703308 VO High-Performance Computing
The 13 Dwarfs of HPC

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Overview

- The 13 Dwarfs of HPC
  - abstract application categories

Motivation

- MPI API or concepts such as data vs. task parallelism are still pretty low-level characteristics of parallel programs

- we need to be able to recognize higher-level classes of HPC applications and discuss them

- this lecture presents the most prominent classes of HPC applications
  - many new applications you encounter will fit into these categories or are a combination of them

How and why are dwarfs defined?

- group applications by similarity in computation and data structures
  - first published by Asanovic et al in *The Landscape of Parallel Computing Research: A View from Berkeley*
  - https://www2.eecs.berkeley.edu/Pubs/TechRpts/2006/EECS-2006-183.pdf

- purely algorithmic, implementation-independent
  - enables cross-platform reasoning and cross-application knowledge/resource sharing (e.g. libraries)

- serve as small, abstract, high-level benchmarks for studying new
  - programming models
  - communication patterns
  - hardware architectures, topologies
  - …

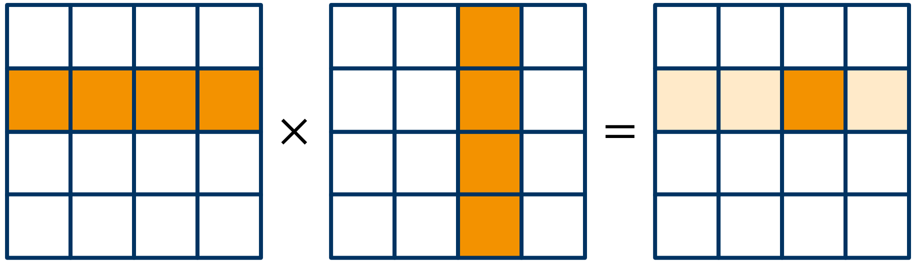
- used to kick off innovation in all of these aspects

7 original dwarfs of HPC

What are we going do discuss?	What have you already heard?
1. Dense Linear Algebra	matrix mul (first MPI lecture)
2. Sparse Linear Algebra	
3. Spectral Methods	
4. N-body Methods	N-body
5. Structured Grids	heat stencil
6. Unstructured Grids	
7. Monte Carlo Methods	Monte Carlo π

Dense linear algebra

- data is stored in densely-populated matrices (or vectors)
  - data is stored uncompressed (“as is”)
  - data access via strides, often unit stride



- e.g. matrix multiplication, LU decomposition, Gauss-Seidel, …
- rarely done manually, there are a TON of libraries out there

Dense linear algebra: characteristics

- naïve implementations usually memory bound
  - remember: memory wall!
  - caches and prefetching helps
- simple but significant data structure
  - stride often enables/prevents vectorization (SIMD)
  - fastest-changing index affects cache efficiency (hence matrices are often transposed)
- still the default measure for performance in HPC
  - e.g. TOP500 uses HPL, a high performance LINPACK benchmark
  - but nowadays not the only one (e.g. HPCG)

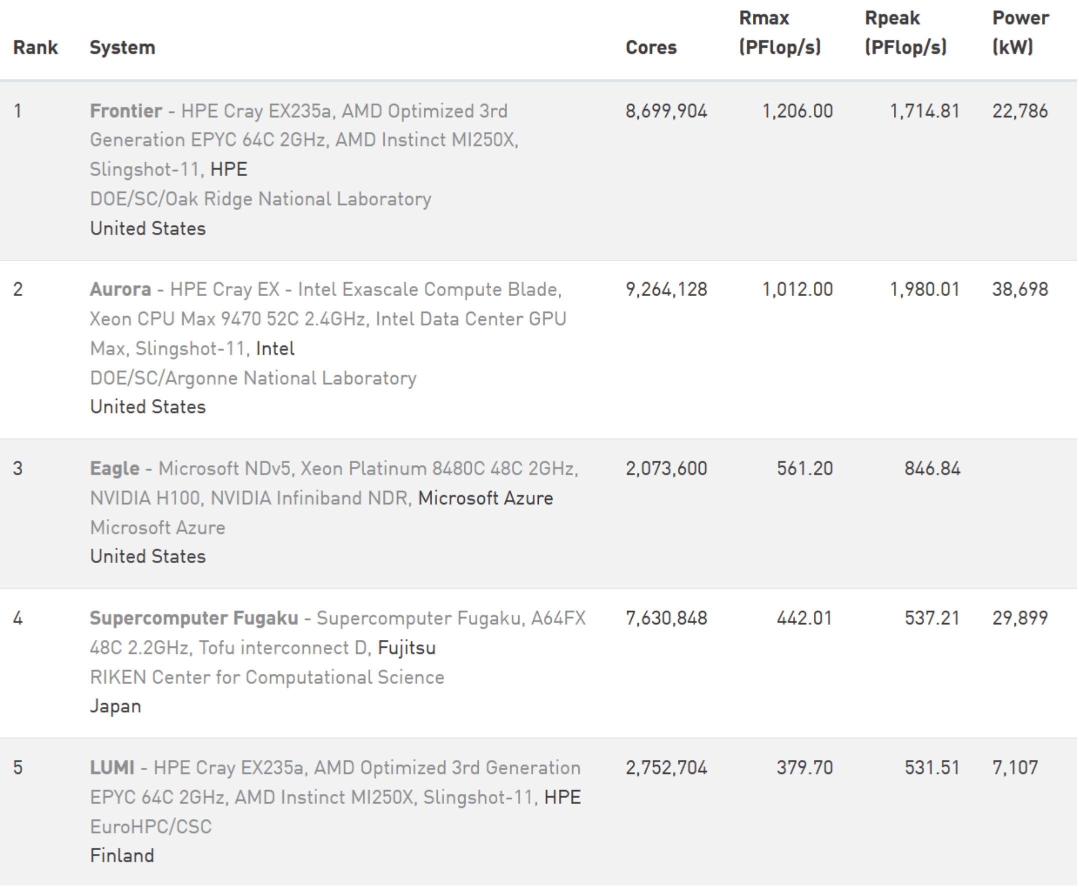
```
for (int i = 0; i < N; ++i) {
  for (int j = 0; j < N; ++j) {
    double tmp = 0.0;
    for (int k = 0; k < N; ++k) {
      tmp += A[i][k] * B[k][j];
    }
    result[i][j] = tmp;
  }
}
```

```
vgatherqpd ymm0{k2}, [rax+ymm5*1]
vmulpd  ymm0, ymm0, YMMWORD PTR [rdx+rdi]
...
```

Side note: TOP500 list: Rmax vs. Rpeak

- Rmax: achieved by software
  - high performance linpack (HPL) benchmark
  - linear algebra stress-testing

- Rpeak: achievable by hardware
  - product of: number of FP units per CPU, their FP instructions per cycle, clock frequency, and number of CPUs



Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,206.00	1,714.81	22,786
2	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	9,264,128	1,012.00	1,980.01	38,698
3	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	
4	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
5	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,752,704	379.70	531.51	7,107

