L5: HPC for AI applications & Environmental impact of computation

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2. Introduction to AI applications
3. Environmental impact of computation
4. Energy consumption of HPC
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6. More frugal computing?

HPC for AI & Environmental impact of computation

Introduction to AI applications

AI Renaissance: Neural Networks

- 2012: **AI renaissance** brought by increased data availability and computation ressources
  - 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**

Objectives

- 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

- Neural networks are composed of layers of neurons
- Each neuron computes a weighted sum of its inputs followed by a non-linear activation function f

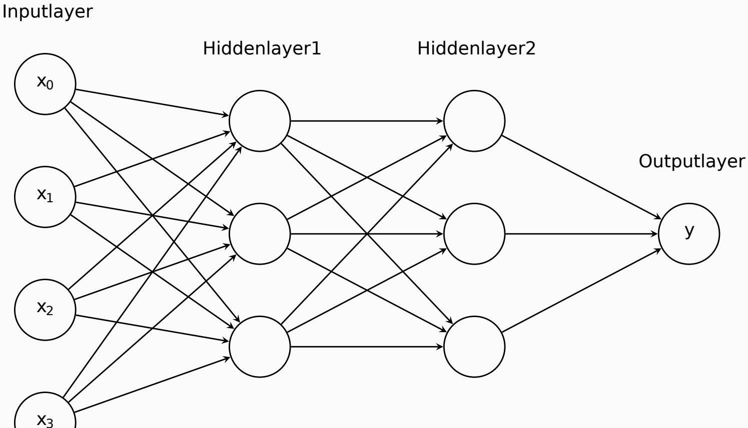
$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \rightarrow \textbf{neuron} \rightarrow y$$

$$y = f\left(\sum_i w_i x_i + b\right)$$

- Common activation functions: ReLU, sigmoid, ...
- **Perceptron**: single layer of neurons (1958 Rosenblatt)

Architectures

- Different architectures for different tasks:
  - Fully connected layers
  - Convolutional layers
  - Recursive layers
  - Transformers (attention mechanism)



Inference

- Inference: use the trained model to make predictions on new data
- Forward pass through the network:
  - For each layer, compute the weighted sum and apply activation function
  - The weighted sum is a matrix-vector multiplication for fully connected layers and convolutions (often implemented as GEMM).

Two layer network

Layer 1:

- X: input data [K × B] → K features, B batch size
- W_1: weights [H × K] → H hidden units
- b_1: bias [H × 1]

Layer 2:

- W_2: weights [O × H] → O outputs
- b_2: bias [O × 1]

ReLU $f(x) = max(0, x)$, $f'(x) = 1_{x>0}$

Forward inference

- Layer 1 Pre-activation hidden (GEMM, H×K × K×B → H×B)

$$Z_1 = W_1 \cdot X + B_1$$

- Layer 1 Activation - ReLU (elementwise)

$$H = f(Z_1)$$

- Layer 2 Output pre-activation (GEMM, O×H × H×B → O×B)

$$Z_2 = W_2 \cdot H + B_2$$

- Layer 2 Activation - ReLU (elementwise)

$$Y = f(Z_2)$$

- Forward is dominated by the two large GEMMs Z1 and Z2.

Training

- Training: adjust weights W and biases b to minimize a loss function L over a training dataset
- Use **backpropagation** to compute gradients on each layer (chain rule)
- Example with one neuron and MSE loss:

$$y = f(w_1 x_1 + w_2 x_2 + b)$$

$$L = (y - y_{true})^2$$

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial y} \cdot \frac{\partial y}{\partial w_1} = 2(y - y_{true}) \cdot f'(w_1 x_1 + w_2 x_2 + b) \cdot x_1$$

- Backward pass can be efficiently implemented using automatic differentiation and matrix multiplications.

Stochastic Gradient Descent

- Use **stochastic gradient descent** to update weights:

$$w_1 \leftarrow w_1 - \eta \cdot \frac{\partial L}{\partial w_1}$$

$$w_2 \leftarrow w_2 - \eta \cdot \frac{\partial L}{\partial w_2}$$

$$b \leftarrow b - \eta \cdot \frac{\partial L}{\partial b}$$

- η is the learning rate
- Repeat for many epochs over the training dataset

Training

1. Forward pass to compute H and Y
2. Compute loss $L(Y, Y_{true})$
3. Backward pass to compute gradients.

The backward pass is also dominated by GEMMs.

