FRIEDRICH-ALEXANDER
UNIVERSITÄT
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COMPRESSIBLE LATTICE BOLTZMANN SOLVER CPU BENCHMARK

MuCoSim WS 2023/24

PHASE: 2

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Introduction: Summary

- Lattice Boltzmann Method(LBM) commonly adopt a structured grid in practice.

"Represented by a regular grid; points on grid are conceptually updated together. It has high spatial locality"'[1]

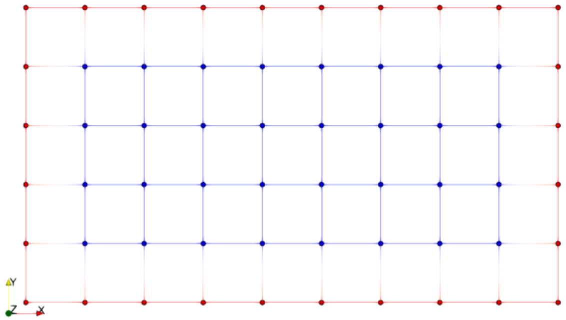


Figure 1: Exemplary structured grid

- Naturally adapted to parallel processes computing. [3].
- The "Collide and Stream" algorithms.

$$\boldsymbol{f}_i^*(\boldsymbol{x},\boldsymbol{t}) = \boldsymbol{f}_i(\boldsymbol{x},\boldsymbol{t}) + \Omega_i(\boldsymbol{x},\boldsymbol{t}) \qquad \boldsymbol{f}_i(\boldsymbol{x}+\boldsymbol{c}_i\Delta \boldsymbol{t},\boldsymbol{t}+\Delta \boldsymbol{t}) = \boldsymbol{f}_i^*(\boldsymbol{x},\boldsymbol{t})$$

- Compressible LBM → $\boldsymbol{f_i^{eq}}$ using discreate entropy function by formulating a minimization problem.

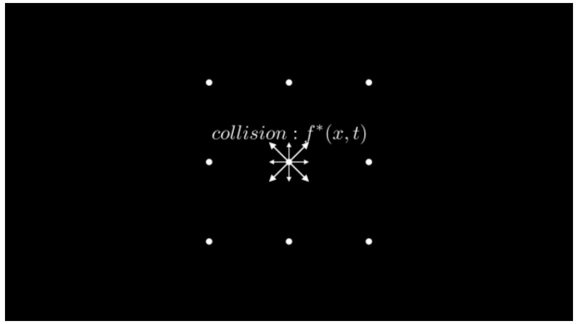


Figure 02: Collide and Stream

- 2 pdfs' to integrate energy equation apart from the mass, and momentum equations.
- The present solver based on Entropic Lattice Boltzmann Method (ELBM)

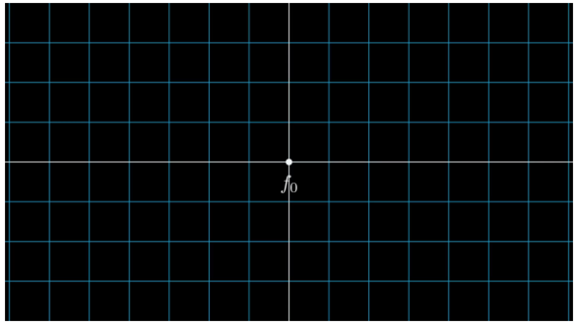


Figure 03: f and g populations in a lattice node

git@gitlab.cs.fau.de:yh54ojyn/mucosim.git

Test system & CLBM solver

Algorithm

- Solver is based on C++ with OpenMP and build using Cmake 3.23.1.
- Input parameter file defines the simulation properties.
- For benchmarking, a 2D shock tube simulation is considered.
- Stencil configuration : D2Q9 (D2Q9 X 2 in one LB node);
- Domain size : 3000 x 3000 lattice nodes

Tools

- LIKWID version : 5.3.0
- LIKWID flags : likwid-perfctr -g MEM/ENERGY/MEM_DP
  : likwid-topology

Compiler

- GNU g++
- compiler flags : -O3 –march=native –mavx –ftree-vectorize

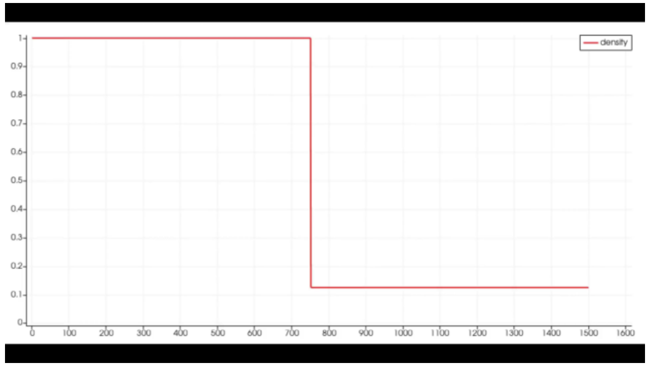


Figure 05: Results for density variation of air inside a 2D shock tube using CLBM solver

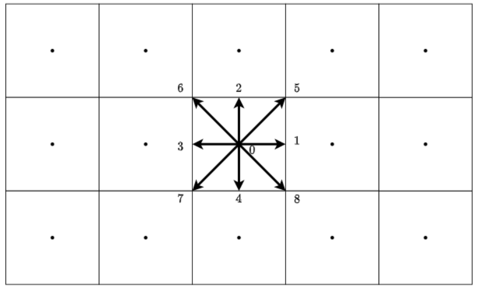


Figure 04:Lattice with D2Q9 stencil

Test system

Name	Fritz
Processor	Intel Xeon Platinum 8360Y
Micro architecture	Icelake
Frequency [GHz]	2.4
Cores	72
Sockets	2 (No SMT)
NUMA domains	4
Main memory [GB]	256
Thermal design power [W]	250

Issues: Phase01

- According to single core performance, domain size of 500x500 fits to L3 cache.
- Bad scaling behaviour after the second socket.
- Total memory bandwidth and performance has a saturating trend in 1st NUMA domain.
- expf4; calculation of exponential function using math.h library is critical inside the newtonRaphson kernel.

Grouping: Function / Call Stack

Function / Call Stack	CPU Time	Module	Function (I
expf64	1687.306s	libm.so.6	expf64
↖ j23 ← newtonRaphson._omp_fn.17	261.509s	CLBM	j23(node&)
↖ j13 ← newtonRaphson._omp_fn.17	255.705s	CLBM	j13(node&)
↖ j33 ← newtonRaphson._omp_fn.17	131.396s	CLBM	j33(node&)
↖ func2 ← newtonRaphson._omp_fn.17	128.771s	CLBM	func2(node&, double)
↖ j22 ← newtonRaphson._omp_fn.17	128.538s	CLBM	j22(node&)
↖ j21 ← newtonRaphson._omp_fn.17	127.912s	CLBM	j21(node&)
↖ j11 ← newtonRaphson._omp_fn.17	127.344s	CLBM	j11(node&)
↖ func3 ← newtonRaphson._omp_fn.17	126.925s	CLBM	func3(node const&, double)
↖ j12 ← newtonRaphson._omp_fn.17	126.888s	CLBM	j12(node&)
↖ func1 ← newtonRaphson._omp_fn.17	121.991s	CLBM	func1(node&, double)
calcGeq._omp_fn.5	95.709s	CLBM	calcGeq._omp_fn.5
[No call stack information]	54.618s		
stream._omp_fn.15	679.169s	CLBM	stream._omp_fn.15
collision._omp_fn.9	610.130s	CLBM	collision._omp_fn.9
calcQuasiEqG._omp_fn.8	505.590s	CLBM	calcQuasiEqG._omp_fn.8
resetDDFshitS._omp_fn.11	475.925s	CLBM	resetDDFshitS._omp_fn.11
pTensor._omp_fn.6	425.356s	CLBM	pTensor._omp_fn.6
swap._omp_fn.16	422.428s	CLBM	swap._omp_fn.16
pEqTensor._omp_fn.7	410.548s	CLBM	pEqTensor._omp_fn.7
calcGeq._omp_fn.5	323.667s	CLBM	calcGeq._omp_fn.5
calcFeq._omp_fn.4	256.802s	CLBM	calcFeq._omp_fn.4
func@0x770e4	248.515s	libm.so.6	func@0x770e4
func@0x1dfd4	227.869s	libgomp.so.1	func@0x1dfd4
setWeights._omp_fn.3	214.170s	CLBM	setWeights._omp_fn.3

Figure 6: Vtune hotspot results..

