Title: Efficient numerical methods for modern computing systems

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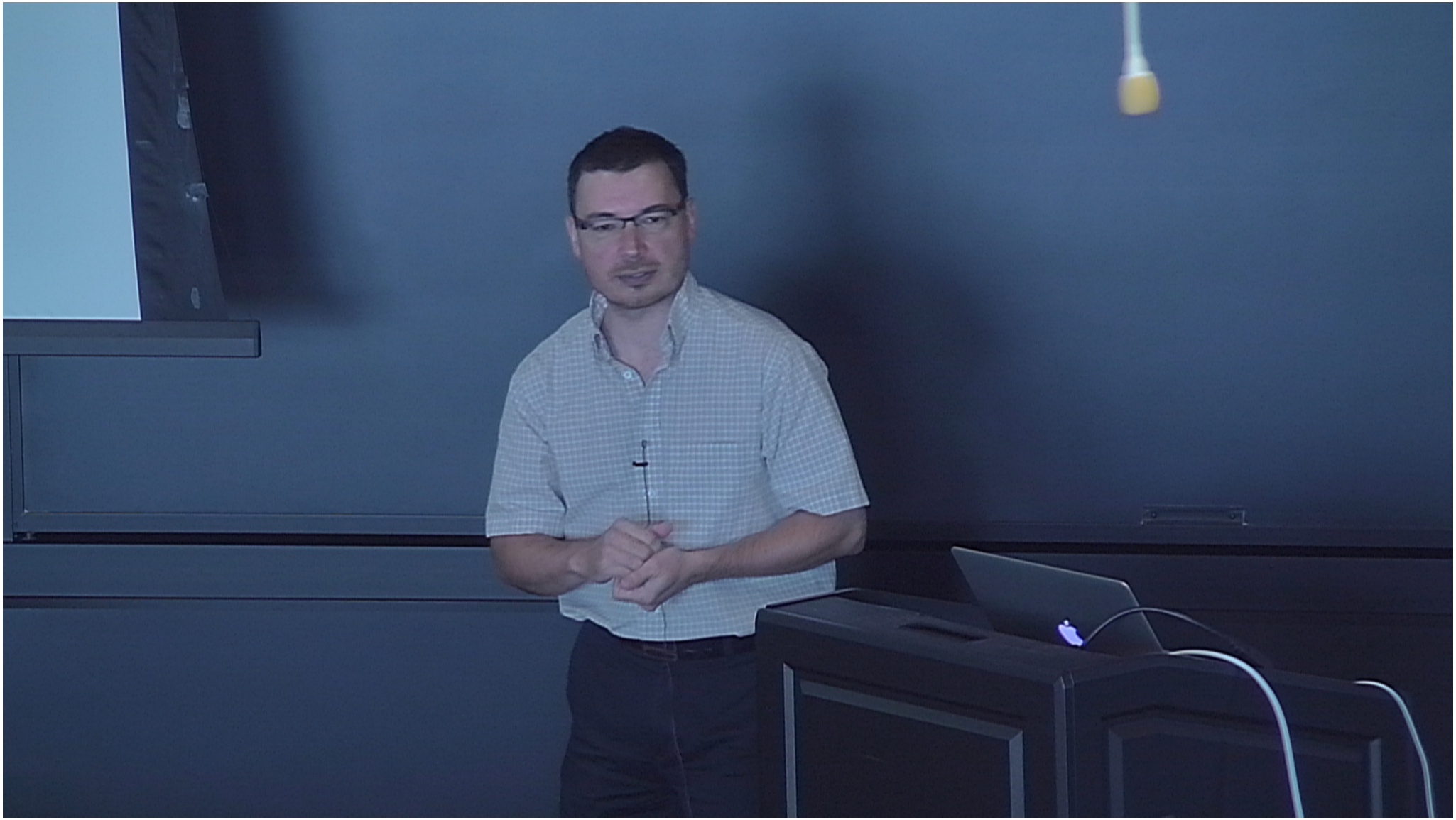
Abstract:



