

L5: HPC for AI applications & Environmental impact of computation

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2. Introduction to AI applications
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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

Short introduction to Neural Networks

- 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

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

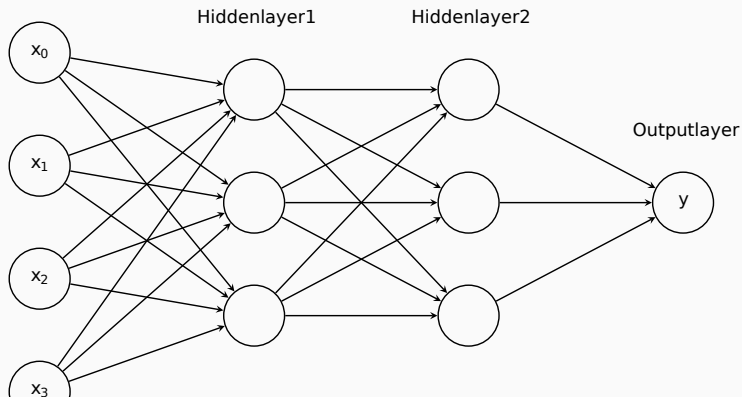
$$y = f \left(\sum_i w_i x_i + b \right)$$

- 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)

Inputlayer



- 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 $[K \times B] \rightarrow K$ features, B batch size
- W_1 : weights $[H \times K] \rightarrow H$ hidden units
- b_1 : bias $[H \times 1]$

Layer 2:

- W_2 : weights $[O \times H] \rightarrow O$ outputs
- b_2 : bias $[O \times 1]$

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

Forward inference

- Layer 1 Pre-activation hidden (GEMM, $H \times K \times K \times B \rightarrow H \times B$)

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

- Layer 1 Activation - ReLU (elementwise)

$$H = f(Z_1)$$

- Layer 2 Output pre-activation (GEMM, $O \times H \times H \times B \rightarrow O \times B$)

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

- Layer 2 Activation - ReLU (elementwise)

$$Y = f(Z_2)$$

- Forward is dominated by the two large GEMMs Z_1 and Z_2 .

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:

$$y = f(w_1x_1 + w_2x_2 + b)$$

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

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial y} \cdot \frac{\partial y}{\partial w_1} = 2(y - y_{true}) \cdot f'(w_1x_1 + w_2x_2 + b) \cdot x_1$$

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

- 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

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.

- 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

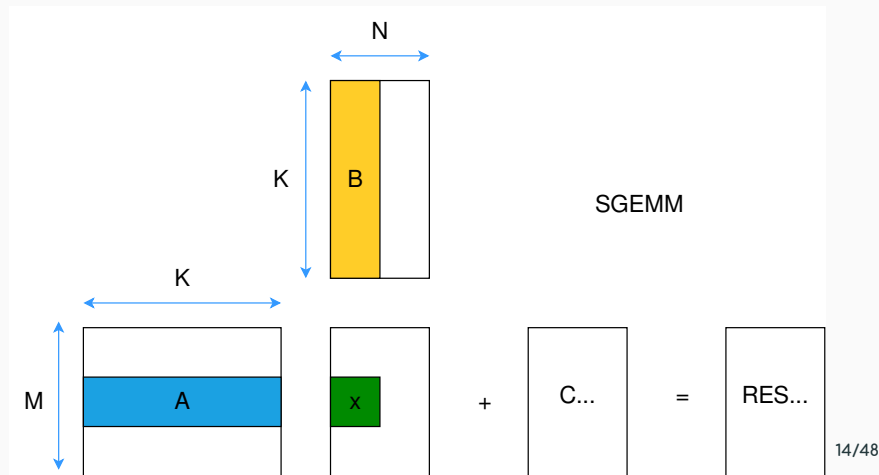
class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.fc1 = nn.Linear(28*28, 512)
        self.fc2 = nn.Linear(512, 10)

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

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

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 given (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 $\geq N \times 4B$
 - BAD: For a given (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

