HPC-Performance
Intel® VTune™ Profiler

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intel®

Intel® VTune Profiler -

More Complete HPC Performance Overview

MPI metrics added to HPC analysis

MPI Imbalance Metric

- Metric for performance of rank on critical path
- Computational bottlenecks and outlier rank behavior now available in VTune Profiler
- For communication pattern problems between ranks use Intel® Trace Analyzer and Collector (ITAC)

Threading: CPU Utilization

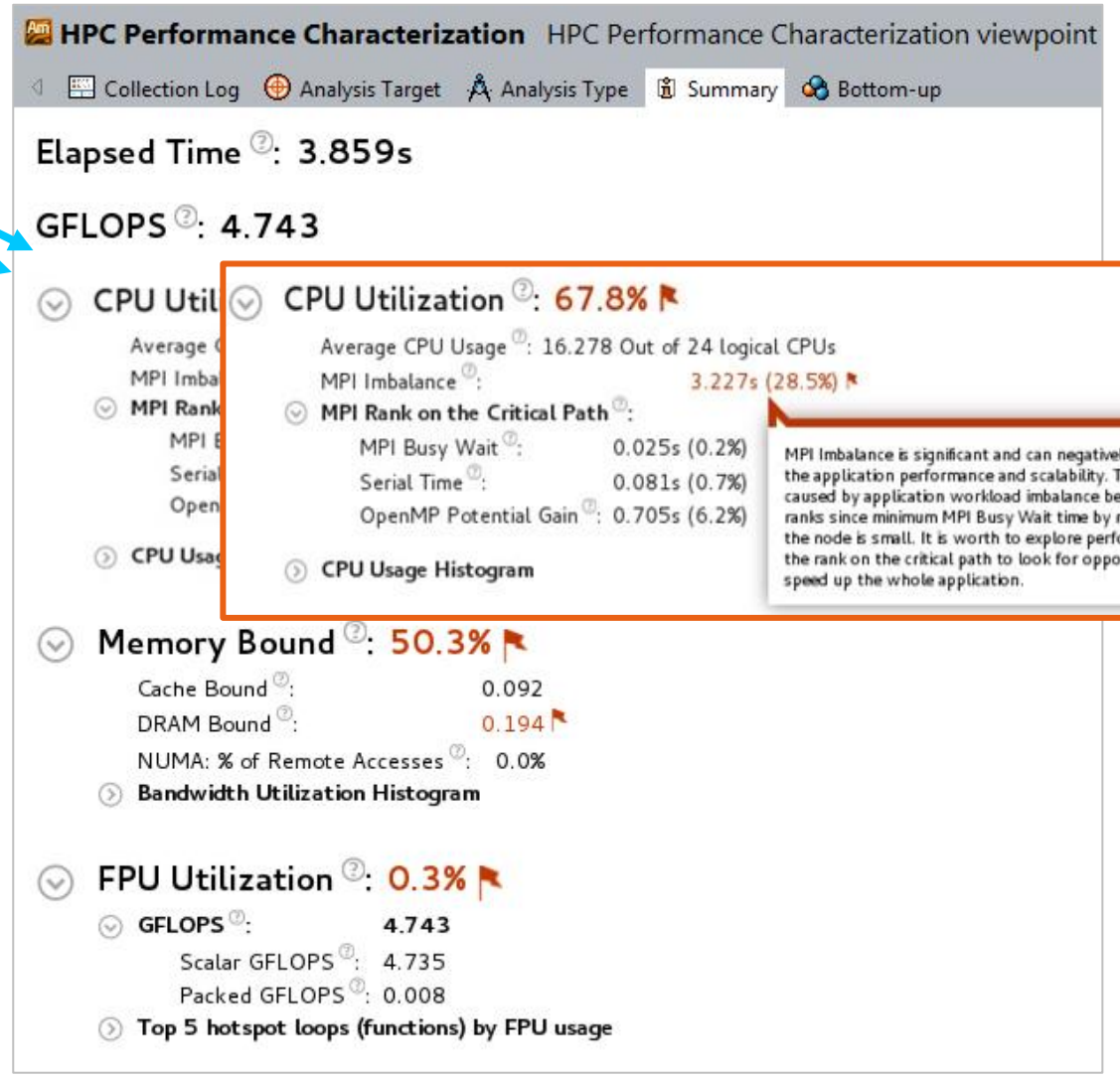
- Serial vs. Parallel time
- Top OpenMP regions by potential gain
- Tip: Use hotspot OpenMP region analysis for more detail

Memory Access Efficiency

- Stalls by memory hierarchy
- Bandwidth utilization
- Tip: Use Memory Access analysis

Vectorization: FPU Utilization

- FLOPS† estimates from sampling
- Tip: Use Intel Advisor for precise metrics and vectorization optimization



† For 3rd, 5th, 6th Generation Intel® Core™ processors and second generation Intel® Xeon Phi™ processor code named Knights Landing.

Three Keys to HPC Performance:

