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]

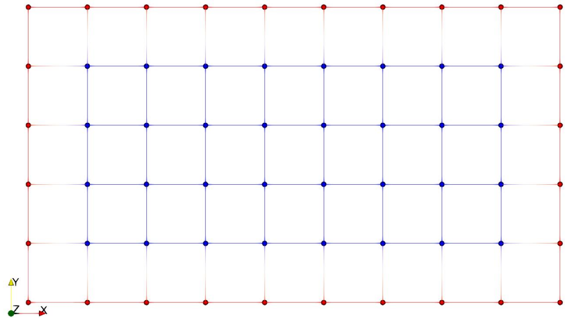


Figure 1: Exemplary structured grid

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

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

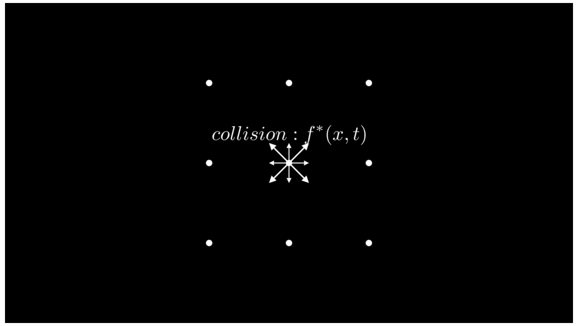


Figure 02: Collide and Stream

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

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

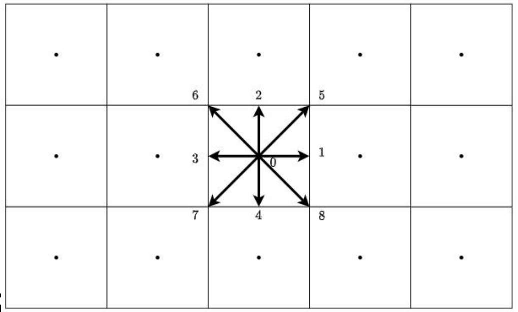


Figure 04:Lattice with D2Q9 stencil

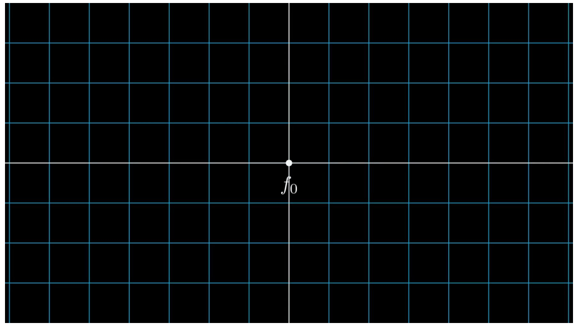


Figure 03: f and g populations in a lattice node

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

Test system & CLBM solver

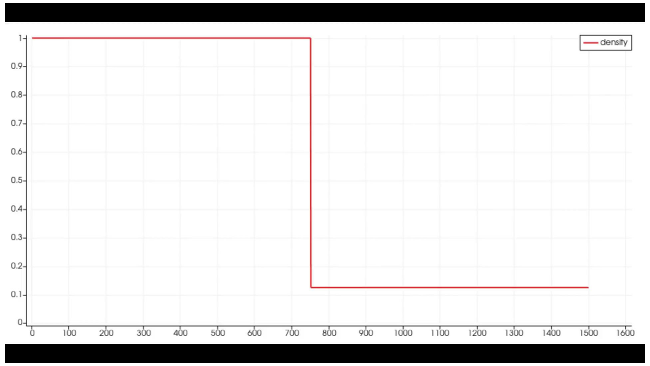


Figure 05: Results for density variation of air inside a 2D shock tube using CLBM solver

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)

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

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 doamin 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..

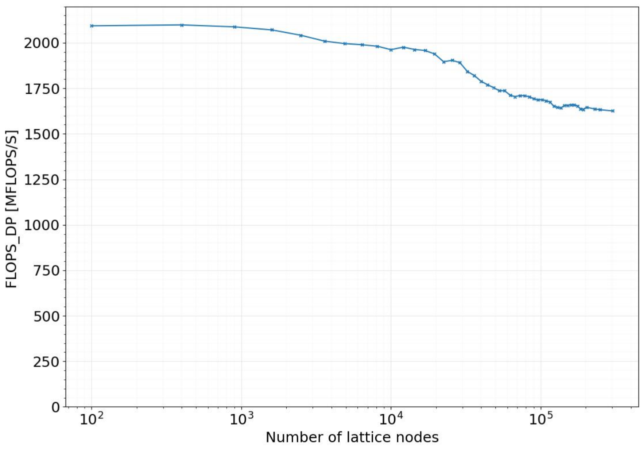


Figure 7: single core performance for fixed 2.4GHz.

BAD IMPLEMENTATION?
NEED CODE OPTIMIZATIONS?
OpenMP sheduling?

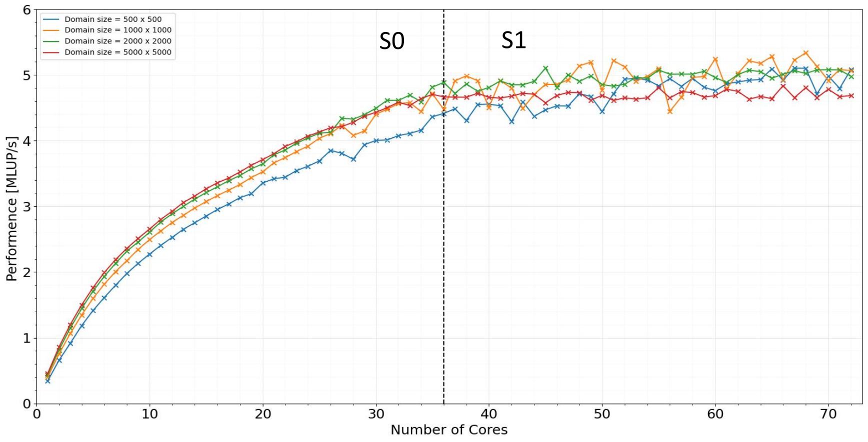


Figure 6: Performance saturation in one node. (phase:01)

