

L5: HPC for AI applications & Environmental impact of computation

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1. HPC for AI & Environmental impact of computation
2. Introduction to AI applications
3. Environmental impact of computation
4. Energy consumption of HPC
5. AI energy and computation costs
6. More frugal computing?

HPC for AI & Environmental impact of computation

Introduction to AI applications

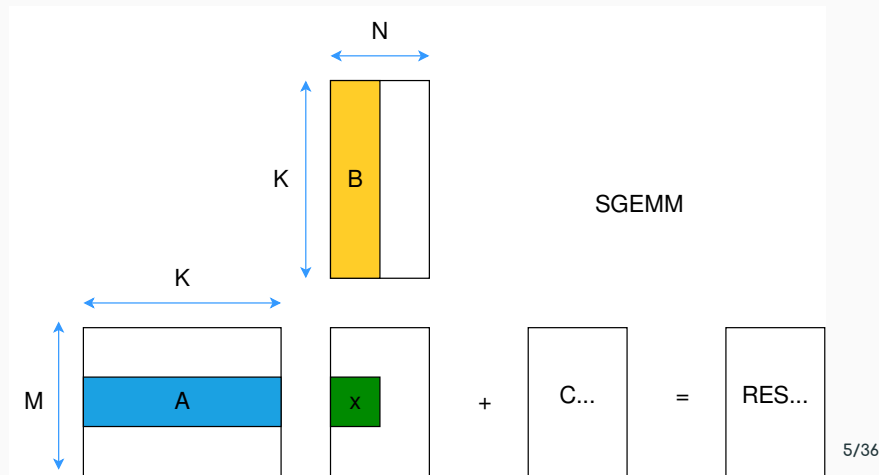
- 2012: **AI renaissance** brought by increased data availability and computation resources
 - breakthroughs in multiple domains
 - many innovations: algorithms, specialized processors, optimizations
- Most systems use **neural networks**:
 - Training (stochastic gradient descent + backpropagation)
 - Inference (forward pass)
- For both, **the bottleneck is matrix multiplication**

- Explain why dense linear algebra (GEMM) dominates NN compute
- Core SGEMM kernel ideas and common optimizations
- Use Roofline model to identify bottlenecks
- Understand mixed precision & quantization tradeoffs for energy/perf

SGEMM

Single-precision General Matrix-Matrix multiplication (SGEMM):

$$RES = A \times B + C$$



Naive SGEMM implementation (pseudocode)

```
// Initialize RES to C
for (i = 0; i < M; i++)
    for (j = 0; j < N; j++)
        RES[i][j] = C[i][j];

// Matrix multiply
for (i = 0; i < M; i++) {
    for (j = 0; j < N; j++) {
        for (k = 0; k < K; k++) {
            RES[i][j] += A[i][k] * B[k][j];
        }
    }
}
```

- FLOPS: $2 \times M \times N \times K$
- Memory: $4 \times (M \times K + K \times N + M \times N)$ bytes

order in memory \rightarrow

$$\begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix}$$

- Stride in accessing B (column-major)
 - Poor spatial locality
 - Difficult to vectorize
 - Cache misses for large matrices (reuse distance too large)
- **Low arithmetic intensity:** ≈ 0.5 FLOP/byte for large matrices

Reordering loops (i,k,j)

- Sums $RES[i][j] += A[i][k] * B[k][j]$; are independent \rightarrow reorder loops:

```
for (i = 0; i < M; i++)  
  for (k = 0; k < K; k++)  
    for (j = 0; j < N; j++)  
      RES[i][j] += A[i][k] * B[k][j];
```

- $A[i][k]$ does not depend on $j \rightarrow$ load once, reuse N times
- RES and B accesses are now stride-1 (row-major)

```
for (i = 0; i < M; i++)  
  for (k = 0; k < K; k++) {  
    const float temp = A[i][k];  
    for (j = 0; j < N; j++)  
      RES[i][j] += temp * B[k][j];  
  }
```

- Better spatial locality and easier to vectorize

Inner loop assembly for (i,k,j) ordering with AVX (8 float in a vector):

```
.loop:                                # Inner loop
    vmovss  xmm0, DWORD PTR A[i][k]  # Load A[i][k]
    vbroadcastss ymm0, xmm0          # Broadcast scalar to
    all lanes                        # all lanes
    vmovaps ymm1, YMMWORD PTR B[k][j] # Load B[k][j:j+8]
    vfmadd231ps ymm2, ymm1, ymm0      # Fused multiply-add
    vmovaps YMMWORD PTR RES[i][j], ymm2 # Store RES[i][j:j+8]
    add     j, 8                     # Increment j by 8 (
    vector width)                    #
    cmp     j, N                     # Compare j with N
    jl      .loop                    # Loop if j < N
```