Taken from the June 2024 list of the Top500

Dense linear algebra: optimizations

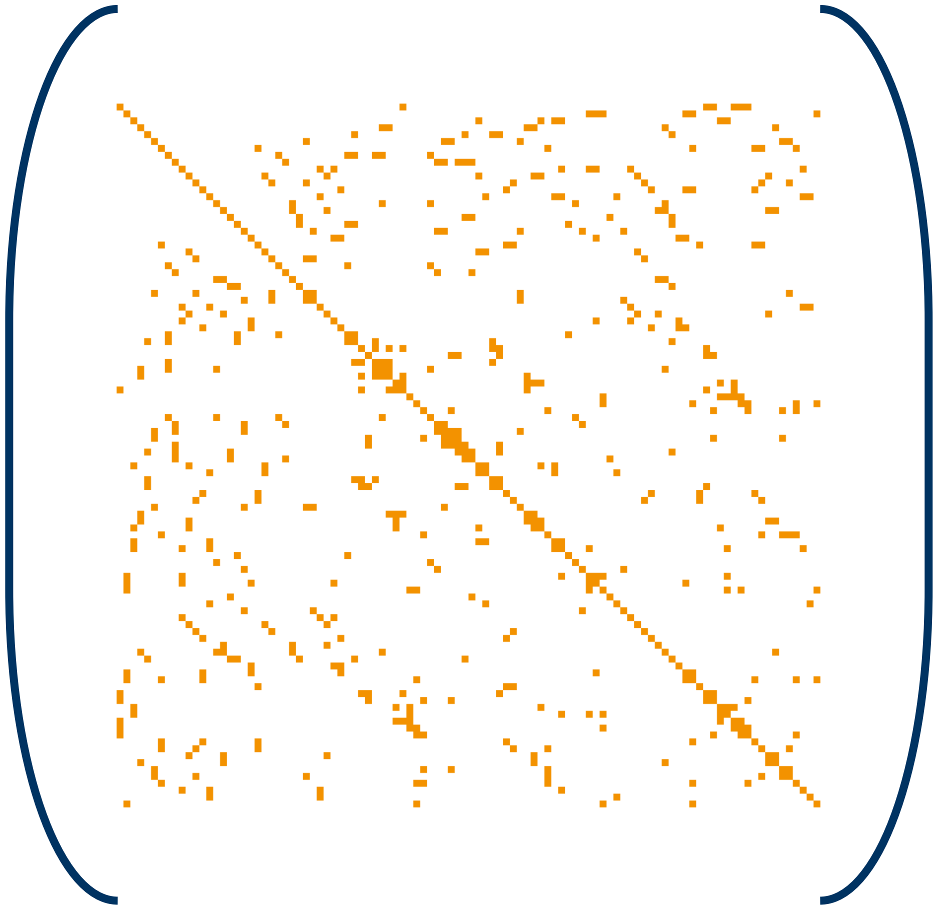
- loop blocking or tiling
  - do not work on single elements but smaller blocks (e.g. 2x2 or 32x32)
  - exploits locality and cache
  - also, lots of other HOTs (Higher Order Transformations)
- vectorization (SIMD, e.g. SSE/AVX)
  - might entail modifications, e.g. transposing matrix A or B in matrix mul
- hardware-specific instructions
  - e.g. fused multiply-add (FMA)

```
for (int ii = 0; ii < N; ii += ib) {
 for (int jj = 0; jj < N; jj += jb) {
  for (int k = 0; k < N; ++k) {
   for (int i = ii; i < ii+ib; ++i) {
    for (int j = jj; j < jj+jb; ++j) {
      // ... process single tile
    }
   }
  }
 }
}
```

Sparse linear algebra

- data is stored in sparsely-populated matrices (or vectors)
  - (vast) majority of data is zero
  - data is stored in compressed format
  - data often accessed indirectly via indices

- e.g. conjugate gradient, Google’s PageRank, data mining



Sparse linear algebra: characteristics

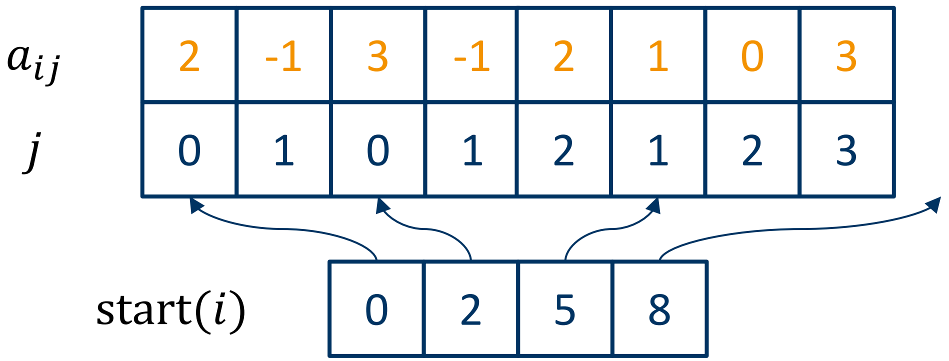
- computationally or memory limited
  - depends on sparsity of data, data structure representation and algorithm
- different data structures available
  - e.g. coordinate scheme (COO) or “triplet format” or similar: (i, j, a_{ij})
  - array of structs (AoS) vs. struct of arrays (SoA)
  - not necessarily sorted!

```
typedef struct sparseElement {
    int i; int j; double value;
} sparseElement;
sparseElement sparseMatrix[SIZE];
sparseMatrix[0].i = 0;

// ############## vs. ##############

typedef struct sparseMatrixT {
    int i[SIZE]; int j[SIZE];
    double values[SIZE];
} sparseMatrixT;
sparseMatrixT sparseMatrix;
sparseMatrix.i[0] = 0;
```

Sparse linear algebra: optimizations

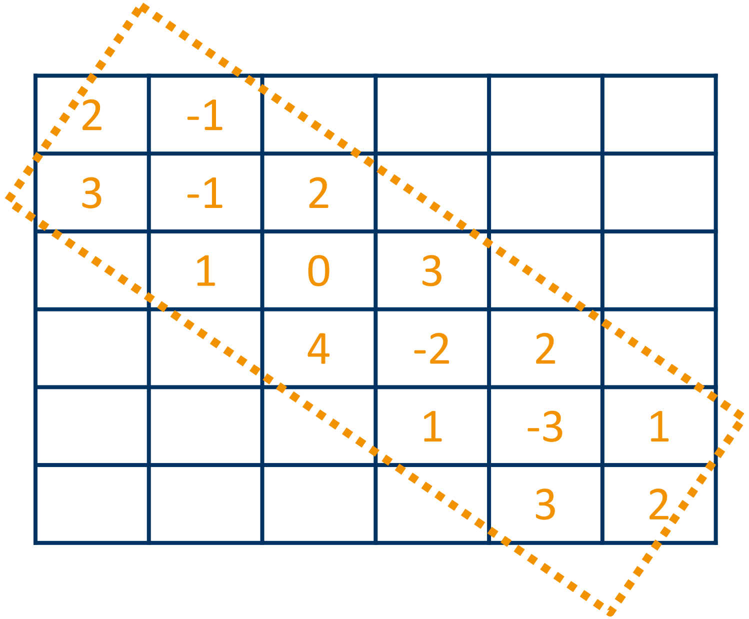
- compressed row storage (CRS)
  - two arrays of size N
  - one holds a_{ij}, the other j
  - third array points to start of row i in j
  - smaller memory footprint than COO
    - $2N + (m + 1)$ vs. $3N$

- variants
  - column-major variant (CCS)
  - store small blocks (2x2 or 4x4) instead of single elements, improves SIMDness
  - compressed diagonal storage (CDS)
    - use domain-specific knowledge!