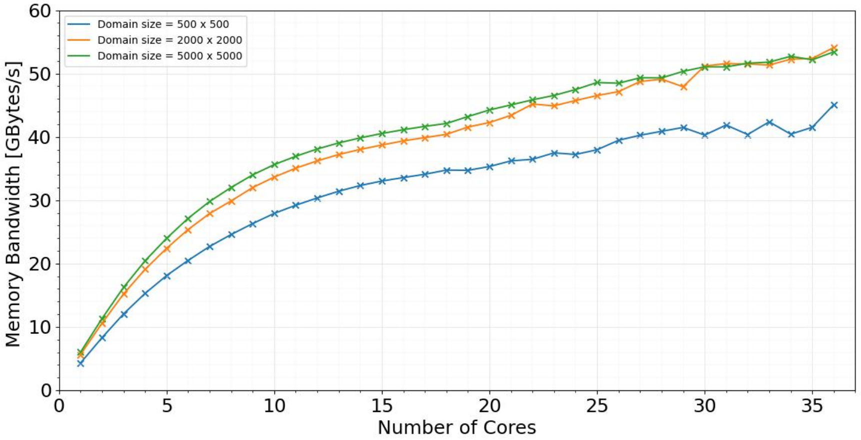


Figure 8: Memory bandwidth saturation in one node. (phase:01)

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, modifiedthe newtonRapson subroutines.
- Further, experimented OpenMP sheduling 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.

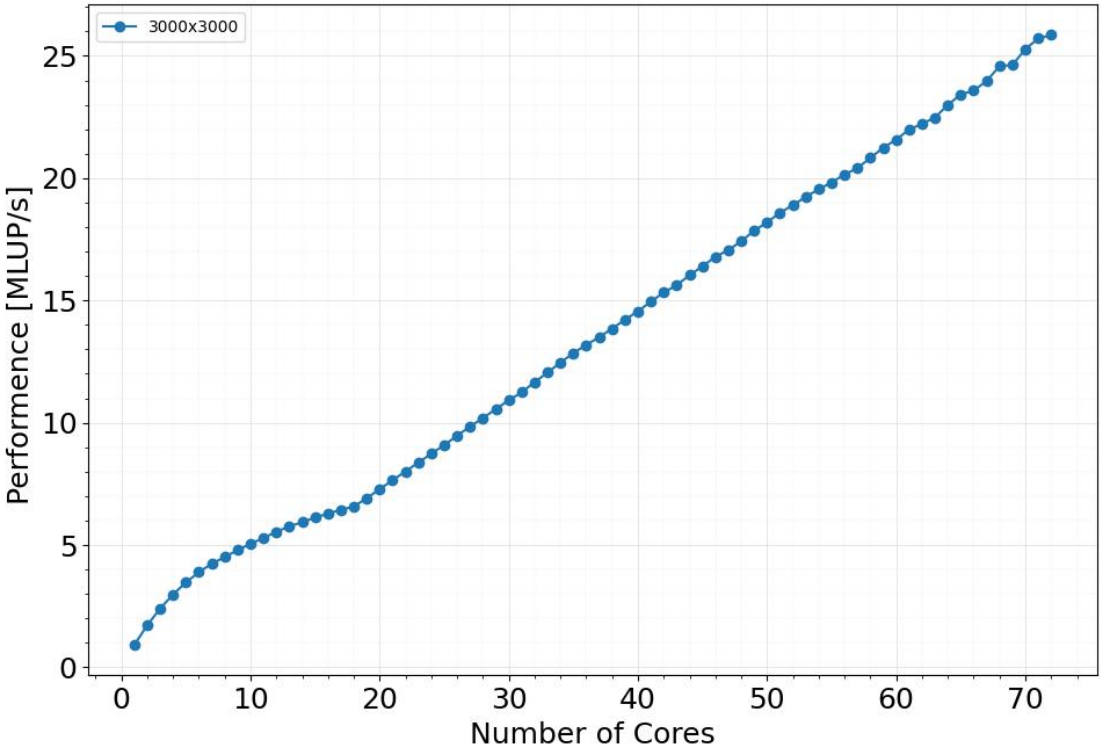


Figure 7: Performance measurements in one node at 2.4 GHz

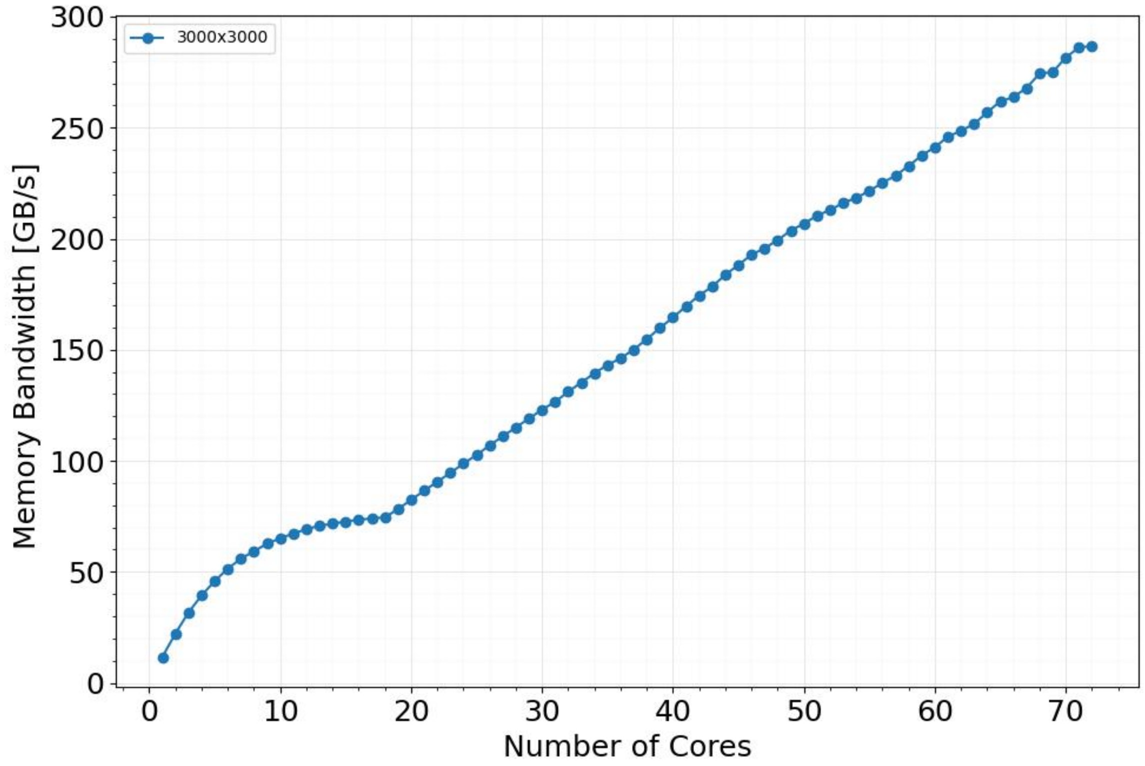


Figure 8: Memory bandwidth measurements in one node at 2.4 GHz

- Memory Bandwidth also saturates in 1st NUMA domain. (74.5 GB/s).
- single core performance is ~2x compared to phase 01.

