GPUs

A bit of history

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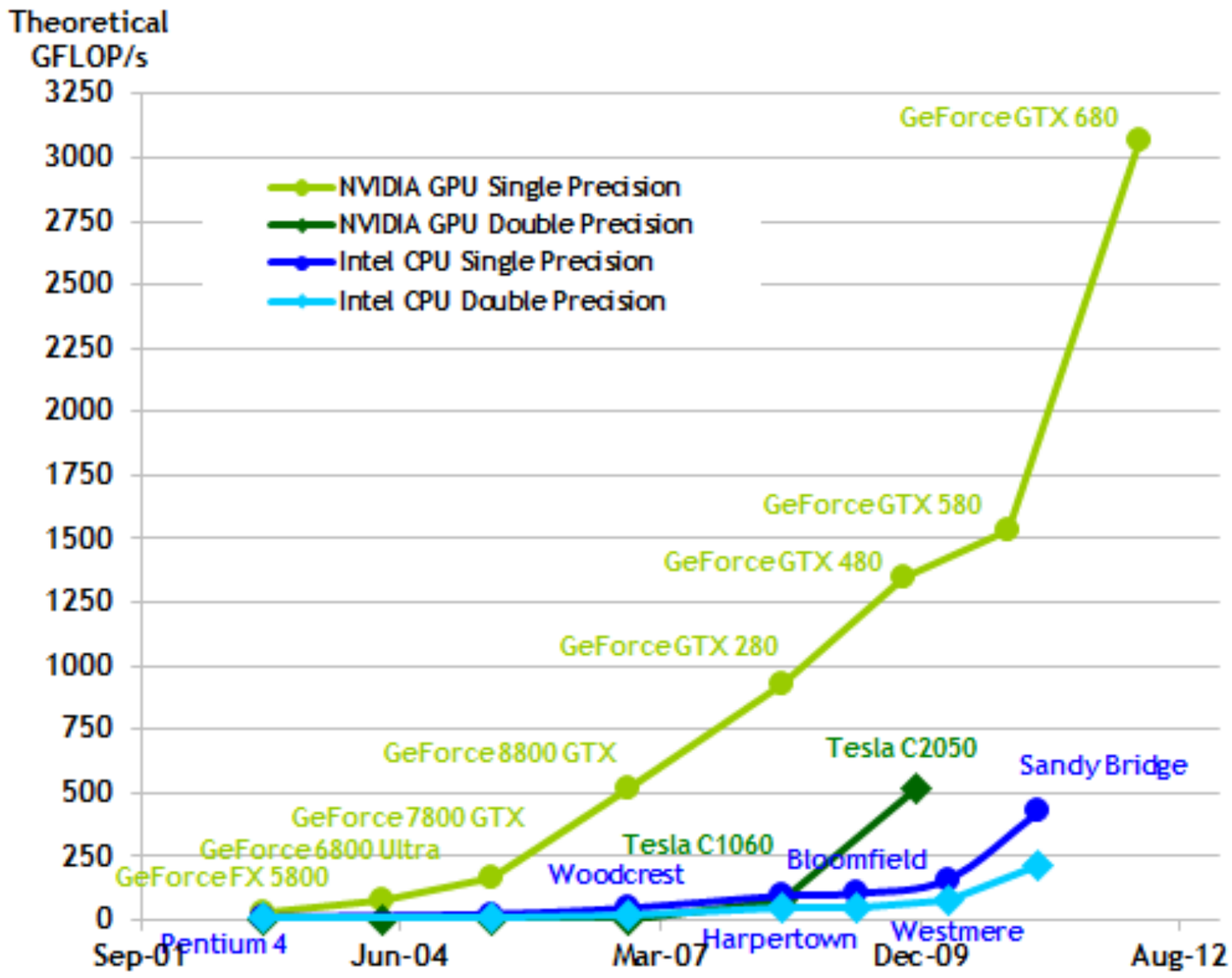
- First GPGPU applications were developed via Shader techniques
- CUDA / OpenCL became the first set of languages written specifically compute purposes