- Temporal locality analysis:
 - GOOD: $A[i][k]$ reused in the inner loop, reuse distance 1.
 - MEDIUM: For a fixed (i, j) , each $RES[i][j]$ revisited once per k .
So reuse distance K (one full row).
 - To keep RES in cache between uses you would need cache $\geq K \times 4B$
 - BAD: For a fixed (k, j) , $B[k][j]$ used once per i . So reuse distance $K \times N$ (entire B matrix).
 - To keep B in cache between uses you would need cache $\geq K \times N \times 4B$
- Still poor temporal locality for large matrices
- Solution: tiling / blocking to increase reuse

Blocking (tiling)

- Idea: operate on sub-matrices blocks that fit in cache

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \times \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{bmatrix}$$

```
#define BS 64 // Block size
// Loop over blocks
for (ii = 0; ii < M; ii += BS)
    for (kk = 0; kk < K; kk += BS)
        for (jj = 0; jj < N; jj += BS)

            // Operate on blocks A[ii:ii+BS, kk:kk+BS],
            // B[kk:kk+BS, jj:jj+BS], RES[ii:ii+BS, jj:jj+BS]
            for (i = ii; i < min(ii+BS, M); i++)
                for (k = kk; k < min(kk+BS, K); k++)
                    for (j = jj; j < min(jj+BS, N); j++)
                        RES[i][j] += A[i][k] * B[k][j];
```

- Each block operation is independent → parallelize over blocks

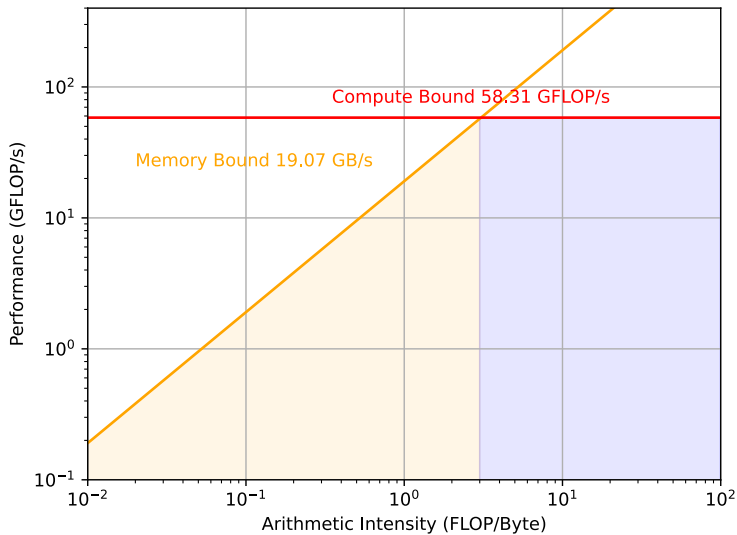
```
#pragma omp parallel for collapse(3)
for (ii = 0; ii < M; ii += BS)
    for (jj = 0; jj < N; jj += BS)
        for (kk = 0; kk < K; kk += BS)
            // Block multiplication as before
```

- Each thread works on its own block → no false sharing
- Synchronization only at the end of the parallel region
- NUMA considerations: pin threads to cores, allocate memory close to threads
- Load balancing: static scheduling usually works well for large matrices