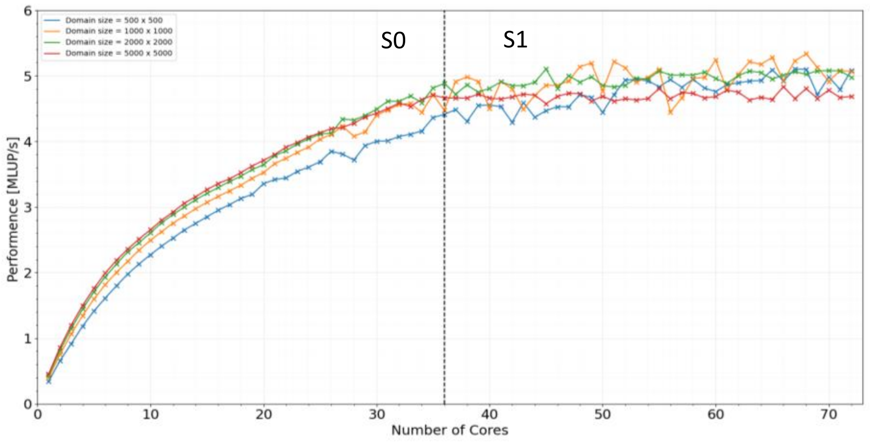


Figure 6: Performance saturation in one node. (phase:01)

BAD IMPLEMENTATION?
NEED CODE OPTIMIZATIONS?
OpenMP scheduling?

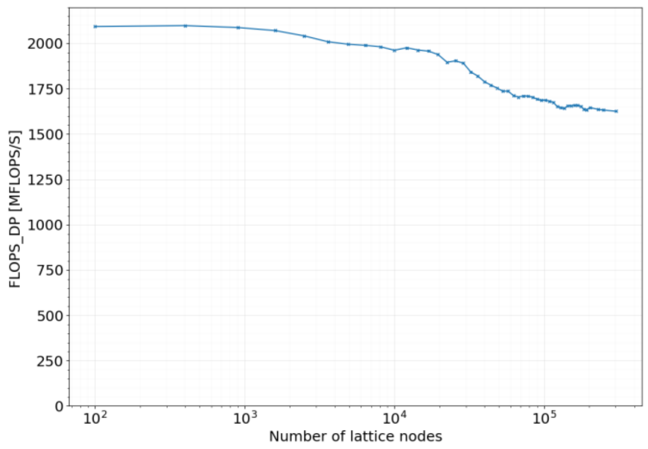


Figure 7: single core performance for fixed 2.4GHz.

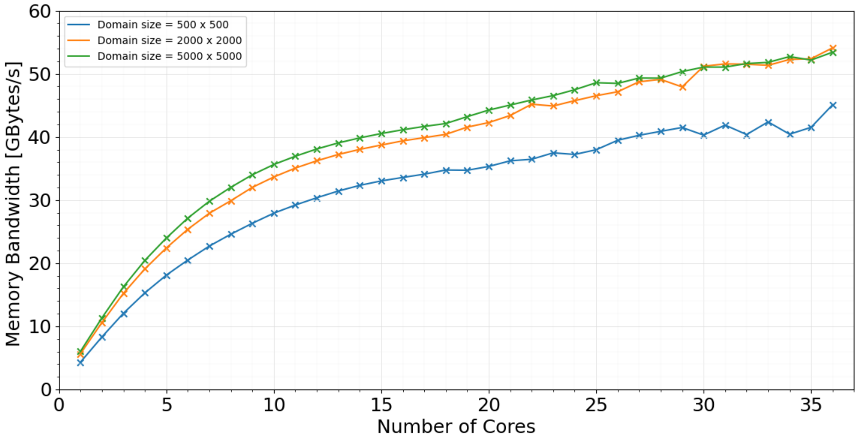


Figure 8: Memory bandwidth saturation in one node. (phase:01)

Issues: Phase01

- According to the initial profiling results; investigated possible issues in newtonRaphson kernel.

- Repeated calls for expf4 unnecessarily.
  - ✓ Since it's the hotpost, investigated the possible code optimizations.
  - ✓ Therefore, modified the newtonRapson subroutines.

- Further, experimented OpenMP scheduling chunk size.
  - ✓ High OpenMP overhead for small domain sizes.
  - ✓ Tried performance vs chunk size investigations
  - ✓ Use the static sheduling.
  - ✓ Found out that peformance is better in default settings compared to settings with chunk size.

- Ready for phase to tests.

Strong scaling.

- Better strong scaling results compared to phase 01
- Performance saturation in 1st NUMA domain.
- Maximum performance of ~26 MLUP/S with using full node.