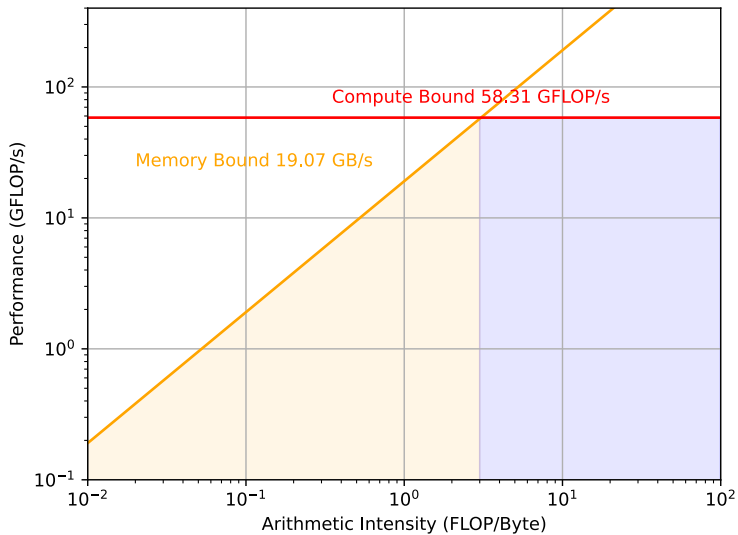
```
#pragma omp parallel for collapse(3)
for (ii = 0; ii < M; ii += BS)
    for (jj = 0; jj < N; jj += BS)
        for (kk = 0; kk < K; kk += BS)
            // Block multiplication as before
```

- 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

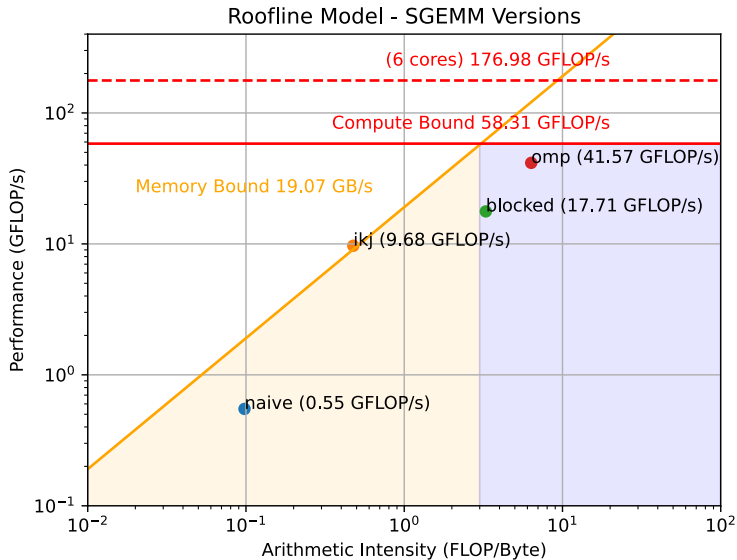
- Highly optimized SGEMM implementations exist:
 - OpenBLAS, Intel MKL for CPU
 - NVIDIA cuBLAS for GPU
- Implementations use blocking, vectorization, parallelization, and many architecture-specific optimizations
- Libraries are carefully tuned for different sizes and shapes of matrices.
- Autotuners (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

- 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)



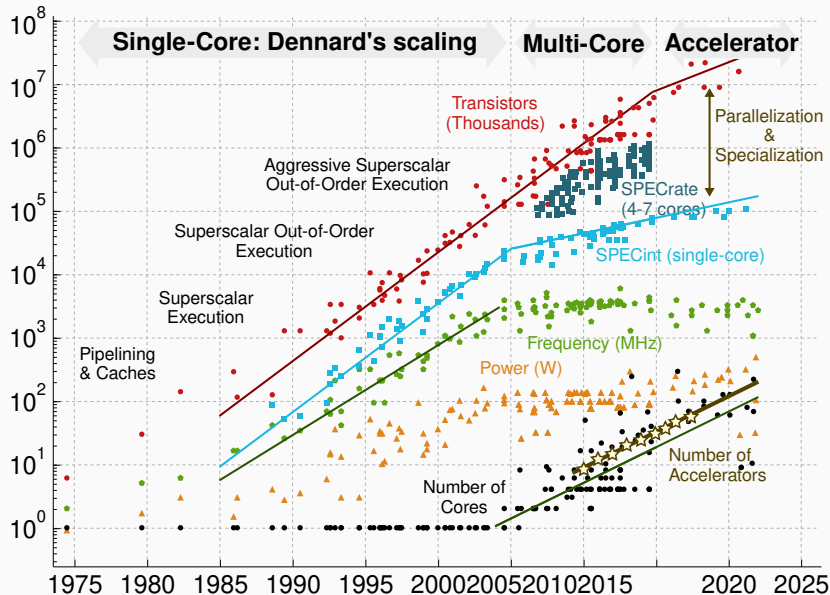
- The ICT sector consumes $\approx 5\%$ of the energy worldwide
- It accounts for **1.8% - 2.8%** of emitted GHG [Freitag, 2021]:
 - Accounts for embodied emissions.
 - Shadow energy during the whole life-cycle: mining, fabrication, transportation, recycling.
- GHG emissions are only one of the sustainability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



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

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} \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.