Performance over the years



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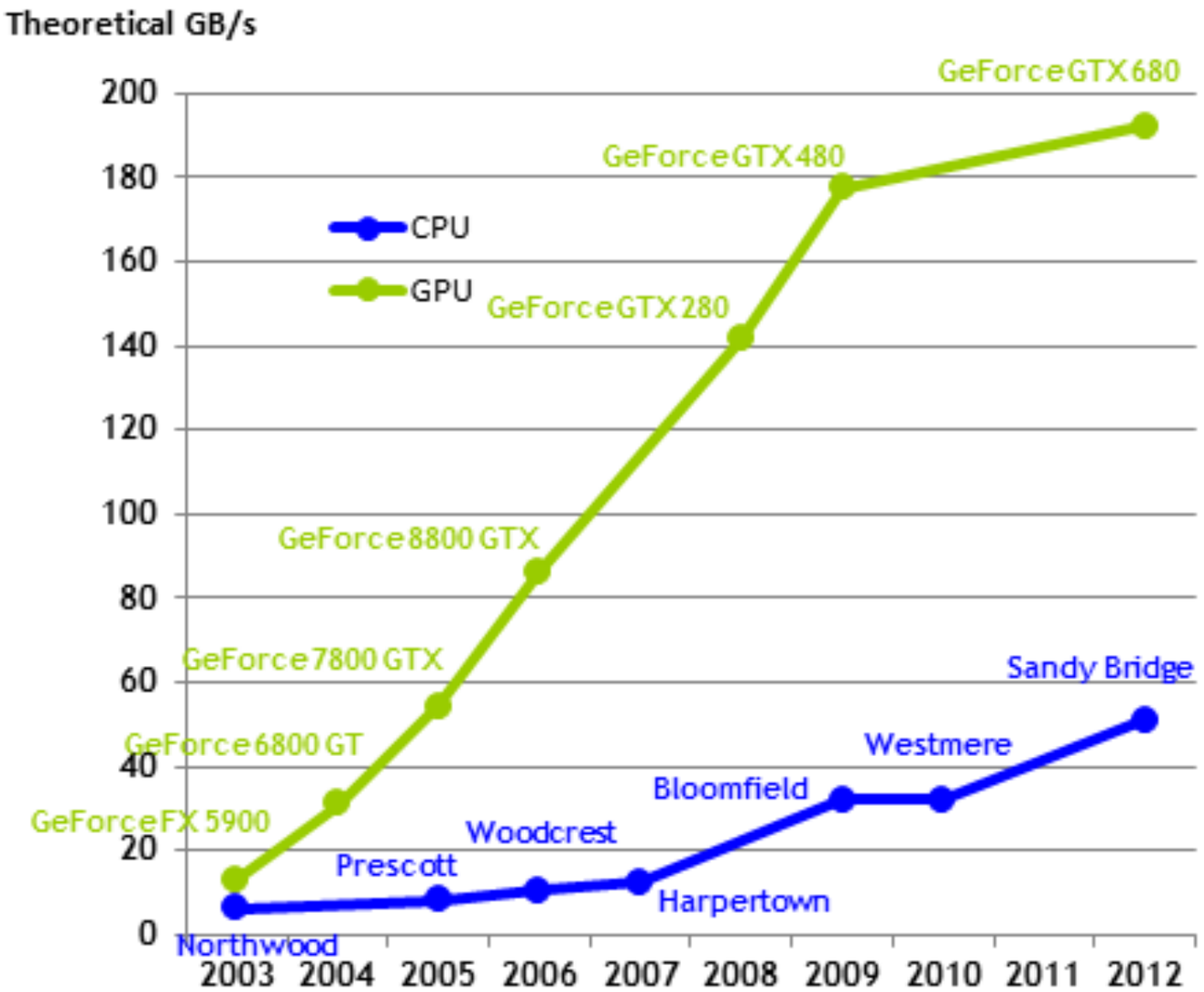
