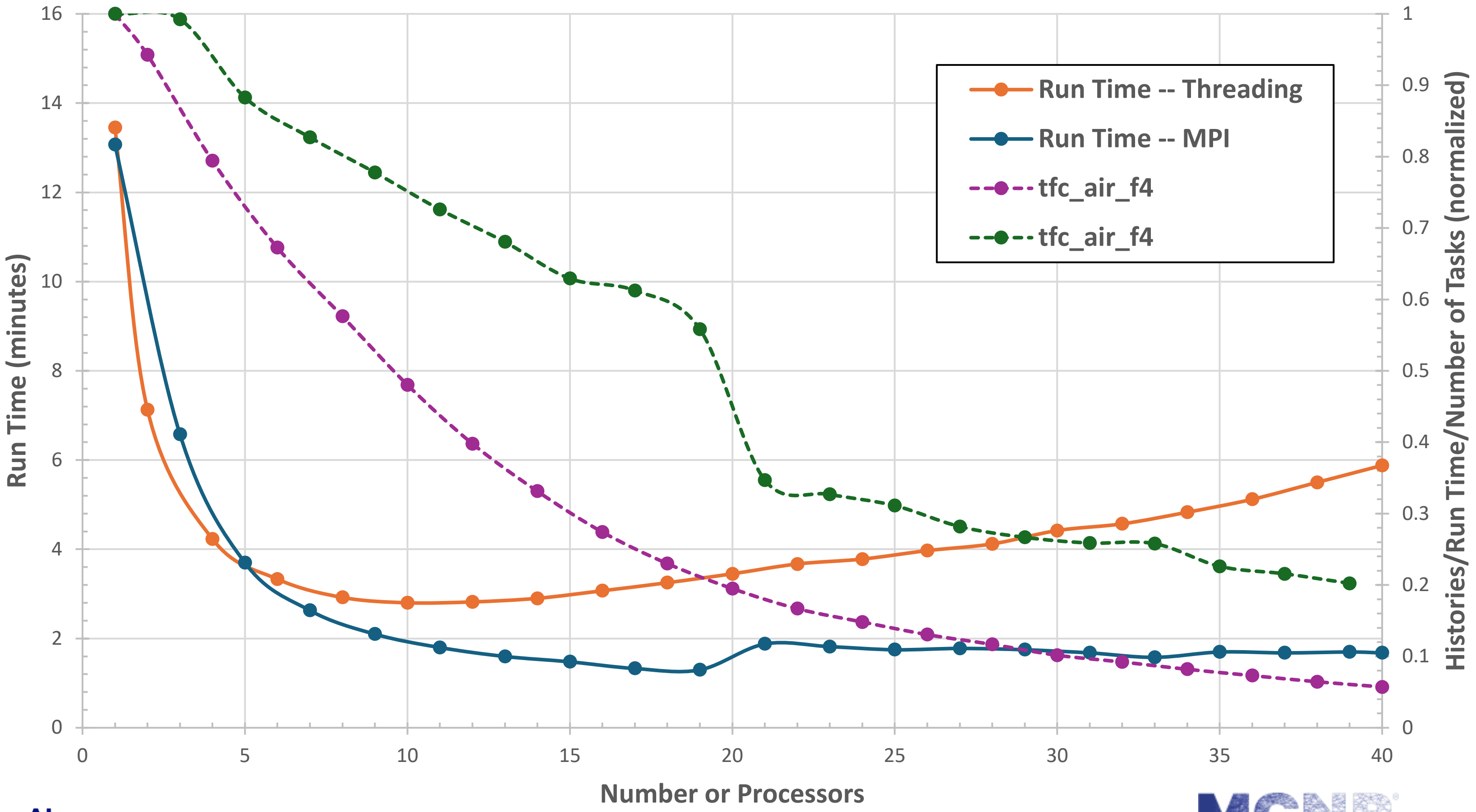
```
Transport neutrons through void, tallying using F4 tallies
c  Air cells
2001  1  -1.29300E-03  -2101        30 -32  imp:n=1  $imp:n= 1
2002  1  -1.29300E-03 -2102  2101  30 -32  imp:n=1  $imp:n= 2
2003  1  -1.29300E-03 -2103  2102  30 -32  imp:n=1  $imp:n= 4
2004  1  -1.29300E-03 -2104  2103  30 -32  imp:n=1  $imp:n= 8
2005  1  -1.29300E-03 -2105  2104  30 -32  imp:n=1  $imp:n= 16
2006  1  -1.29300E-03 -2106  2105  30 -32  imp:n=1  $imp:n= 32
2007  1  -1.29300E-03 -2107  2106  30 -32  imp:n=1  $imp:n= 64
2008  1  -1.29300E-03 -2108  2107  30 -32  imp:n=1  $imp:n= 128
2009  1  -1.29300E-03 -2109  2108  30 -32  imp:n=1  $imp:n= 256
2010  1  -1.29300E-03 -2110  2109  30 -32  imp:n=1  $imp:n= 512
2011  1  -1.29300E-03 -2111  2110  30 -32  imp:n=1  $imp:n= 1024
2012  1  -1.29300E-03 -2112  2111  30 -32  imp:n=1  $imp:n= 2048
2013  1  -1.29300E-03 -2113  2112  30 -32  imp:n=1  $imp:n= 4096
2014  1  -1.29300E-03 -2114  2113  30 -32  imp:n=1  $imp:n= 8192
2015  1  -1.29300E-03 -2115  2114  30 -32  imp:n=1  $imp:n= 16384

................
f104:n  2001 2002 2003 2004 2005 2006 2007 2008 2009 2010
       2011 2012 2013 2014 2015 2016 2017 2018 2019 2020
       2021 2022 2023 2024 2025
f114:n 3001 3002 3003 3004 3005 3006 3007 3008 3009 3010
       3011 3012 3013 3014 3015 3016 3017 3018 3019 3020
       3021 3022 3023 3024 3025
e0 1e-6 999ilog 15
t0 1 98i 1e6
cf104 2010
```