Efficient numerical methods for modern computing systems

Erik Schnetter

Renormalization in Background Independent Theories: Foundations and Techniques

Perimeter Institute, September 30, 2015

Efficient numerical methods for modern computing systems

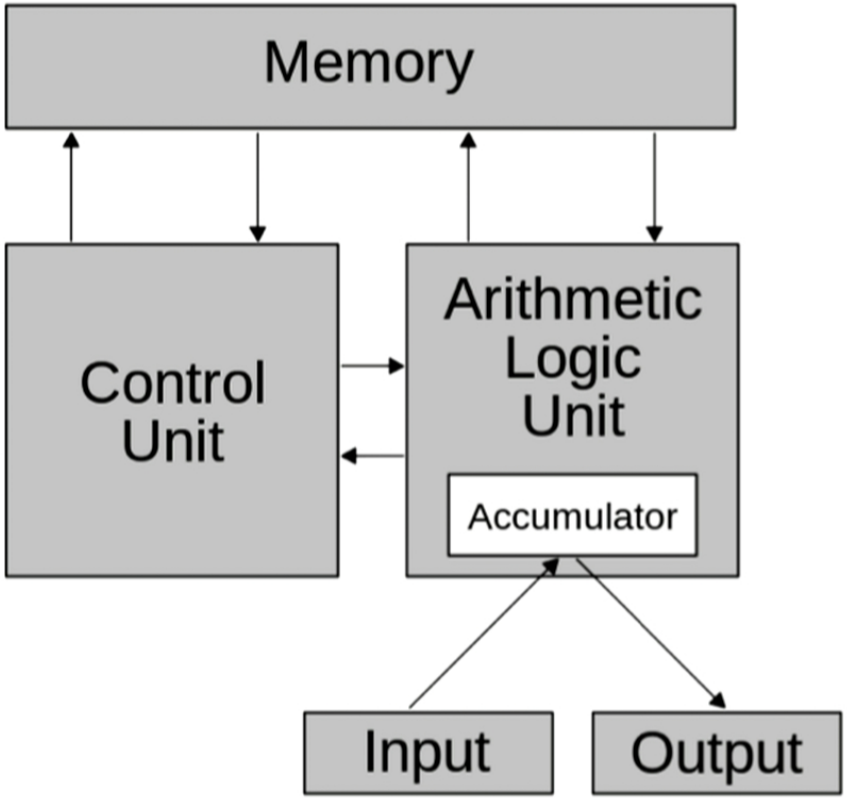
- High-level introduction to computational methods

1. Computing architecture ("what is a computer and how does it work")
2. Numerical analysis ("how do I solve a PDE on a computer")

Algorithm Development

- Naïve idea:
  - Von Neumann (and others) developed a theoretical model of computing
  - Take an algorithm ("constructive proof"), map it to this model, implement it in a computer language, done
- In practice:
  - What is possible (and what is efficient) is not determined by an abstract model, but by current-day hardware technology
  - "Good" algorithms today look very different than 20 years ago
  - (... not because people today are more clever!)