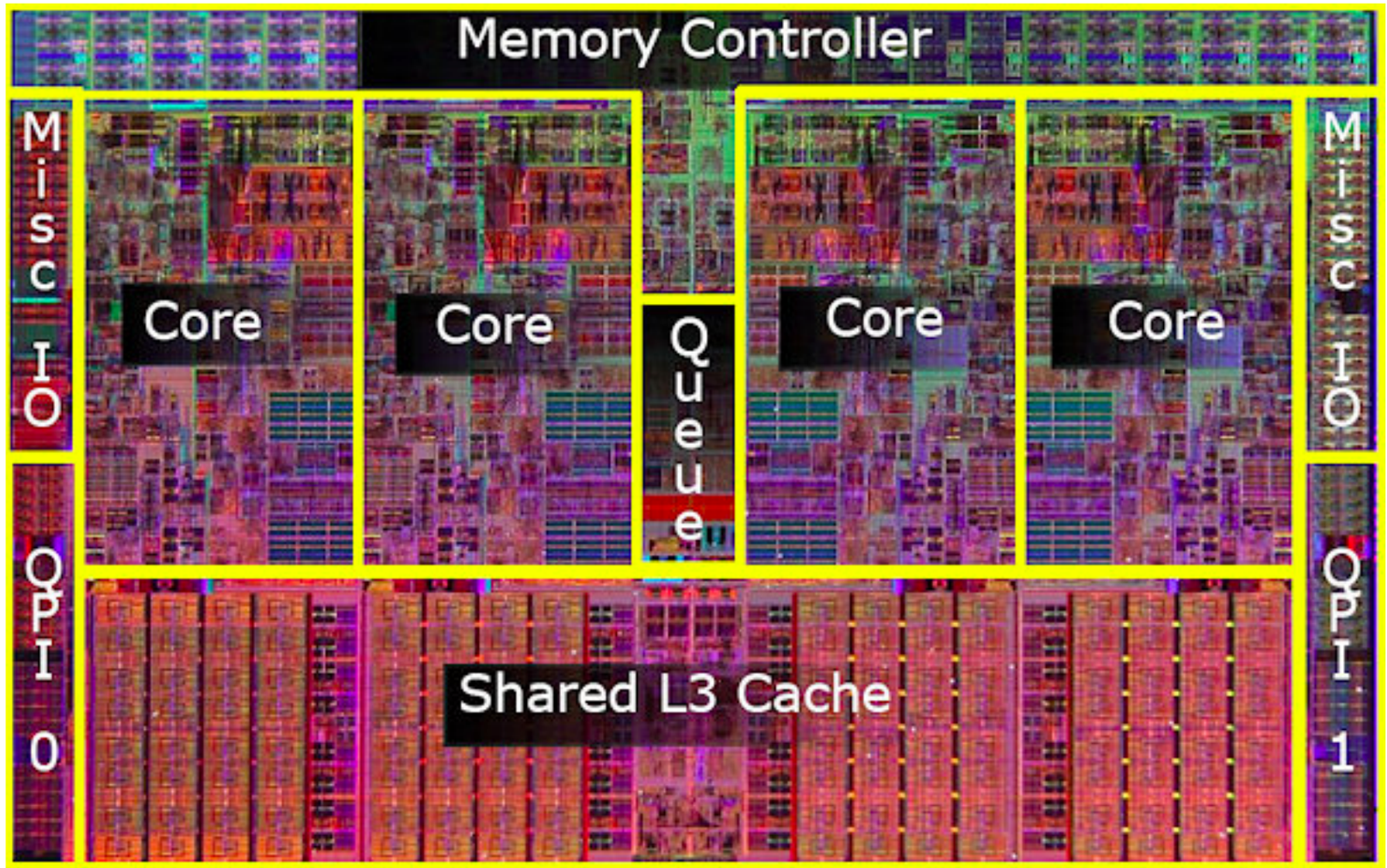
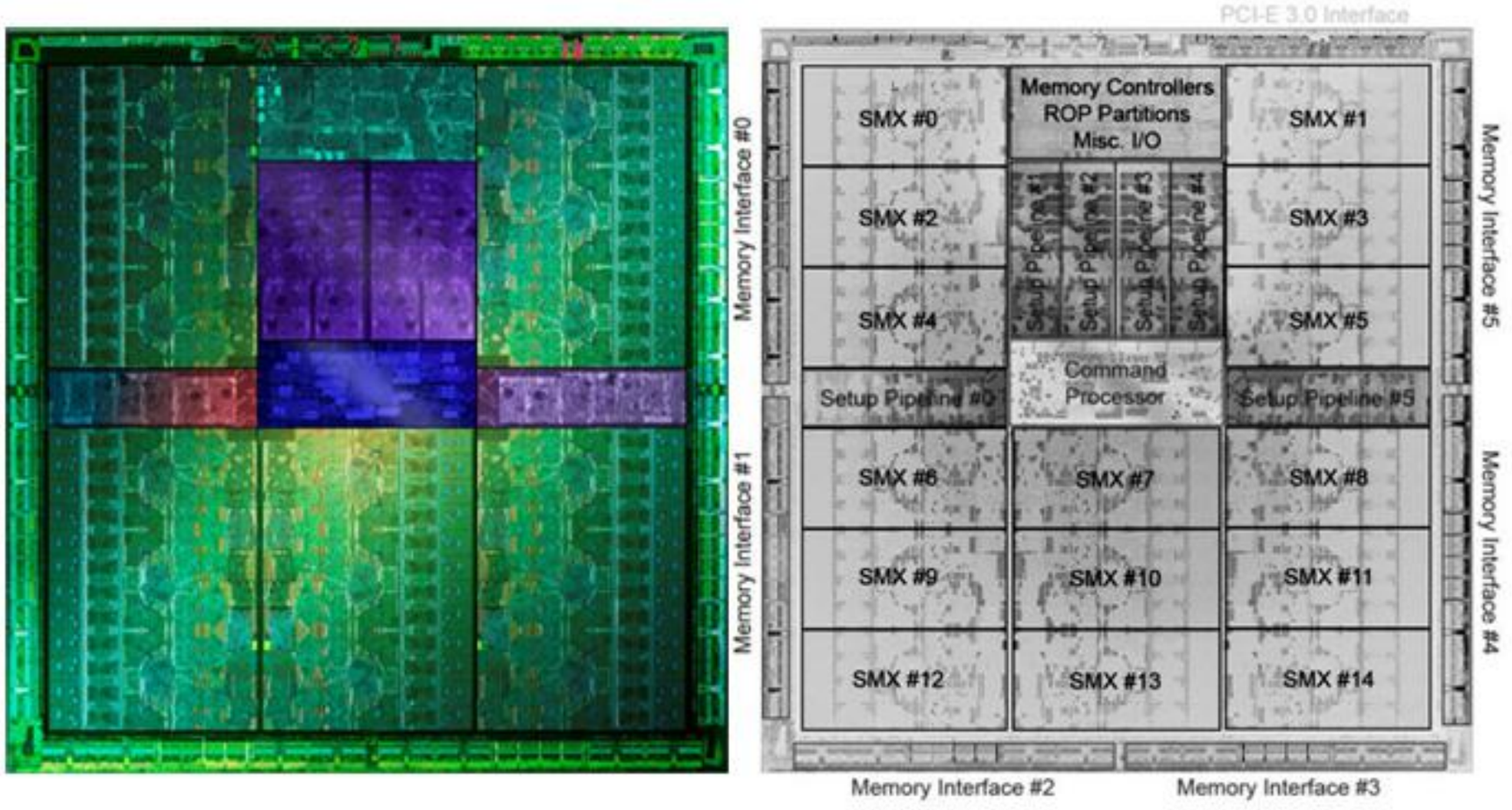