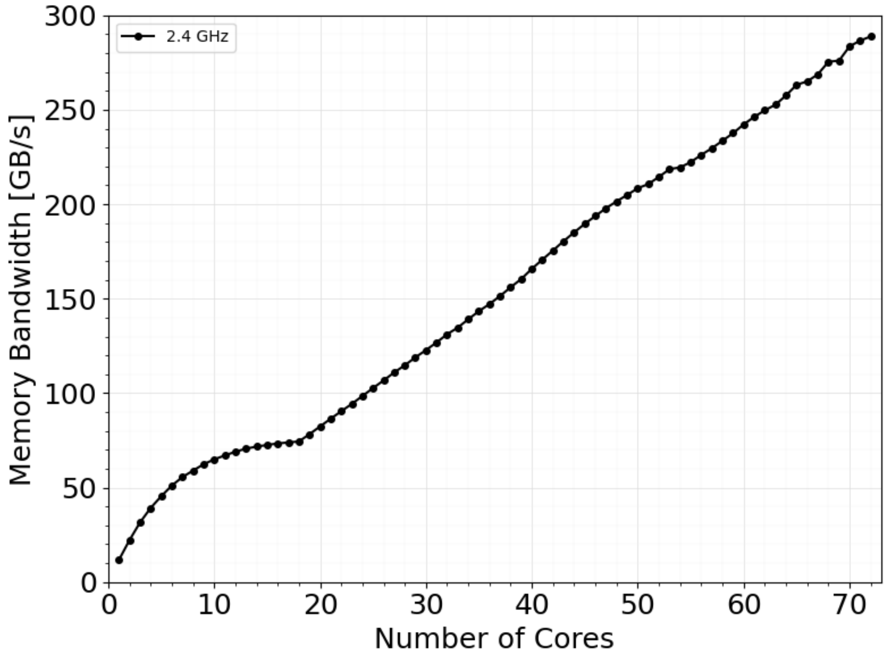


Figure 9: Performance measurements in one node at 2.4 GHz

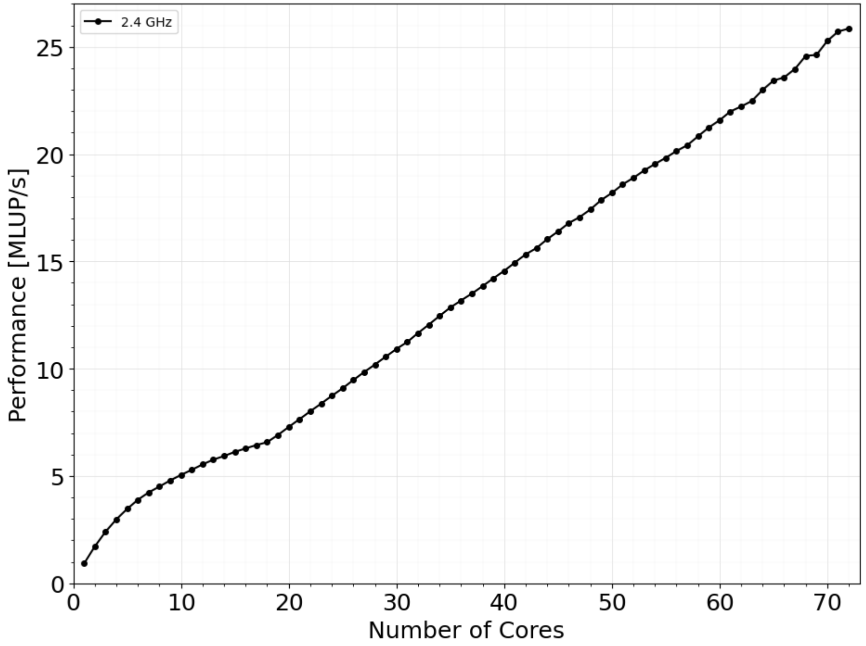


Figure 10: Memory bandwidth measurements in one node at 2.4 GHz

- Memory Bandwidth also saturates in 1st NUMA domain. (74.5 GB/s).
- Single core performance is ~3x compared to phase 01.

Profiling

Elapsed Time: 114.938s

- CPU Time: 7763.840s
- Total Thread Count: 72
- Paused Time: 0s

Top Hotspots

This section lists the most active functions in your application. Optimizing these hotspot functions typically results in improving overall application performance.

Function	Module	CPU Time	% of CPU Time
stream._omp_fn.18	CLBM	769.654s	9.9%
collision._omp_fn.12	CLBM	685.792s	8.8%
resetDDFshitS._omp_fn.14	CLBM	631.249s	8.1%
swap._omp_fn.23	CLBM	591.541s	7.6%
calcQuasiEqG._omp_fn.10	CLBM	576.830s	7.4%
[Others]	N/A*	4508.774s	58.1%

*N/A is applied to non-summable metrics.

Figure 11: Vtune Hotspot results.

- Focused kernels considering energy measurements
  - ✓ Stream
  - ✓ Collision
  - ✓ calcQuasiEqG
  - ✓ newtonRaphson

Welcome × | hotspots_sudesh_72.f0454.nhr.fau.de ×

Hotspots

Analysis Configuration | Collection Log | Summary | Bottom-up | Caller/Callee | Top-down Tree | Flame Graph | Platform

Grouping: Function / Call Stack

Function / Call Stack	CPU Time ▼	Module	Function (Full)	Source File	Start Address
stream._omp_fn.18	769.654s	CLBM	stream._omp_fn.18		0x404ce0
collision._omp_fn.12	685.792s	CLBM	collision._omp_fn.12		0x4042d0
resetDDFshitS._omp_fn.14	631.249s	CLBM	resetDDFshitS._omp_fn.14		0x404570
swap._omp_fn.23	591.541s	CLBM	swap._omp_fn.23		0x406e60
calcQuasiEqG._omp_fn.10	576.830s	CLBM	calcQuasiEqG._omp_fn.10		0x403e40
expf64	574.681s	libm.so.6	expf64		0xfb40
calc_parameters_from_PDF._omp_fn.5	513.967s	CLBM	calc_parameters_from_PDF._omp_fn.5		0x406fe0
pTensor._omp_fn.8	472.088s	CLBM	pTensor._omp_fn.8		0x403900
pEqTensor._omp_fn.9	459.827s	CLBM	pEqTensor._omp_fn.9		0x403ba0
func@0x1dfd4	456.211s	libgomp.so.1	func@0x1dfd4		0x1dfd4
calcFeq._omp_fn.6	312.084s	CLBM	calcFeq._omp_fn.6		0x403380
calcGeq._omp_fn.7	307.521s	CLBM	calcGeq._omp_fn.7		0x403520
allfuncs	305.787s	CLBM	allfuncs(node const&, double, double*)		0x409d50
newtonRaphson._omp_fn.24	297.915s	CLBM	newtonRaphson._omp_fn.24		0x409fb0
setWeights._omp_fn.4	269.078s	CLBM	setWeights._omp_fn.4		0x403280
calcRelaxationFactors._omp_fn.11	222.741s	CLBM	calcRelaxationFactors._omp_fn.11		0x4041b0
pow	171.325s	libm.so.6	pow		0xf3f0
func@0x1de24	52.950s	libgomp.so.1	func@0x1de24		0x1de24
func@0x401bb0	25.340s	CLBM	func@0x401bb0		0x401bb0
func@0x770e4	21.810s	libm.so.6	func@0x770e4		0x770e4
createFlags._omp_fn.0	8.784s	CLBM	createFlags._omp_fn.0		0x402d20
func@0x1ca74	6.797s	libgomp.so.1	func@0x1ca74		0x1ca74

Figure 12: Vtune call stack

- Now the stream and collision kernels plays a critical role as in standard LBM schemes.
- According to literature, there was a strong focus for the root finding scheme considering compressible LBM performance [4].