Profiling

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

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 9: Vtune Hotspot results.

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 10: 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

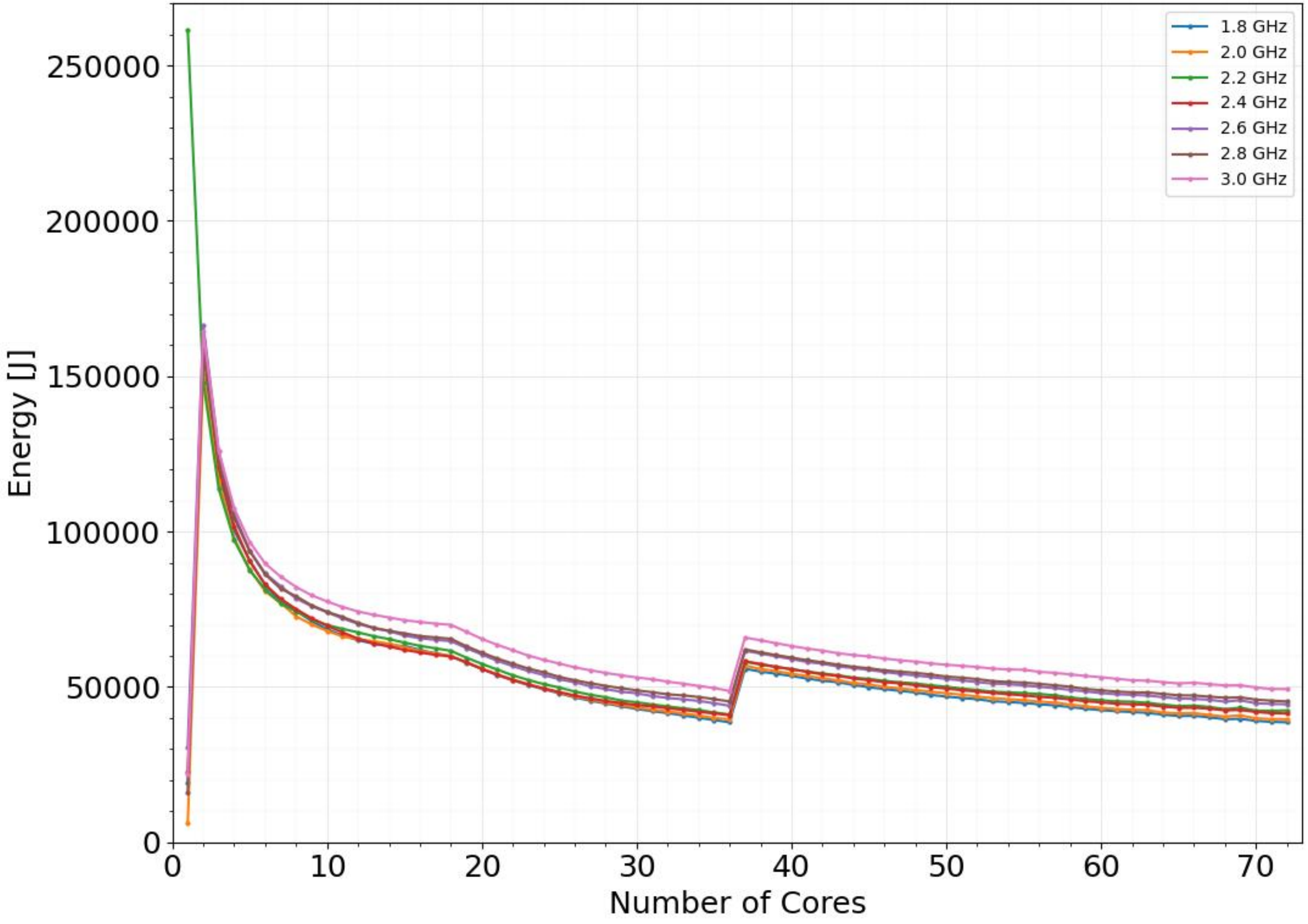


Figure 10: Energy measurements in one node

- An unusual behaviour can be observed at single core power measurment.
  - ✓ This behaviour persists for serveral 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 second optimum point at 1st socket.
- Sudden energy jump when moving to second socket before decrase 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