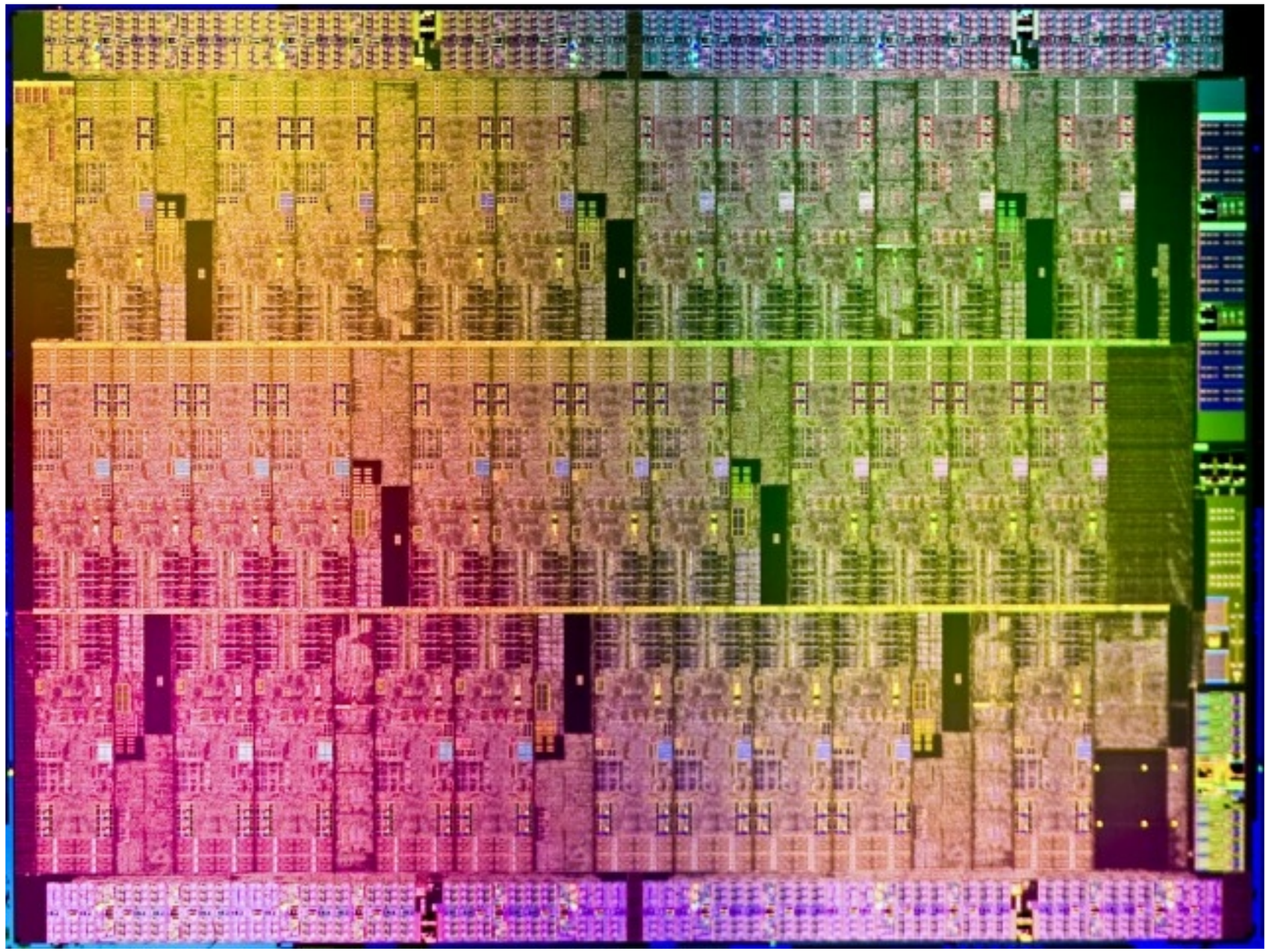
CPU Architecture



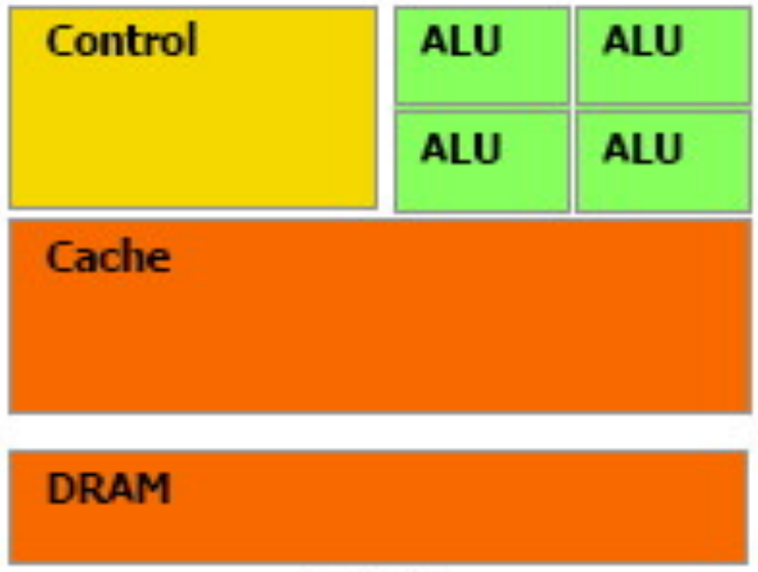
GPU Architecture



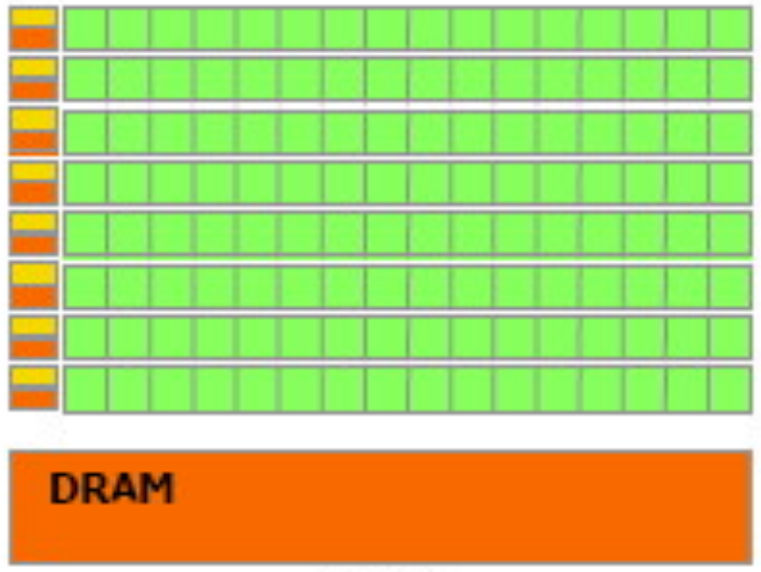
Any Guesses?



Allocation of Transistors



CPU



GPU

Memory Space

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- Memory Management is critical!

Programming Paradigm

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- if() statements create divergence

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- Pre-mature optimization

Algorithms

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  - Ideal: do same amount of total work as serial counter part
  - Less Ideal: do a bit of extra work