a_{ij}	2	-1	3	-1	2	1	0	3
j	0	1	0	1	2	1	2	3

start(i)	0	2	5	8

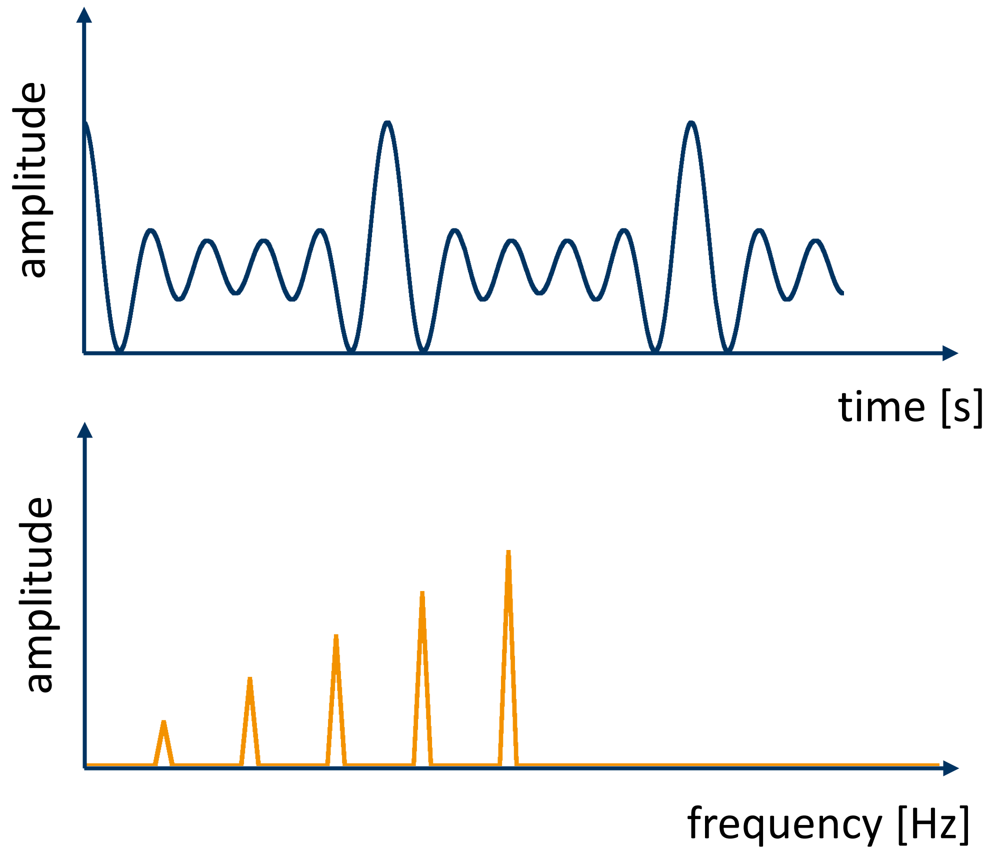


2	-1				
3	-1	2			
	1	0	3		
		4	-2	2	
			1	-3	1
				3	2

Spectral methods

- data in frequency domain, not time or space
  - can include multiple stages of computations alternating between local and global communication

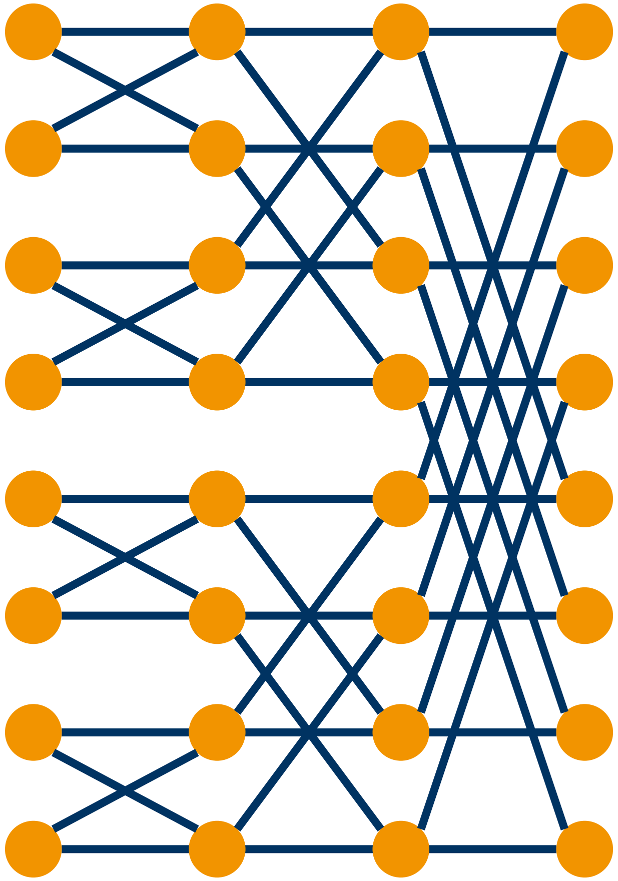
- e.g. fast Fourier transform (FFT), audio and video signal processing
  - e.g. “focus hunting” in contrast-based autofocus of photo/video cameras



Spectral methods: characteristics

- usually implemented using butterfly patterns
  - multiple stages of multiply-add
  - often latency limited due to global communication patterns (e.g. all-to-all)

- often resemble structured or unstructured grid methods after transformation to frequency domain



Spectral methods: optimizations

- requires optimization of the transformation to frequency domain
  - relies on transposing data efficiently

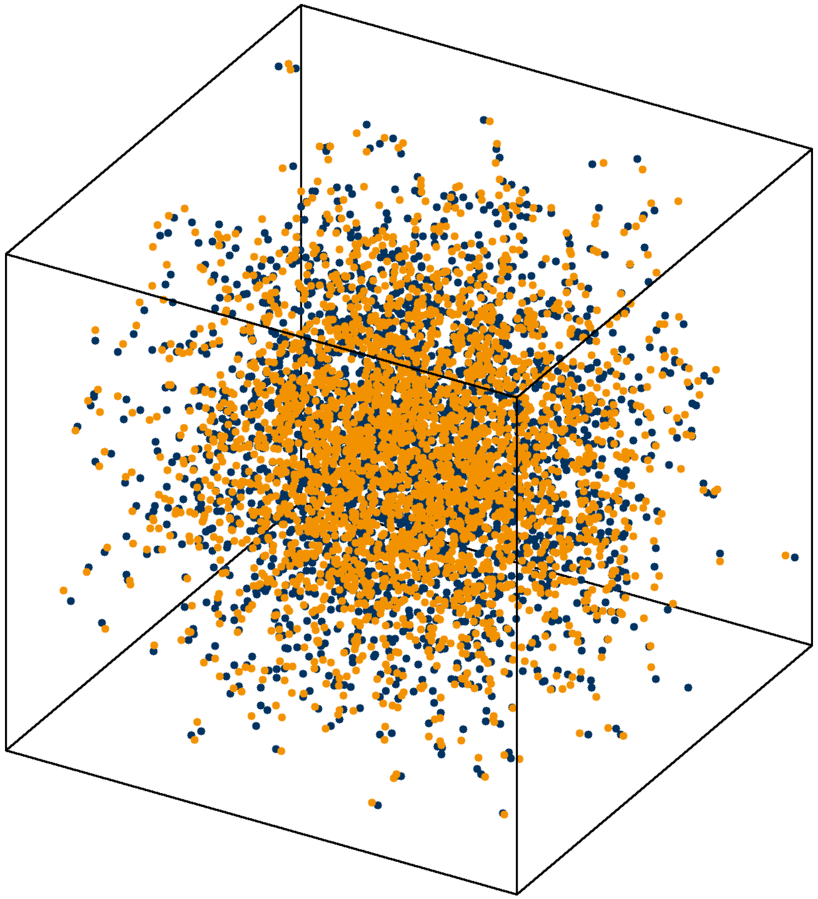
- afterwards, consider similar optimizations as for (un)structured grids