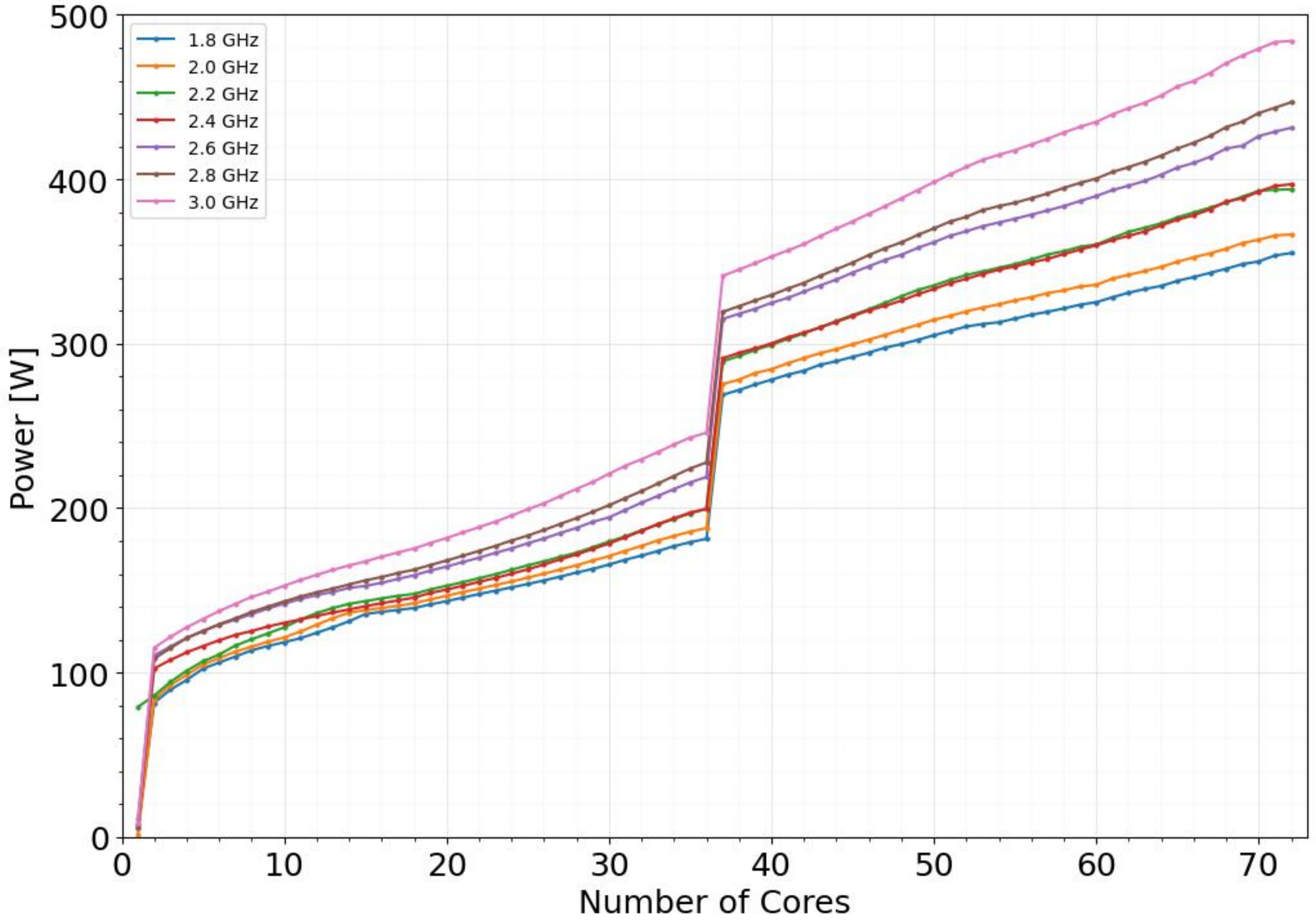


Figure 10: Power measurements in one node

- 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.

Energy and power measurements; main

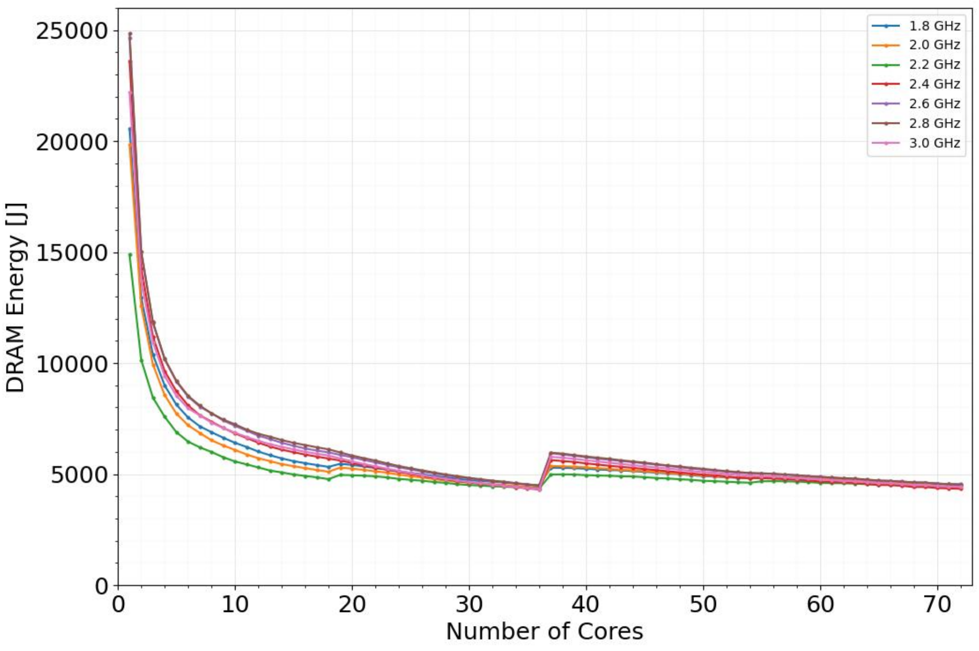


Figure 11: DRAM Energy measurements in one node

- DRAM energy measurements do not show an unexpected behaviour at single core measurements all the time.
- 2.2 GHz seems to be the lowset energy curve for a wider domain.
- The DRAM energy contribution to the total energy is in the range of 5%-11%.

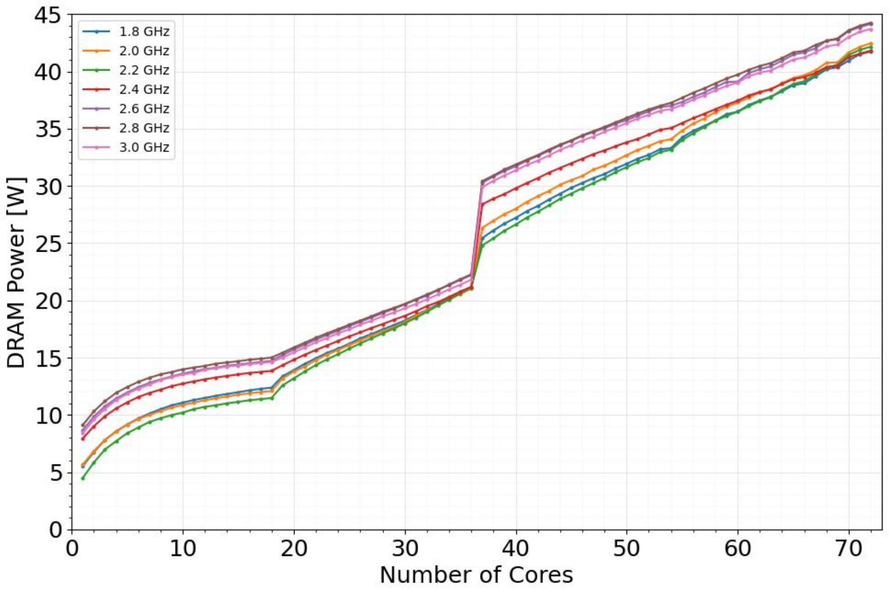


Figure 11: DRAM Power measurements in one node

- 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[5][6].
  - ✓ EDP is the gradient of a line passing through in z-plot.
- First socket measurements is taken for the Z-plot.