Threading, Memory Access, Vectorization – Intel VTune™ Profiler

Threading: CPU Utilization

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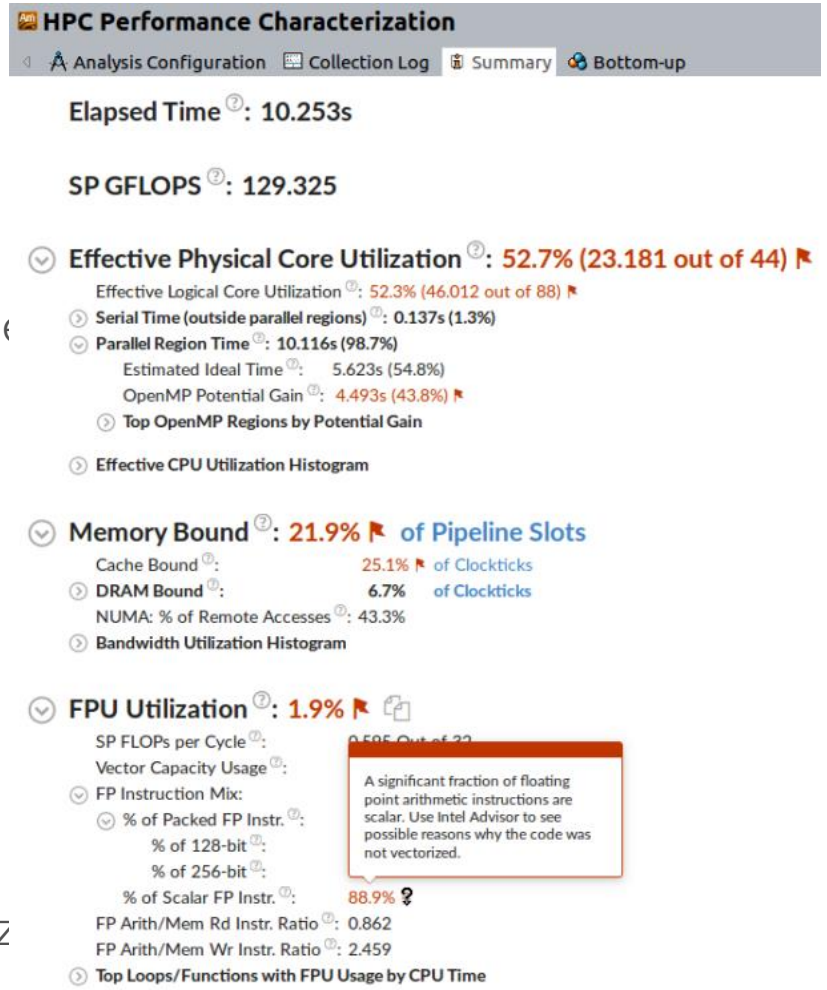
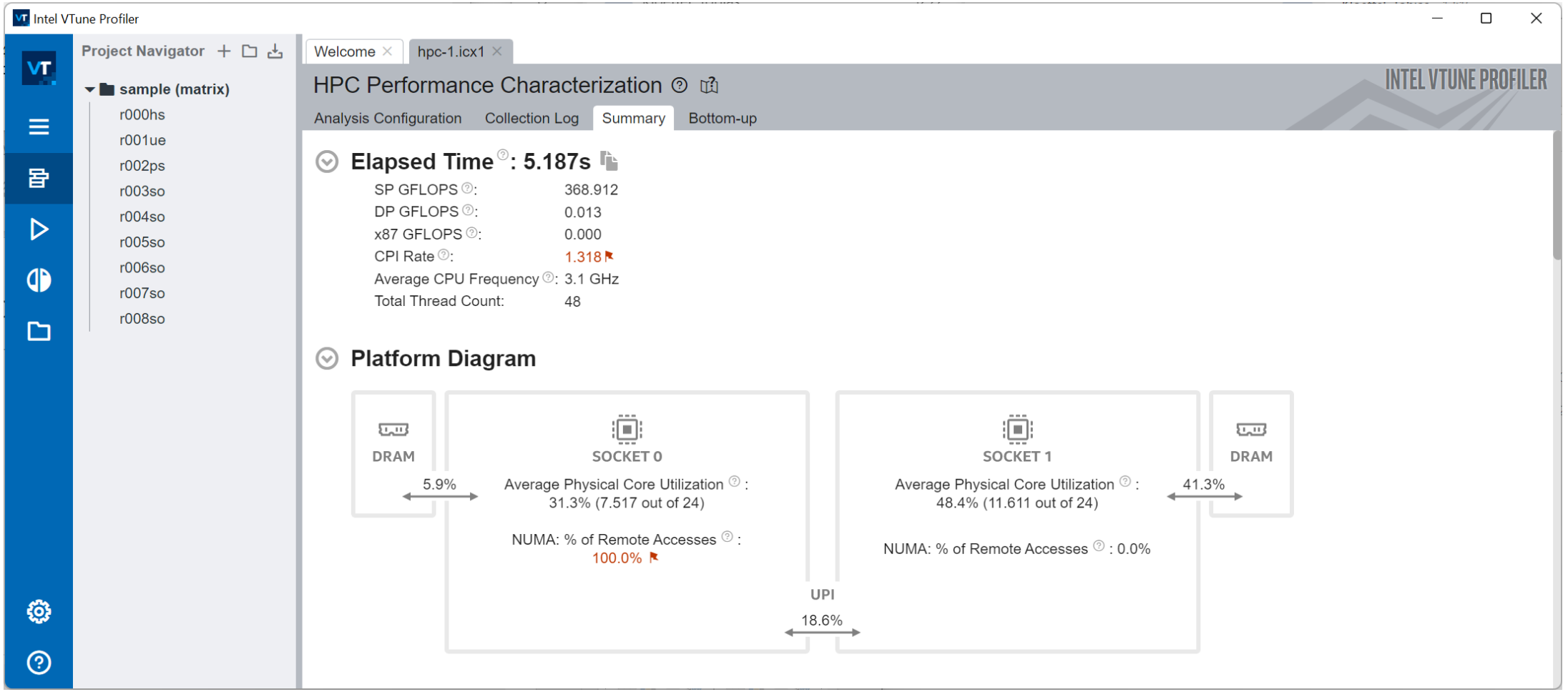
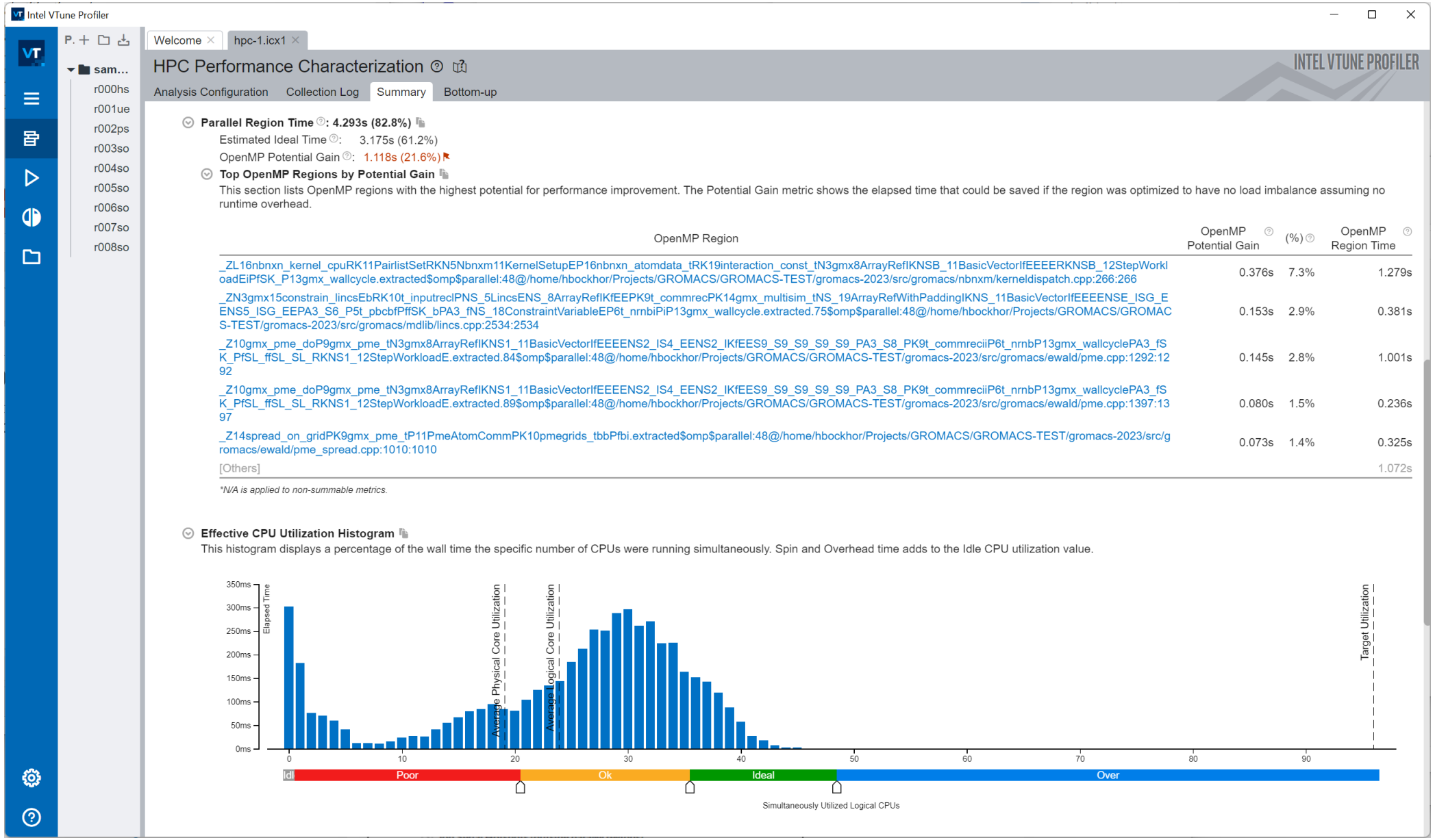
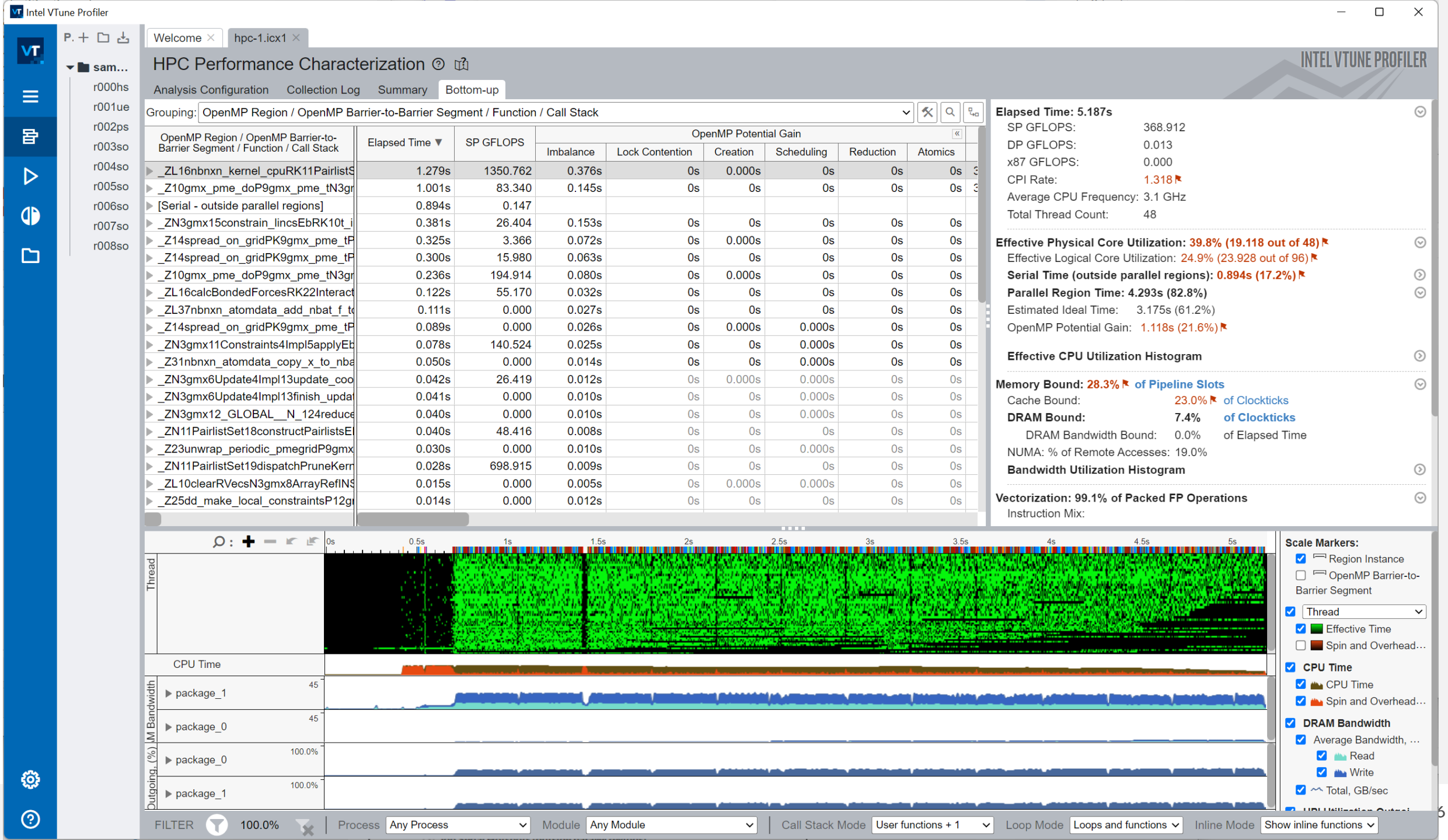