Von Neumann Architecture



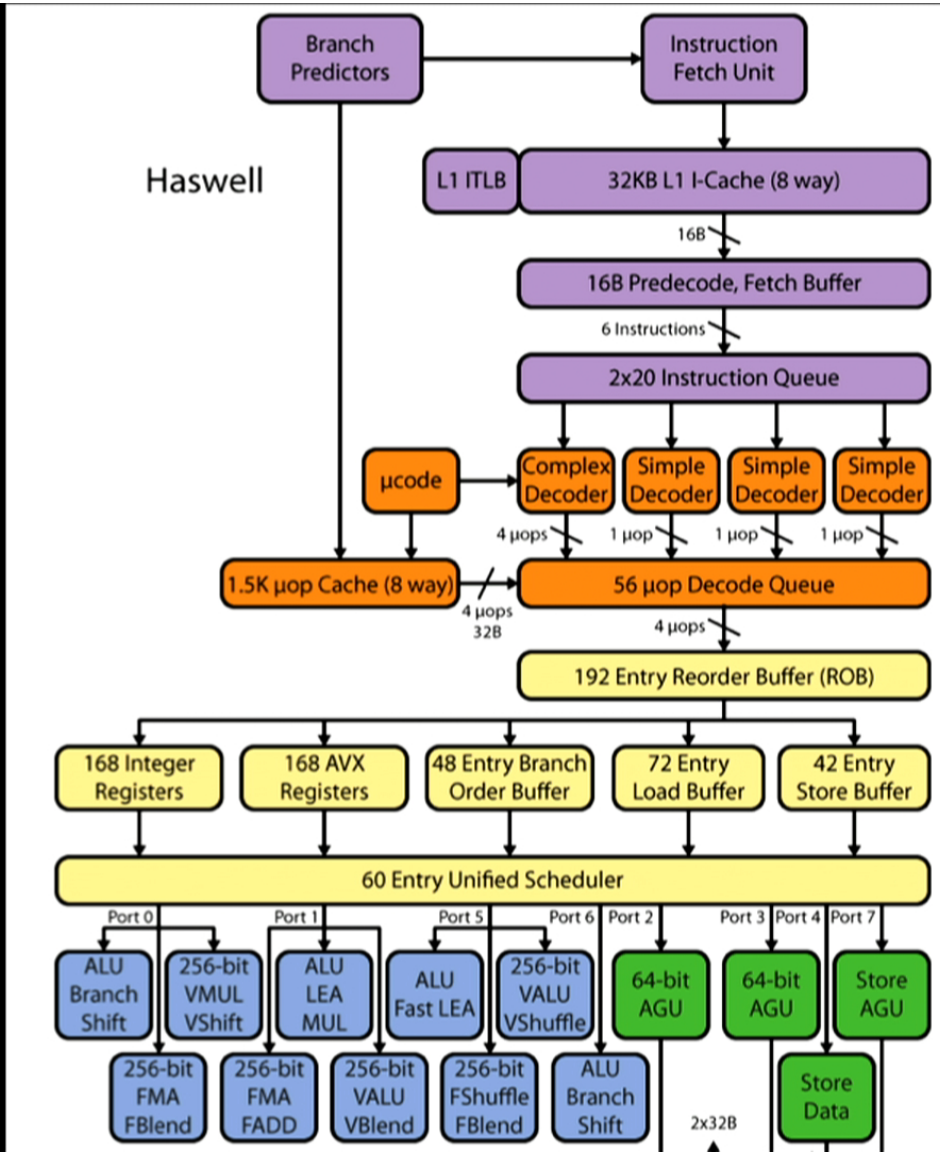
Sequential Execution:

x := a + b

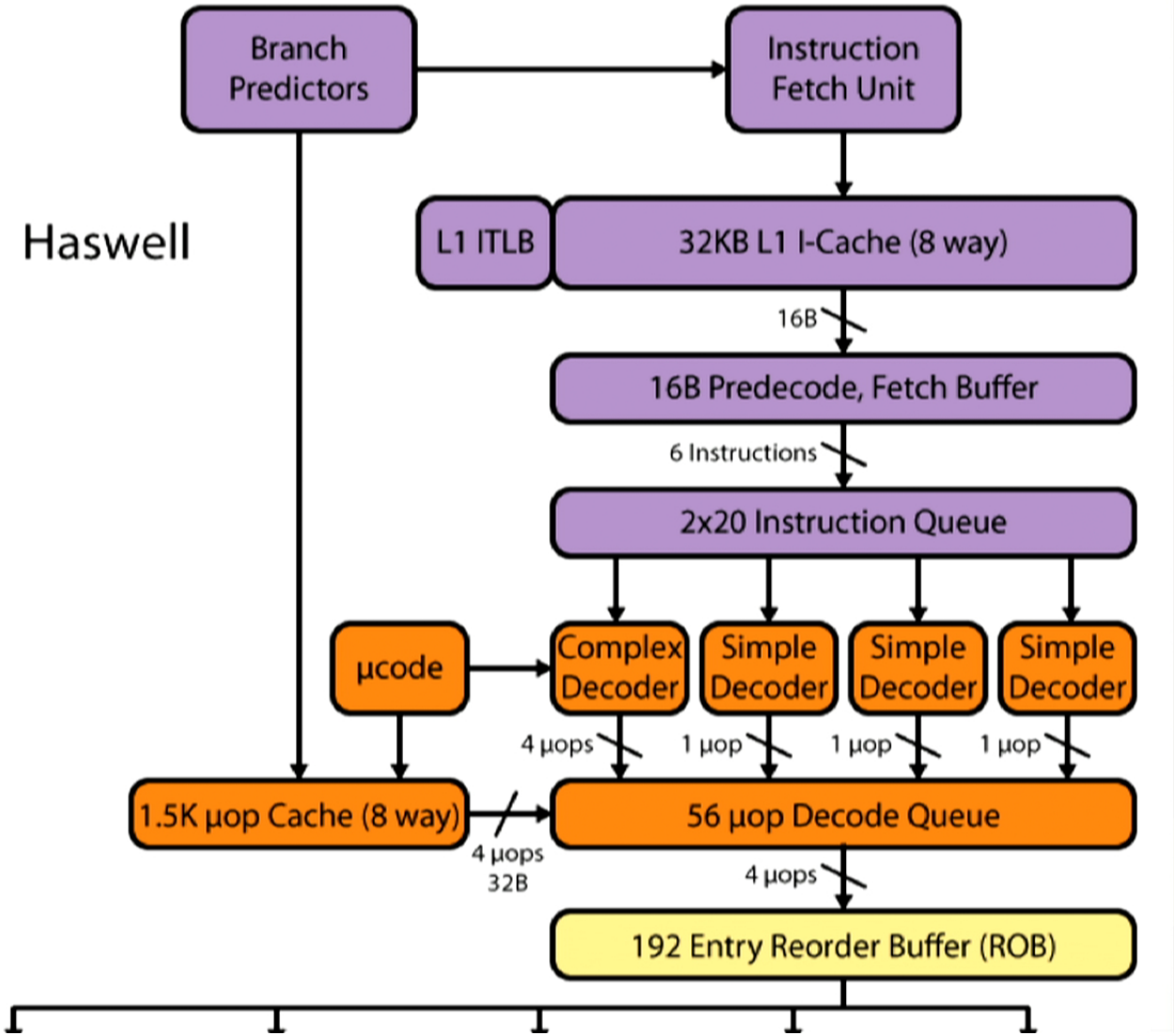
1. read instruction
2. read a
3. read b
4. add
5. write x

