



Programming Techniques for Supercomputers Tutorial

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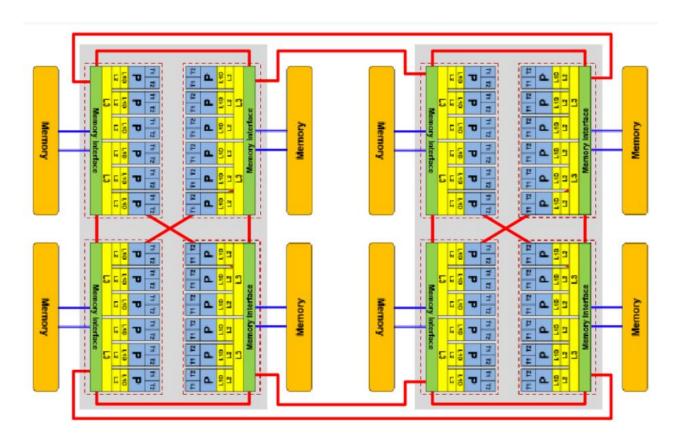
Sommersemester 2025



Scaling behavior a) Topology

2 sockets

- 4 ccNUMA domains per socket
- 8 ccNUMA domains total



Scaling behavior b) Memory Bandwidth

• We reach $\sim 260 [GB/s]$ with full node

To include write-allocates

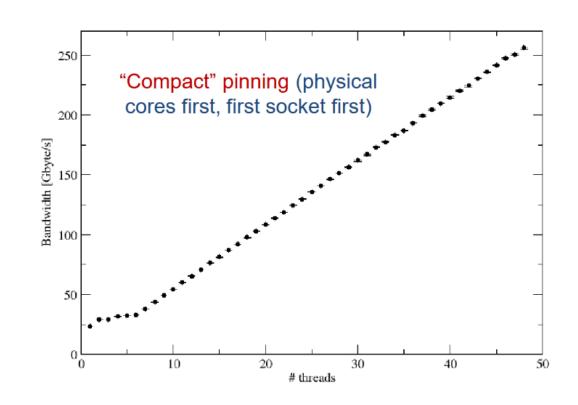
Our hardware capable of achieving

$$\boldsymbol{b_{s, Total}} = 260 * \left(\frac{4}{3}\right) \left[\frac{GB}{s}\right] \approx 347 \left[\frac{GB}{s}\right]$$

Each ccNUMA domain can achieve

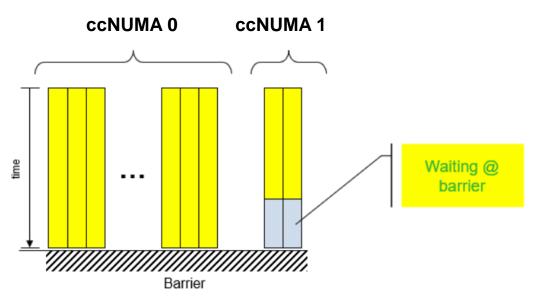
$$\boldsymbol{b_{s, ccNUMA}} = \frac{347}{8} \left[\frac{GB}{s} \right] \approx 43.4 \left[\frac{GB}{s} \right]$$

```
#pragma omp parallel for
for(int i=0; i<N; ++i)
   a[i] = b[i] + s * c[i];</pre>
```