HPC-Performance




Intel VTune Profiler
Welcome
hpc-1.icx1
HPC Performance Characterization
INTEL VTUNE PROFILER
Analysis Configuration
Collection Log
Summary
Bottom-up
Parallel Region Time: 4.293s (82.8%)
Estimated Ideal Time: 3.175s (61.2%)
OpenMP Potential Gain: 1.118s (21.6%)
Top OpenMP Regions by Potential Gain
This section lists OpenMP regions with the highest potential for performance improvement. The Potential Gain metric shows the elapsed time that could be saved if the region was optimized to have no load imbalance assuming no runtime overhead.
OpenMP Region
OpenMP Potential Gain
(%)
OpenMP Region Time
_ZL16nbnxn_kernel_cpuRK11PairlistSetRKN5Nbnxm11KernelSetupEP16nbnxn_atomdata_tRK19interaction_const_tN3gmx8ArrayRefIKNSB_11BasicVectorIfEEEERKNSB_12StepWorkloadEiPfSK_P13gmx_wallcycle.extractedompparallel:48@/home/hbockhor/Projects/GROMACS/GROMACS-TEST/gromacs-2023/src/gromacs/nbnxm/kerneldispatch.cpp:266
0.376s 7.3% 1.279s
_ZN3gmx15constrain_lincsEbRK10t_inputreclPNS_5LincsENS_8ArrayRefIKfEEPK9t_commrecPK14gmx_multisim_tNS_19ArrayRefWithPaddingIKNS_11BasicVectorIfEEEENSE_ISG_EENS5_ISG_EEPA3_S6_P5t_pbcbfPffSK_bPA3_fNS_18ConstraintVariableEP6t_nrnbiPiP13gmx_wallcycle.extracted.75ompparallel:48@/home/hbockhor/Projects/GROMACS/GROMACS-TEST/gromacs-2023/src/gromacs/mdlib/lincs.cpp:2534:2534
0.153s 2.9% 0.381s
_Z10gmx_pme_doP9gmx_pme_tN3gmx8ArrayRefIKNS1_11BasicVectorIfEEEENS2_IS4_EENS2_IKfEES9_S9_S9_S9_S9_PA3_S8_PK9t_commreciiP6t_nrnbP13gmx_wallcyclePA3_fSK_PfSL_ffSL_SL_RKNS1_12StepWorkloadE.extracted.84ompparallel:48@/home/hbockhor/Projects/GROMACS/GROMACS-TEST/gromacs-2023/src/gromacs/ewald/pme.cpp:1292:1292
0.145s 2.8% 1.001s
_Z10gmx_pme_doP9gmx_pme_tN3gmx8ArrayRefIKNS1_11BasicVectorIfEEEENS2_IS4_EENS2_IKfEES9_S9_S9_S9_S9_PA3_S8_PK9t_commreciiP6t_nrnbP13gmx_wallcyclePA3_fSK_PfSL_ffSL_SL_RKNS1_12StepWorkloadE.extracted.89ompparallel:48@/home/hbockhor/Projects/GROMACS/GROMACS-TEST/gromacs-2023/src/gromacs/ewald/pme.cpp:1397:1397
0.080s 1.5% 0.236s
_Z14spread_on_gridPK9gmx_pme_tP11PmeAtomCommPK10pmegrids_tbbPfbi.extractedompparallel:48@/home/hbockhor/Projects/GROMACS/GROMACS-TEST/gromacs-2023/src/gromacs/ewald/pme_spread.cpp:1010:1010
0.073s 1.4% 0.325s
[Others]
1.072s
*N/A is applied to non-summable metrics.
Effective CPU Utilization Histogram
This histogram displays a percentage of the wall time the specific number of CPUs were running simultaneously. Spin and Overhead time adds to the Idle CPU utilization value.
Elapsed Time
Average Physical Core Utilization
Average Logical Core Utilization
Target Utilization
Idle
Poor
Ok
Ideal
Over
Simultaneously Utilized Logical CPUs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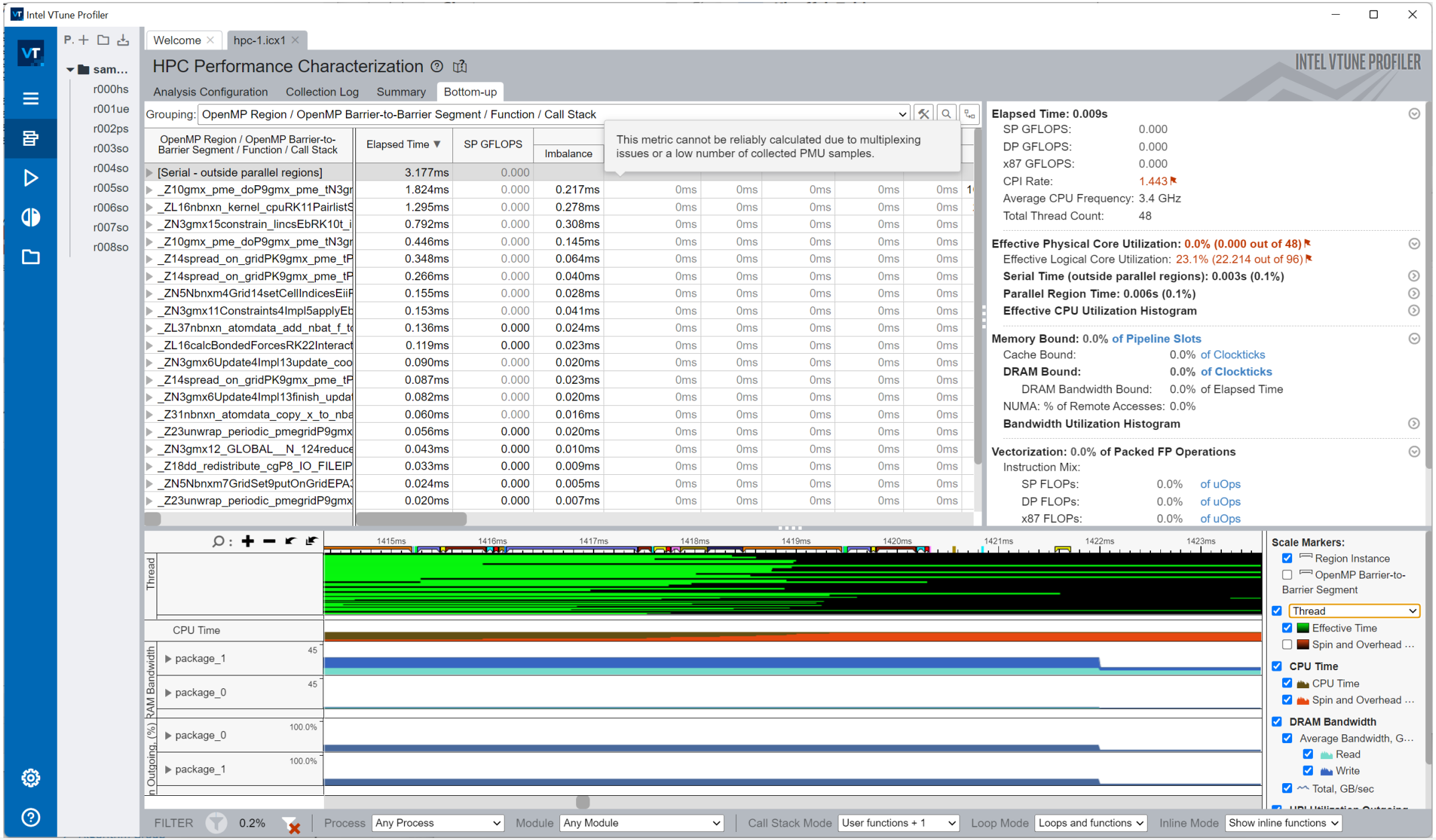
OpenMP Region / OpenMP Barrier-to-Barrier Segment / Function / Call Stack
Elapsed Time
SP GFLOPS
OpenMP Potential Gain
Imbalance
Lock Contention
Creation
Scheduling
Reduction
Atomics
_ZL16nbnxn_kernel_cpuRK11PairlistS 1.279s 1350.762 0.376s 0s 0.000s 0s 0s 0s
_Z10gmx_pme_doP9gmx_pme_tN3gr 1.001s 83.340 0.145s 0s 0s 0s 0s 0s
[Serial - outside parallel regions] 0.894s 0.147
_ZN3gmx15constrain_lincsEbRK10t_i 0.381s 26.404 0.153s 0s 0s 0s 0s 0s
_Z14spread_on_gridPK9gmx_pme_tP 0.325s 3.366 0.072s 0s 0.000s 0s 0s 0s
_Z14spread_on_gridPK9gmx_pme_tP 0.300s 15.980 0.063s 0s 0s 0s 0s 0s
_Z10gmx_pme_doP9gmx_pme_tN3gr 0.236s 194.914 0.080s 0s 0.000s 0s 0s 0s
_ZL16calcBondedForcesRK22Interact 0.122s 55.170 0.032s 0s 0s 0s 0s 0s
_ZL37nbnxn_atomdata_add_nbat_f_t 0.111s 0.000 0.027s 0s 0s 0s 0s 0s
_Z14spread_on_gridPK9gmx_pme_tP 0.089s 0.000 0.026s 0s 0.000s 0.000s 0s 0s
_ZN3gmx11Constraints4Impl5applyEb 0.078s 140.524 0.025s 0s 0s 0.000s 0s 0s
_Z31nbnxn_atomdata_copy_x_to_nba 0.050s 0.000 0.014s 0s 0s 0.000s 0s 0s
_ZN3gmx6Update4Impl13update_coo 0.042s 26.419 0.012s 0s 0.000s 0.000s 0s 0s
_ZN3gmx6Update4Impl13finish_updat 0.041s 0.000 0.010s 0s 0s 0.000s 0s 0s
_ZN3gmx12_GLOBAL__N_124reduce 0.040s 0.000 0.010s 0s 0s 0.000s 0s 0s
_ZN11PairlistSet18constructPairlistsEl 0.040s 48.416 0.008s 0s 0s 0s 0s 0s
_Z23unwrap_periodic_pmegridP9gmx 0.030s 0.000 0.010s 0s 0s 0.000s 0s 0s