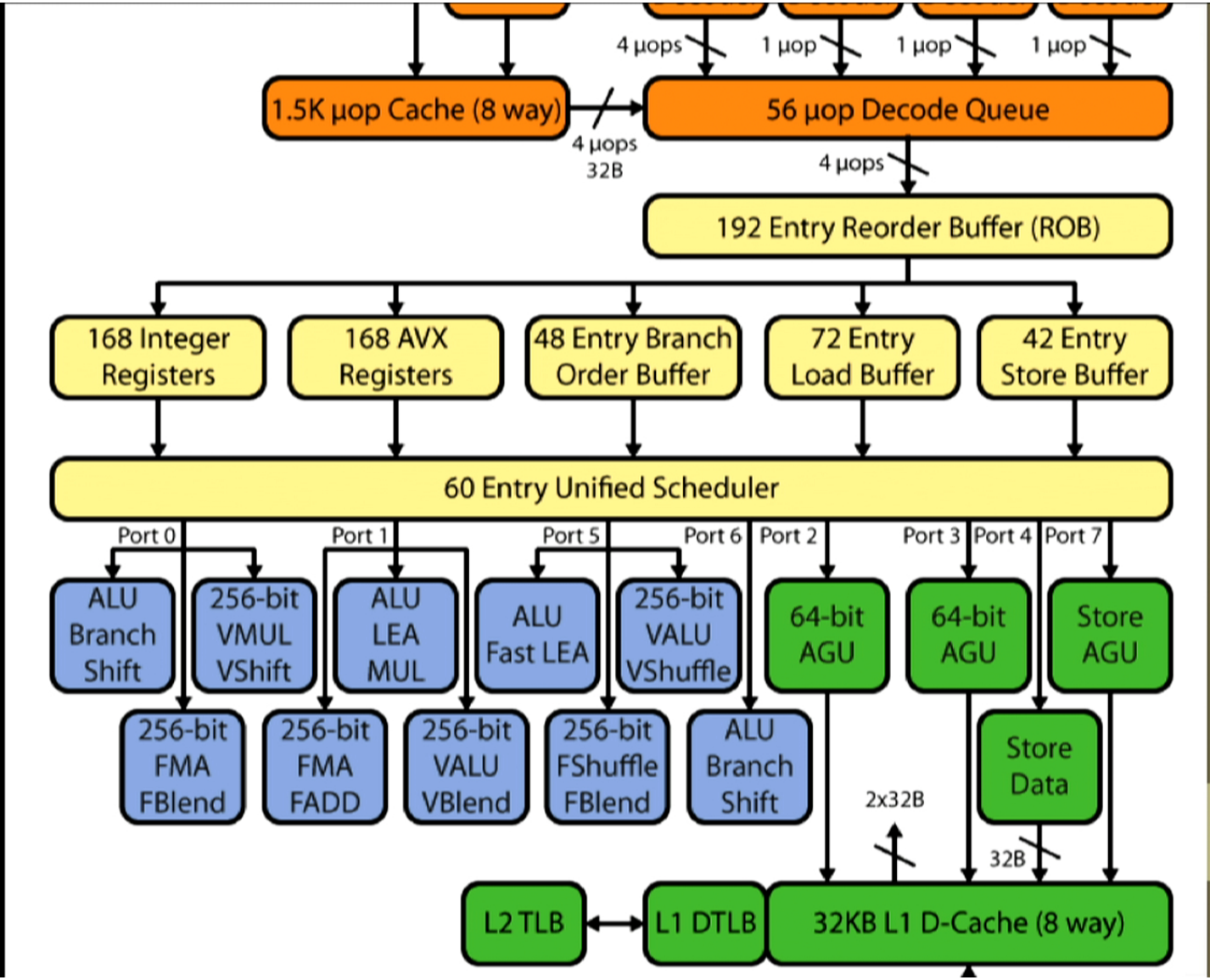
[Wikipedia]

Modern Intel processor



[IDF 2012]