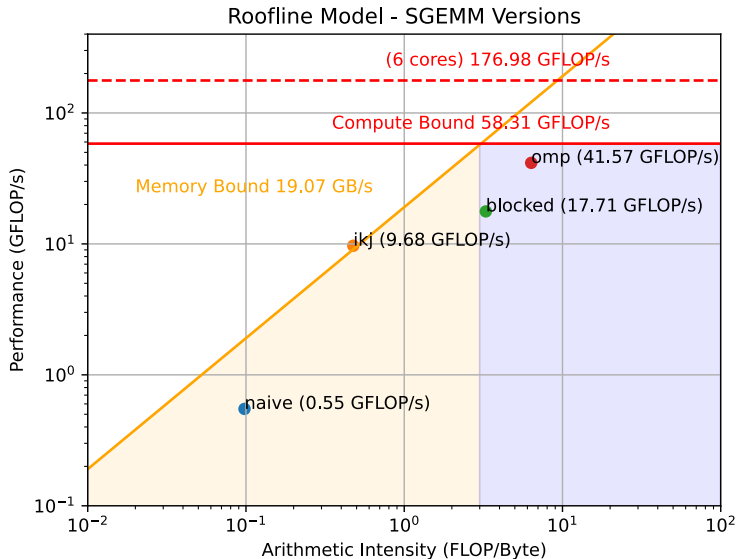
- Highly optimized SGEMM implementations exist:
 - OpenBLAS, Intel MKL for CPU
 - NVIDIA cuBLAS for GPU
- Implementations use blocking, vectorization, parallelization, and many architecture-specific optimizations
- Libraries are carefully tuned for different sizes and shapes of matrices.
- Autotuners (e.g., ATLAS, TVM, MLKAPS) can generate optimized code for specific hardware and problem sizes.

- Hypothesis: performance is limited by either compute or memory bandwidth
 - performance: FLOP/s (vertical axis)
 - memory bandwidth: Bytes/s
 - arithmetic intensity: FLOP/byte (horizontal axis)
- Simple visual model to understand bottlenecks

Roofline model - Bounds



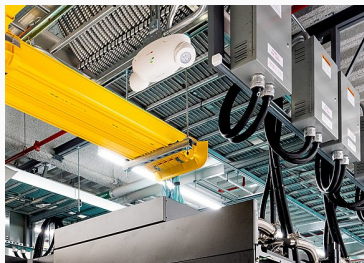
Roofline model - SGEMM analysis



Environmental impact of computation

Introduction

- Major ecological crisis: French roadmap targets carbon neutrality in 2050 (Stratégie Nationale Bas Carbone).
- Requires a **40% energy consumption reduction**.
- HPC part of the solution: modeling and improving complex systems
- HPC part of the problem: Frontier system at ORNL
 - More than 10^{18} floating point operations per second
 - Consumes 21MW: the energy of a small town (16 000 french houses)



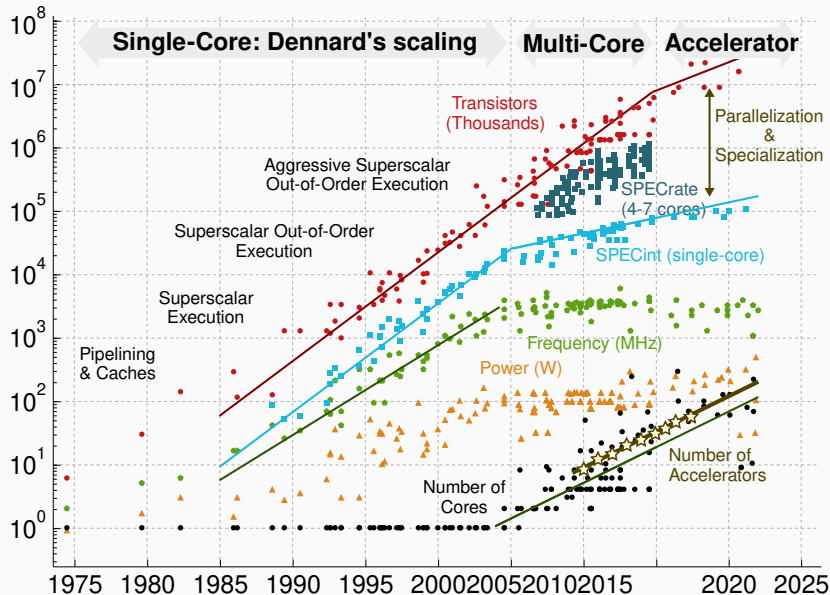
- The ICT sector consumes $\approx 5\%$ of the energy worldwide
- It accounts for **1.8% - 2.8%** of emitted GHG [Freitag, 2021]:
 - Accounts for embodied emissions.
 - Shadow energy during the whole life-cycle: mining, fabrication, transportation, recycling.
- GHG emissions are only one of the sustainability issues
 - rare-earth mining and waste disposal (eg. Agbogbloshie).
 - human-right abuses, health issues, pollution.
- This presentation focus on energy consumption of HPC

What about renewable energies?