_ZN11PairlistSet19dispatchPruneKern 0.028s 698.915 0.009s 0s 0s 0s 0s 0s
_ZL10clearRVecsN3gmx8ArrayRefIN 0.015s 0.000 0.005s 0s 0.000s 0.000s 0s 0s
_Z25dd_make_local_constraintsP12gr 0.014s 0.000 0.012s 0s 0s 0s 0s 0s
Elapsed Time: 5.187s
SP GFLOPS: 368.912
DP GFLOPS: 0.013
x87 GFLOPS: 0.000
CPI Rate: 1.318
Average CPU Frequency: 3.1 GHz
Total Thread Count: 48
Effective Physical Core Utilization: 39.8% (19.118 out of 48)
Effective Logical Core Utilization: 24.9% (23.928 out of 96)
Serial Time (outside parallel regions): 0.894s (17.2%)
Parallel Region Time: 4.293s (82.8%)
Estimated Ideal Time: 3.175s (61.2%)
OpenMP Potential Gain: 1.118s (21.6%)
Effective CPU Utilization Histogram
Memory Bound: 28.3% of Pipeline Slots
Cache Bound: 23.0% of Clockticks
DRAM Bound: 7.4% of Clockticks
DRAM Bandwidth Bound: 0.0% of Elapsed Time
NUMA: % of Remote Accesses: 19.0%
Bandwidth Utilization Histogram
Vectorization: 99.1% of Packed FP Operations
Instruction Mix:
0s 0.5s 1s 1.5s 2s 2.5s 3s 3.5s 4s 4.5s 5s
Thread
CPU Time
DRAM Bandwidth
package_1
package_0
Outgoing... (%)
100.0%
Scale Markers:
Region Instance
OpenMP Barrier-to-Barrier Segment
Thread
Effective Time
Spin and Overhead...
CPU Time
CPU Time
Spin and Overhead...
DRAM Bandwidth
Average Bandwidth, ...
Read
Write
Total, GB/sec
FILTER 100.0%
Process Any Process
Module Any Module
Call Stack Mode User functions + 1
Loop Mode Loops and functions
Inline Mode Show inline functions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OpenMP Region / OpenMP Barrier-to-Barrier Segment / Function / Call Stack
Elapsed Time
SP GFLOPS
Imbalance
This metric cannot be reliably calculated due to multiplexing issues or a low number of collected PMU samples.
[Serial - outside parallel regions] 3.177ms 0.000
_Z10gmx_pme_doP9gmx_pme_tN3gr 1.824ms 0.000 0.217ms
_ZL16nbnxn_kernel_cpuRK11PairlistS 1.295ms 0.000 0.278ms
_ZN3gmx15constrain_lincsEbRK10t_i 0.792ms 0.000 0.308ms
_Z10gmx_pme_doP9gmx_pme_tN3gr 0.446ms 0.000 0.145ms
_Z14spread_on_gridPK9gmx_pme_tP 0.348ms 0.000 0.064ms
_Z14spread_on_gridPK9gmx_pme_tP 0.266ms 0.000 0.040ms
_ZN5Nbnxm4Grid14setCellIndicesEiiP 0.155ms 0.000 0.028ms
_ZN3gmx11Constraints4Impl5applyEb 0.153ms 0.000 0.041ms
_ZL37nbnxn_atomdata_add_nbat_f_to 0.136ms 0.000 0.024ms
_ZL16calcBondedForcesRK22Interact 0.119ms 0.000 0.023ms
_ZN3gmx6Update4Impl13update_coo 0.090ms 0.000 0.020ms
_Z14spread_on_gridPK9gmx_pme_tP 0.087ms 0.000 0.023ms
_ZN3gmx6Update4Impl13finish_updat 0.082ms 0.000 0.020ms
_Z31nbnxn_atomdata_copy_x_to_nbs 0.060ms 0.000 0.016ms
_Z23unwrap_periodic_pmegridP9gmx 0.056ms 0.000 0.020ms
_ZN3gmx12_GLOBAL__N_124reduce 0.043ms 0.000 0.010ms
_Z18dd_redistribute_cgP8_IO_FILEIP 0.033ms 0.000 0.009ms
_ZN5Nbnxm7GridSet9putOnGridEPA3 0.024ms 0.000 0.005ms
_Z23unwrap_periodic_pmegridP9gmx 0.020ms 0.000 0.007ms
Elapsed Time: 0.009s
SP GFLOPS: 0.000
DP GFLOPS: 0.000
x87 GFLOPS: 0.000
CPI Rate: 1.443
Average CPU Frequency: 3.4 GHz
Total Thread Count: 48
Effective Physical Core Utilization: 0.0% (0.000 out of 48)
Effective Logical Core Utilization: 23.1% (22.214 out of 96)
Serial Time (outside parallel regions): 0.003s (0.1%)
Parallel Region Time: 0.006s (0.1%)
Effective CPU Utilization Histogram
Memory Bound: 0.0% of Pipeline Slots
Cache Bound: 0.0% of Clockticks
DRAM Bound: 0.0% of Clockticks
DRAM Bandwidth Bound: 0.0% of Elapsed Time
NUMA: % of Remote Accesses: 0.0%
Bandwidth Utilization Histogram
Vectorization: 0.0% of Packed FP Operations
Instruction Mix:
SP FLOPs: 0.0% of uOps
DP FLOPs: 0.0% of uOps
x87 FLOPs: 0.0% of uOps
1415ms 1416ms 1417ms 1418ms 1419ms 1420ms 1421ms 1422ms 1423ms
Thread
CPU Time
DRAM Bandwidth
package_1
package_0
Outgoing (%)
100.0%
Scale Markers:
Region Instance
OpenMP Barrier-to-Barrier Segment
Thread
Effective Time
Spin and Overhead ...
CPU Time
CPU Time
Spin and Overhead ...
DRAM Bandwidth
Average Bandwidth, G...
Read
Write
Total, GB/sec
FILTER 0.2%
Process Any Process
Module Any Module
Call Stack Mode User functions + 1
Loop Mode Loops and functions
Inline Mode Show inline functions