Frameworks

- Popular frameworks: TensorFlow, PyTorch, JAX, ...
- High-level APIs for defining models, automatic differentiation, GPU acceleration

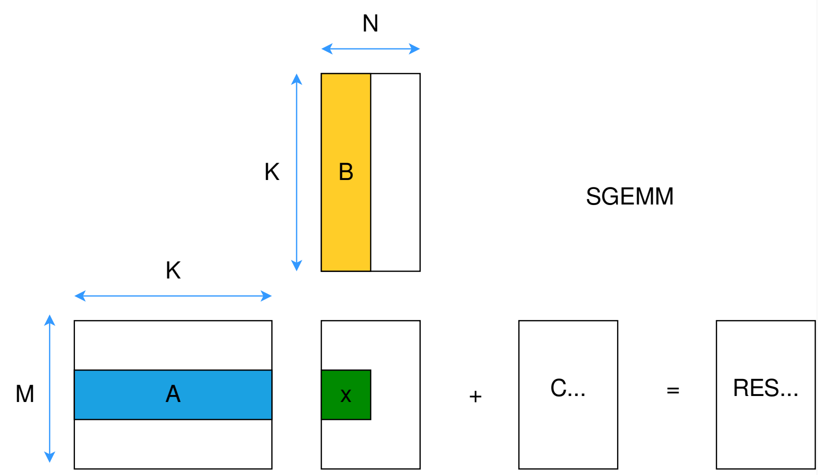
```
# Simple 2-layer NN in PyTorch
import torch
import torch.nn as nn

class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.fc1 = nn.Linear(28*28, 512)
        self.fc2 = nn.Linear(512, 10)

    def forward(self, x):
        x = torch.flatten(x, 1)
        x = torch.relu(self.fc1(x))
        x = torch.relu(self.fc2(x))
        return x
```

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

Locality issues in naive SGEMM

order in memory $\rightarrow$

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

- 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 → 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` → 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

Vectorization

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
    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
```

Problems with (i,k,j) ordering

- 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

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