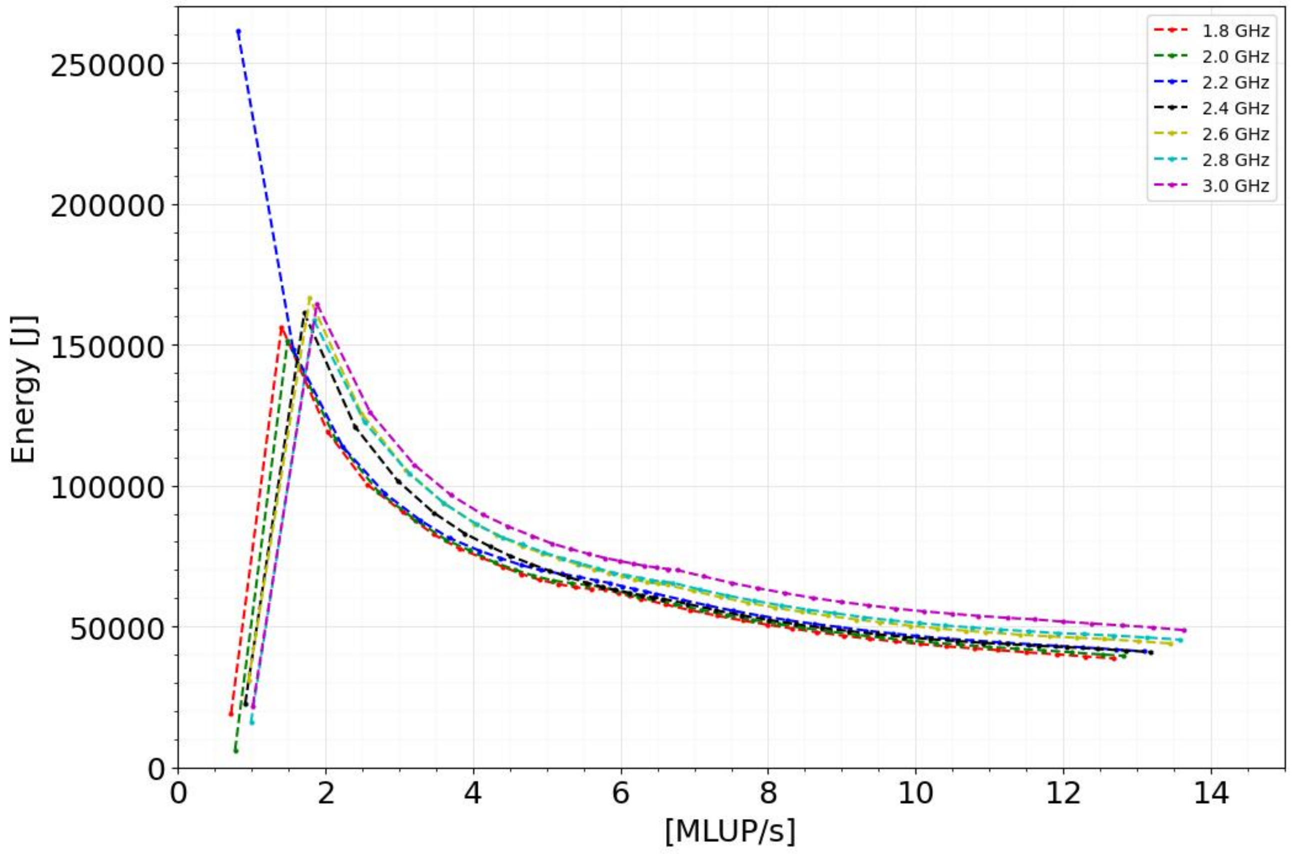


Figure 11: Z-plot considering one socket.