- severely restricted scalability on larger HPC systems
  - ongoing research
  - lots of it in math

N-body methods

- models interactions between discrete, moving points
  - often requires dynamic data structures
  - varying spatial locality
  - movement affects load balance and data access costs

- e.g. galaxy collision simulations, molecular dynamics, protein folding



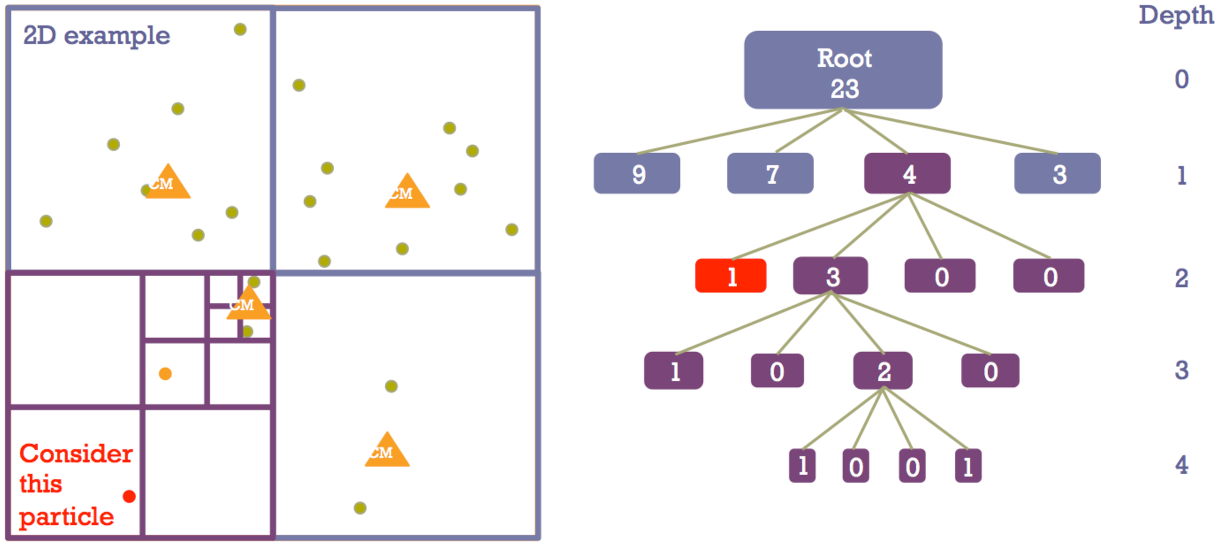
N-body methods: characteristics

- computational effort is an issue
  - $\mathcal{O}(N^2)$ for N particles
  - but also global communication
- lots of hierarchical optimization studies
  - domain decomposition!
  - e.g. Barnes-Hut or fast multipole optimization

- alternative approaches rely on domain-specific knowledge, e.g.
  - ignore long-distance particle interactions
  - store particles in Cartesian topology & only consider particles in neighboring grid cells

N-body methods: optimizations

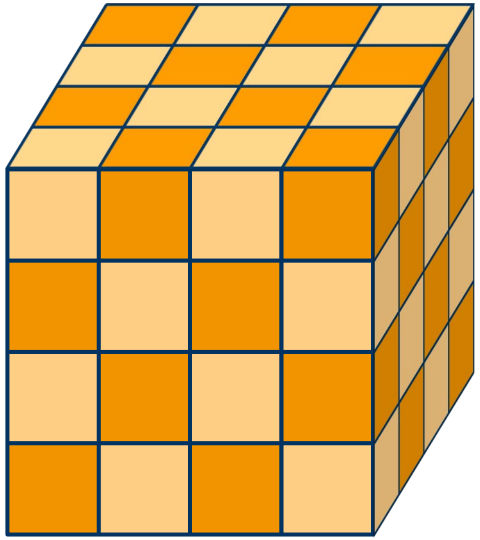
- Barnes-Hut optimization:
  - decompose domain into quadtree (for 2D)
  - aggregate particle effect (e.g. gravitation from mass) for each cell into a single (hypothetical) particle at the center of gravity per cell
  - reduces complexity from $\mathcal{O}(N^2)$ to $\mathcal{O}(N \cdot \log N)$



Structured grids

- model interactions between discrete, fixed points
  - grid structure described by pattern
  - topological information easily derived
  - usually high spatial locality
  - may be subdivided into finer grid ("adaptive")

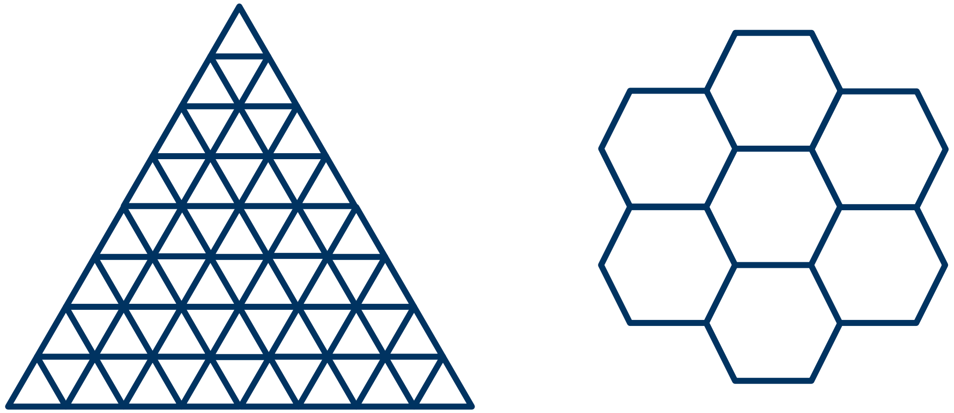
- e.g. heat transfer (stencil), computational fluid dynamics (CFD), octrees