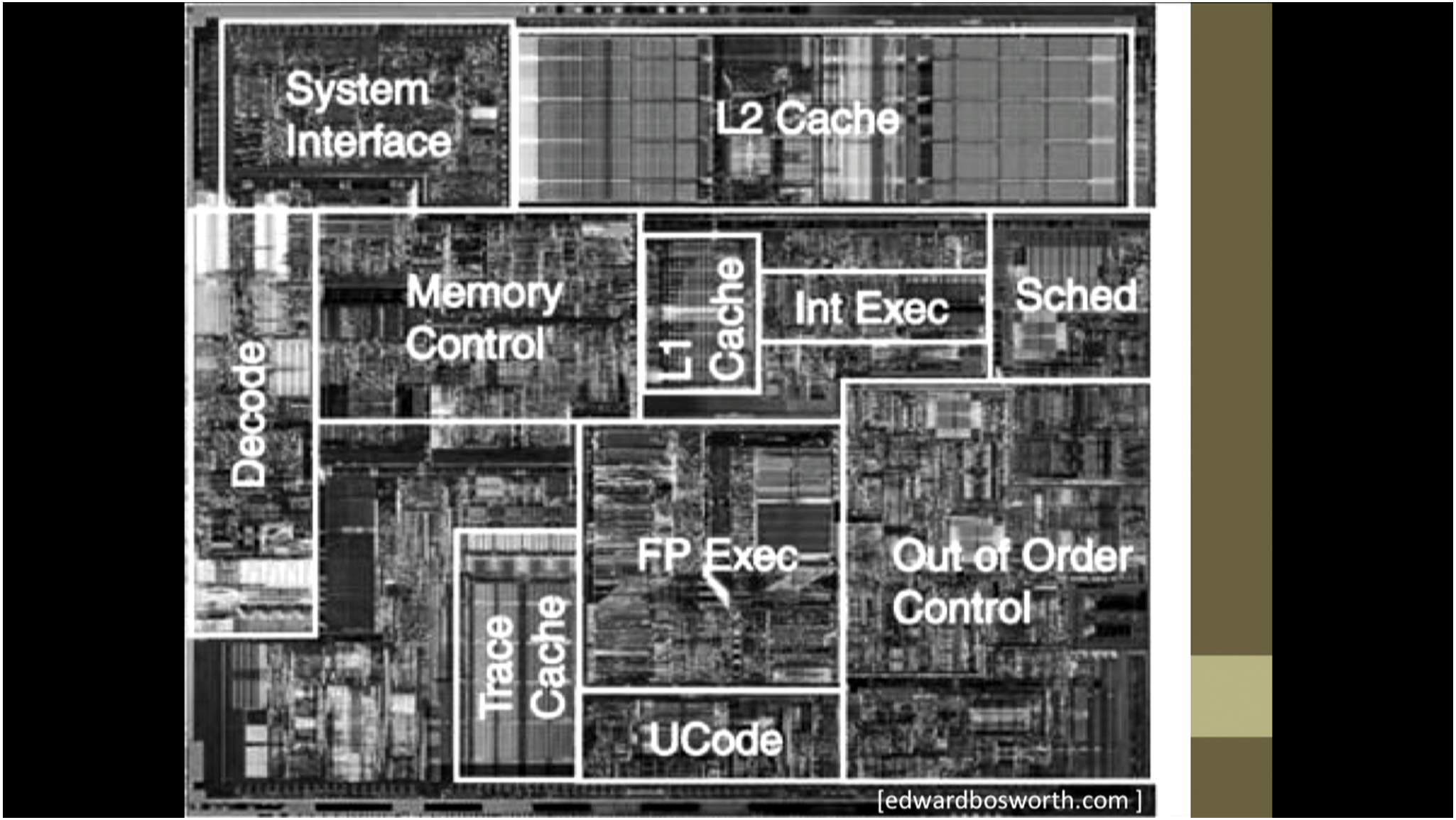

Haswell
Branch Predictors
Instruction Fetch Unit
L1 ITLB
32KB L1 I-Cache (8 way)
16B
16B Predecode, Fetch Buffer
6 Instructions
2x20 Instruction Queue
µcode
Complex Decoder
Simple Decoder
Simple Decoder
Simple Decoder
4 µops
1 µop
1 µop
1 µop
1.5K µop Cache (8 way)
4 µops
32B
56 µop Decode Queue
4 µops
192 Entry Reorder Buffer (ROB)