Energy and power measurements; main

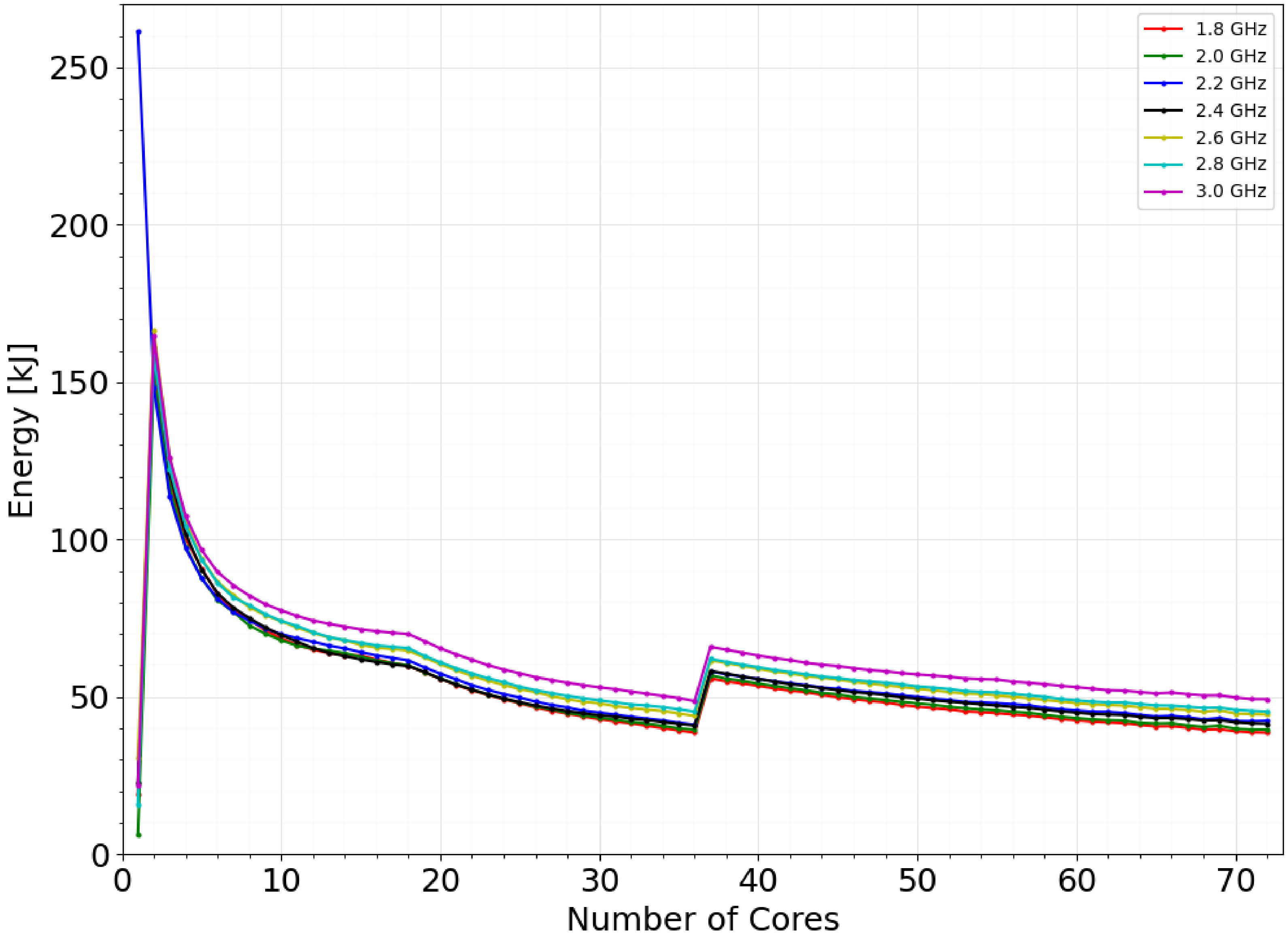


Figure 13: Energy measurements in one node

- An unusual behaviour can be observed at single core power measurement.
  - ✓ This behaviour persists for several data samples
  - ✓ However, for 2.2 GHz, the intended energy measurements can be obtained.
- The energy values have a saturating optimum point at 1st NUMA domain before it reaches a second optimum point at 1st socket.
- Sudden energy jump when moving to second socket before decrease in a quite linear fashion in second socket.
- The frequencies (GHz) 1.8, 2.0, 2.2 and 2.4 shows the lowest CPU energy measurements in first socket.

Energy and power measurements; main

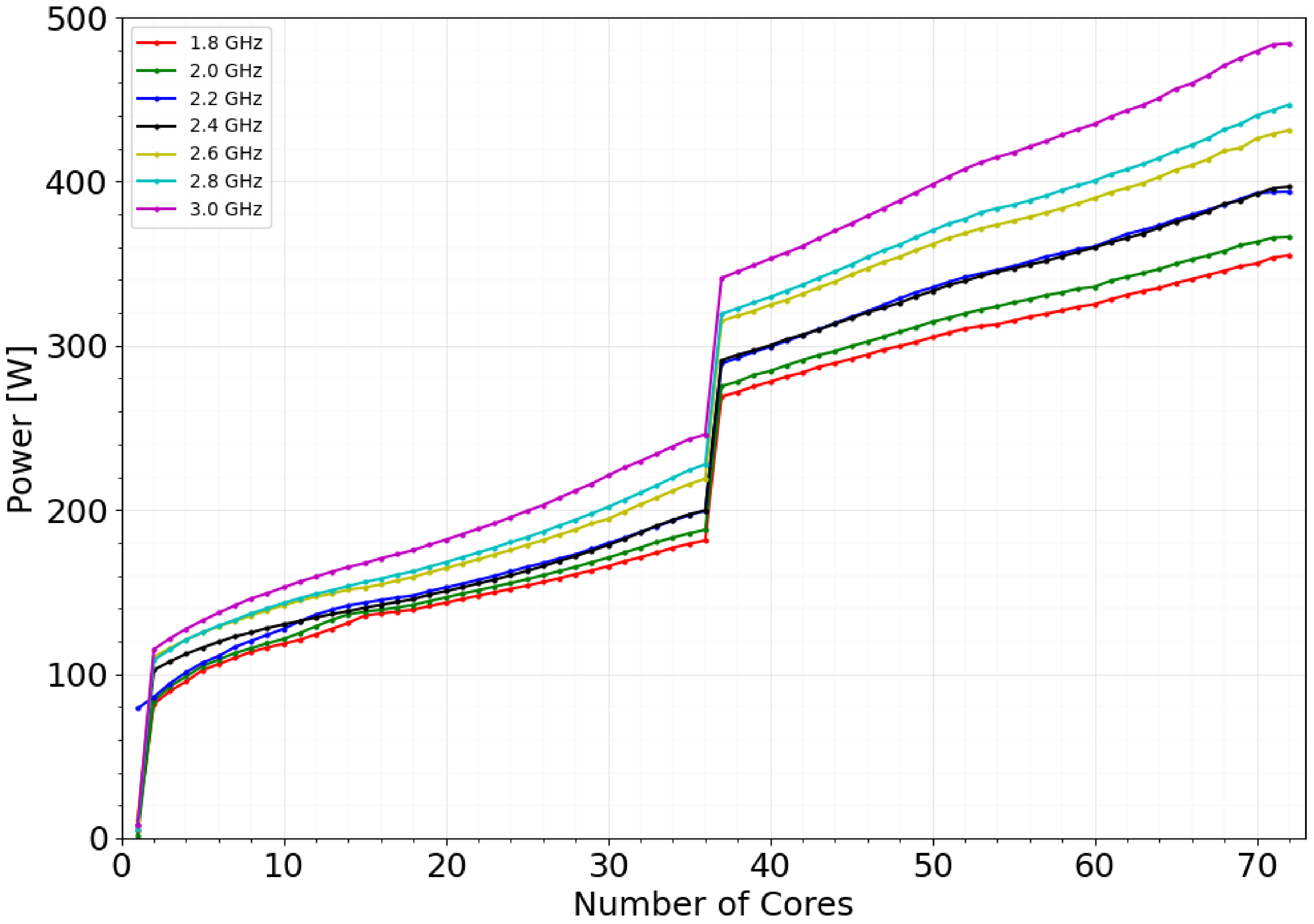


Figure 14: Power measurements in one node

- An unusual behaviour also can be observed at first core power measurment.
- LIKWID-POWERMETER also produced the same results.
- Sudden power jump when moving to second socket.