Example: Prefix Sum

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- Problem:
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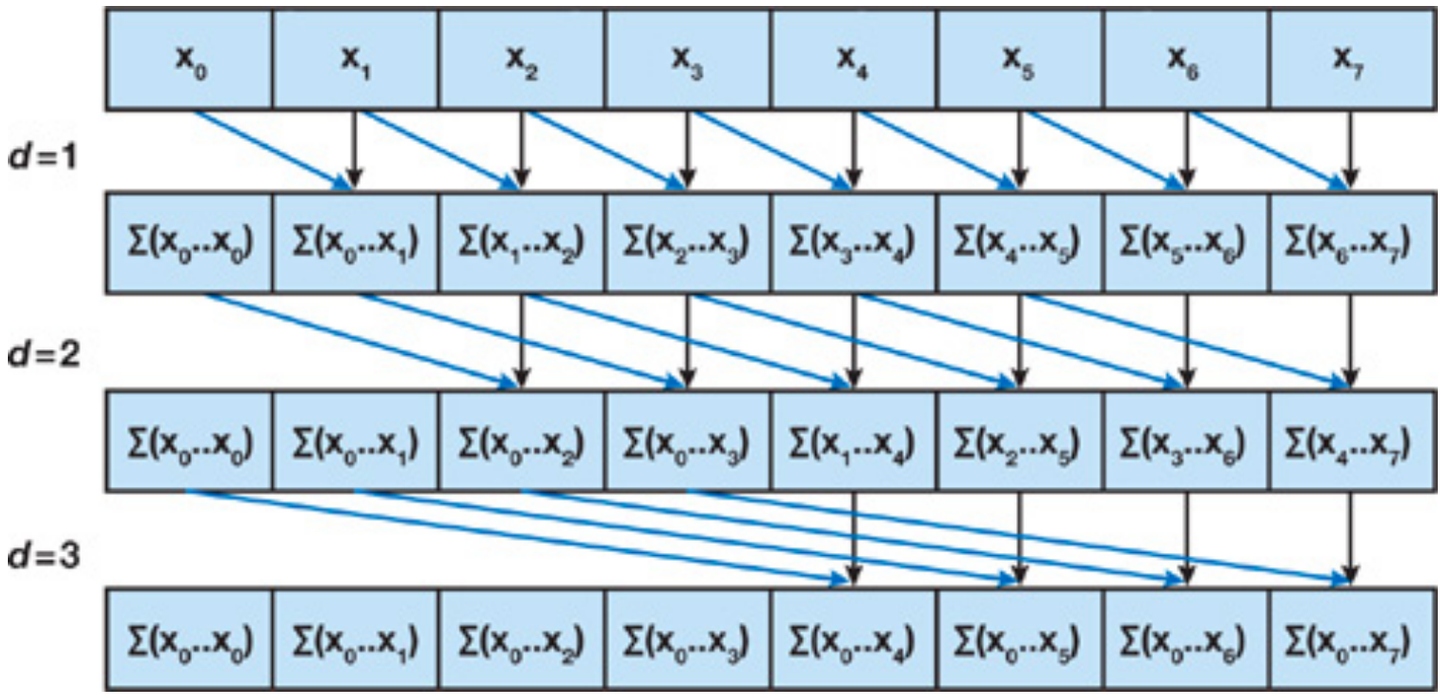
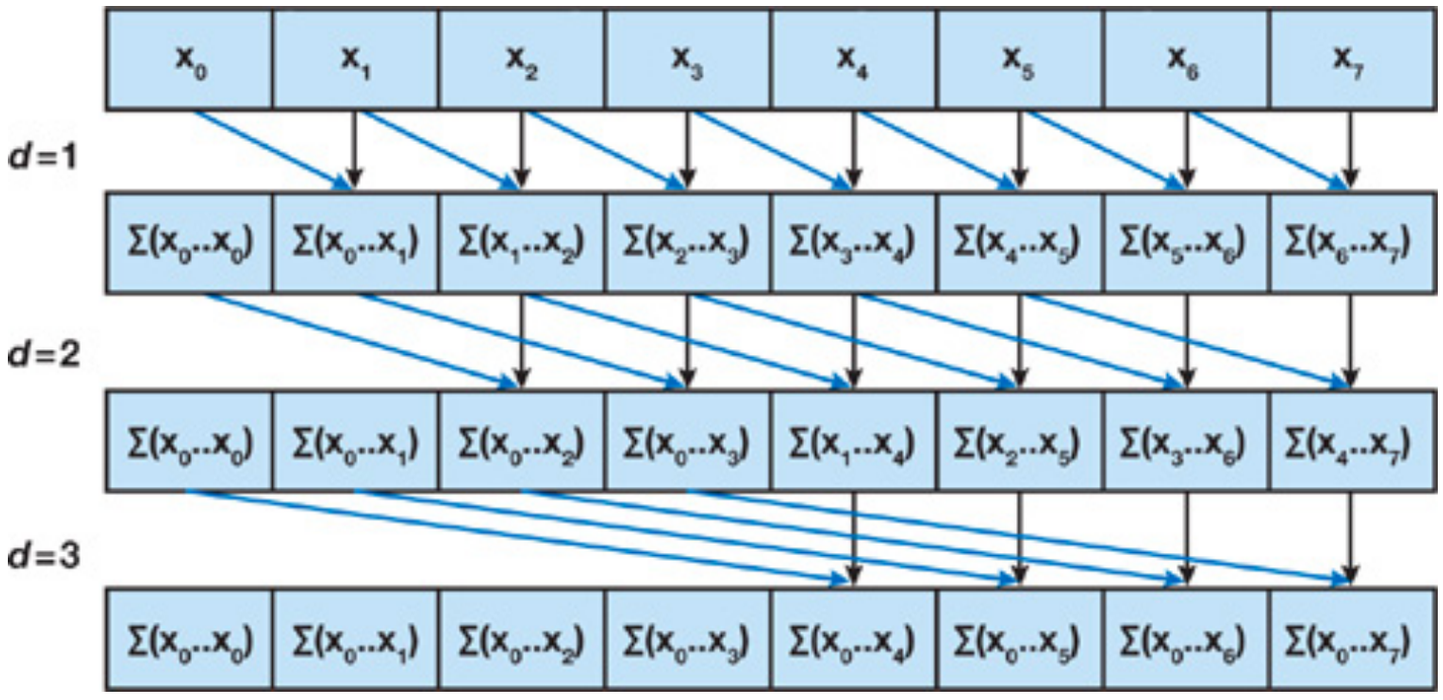
- Trivial for CPU, with total work O(N)