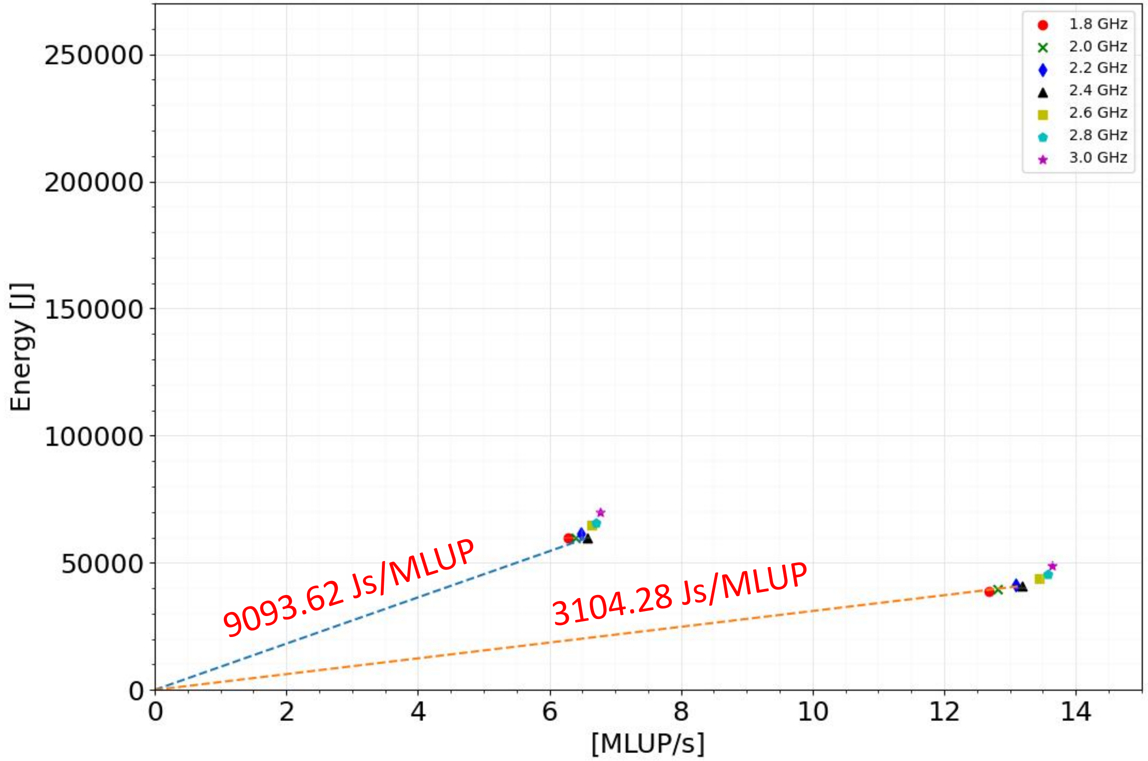


Figure 12: EDP related to 18 and 36 cores at 2.4 GHz

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

Energy Delay Product(EDP)…

- With EDP the trade of between energy and performance can be discribed.

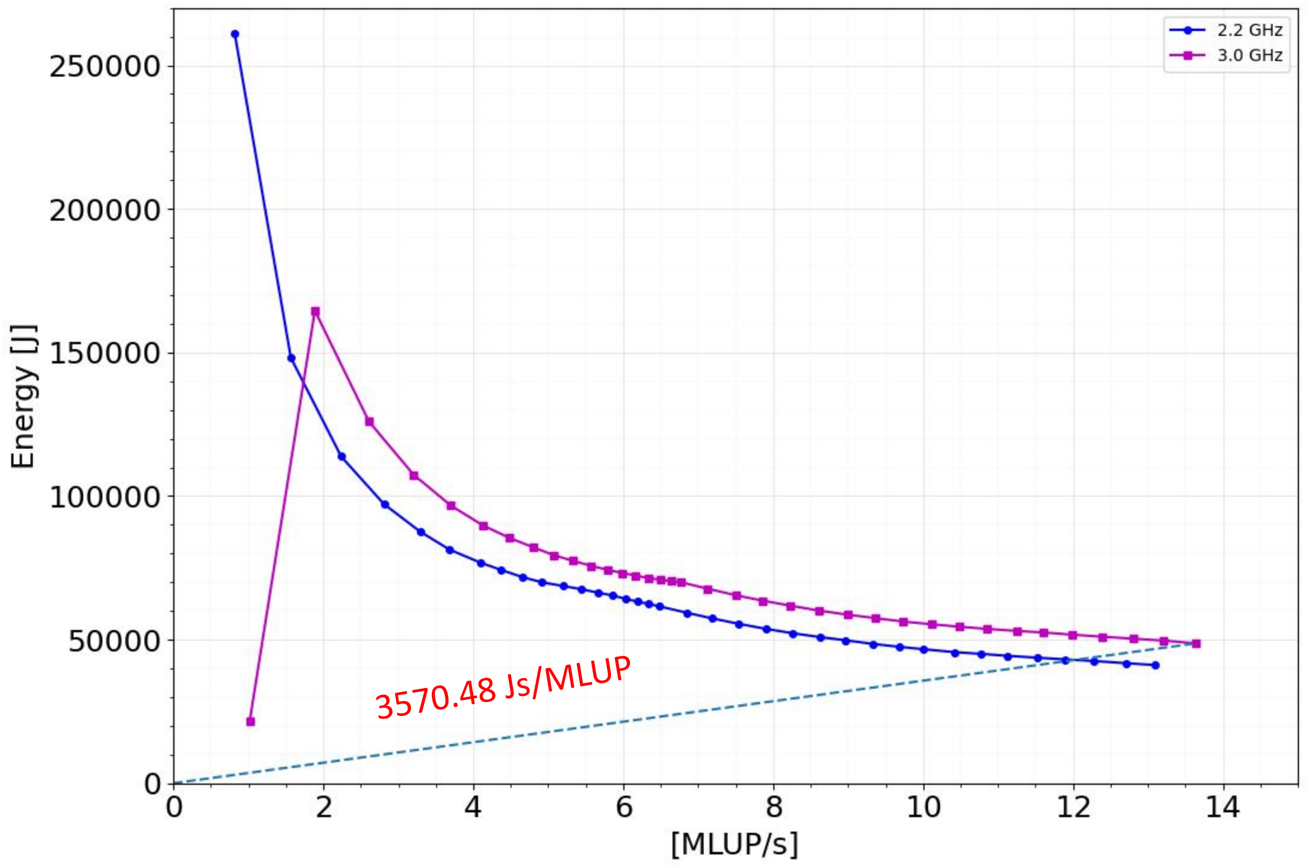


Figure 11: Energy and performance trae-off

- Considering EDP it is vissible that
  - ✓ 33 cores @ 2.2 GHz have the same energy efficiency as the 36 cores @ 3.0 GHz.
  - ✓ But, performance wise it loose nearly 10%.