Tally	Bins
102	5,010,000
114	2,505,000
Total	**7,515,000**

Each task requires an additional 250 MB of memory

Fixed Source With 7.5 Million Tally Bins -- Threading and MPI Performance



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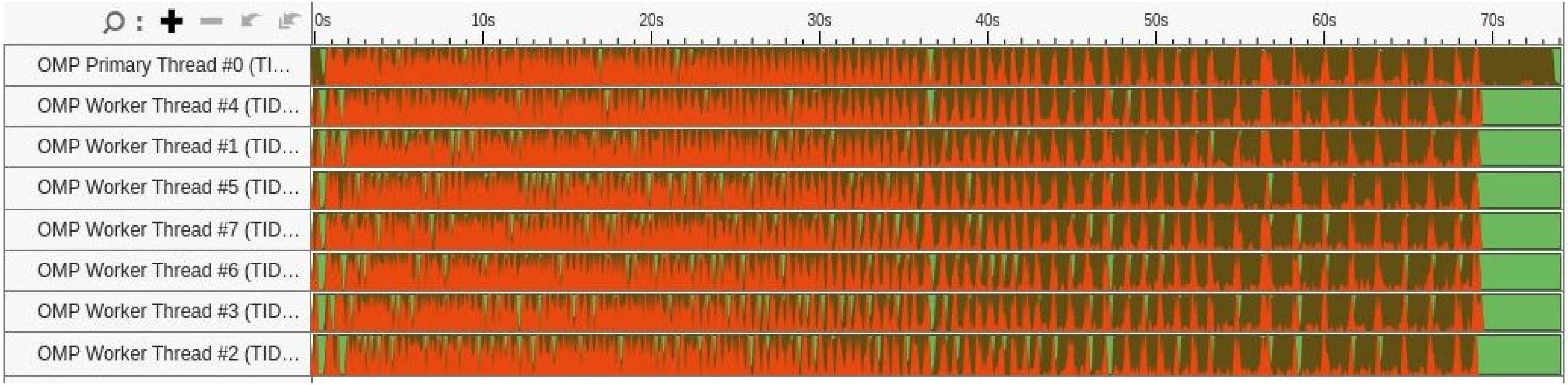
Fixed Source w/ 7.5 M Tally Bins -- CPU Cycle Utilization

8 tasks



Note that the frequency of spin and overhead spikes decrease later in the problem

Running MCNP   Idle   Spin and overhead

Tally Fluctuation Charts

- To calculate a point for the tally fluctuation chart, MCNP stops transporting particles and collects the tally results.

- MCNP begins by calculating TFC points every 1000 histories. But since the TFC chart is limited to 20 points, after MCNP calculates the 20th point, the TFC chart is trimmed down to 10 points and MCNP doubles the number of histories run between the TFC point calculations.

- The initial value of 1000 histories per TFC point can be changed using the 5th entry of the **`PRDMP`** card.
  - MPI runs automatically set this value to **`NPS`**/10.
  - Except for problems with point detectors that use Russian Roulette to limit small contributions **AND** which $\mathbf{k_i}$ on the **`DD`** card is negative. This is the default for F5 tallies.

How to find the best way to run a problem? Test Runs!!

Run time (minutes) using all 40 Logical CPUs			
Parallel setup	Godiva	PWR Initial Core	7.5 M tally bins
nmpi 3, tasks 20	22.67	7.97	9.83
nmpi 5, tasks 10	14.40	5.83	5.82
nmpi 6, tasks 8	19.12	7.80	7.88
nmpi 9, tasks 5	10.70	5.82	5.75
nmpi 11, tasks 4	10.42	5.88	5.82
nmpi 21, tasks 2	10.63	6.08	6.28

Summary

- Discussed how MCNP uses threading and MPI to run problems in parallel

- Parallel timing studies for a few MCNP problems were performed. These studies showed that:
  - MCNP does not take advantage of the extra logical CPU cores provided by hyperthreading
  - Source particles are not process in parallel for criticality problems
  - Increasing the number of histories between TFC points can significantly improve performance in thread only problems

- Conduct several test runs to determine which combination of threading and MPI is the most effective for a problem.