Work Inefficient Parallel Reduction

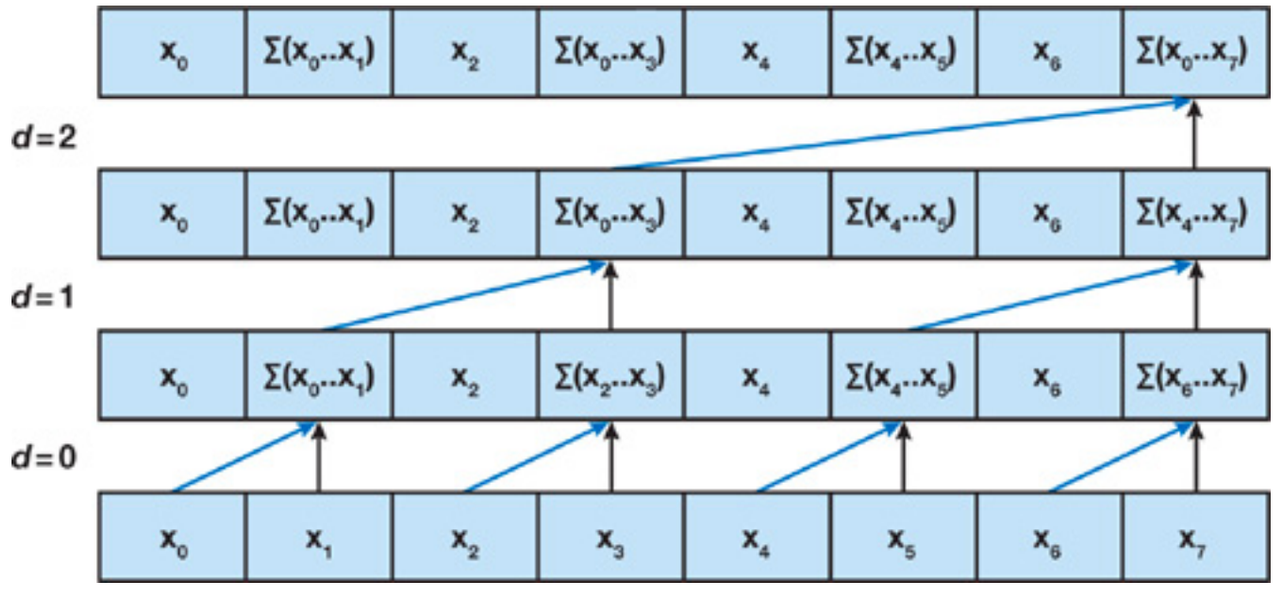


Work Inefficient Parallel Reduction



O(N log N)

Work Efficient Parallel Reduction



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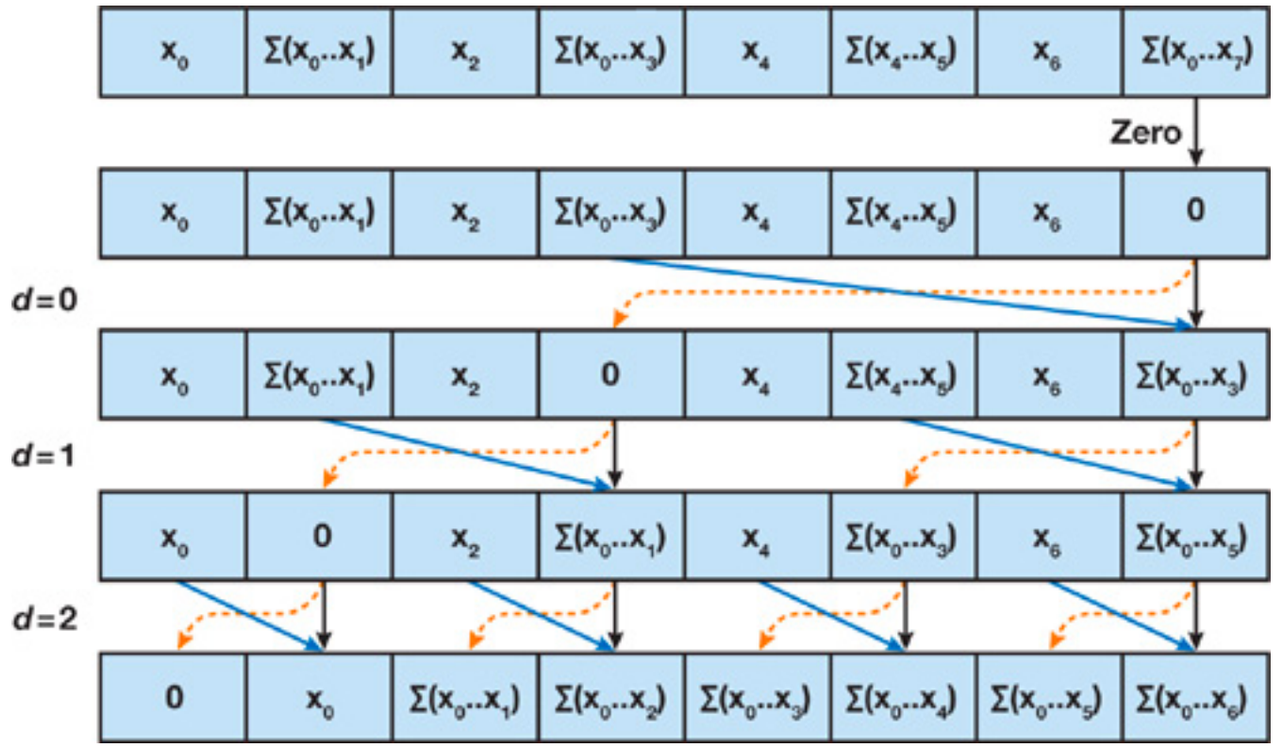