DRAM;Energy and power measurements; main

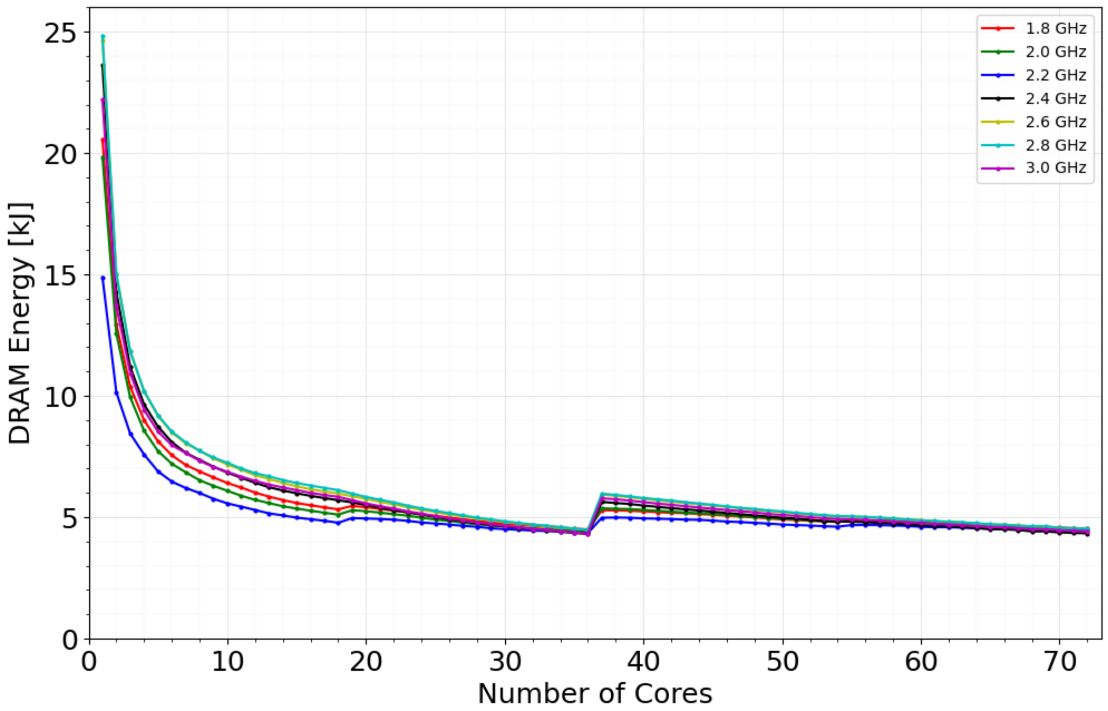


Figure 15: DRAM Energy measurements in one node

DRAM energy measurements do not show an unexpected behaviour at single core measurements all the time.

2.2 GHz seems to be the lowest energy curve for a wider domain.

The DRAM energy contribution to the total energy is in the range of 5%-11%.

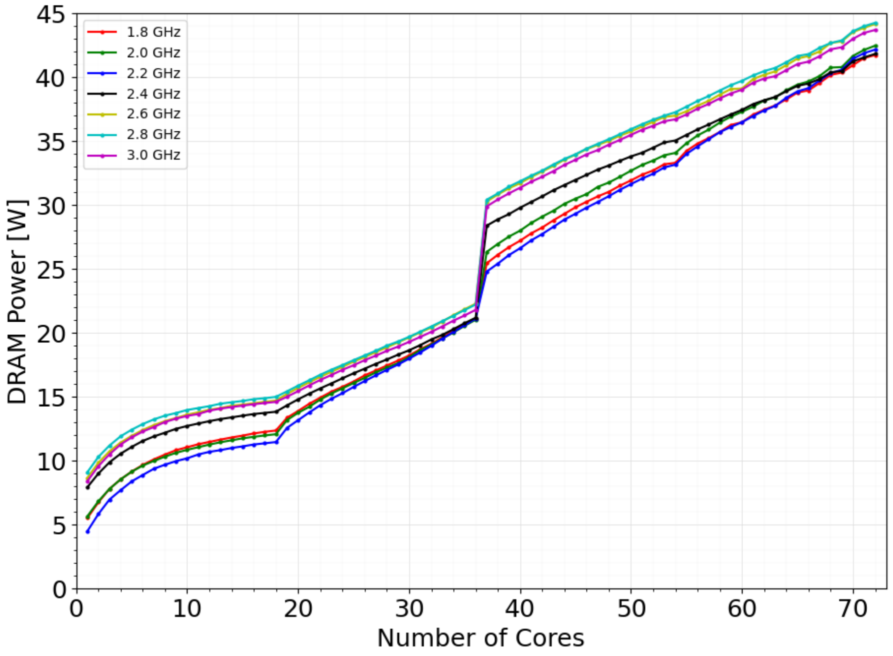


Figure 16: DRAM Power measurements in one node

- First NUMA domain there is a saturating trend considering DRAM power.

Energy Delay Product (EDP)

- Z-plot considers dissipated energy versus any suitable performance metric for a given program.
  - ✓ EDP is the gradient of a line passing through in z-plot.
- First socket measurements are taken for the Z-plot.

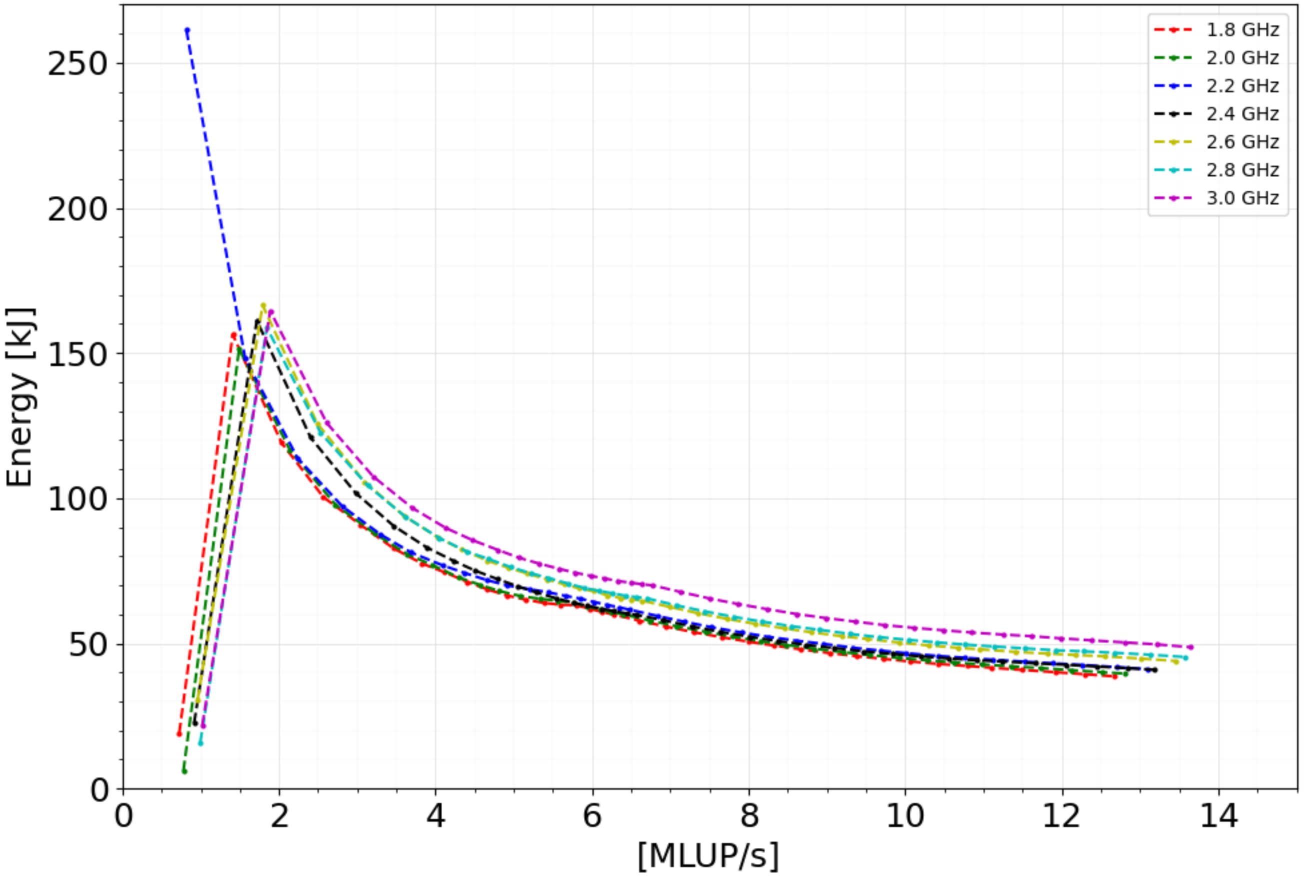


Figure 18: Z-plot considering one socket.