```c
#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];
```

Parallelization

- 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

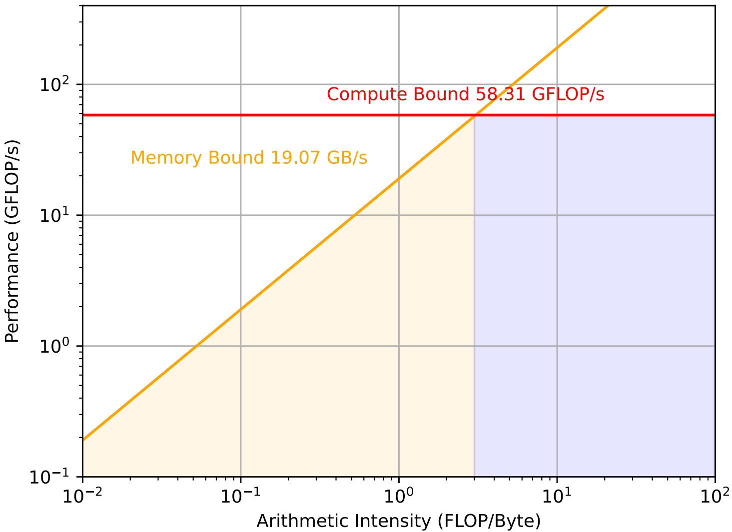
Libraries & autotuners

- 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.

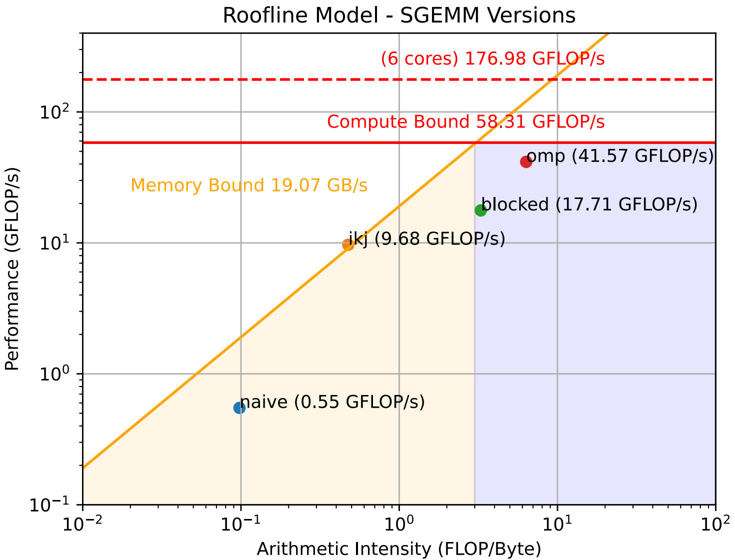
Roofline model - Definitions

- 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)

Environmental impact of computation

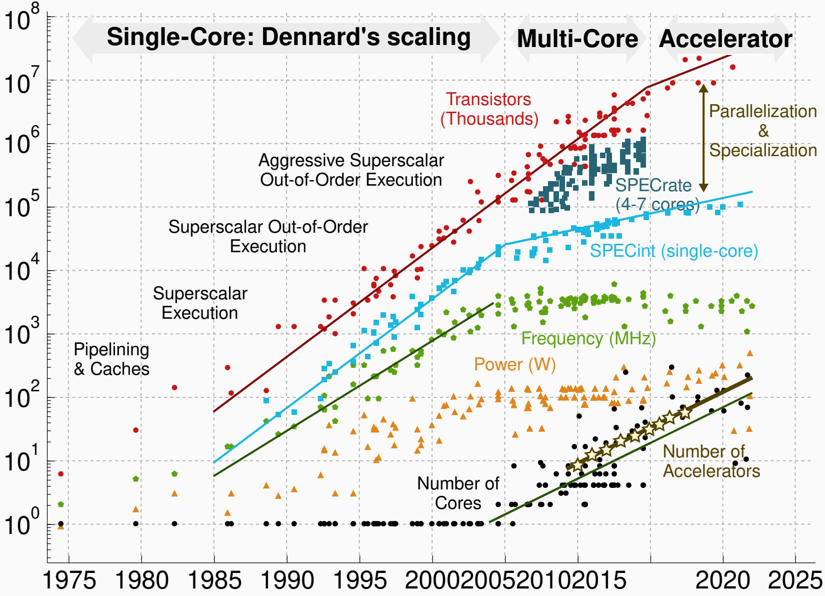
- The ICT sector consumes $\approx$ **5% of the energy** wordwide
- It accounts for **1.8% - 2.8%** of emitted GHG [Freitag, 2021]:
  - Accounts for embodied emissions.
  - Shadow energy during the **whole life-cycle: mining, fabrication, transportation, recycling**.
- GHG emmissions are only one of 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 ressource**
- Decarbonation $\rightarrow$ 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]



C. Batten, M. Horowitz, F. Labonte, O. Shacham, K. Olukotun,L. Hammond, K. Rupp & [Y. Shao, IEEE Micro'15] & [C. Leiserson, Science'20]

Dennard's scaling 1970-2005

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