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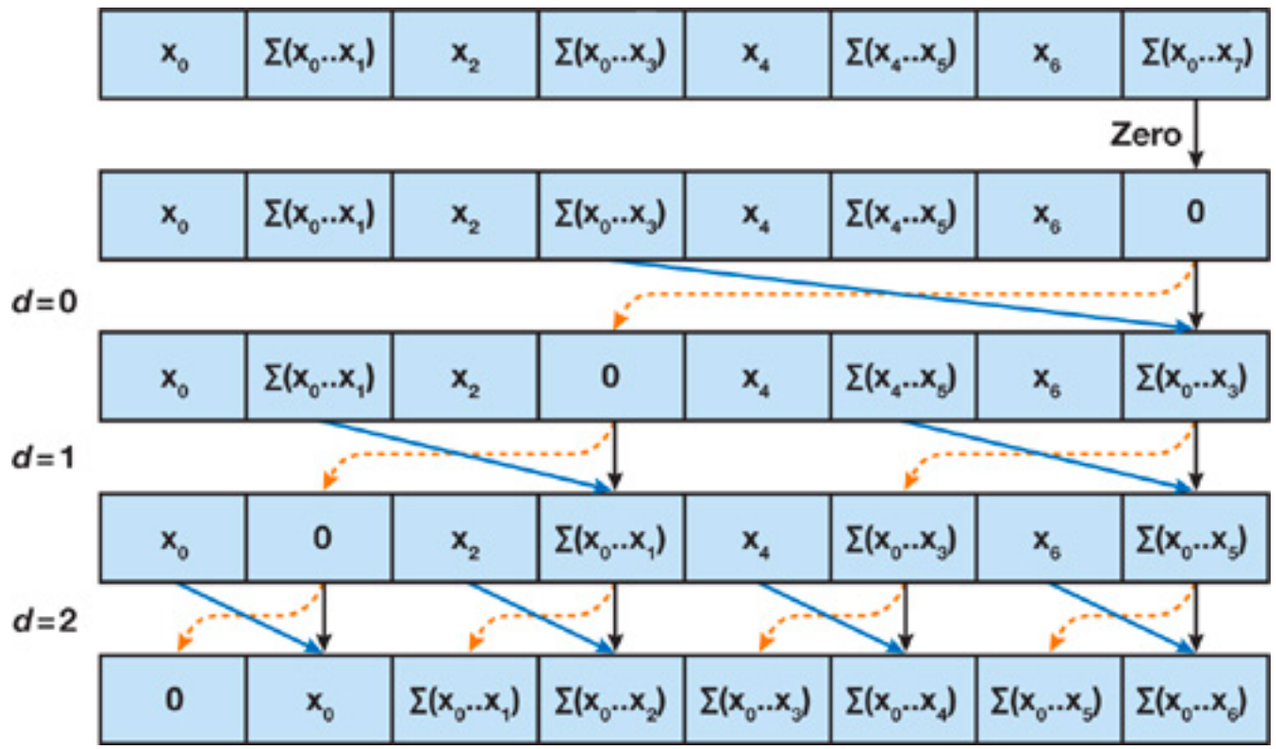

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  - Work inefficient algorithms that adapt well to memory (naive prefix sum)
  - Work efficient algorithms that don't adapt well to memory (eg. neighbourlists)
  - Really lucky if we can find something works well in both cases

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- Maximum Speedup Attainable:
  - S(N) = 1/((1-P)+P/N)
- Very unlikely for a large program to be 100% parallelizable

Algorithms that can be effectively parallelized

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- Reduction, Prefix Sums

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- Radix-based sorting
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- Matrix multiplication, Linear Algebra
- FFTs
- Simple Dynamic Programming

Algorithms with no good parallel solution

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- Many graph search algorithms

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- Quick Sort

Algorithms with no good parallel solution

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- Quick Sort
- Binary Search

Asymmetric Algorithms

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- Compression algorithms (eg. given a Huffman code, encoding is parallelizable, decoding not easily parallelizable.)

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- Compression algorithms (eg. given a Huffman code, encoding is parallelizable, decoding not easily parallelizable.)
- Converting the representation of a large molecule into internal coordinates (bijection from R^3N into Phi/Psi space)

Language Differences

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- CUDA is a language: supports only NVIDIA cards, lots of good documentation
- OpenCL is a standard: supports NVIDIA, ATI, and Intel CPUs and Xeon Phi's