Hotspot measurements

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

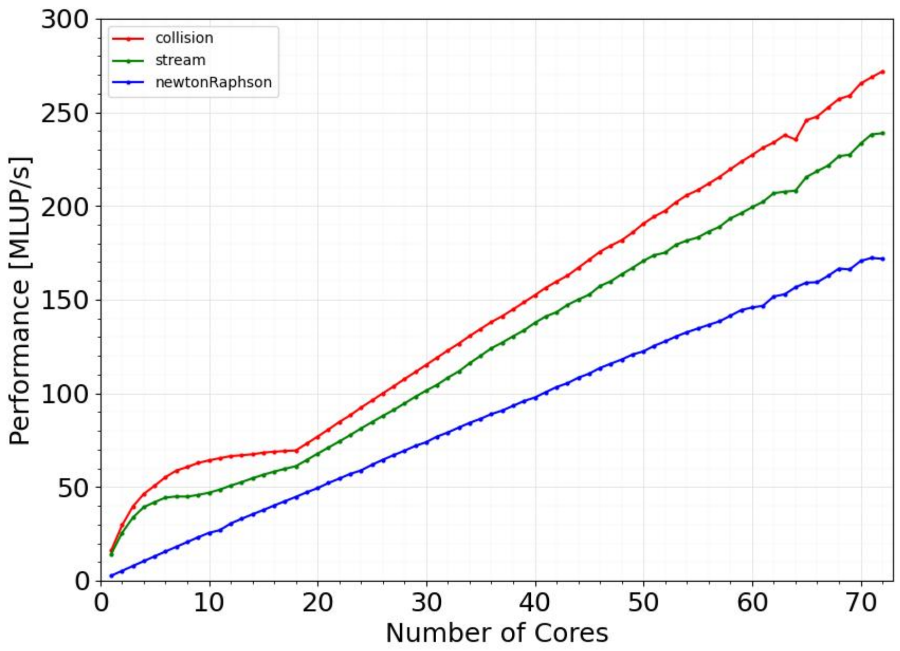


Figure 11: Performance vs. core count

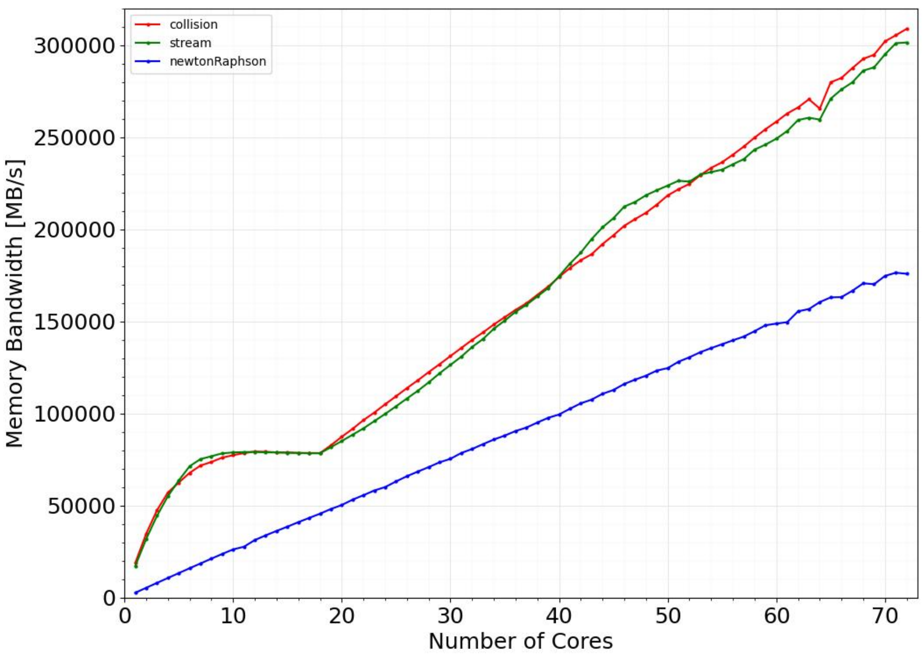
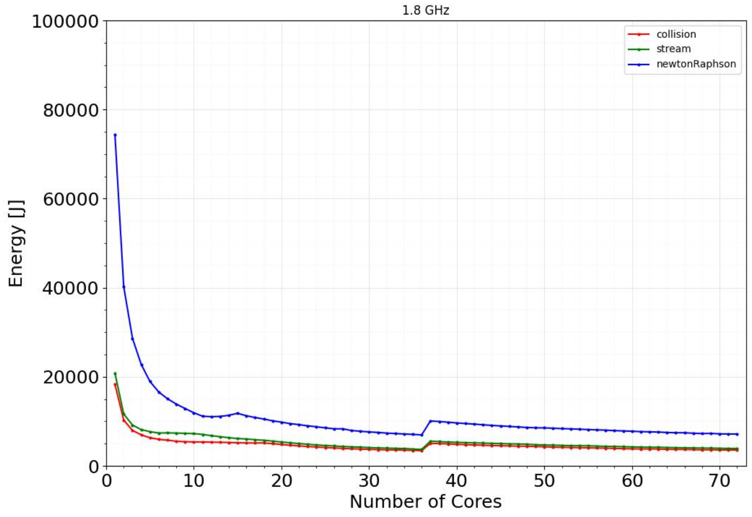


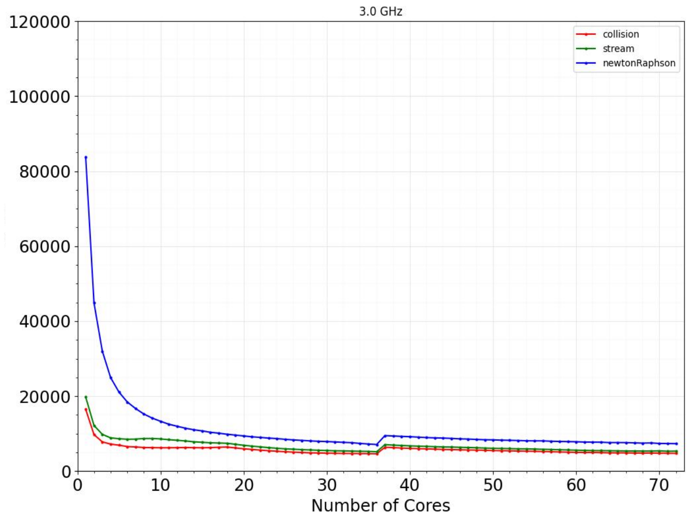
Figure 11: Memory bandwidth vs. core count

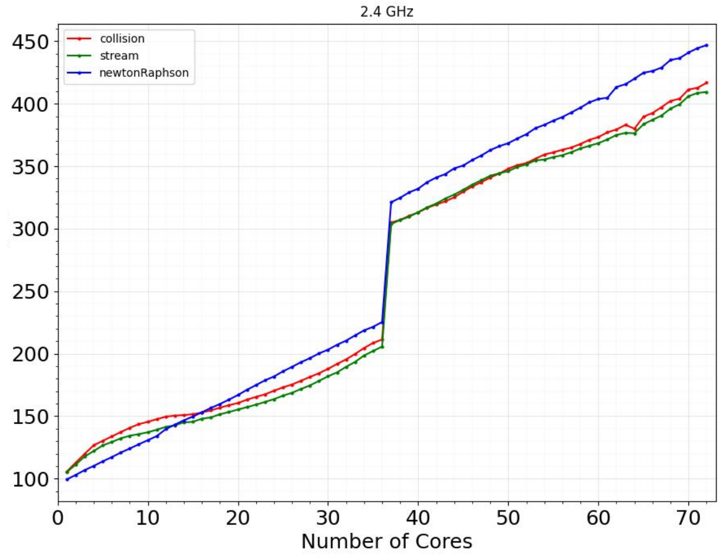
- newtonRaphson kernel does not show any saturation in full node.
- collision and streaming shows the sathrating trend inside the first NUMA doamin.