- 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

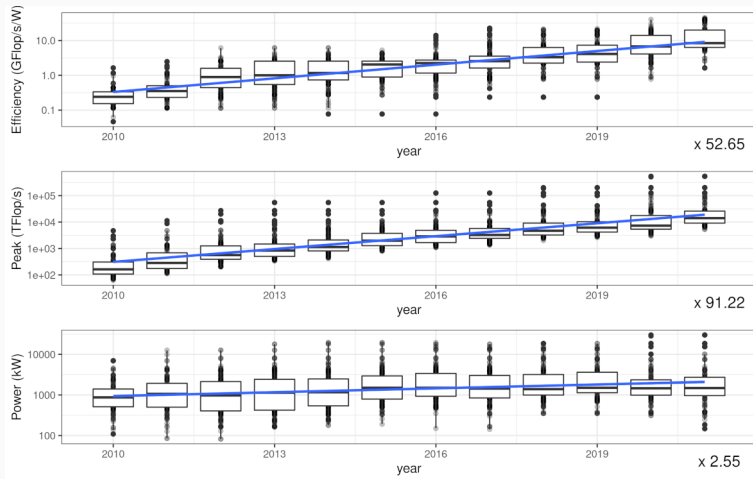


Figure 7: Evolution of TOP 100 systems

Efficiency and Peak computation exponential increase.

- 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]

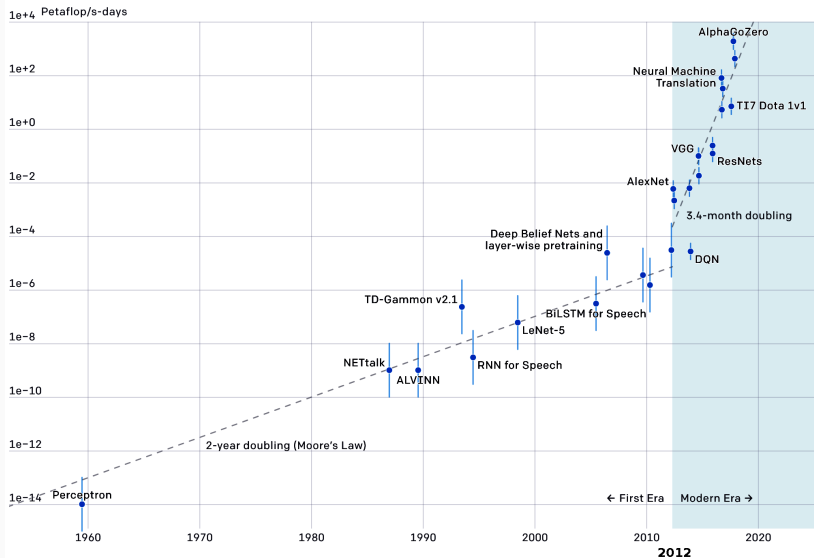
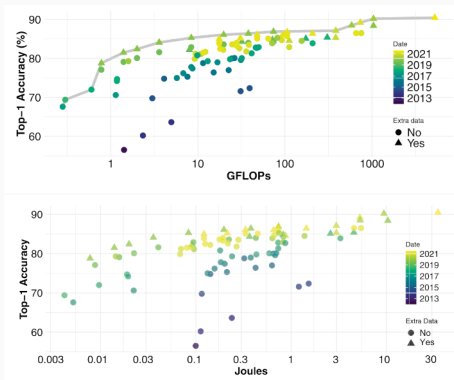


Figure 8: OpenAI, 2020

Should we study training or inference?

- **Training:** huge cost but done once
 - GPT3, 175 billion parameters, ≈ 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