Structured grids: characteristics

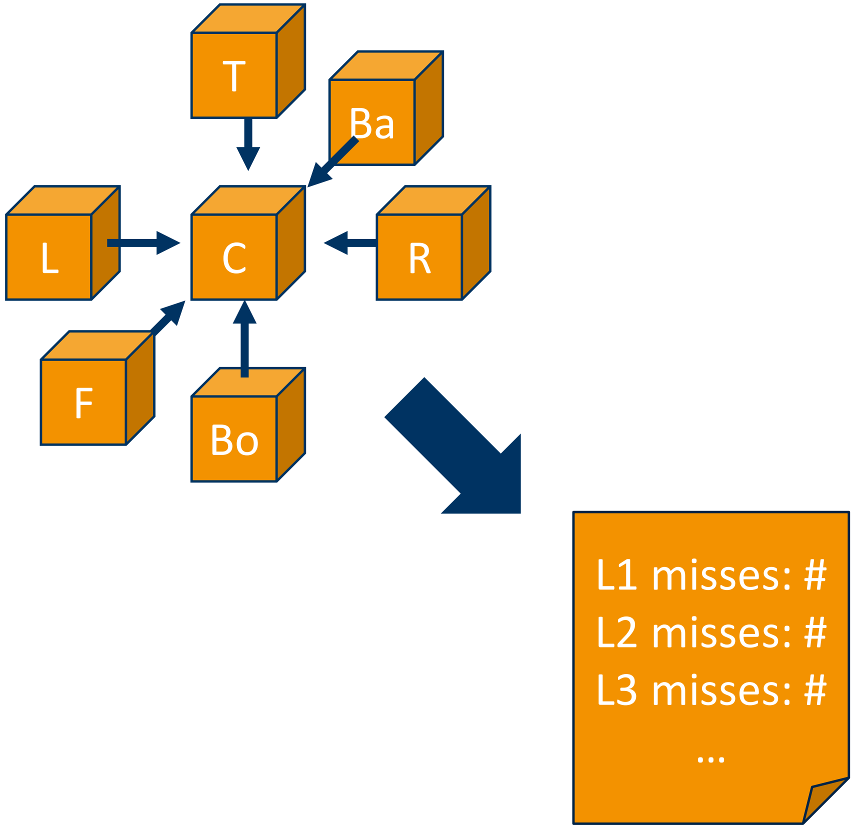
- structured nature is a key aspect
  - similar characteristics compared to dense linear algebra (e.g. row-major vs. column-major)
  - memory access patterns & addresses often predictable, facilitates e.g. prefetching
  - adaptive grids and multi-grids possible
- typically memory bound
  - e.g. 7-point stencil in 3D: load 7 data points for computing a new one
  - local communication only (ghost cell exchange with direct neighbor)

- structured grid does not imply rectangular!



Structured grids: optimizations

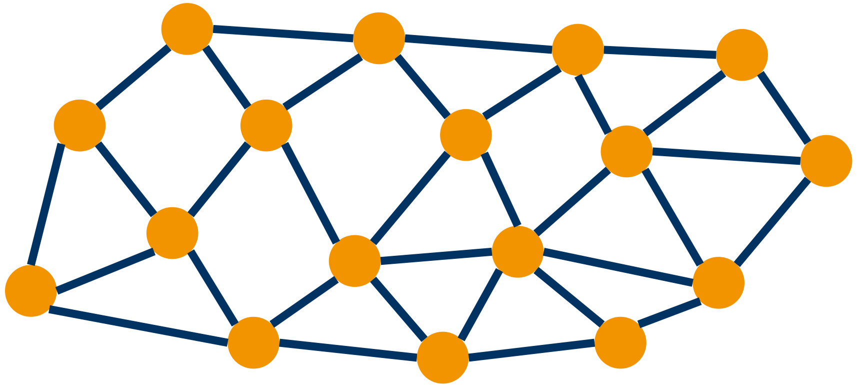
- decomposition, decomposition, decomposition
  - highly dependent on type of grid and specific use case
- structured nature of the problem makes analytic prediction possible
  - performance models and simulators for simple stencil kernels (e.g. Kerncraft)



L1 misses: #
L2 misses: #
L3 misses: #
…

Unstructured grids

- model interactions between discrete, fixed points
  - grid pattern described explicitly by individual connections
  - irregular geometry and topology
  - usually involves multiple levels of indirection when accessing data

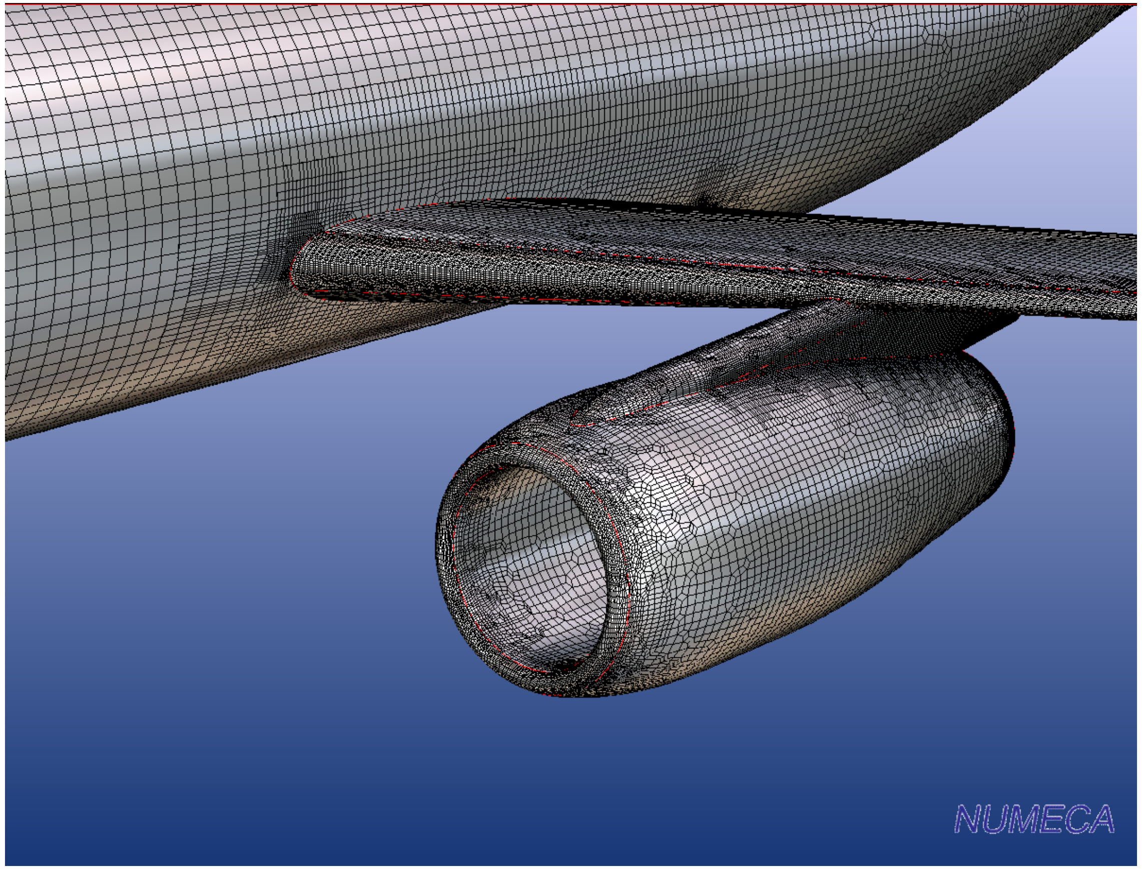


- e.g. computational fluid dynamics (CFD)

Unstructured grids: characteristics

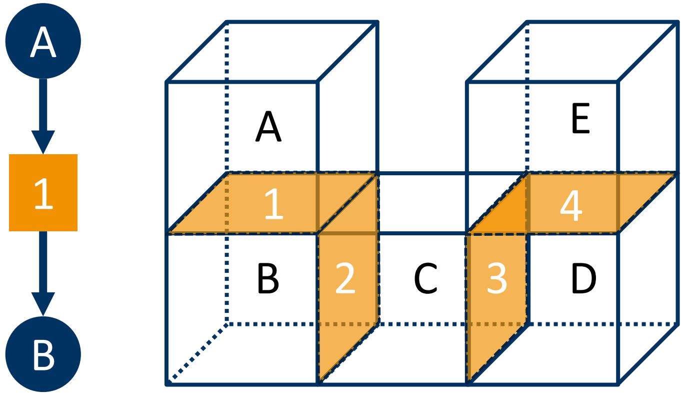
- usually heavily latency bound due to indirect access
  - … = `cells[neighbors[i]]`
  - … = `cell.getNeighbor(i)`
  - also known as “pointer chasing”