- Low-carbon electricity is a **limited** resource
- Decarbonation → huge increase in electricity demand
 - Heating, Transportation, Industry
 - Computing will compete for low-carbon electricity.

Energy consumption of HPC

Evolution of processing units [Batten, 2023]



$$\text{CMOS Power } P = \underbrace{1/2.C.V^2.f}_{P_{\text{dynamic}}} + \underbrace{V.I_{\text{leak}}}_{P_{\text{static}}}$$

For each generation, transistors dimensions reduced by 30%,

- Voltage and capacitance reduced by 30%
- Frequency increases: $\times 1.4 \approx 1/0.7$
- Surface halved: $0.5 \approx 0.7 \times 0.7$
- Power halved: $\Delta P = 0.7 \times 0.7^2 \times 1/0.7 \approx 0.5$

Power per surface unit remains constant but manufacturers double number of transistors and frequency increases:

- Power efficiency doubles every 1.57 years
- Total power increases

- At current scale, leak currents start increasing (P_{static} ↗).
Power wall slows Dennard's scaling.
- Computing demand → **parallelism** and **specialization**.
- Number of cores increases exponentially since 2005.
- Power efficiency still improving:
 - selectively turning-off inactive transistors;
 - architecture design optimizations;
 - software optimizations.

- For domain specific applications, such as AI, specialized accelerators are used
 - Memory and compute units tuned for a specific problem (matrix multiplication) ;
 - Faster and better power efficiency: GPU, TPU, FPGA, ASIC.

Analysis of TOP-100 HPC systems

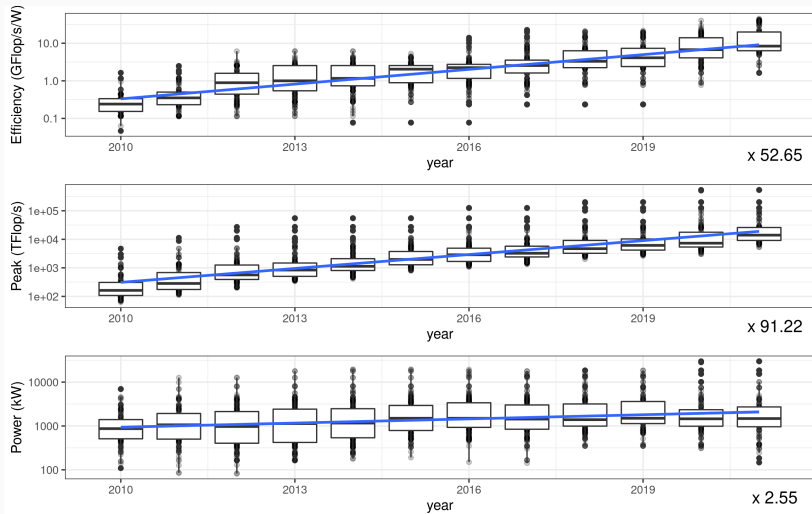


Figure 6: image

- In 1865, Jevons shows that steam engine improvements translate into increased coal consumption.
- In HPC, efficiency gains contribute to the rising computation demand.
 1. net increase of the total power consumption.
- Rebound effects for data-centers [Masanet, 2020]
 1. 6% increase in energy consumption from 2010 to 2018 (255 % increase in nodes).
- **Indirect rebound effects:** computation advances can contribute to the acceleration of other fields.

AI energy and computation costs

Training cost doubles every 3.4 months [OpenAI, 2020]