Multicore 2005-2020

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

AI Accelerators 2020-2024

- 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

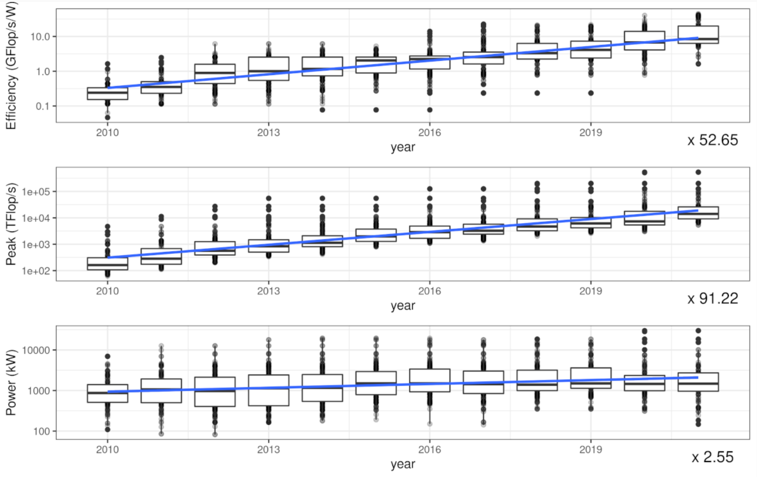


Figure 7: Evolution of TOP 100 systems

Efficiency and Peak computation exponential increase.

Rebound effects

- In 1865, Jevons shows that steam engine improvements translate into increased coal consumption.
- In HPC, efficiency gains contribute to the rising computation demand.
  - **net increase of the total power consumption.**
- Rebound effects for data-centers [Masanet, 2020]
  - 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]

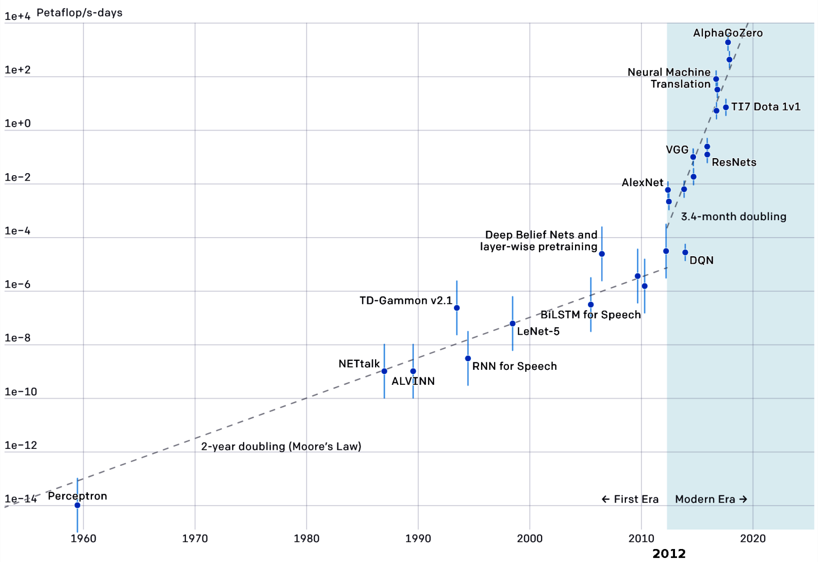
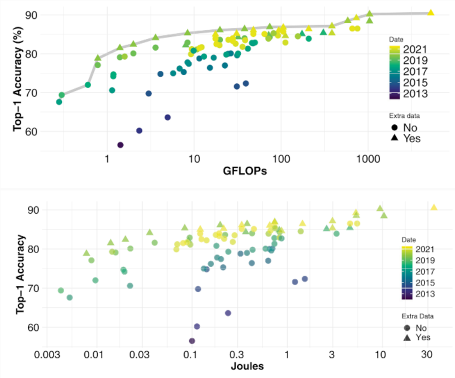


Figure 8: OpenAI, 2020

Should we study training or inference?

- **Training**: huge cost but done once
  - GPT3, 175 billion parameters, $\approx$ 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



Exponential increase in compute for linear accuracy gain
[Desislavov, 2023 / Schwartz, 2019]

More frugal computing?

Smaller precision / Smaller models for AI