- similar problems compared to structured grids, e.g.
  - domain decomposition / adaptivity
  - topological information
  - ghost cell exchange
  - but hardly analytically predictable

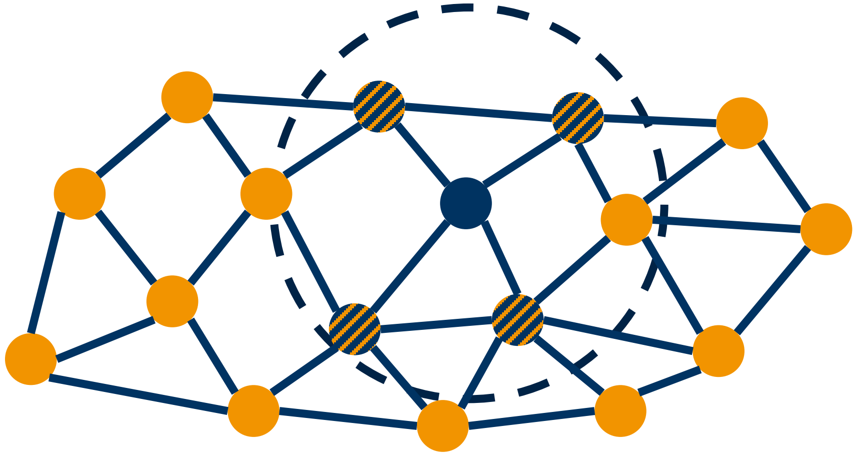


Unstructured grids: optimizations

- problem space discretization and topology
  - which types of grid elements?
  - which types of connections?
  - cells, faces, vertices, edges, …
  - should be efficient to load/store, navigate, and compute

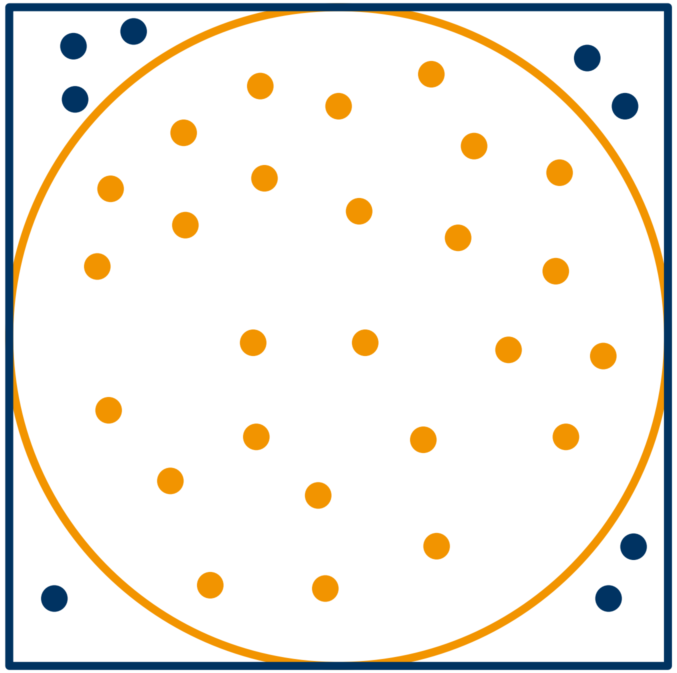


- decomposition, decomposition, decomposition
  - efficient ghost cell exchange required
  - efficient grid navigation e.g. to access neighbors



Monte Carlo methods

- also known as map-reduce
  - process data independently and merge the results
- models statistical evaluation of repeated random trials
  - communication usually insignificant
  - embarrassingly parallel, multiple copies of sequential method
- e.g. numerical integration, quantum many-body problems, ray tracing



Monte Carlo methods: characteristics

- parallelization almost a no-factor
  - similar to multiple sequential programs sharing some resources (e.g. L3 cache, random number generator, thermal envelope of CPU)
  - relatively inexpensive reduction
- depends heavily on sequential speed and shared bottlenecks

Monte Carlo methods: optimizations

- not much to do beyond sequential optimization
  - ILP
  - prefetching
  - vectorization
  - reduce resource contention
    (read: fast random number generation)

- consider different hardware
  - GPUs
  - FPGAs
  - …

- try to decrease cost of evaluating a sample
  - increase number of samples if required

Additional Dwarfs

Additional dwarfs

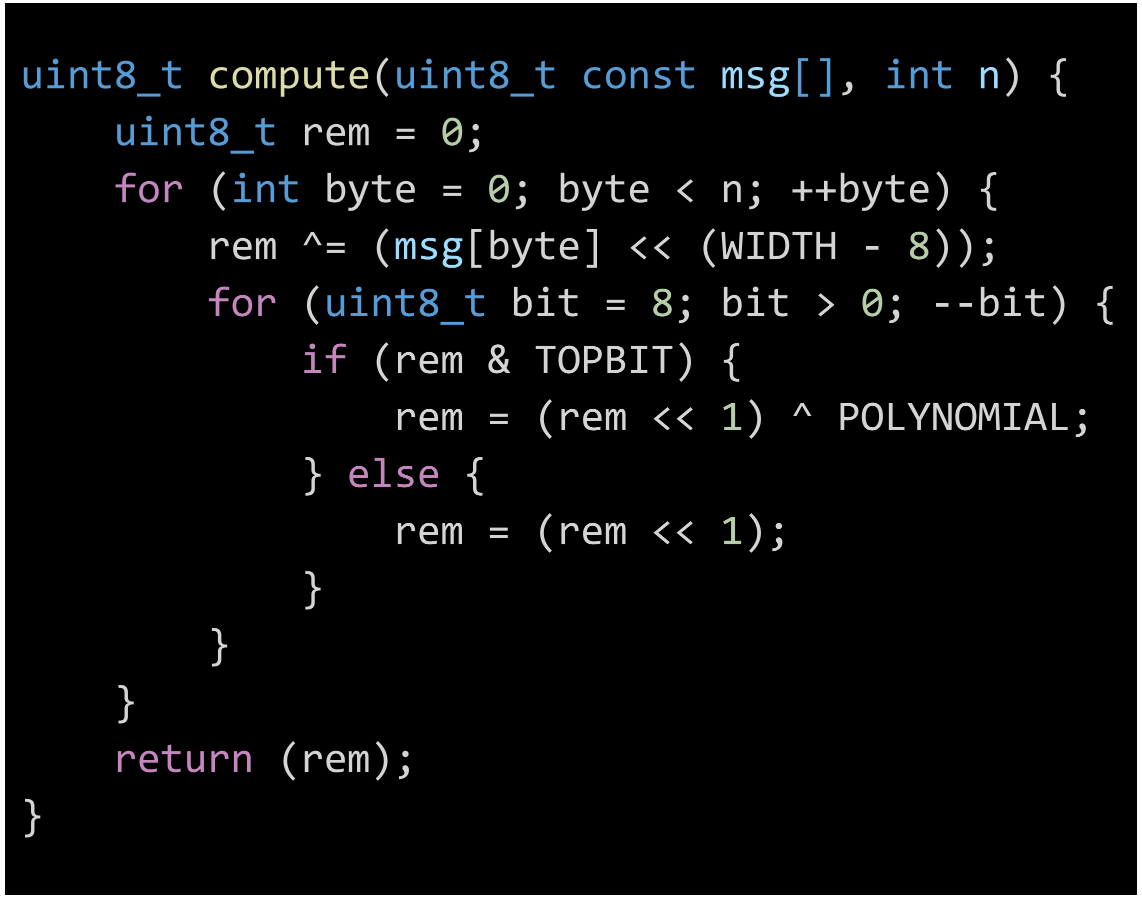
- 8. Combinational Logic
- 9. Graph Traversal
- 10. Dynamic Programming
- 11. Backtrack & Branch+Bound
- 12. Graphical Models
- 13. Finite State Machine