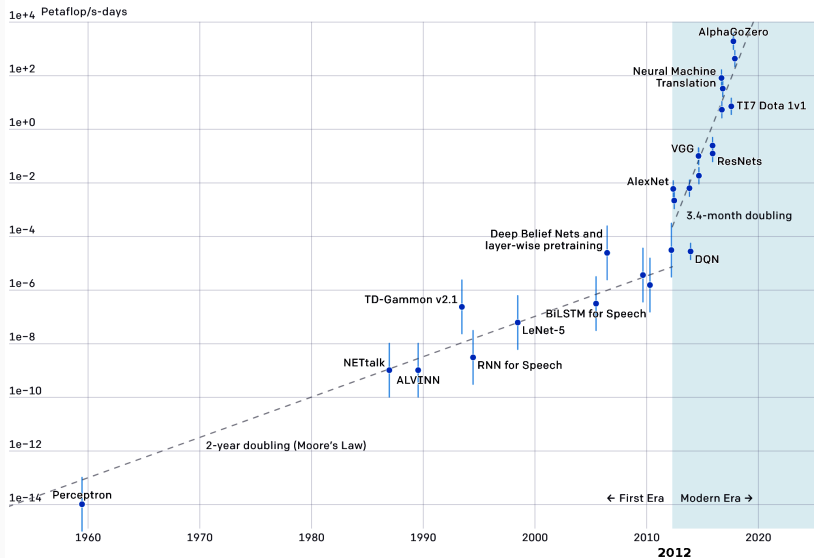
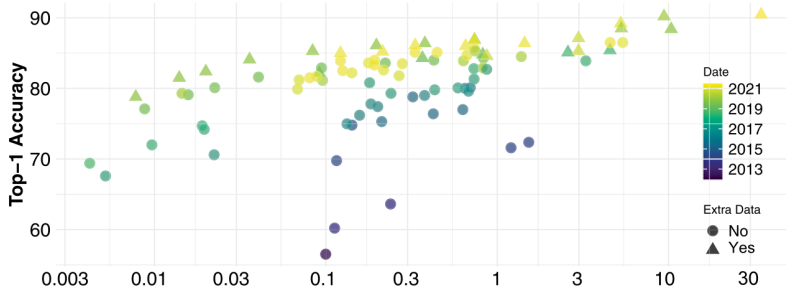
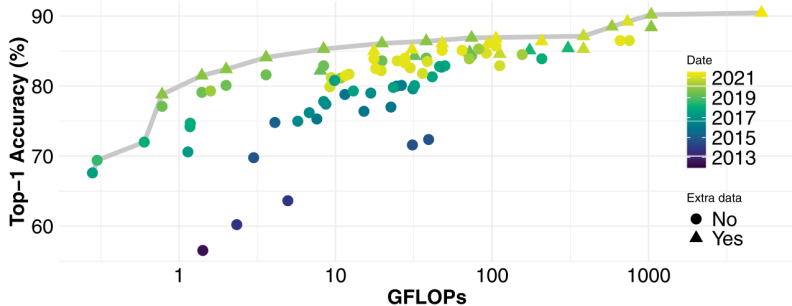


Figure 7: image

Should we study training or inference?

- **Training:** huge cost but done once
 - GPT3, 175 billion parameters, ≈ 314 ZettaFLOP
 - GPT4, 1.7 trillion parameters
- **Inference:** millions of users and requests
 - 80-90% cost of a deployed AI system is spend on inference [NVIDIA, 2019]

Inference cost - Diminishing returns for computer vision



More frugal computing?

Smaller precision / Smaller models for AI

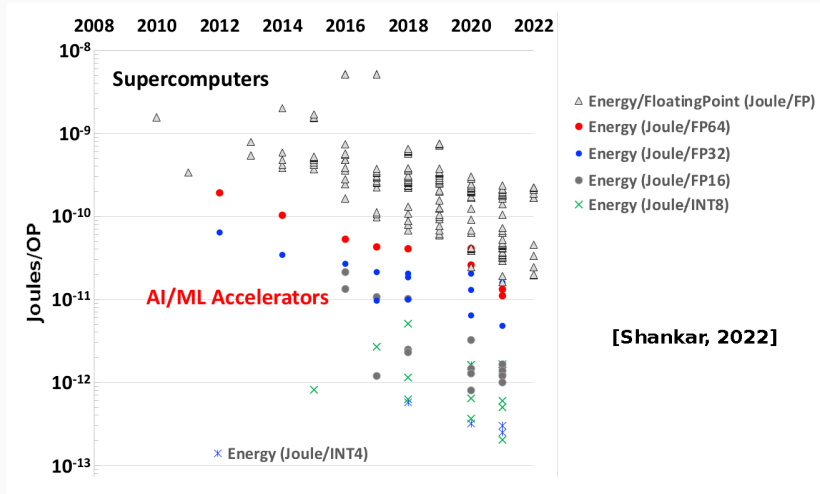
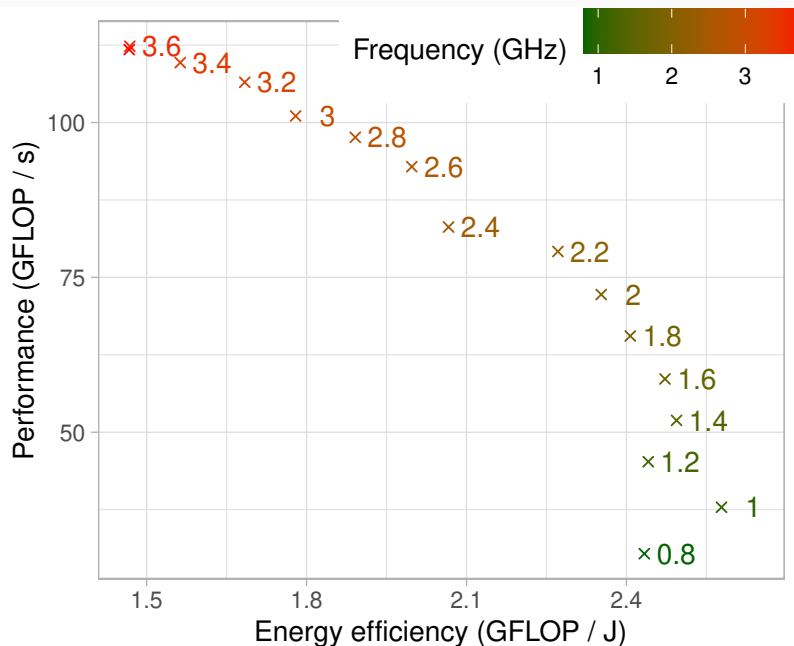