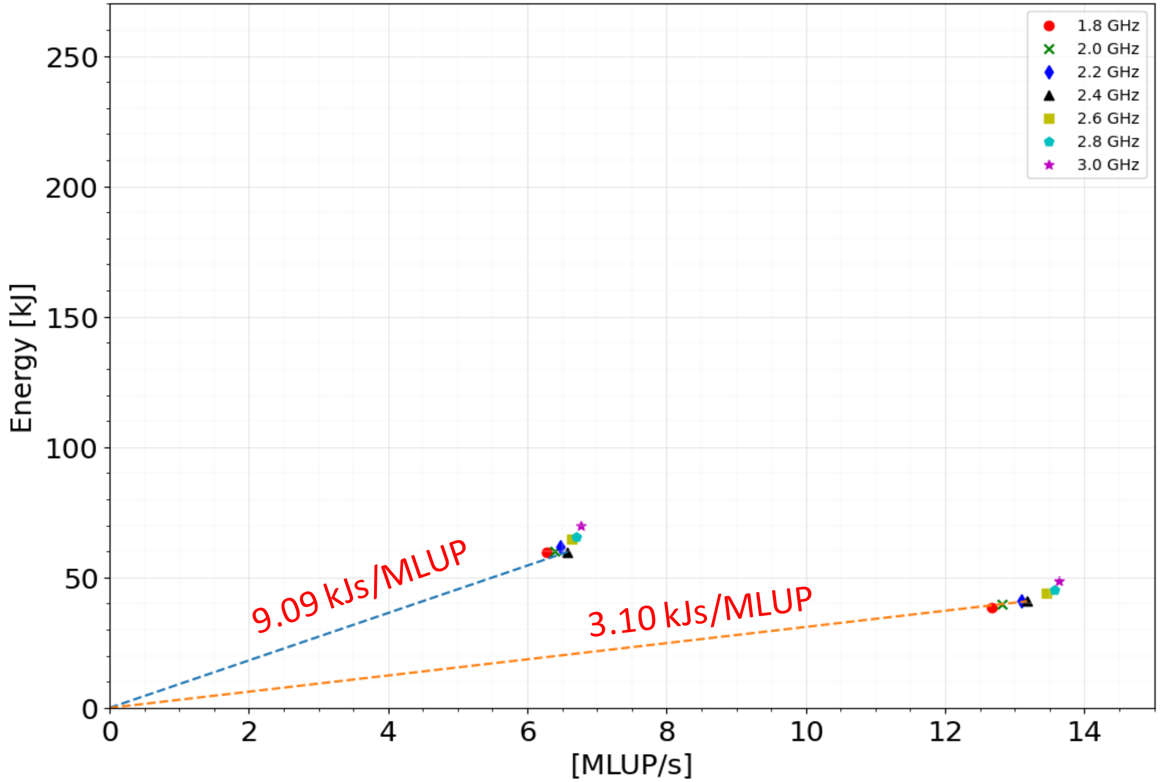


Figure 17: EDP related to 18 and 36 cores at 2.4 GHz

- This verifies the earlier point relating energy with first four frequencies.

Hotspots measurements

- Considered the stream, collision, calcQuasiEqG and newtonRaphson kernels.
- Observed the performance, memory bandwidth saturations and energy contributions.

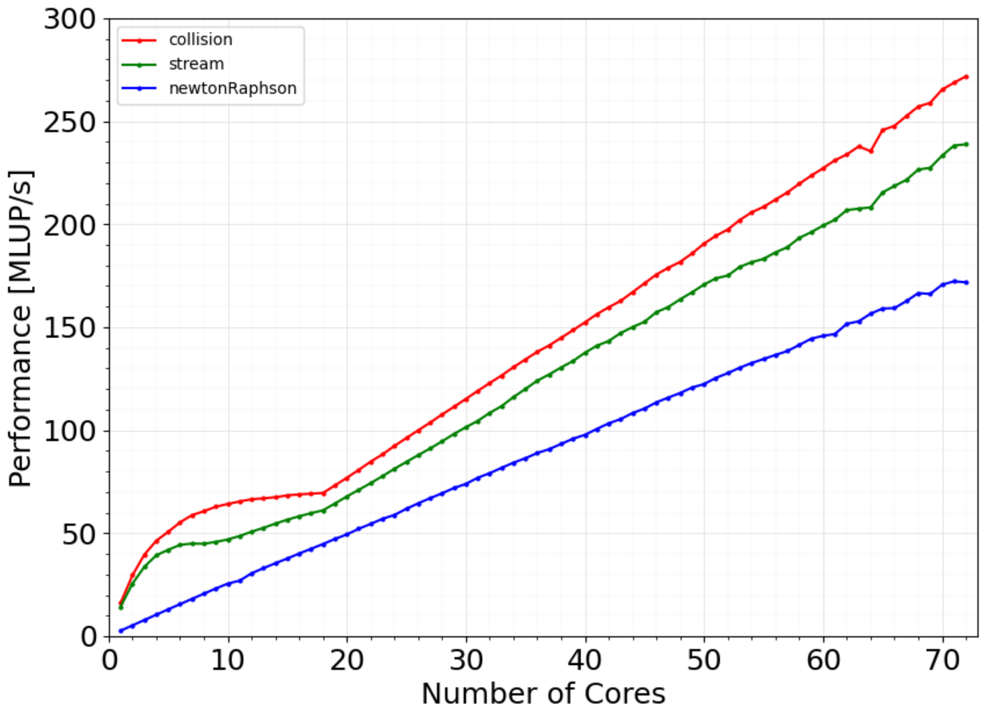


Figure 19: Performance vs. core count

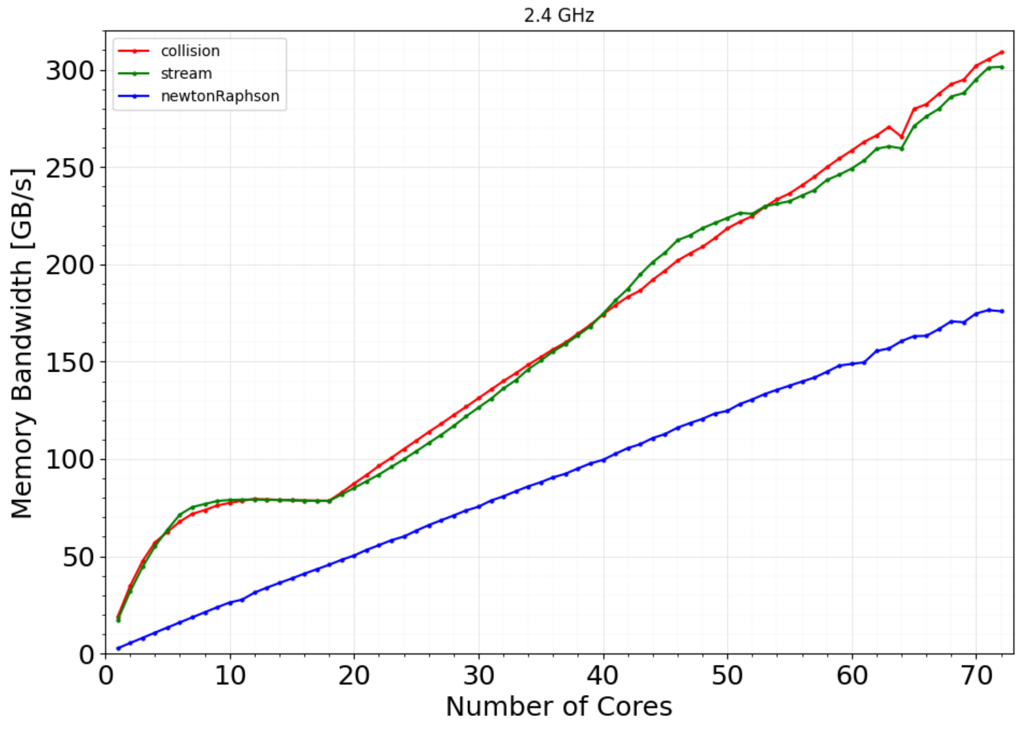
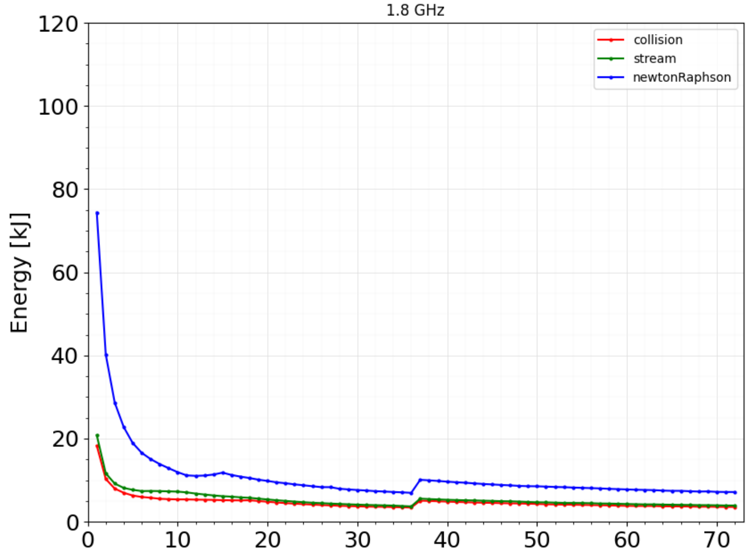