- slightly different focus compared to first 7 dwarfs
  - more (but not exclusively) on integer-heavy applications, machine learning, theoretical problems
  - less on physical processes

Combinational logic

- generally involves performing simple operations on large amounts of integer data
  - e.g. computing cyclic redundancy codes (CRC)

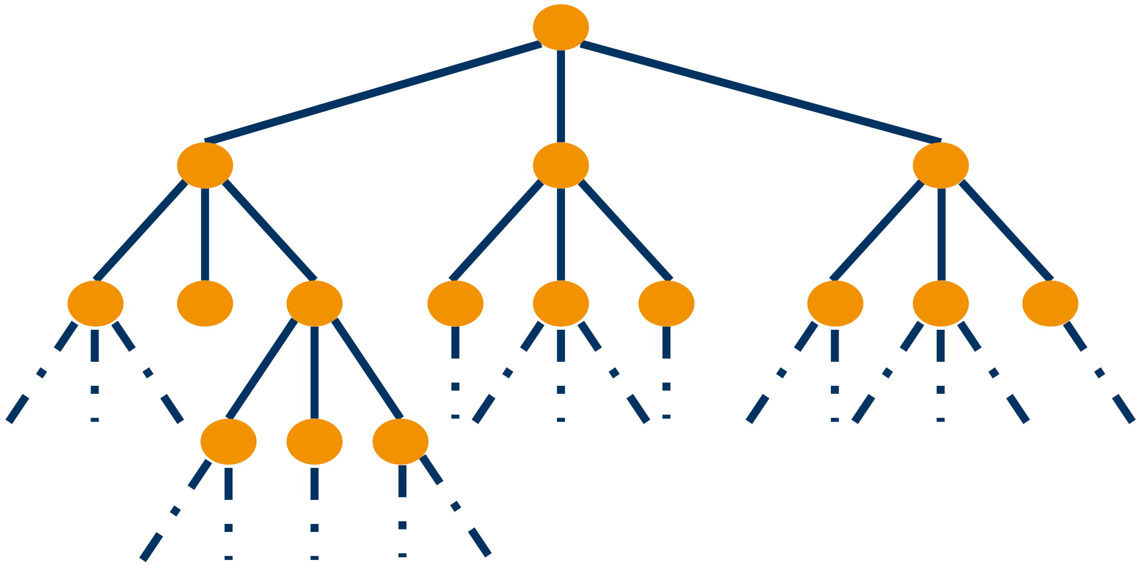
- often parallelizable on multiple levels
  - bit-level parallelism (e.g. x86 popcnt)
  - block-level parallelism



```c
uint8_t compute(uint8_t const msg[], int n) {
    uint8_t rem = 0;
    for (int byte = 0; byte < n; ++byte) {
        rem ^= (msg[byte] << (WIDTH - 8));
        for (uint8_t bit = 8; bit > 0; --bit) {
            if (rem & TOPBIT) {
                rem = (rem << 1) ^ POLYNOMIAL;
            } else {
                rem = (rem << 1);
            }
        }
    }
    return (rem);
}
```

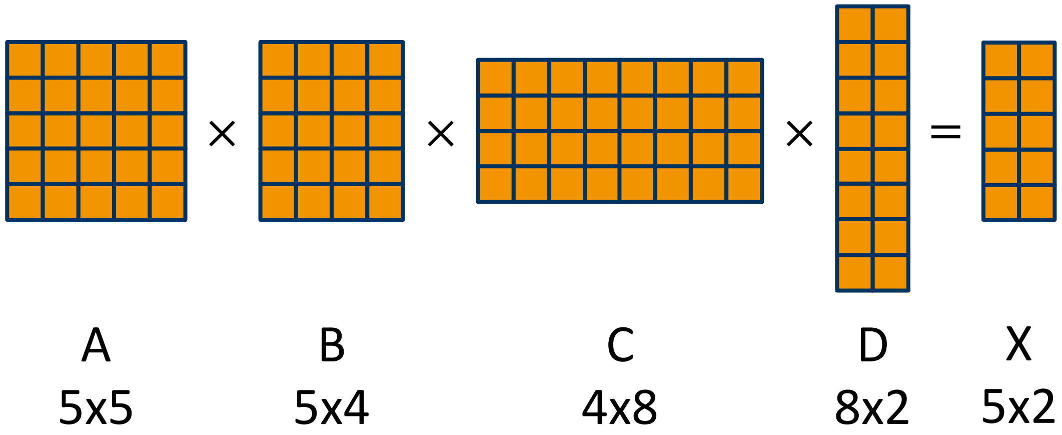
Graph traversal

- traverse a number of objects in a graph and examine characteristics
  - e.g. searching, sorting, collision detection, decision trees, …
  - usually heavy on data reads and lookups, very little computation and output
- parallelizable over different paths in the graph
  - but indirect accesses are heavily latency-bound (c.f. unstructured grids)



Dynamic programming

- method of computing solutions by solving simpler, overlapping sub-problems
  - applicable to problems where optimal result is composed of optimal results of sub-problems
  - e.g. matrix-chain-multiplication
- usually based on memoization
  - solve each sub-problem exactly once
  - store and re-use the result