Figure 8: image

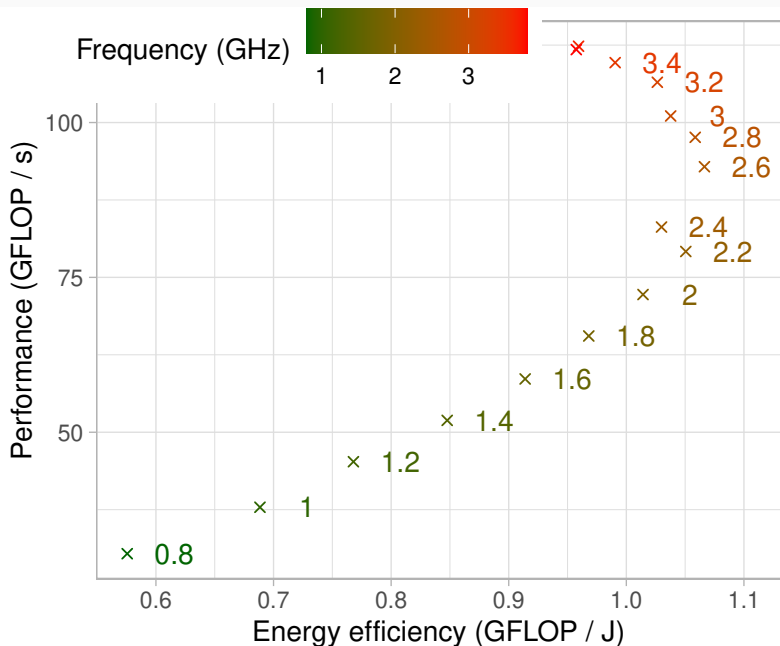
LLM success of smaller models (Llama, Chinchilla) fine-tuned for specific tasks with LoRA.

- Inference cost grows with model complexity
- Simpler models are often more interpretable
 - Traditional science also prefers simpler models
- DNN not necessary for all tasks

DVFS study of LU decomposition



When accounting for the whole system



Need for an interdisciplinary discussion

- AI / HPC can contribute towards sustainability (eg. acceleration of weather forecast models) ... **but its energy cost must be reduced**
- **Efficiency:**
 - Improve hardware and software
 - Use smaller models / smaller precision
- ... subject to rebound effects
- **Frugality in computing:**
 - Balance computation cost vs. outcomes for each task
 - Choose the right sized model
 - Assess the environmental impact

Treatment of febrile children illnesses in dispensaries.

- IMCI: Paper-based decision tree WHO
- e-POCT CART tree tailored to real data on a standalone tablet
 - Final CART tree easy to interpret and manually checked
 - Randomized-trial → better clinical outcomes and antibiotic prescription reduction
- Sophisticated AI that continuously collects patient data and adapts the algorithm ?
 - Increase in hardware and computation costs.
 - Loss in explainability and verification of the algorithm.

- S. Boehm Optimizing, How to Optimize a CUDA Matmul Kernel

References - Environmental impact of computation

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