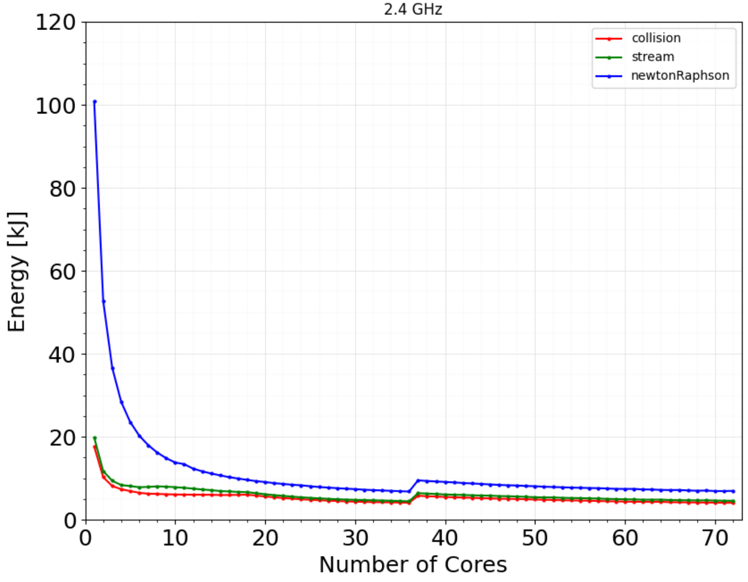
Figure 20: Memory bandwidth vs. core count

- newtonRaphson kernel does not show any saturation in full node.
- collision and streaming shows the saturating trend inside the first NUMA doamin.
- Note that here, MLUP/s have high values. Because we calcultate the same metric with respect to the hotspot runtime. (total runtime >> hotspot runtime; for 2.7 Billion lattice updates)
- Cannot use Flop/s for the representation. Because stream does not have floating point operations.

Hotspots measurements…

- The previously observed, unexpected measurement point at single cores does not appear in energy plots.





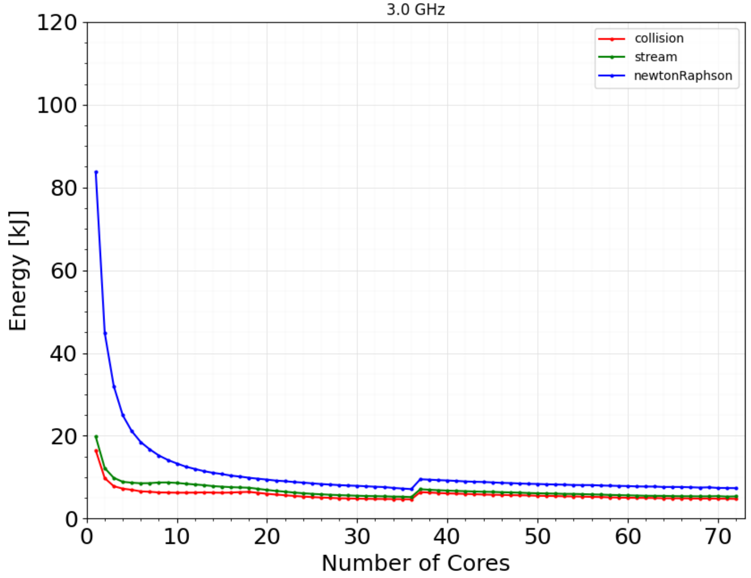


Figure 21: Energy vs. core count

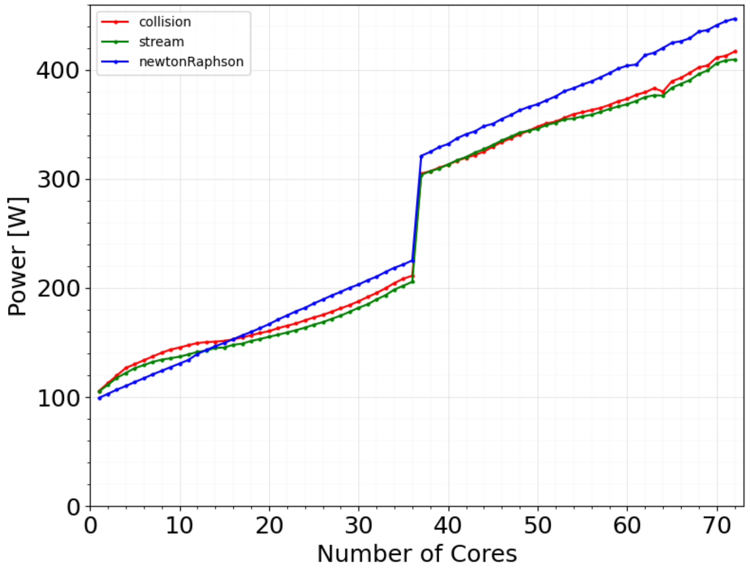


Figure 22: Power vs. core count

- All three kernels contributes 9% - 16% to the main energy measurements.
- newtonRaphson has the highest contribution while showing a scalable performance within the node.
- Both the highest hotspot ranks seems to be having similar variation in terms of power and energy.