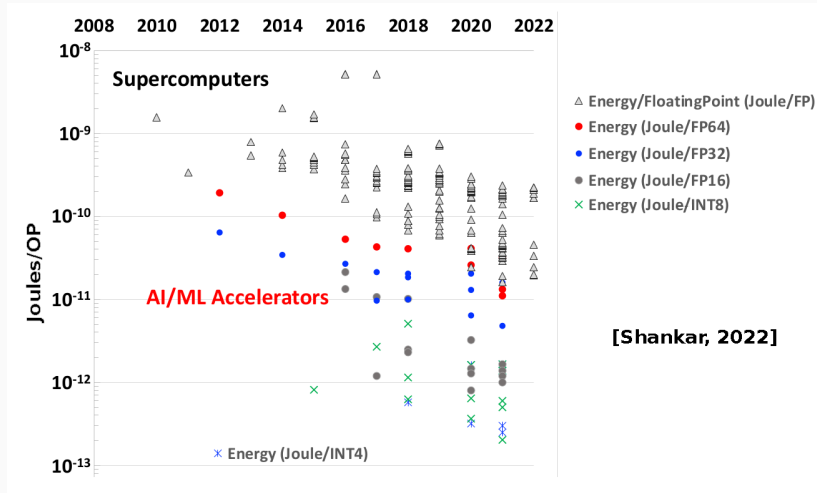


Figure 9: Shankar 2022

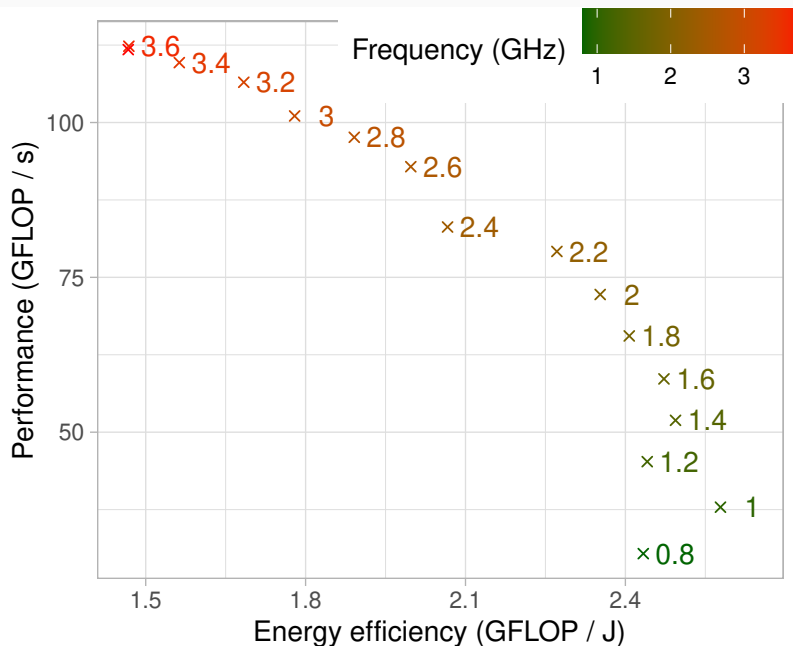
LLM success of smaller models (Llama, Chinchilla) fine-tuned for specific tasks with LoRA.

- 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

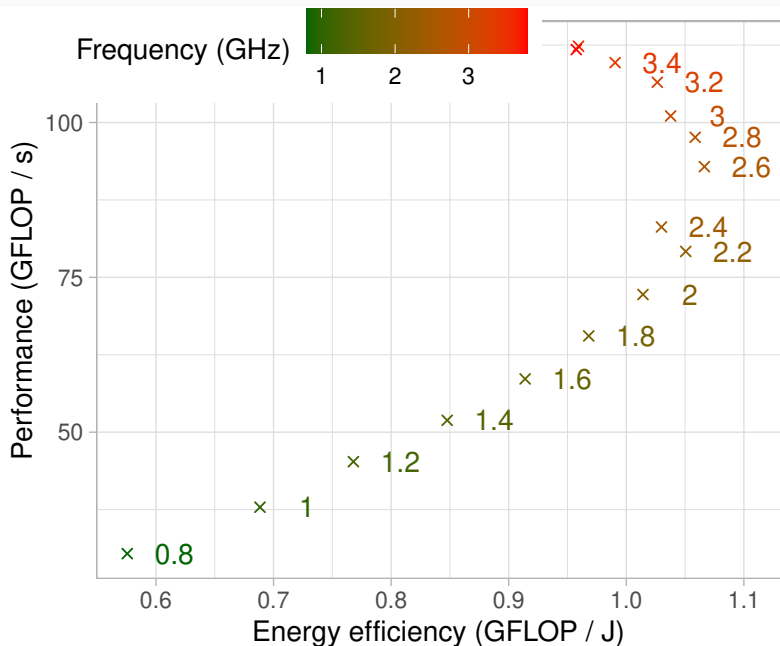
(Thomas Roglin, M1 UVSQ/INTEL internship 2023)

Save energy by computing slower: 1GHz



- 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

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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