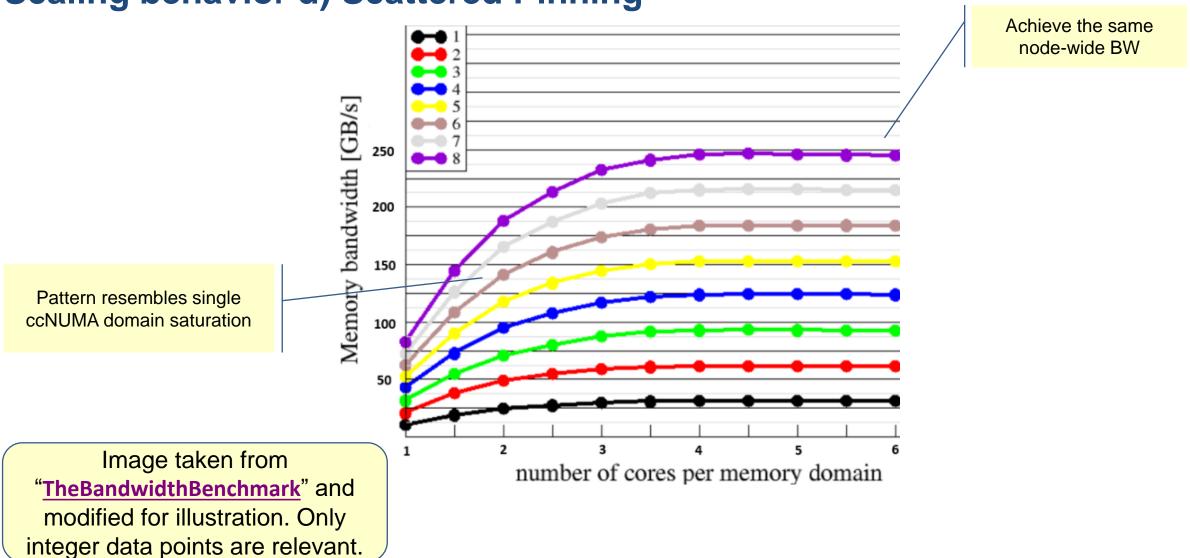
Scaling behavior c) Linear Scalaing

- 1. Every thread has the same workload
- 2. Left ccNUMA domain performance is saturated
- 3. Barrier enforces "speeders" to wait
 - Faster due to more available bandwidth
- Each new speeder contributes a "per-core performance" equal to the average per-core performance of the already-filled domain



Constant contributions => linear scalability

Scaling behavior d) Scattered Pinning



PTfS 2025 Tutorial - Assignment 10

Triangular parallel MVM

Parallelize outer loop to reduce OpenMP overhead

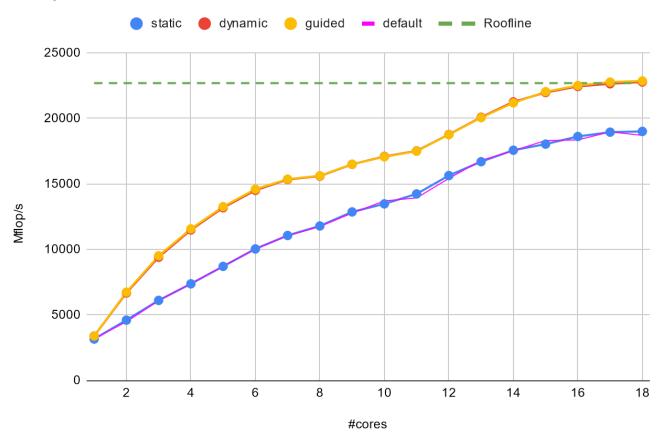
```
#pragma omp parallel private(i,k)
{
  for(k=0; k<niter; k++) {
    #pragma omp for schedule(runtime)
    for(j=0; j<size; ++j)
        for(i=0; i<=j; ++i)
        c[j]=c[j]+a[i+size*j]*b[i];
        if(c[size >> 1]<0.0) whatever();
    }
}</pre>
```

Non-default schedule to improve load balancing

Triangular parallel MVM

-Ofast -xHost -fno-inline -fno-alias -qopenmp

Mflop/s vs. #cores



Performance modeling of a 3D Jacobi smoother

```
#pragma omp parallel private(iter)
 for(iter=0; iter<maxiter; ++iter) {</pre>
    #pragma omp for schedule(runtime) private(j,i)
    for (k=1; k< N-1; ++k) {
      for(j=1; j<N-1; ++j) {
        for(i=1; i<N-1; ++i) {
          f[t1][k][j][i] = 1./6. * (f[t0][k-1][j][i]+ f[t0][k+1][j][i]+
                                     f[t0][k][j-1][i]+ f[t0][k][j+1][i]+
                                     f[t0][k][j][i-1]+ f[t0][k][j][i+1]);
    #pragma omp single
      swap(t0,t1);
```

Performance modeling of a 3D Jacobi smoother b) Data Layout

- Swap from f[t][k][j][i] -> f[k][j][i][t]?
- Problem 1: Read and write streams are interleaved
 - ALL cache lines are modified
 - RHS data must be read, and then written to memory again!
- Problem 2: Poor SIMD utilization
 - Requires shuffling around data in SIMD registers

Performance modeling of a 3D Jacobi smoother c) Performance

•
$$b_S = 41 \left[\frac{GB}{S} \right]$$
, $(L3\$)$ $CS = 25 \left[MiB \right]$ — L2 not considered on IVB (inclusive \$)

■
$$N = 350 \rightarrow (2 \times 350^3 \times 8)[B] = 686 [MB] \rightarrow \text{out-of-cache working set}$$

• LC:
$$10 \times 350^2 \times 3 \times 8 [B] = 29.4 [MB] > CS/2$$

- LC broken in L3 \rightarrow $B_c = 40 [B/LUP]$
- $P = b_s/B_c = 1025 [MLUP/s]$

Only hold 10+2 layers total!

- OMP_SCHEDULE = static,1
 - L3\$-LC: $(10 + 2) \times 350^2 \times 8[B] = 11.8[MB] < CS/2$
 - LC holds in L3 \rightarrow $B_c = 24 [B/LUP]$
 - $P = b_s/B_c = 1708 [MLUP/s]$