Get The Data You Need

Tune OpenMP for Efficiency and Scalability

- Typical Questions:

Q: *"I put in pragmas, but why is my speed up far from linear?"*

A: Parallelization inefficiency

Q: *"I ran my app on a system with more cores but why does it run less efficiently than on the system with fewer cores?"*

A: Scalability issues

- Data Needed:

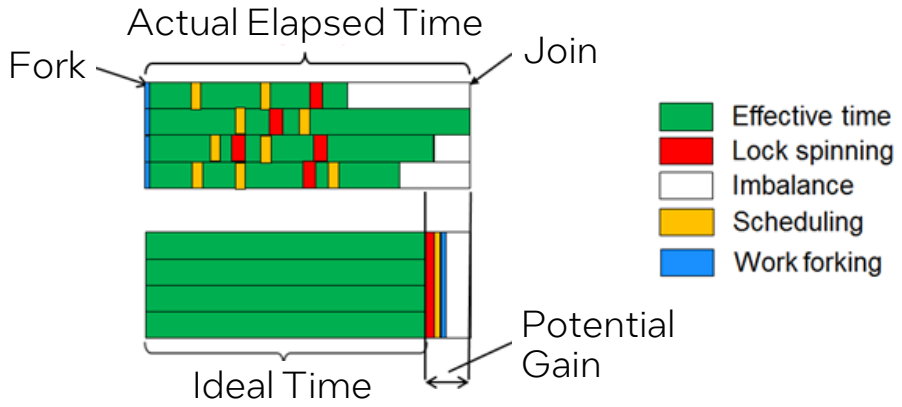
1) Is the serial time of my application significant enough to prevent scaling?
2) How much gain can be achieved by tuning OpenMP?
3) Which OpenMP regions / loops / barriers will benefit most from tuning?
4) What are the inefficiencies with each region?