Hotspot measurements…

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







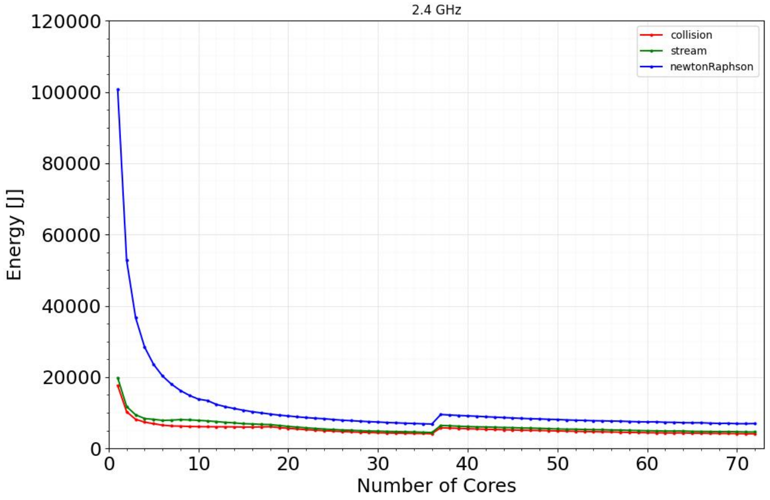


Figure 11: Energy vs. core count

Figure 11: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.

- Bothe the highest hotspot ranks seems to be have similiar variation in terms of power and energy.

Roofline modelling

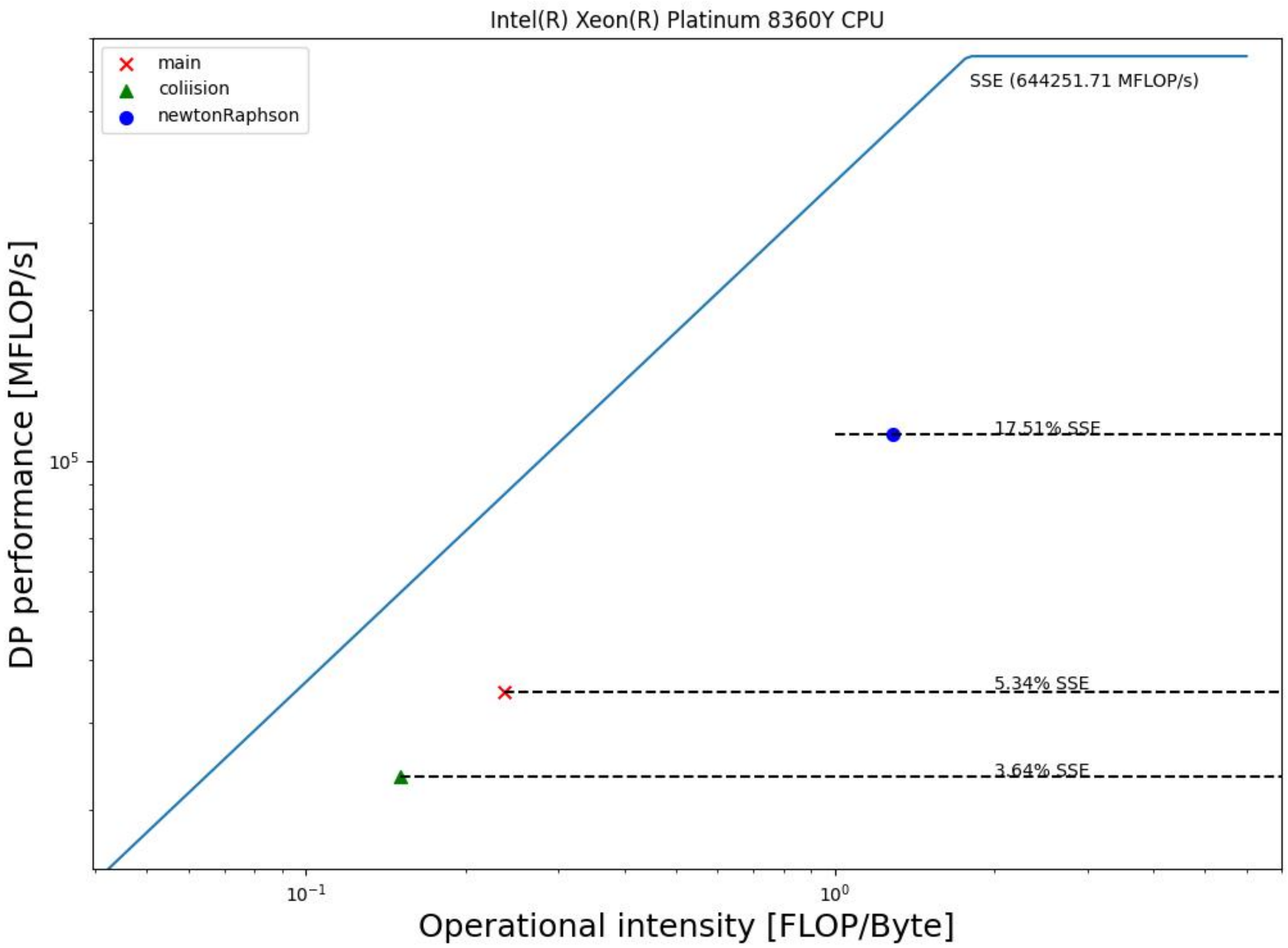


Figure 11: Roofline diagram.

- LIKWID-bench tool is utilized to construct the
- empherical roofline diagram [7].
- Maximum performance is related to the SSE FLOPS.
- Maximum data throughput is related to the likwid-bench load_sse
- 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.
- 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%.
- Investigation of optimal energy point for the present implementation.
- According to the roofline analysis the application has arbitrary horizontal roofs.
  - ✓ Thers is more room for code optimization.
- Root finding scheme has less significance interms of performance, even though root finding algorithm was the highlight in previous literature regarding , this LBM regime.

Reference

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