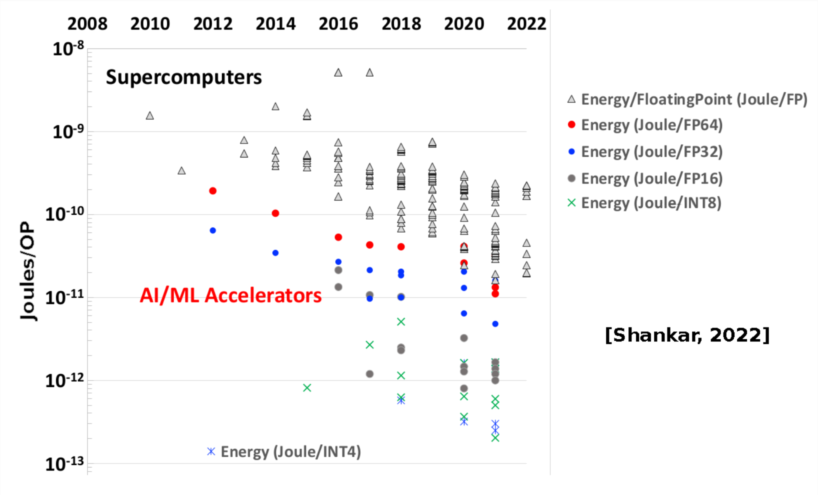


Figure 9: Shankar 2022

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

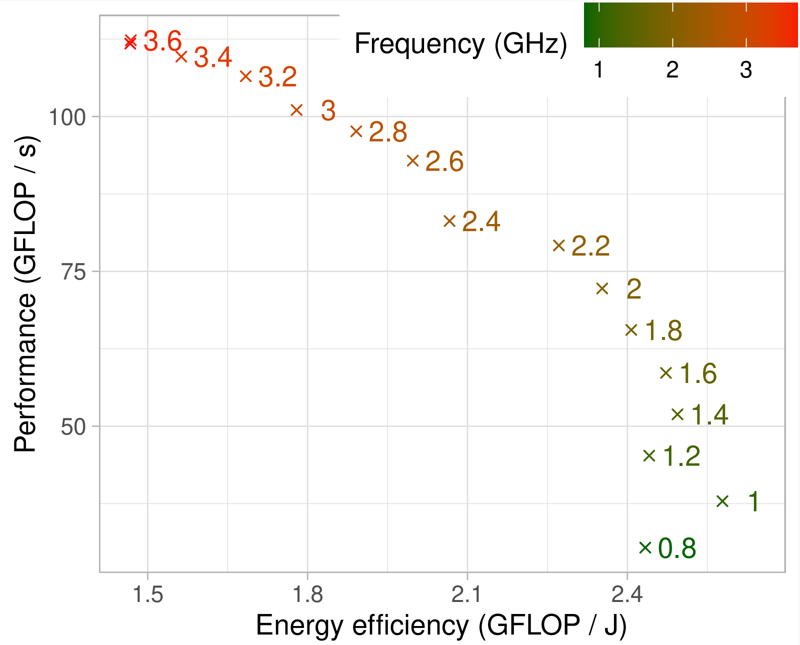
Tradeoff: Model complexity - Cost - Explainability

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

- Knights Mill 72 cores
- Intel MKL dgetrf
- $n \in [1000, 3000]$
- RAPL estimation

(Thomas Roglin, M1 UVSQ/INTEL internship 2023)

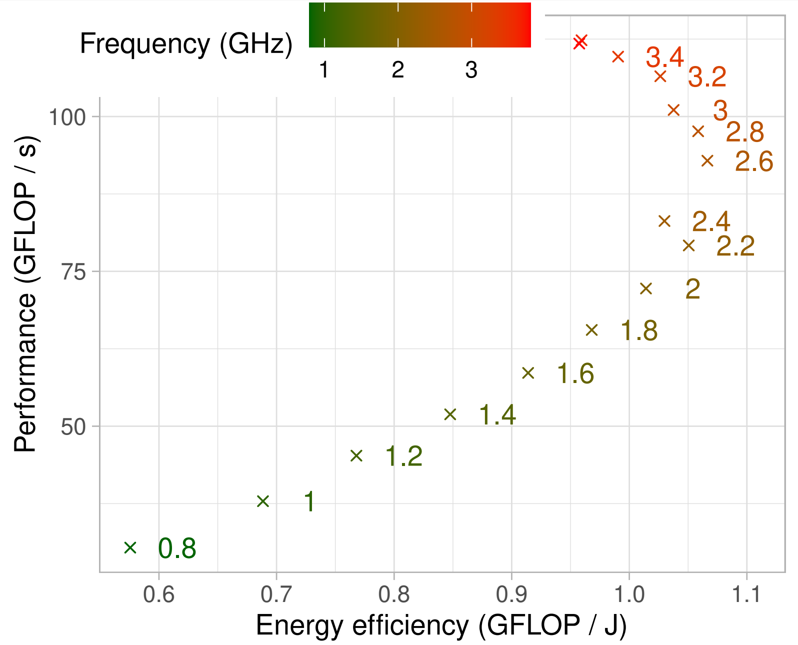
Save energy by computing slower: 1GHz



When accounting for the whole system

- Model: RAPL + **40W**
- System power dominates at low frequencies

Race to idle: 2.6 GHz compute faster and turn off machine



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

Exemple: e-health solution in Tanzania [d'Acremont, 2021]

Treatment of febrile children illnesess 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 $\rightarrow$ 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.

References - HPC for AI applications

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References - Environmental impact of computation

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