Tune OpenMP for Efficiency and Scalability

See the wall clock impact of inefficiencies, identify their cause

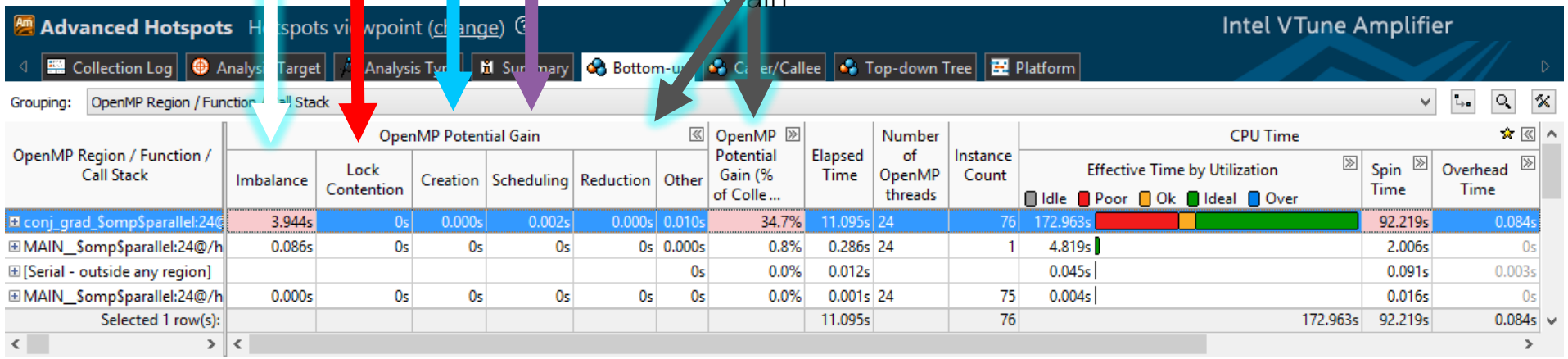
Focus On What's Important

- What region is inefficient?
- Is the potential gain worth it?
- Why is it inefficient?
  Imbalance? Scheduling? Lock spinning?
- Intel® Xeon Phi systems supported



RK: Remove Xeon Phi

Imbalance Lock Fork Scheduling Potential Gain



What is Hindering Parallel Performance?

VTune™ Profiler Identifies Parallel Region Inefficiencies

Advanced Hotspots Hotspots viewpoint (change)

Collection Log | Analysis Target | Analysis Type | Summary | Bottom-up | Caller/Callee | Top-down Tree | Tasks and Frames

Grouping: OpenMP Region / Function / Call Stack

OpenMP Region / Function / Call Stack	OpenMP Potential Gain						OpenMP Potential Gain (% of Collection Time)					
	Imbalance	Lock Con...	Crea...	Sch...	Red...	Other	Imbalance (%)	Lock Con...	Crea... (%)	Sch... (%)	Red... (%)	Other (%)
conj_grad_ompparallel:24@/home/vtune/work/apps/NPB/NPB3.3.1/NPB3.3-OMP/CG/cg.f:514:695	3.944s	0s	0.000s	0.002s	0.000s	0.010s	34.6%	0.0%	0.0%	0.0%	0.0%	0.1%
MAIN__ompparallel:24@/home/vtune/work/apps/NPB/NPB3.3.1/NPB3.3-OMP/CG/cg.f:185:231	0.086s	0s	0s	0s	0s	0.000s	0.8%	0.0%	0.0%	0.0%	0.0%	0.0%
[Serial - outside any region]						0s						0.0%
MAIN__ompparallel:24@/home/vtune/work/apps/NPB/NPB3.3.1/NPB3.3-OMP/CG/cg.f:339:345	0.000s	0s	0s	0s	0s	0s	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
MAIN__ompparallel:24@/home/vtune/work/apps/NPB/NPB3.3.1/NPB3.3-OMP/CG/cg.f:361:365	0.000s	0s	0s	0s	0s	0s	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
MAIN__ompparallel:24@/home/vtune/work/apps/NPB/NPB3.3.1/NPB3.3-OMP/CG/cg.f:263:269	0.000s	0s	0s	0s	0s	0s	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%

Imbalance

Advanced Hotspots Hotspots viewpoint (change)

Collection Log | Analysis Target | Analysis Type | Summary | Bottom-up | Caller/Callee | Top-down Tree | Tasks and Frames

Grouping: OpenMP Region / Function / Call Stack

OpenMP Region / Function / Call Stack	OpenMP Potential Gain						OpenMP Potential Gain (% of Collection Time)					
	Imbalance	Lock Con...	Creation	Scheduling	Reduc...	Other	Imbalance (%)	Lock Con...	Crea... (%)	Scheduling (%)	Red... (%)	Other (%)
conj_grad_ompparallel:24@/home/vtune/work/apps/NPB/NPB3.3.1/NPB3.3-OMP/CG/cg.f:514:695	0.206s	0s	0.000s	3.128s	0.001s	0.002s	1.7%	0.0%	0.0%	25.9%	0.0%	0.0%
MAIN__ompparallel:24@/home/vtune/work/apps/NPB/NPB3.3.1/NPB3.3-OMP/CG/cg.f:185:231	0.075s	0.000s	0s	0s	0s	0.000s	0.6%	0.0%	0.0%	0.0%	0.0%	0.0%
[Serial - outside any region]						0s						0.0%
MAIN__ompparallel:24@/home/vtune/work/apps/NPB/NPB3.3.1/NPB3.3-OMP/CG/cg.f:339:345	0.000s	0s	0s	0s	0s	0.000s	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%

Likely culprit:

Dynamic scheduling overhead

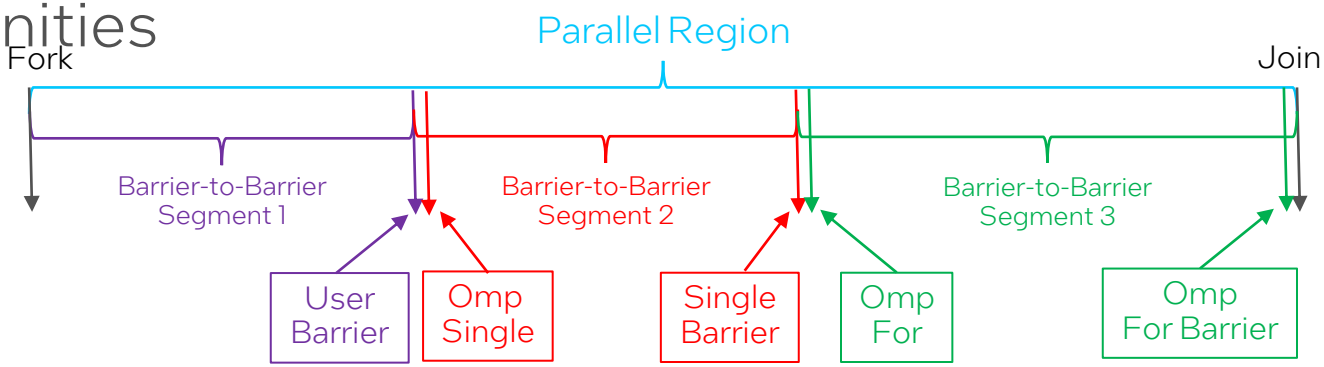
Tune OpenMP for Efficiency and Scalability

See inside each parallel region – Understand the cause of inefficiency

Detailed Barrier to Barrier Analysis

- Tune each segment separately
- Easier to see tuning opportunities

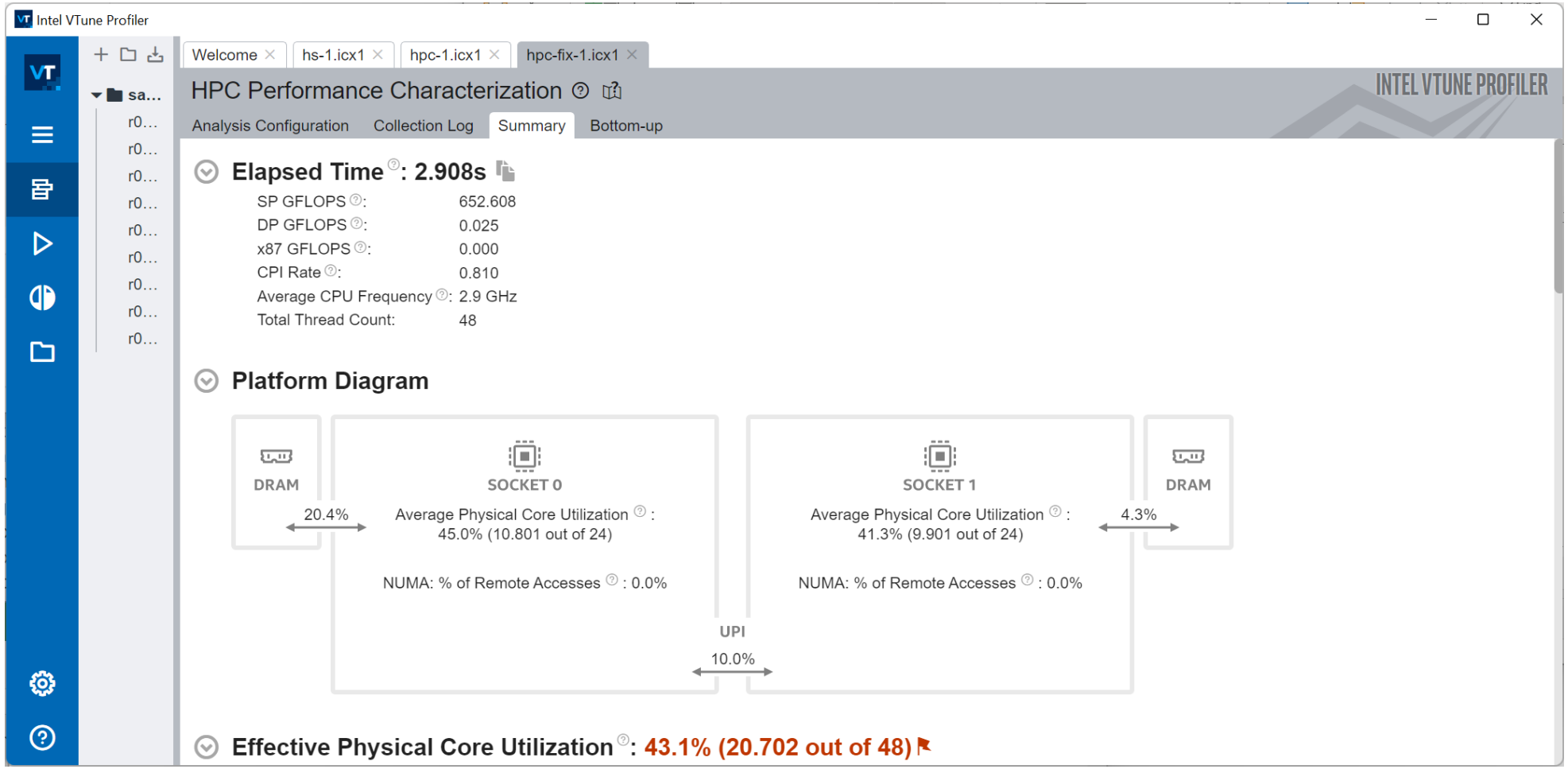
```
#pragma omp parallel
{
  …
#pragma omp barrier
#pragma omp single
    {
      …
    }
#pragma omp for
    {
```



Grouping: OpenMP Region / OpenMP Barrier-to-Barrier Segment / Function / Call Stack

OpenMP Region / OpenMP Barrier-to-Barrier Segment / Function / Call Stack	OpenMP Potential Gain						OpenMP Potential Gain (% of Collection ...
	Imbalance	Lock Contention	Creation	Scheduling	Reduction	Other	
3.3-OMP/CG/cg.f:514:695	3.944s	0s	0.000s	0.002s	0.000s	0.010s	34.7%
NPB3.3.1/NPB3.3-OMP/CG/cg.f:580	3.725s	0s	0s	0.000s	0s	0.008s	32.8%
NPB3.3.1/NPB3.3-OMP/CG/cg.f:683	0.149s	0s	0s	0s	0s	0.000s	1.3%
NPB3.3.1/NPB3.3-OMP/CG/cg.f:664	0.014s	0s	0s	0.000s	0s	0.000s	0.1%

Using KMP_AFFINITY=compact,1



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