Roofline modelling

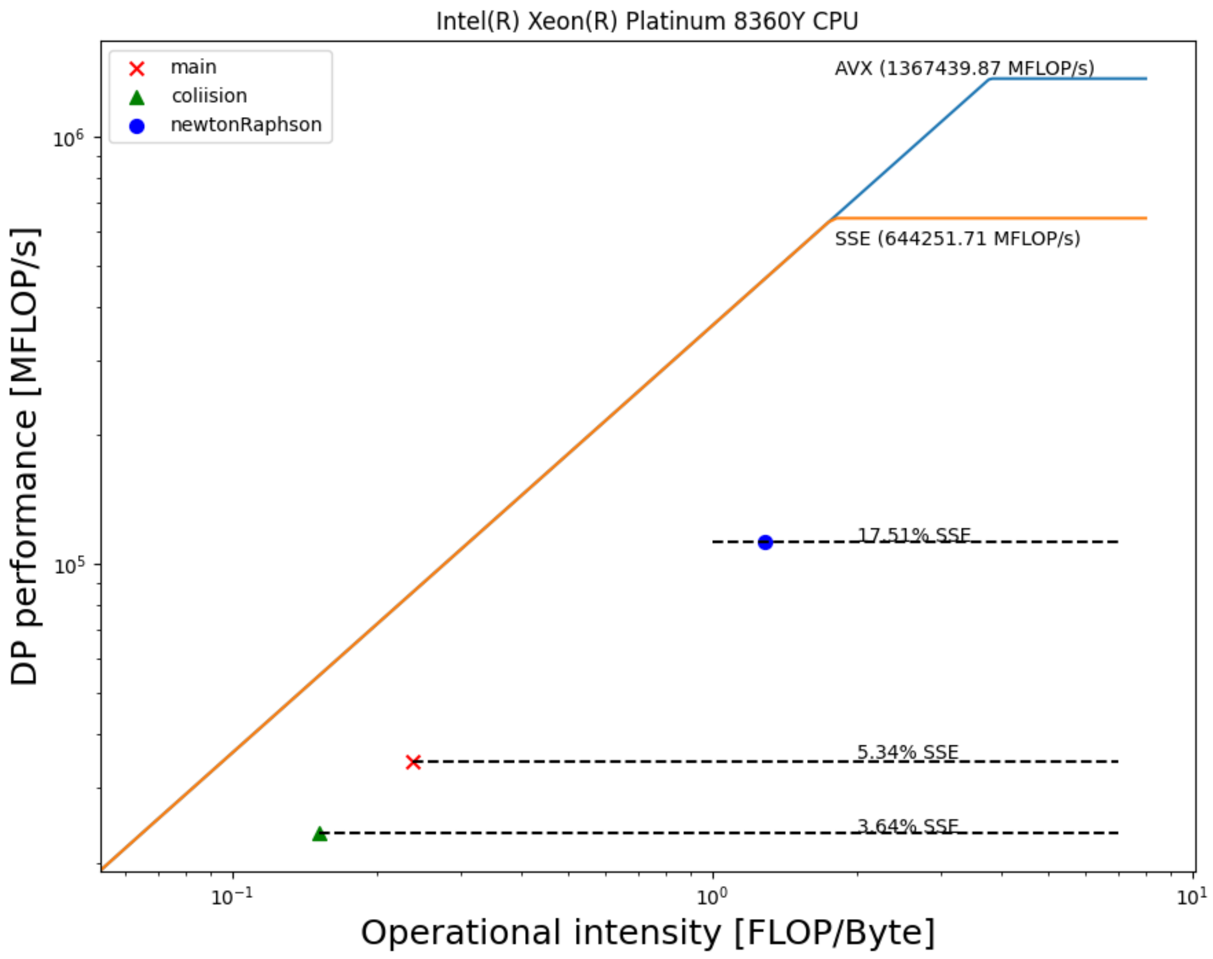


Figure 22: Roofline diagram.

- LIKWID-bench tool is utilized to construct the empherical roofline diagram [7].
- Maximum performance is related to the AVX FLOPS.
- Maximum data throughput is related to the likwid-bench load_avx
- Here the performance metric is double precision performance.
- Stream kernal does not have any flops.
- CLBM application is close to memory bound.

Remarks.

- This is the first kind of benchmarking effort considering LBM in compressible supersonic flow
- CLBM 2D test application shows scalable performance.
- Solver is close to memory bound. According to the roofline analysis, the application has arbitrary horizontal roofs.
  - ✓ May be more opportunity to increase bandwidth utilization, for example by using SIMD instructions in the newtonRaphson routine.
- Optimal energy can be observed at the first socket in fritz node considering 1.8 GHz, 2.0 GHz, 2.2 GHz and 2.4 GHz
  - ✓ EDP results verified the point above.
- DRAM energy contribution to the total energy is 5%-11%.
- Root finding scheme has less significance in terms of performance, even though root finding algorithm was the highlight in previous literature regarding, this LBM regime.

Reference

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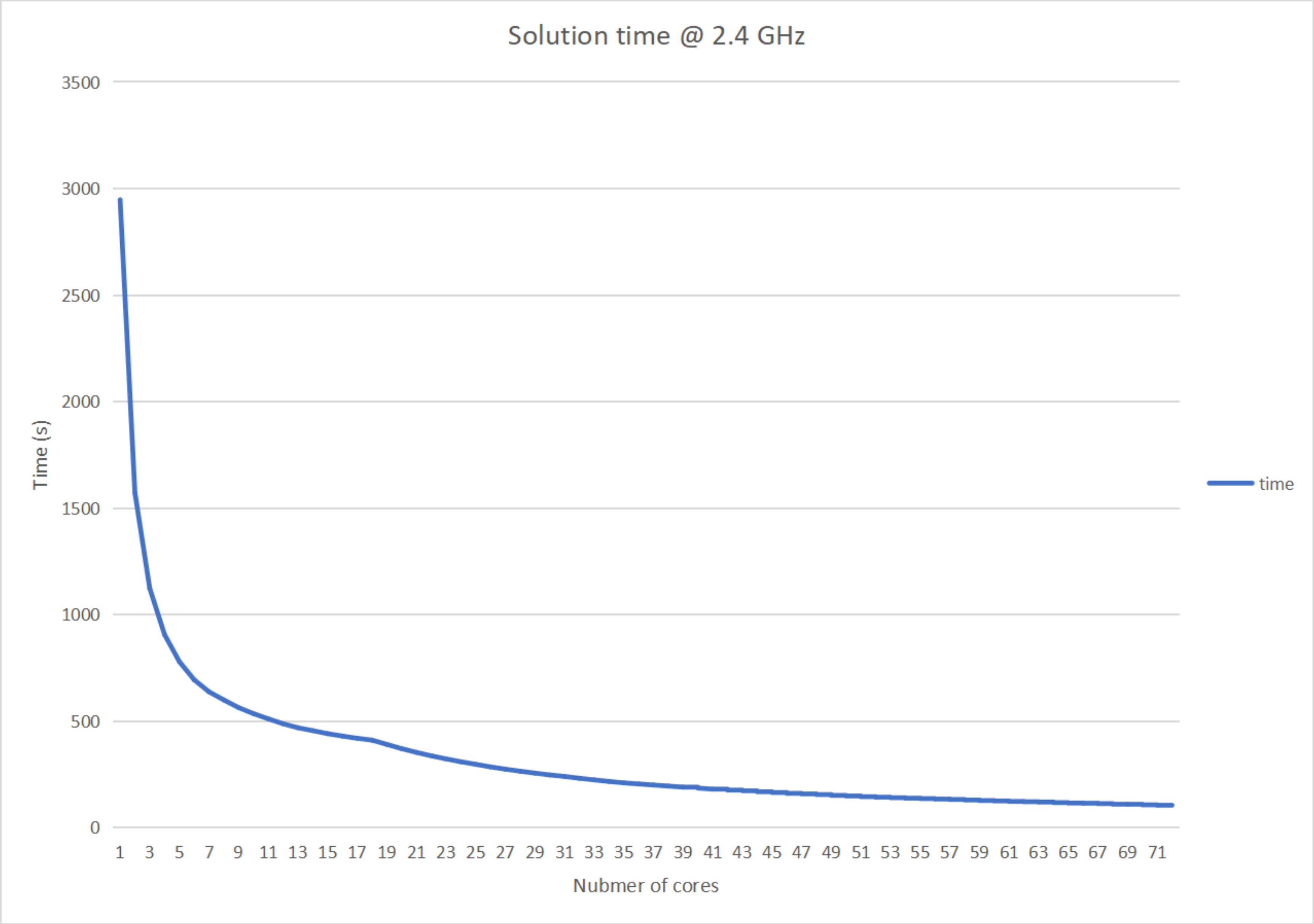
7. https://github.com/RRZE-HPC/likwid/wiki/Tutorial:-Empirical-Roofline-Model

Thank you!

Appendix



Solution time @ 2.4 GHz
3500
3000
2500
2000
1500
1000
500
0
Time (s)
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37 39 41 43 45 47 49 51 53 55 57 59 61 63 65 67 69 71
Nubmer of cores
time

OpenMP_chunk_size