$A \times \big(B \times (C \times D)\big) = X$ 154 ops

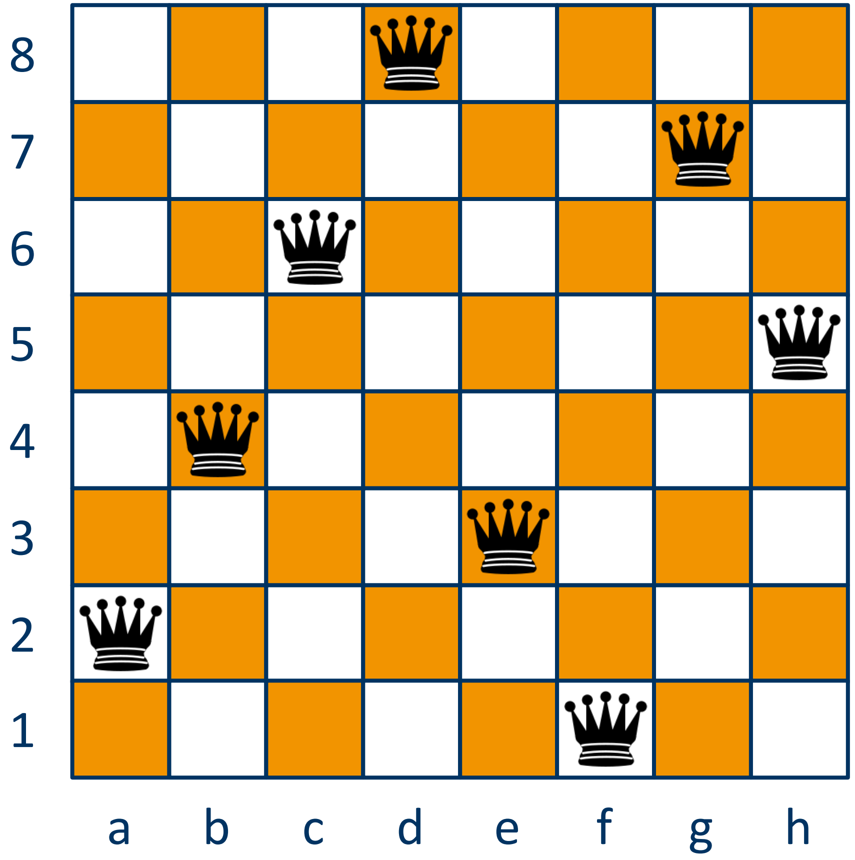
$(A \times B) \times (C \times D) = X$ 204 ops

$\big((A \times B) \times C\big) \times D = X$ 340 ops

Backtrack & Branch+Bound

- search and optimization problems for very large problem spaces
  - incrementally build solution but discard if determined unsuitable
  - e.g. n-queens problem

- use divide & conquer strategy:
  - break down complex problem into smaller sub-problems until they become solvable
  - solve sub-problems in parallel



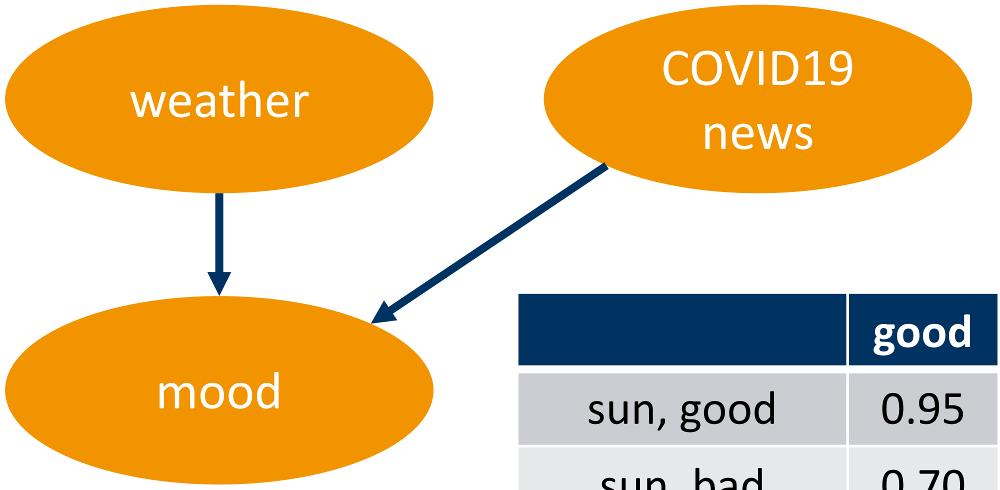
Probabilistic graphical models

- represent graphs consisting of random variables as nodes and dependencies as edges
  - e.g. Bayesian networks, Hidden Markov models

- ongoing research in math and computer science regarding parallelization and optimization

sun	rain
0.40	0.60

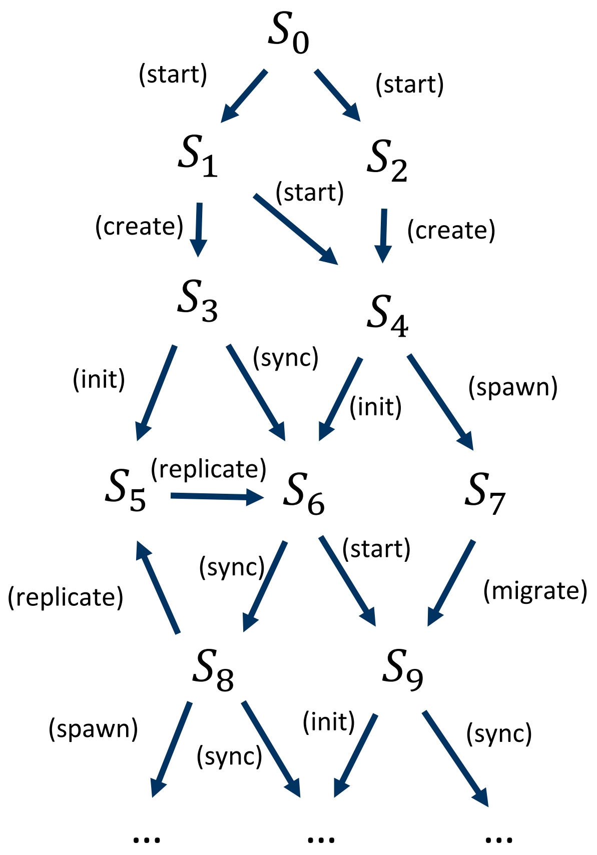
good	bad
0.90	0.10



	good	bad
sun, good	0.95	0.05
sun, bad	0.70	0.30
rain, good	0.75	0.25
rain, bad	0.10	0.90

Finite state machines

- represent interconnected set of states to be moved among
  - e.g. parsers
- can sometimes be decomposed into multiple state machines that act in parallel
  - ongoing research



Literature material

- White Paper by Berkeley University: „The Landscape of Parallel Computing Research: A View from Berkeley” from 2006: https://www2.eecs.berkeley.edu/Pubs/TechRpts/2006/EECS-2006-183.pdf
- Holds more detailed descriptions and related aspects

Note the focus on scientific problems

- MPI can be (and is!) used to implement also
  - distributed-memory runtime systems
  - emulate shared memory runtime systems on distributed memory (e.g. PGAS)
  - provide the connecting parallelism layer for shared-memory or sequential systems
    - e.g. use multiple accelerators in separate compute nodes (Celerity project @ UIBK)
    - extend shared memory parallelism to distributed memory (MPI+X)
    - …

- still, the majority of codes is of scientific computing nature

Side note: Portability

- functional portability
  - program runs on different hardware and produces correct results
  - hardware architecture, compiler, libraries, etc.
  - usually not hard to achieve (mostly x86/ARM + GPUs)

- performance (also “non-functional”) portability
  - program runs efficiently on different hardware and is considered “fast”
  - no exact definition, topic of ongoing research

Summary

- 13 Dwarfs of HPC
  - abstract application categories
  - facilitate cross-platform reasoning and cross-application component reuse
  - 7 older ones, most well-studied physics problems
  - 6 newer ones, partially of theoretical nature, subject to ongoing research
  - give a broad perspective on HPC potential and limitations

Image Sources

- Dwarfs: http://pngimg.com/download/47261, http://rpgmke.wikidot.com/moonshae-isles-campaign
- Barnes-Hut: http://portillo.ca/nbody/barnes-hut/
- Unstructured Mesh: https://resourcearea.cpu-24-7.com/en/numeca_welcome
- CRC: https://barrgroup.com/Embedded-Systems/How-To/CRC-Calculation-C-Code