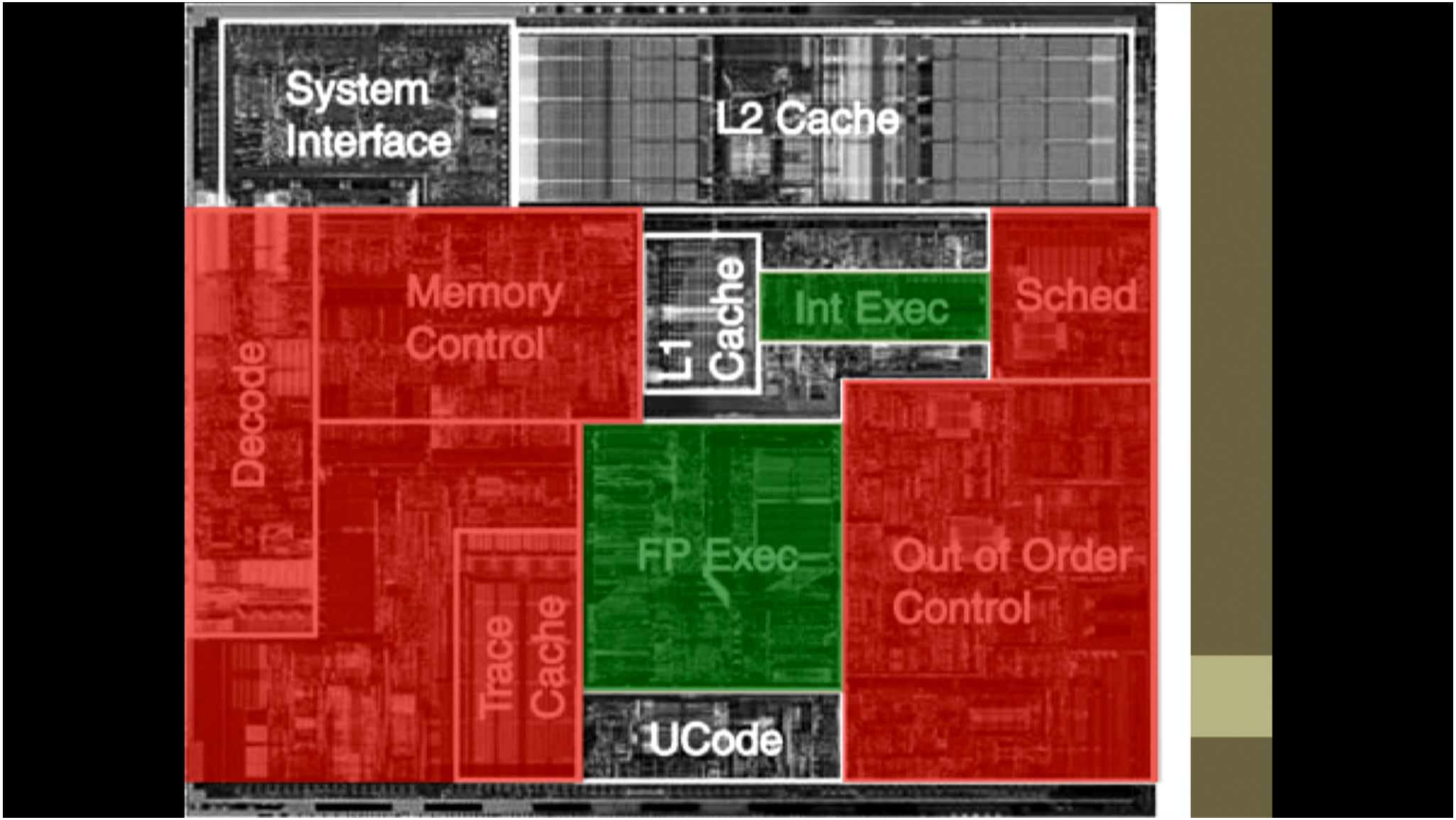

4 µops
1 µop
1 µop
1 µop
1.5K µop Cache (8 way)
4 µops
32B
56 µop Decode Queue
4 µops
192 Entry Reorder Buffer (ROB)
168 Integer Registers
168 AVX Registers
48 Entry Branch Order Buffer
72 Entry Load Buffer
42 Entry Store Buffer
60 Entry Unified Scheduler
Port 0
Port 1
Port 5
Port 6
Port 2
Port 3
Port 4
Port 7
ALU Branch Shift
256-bit VMUL VShift
ALU LEA MUL
ALU Fast LEA
256-bit VALU VShuffle
64-bit AGU
64-bit AGU
Store AGU
256-bit FMA FBlend
256-bit FMA FADD
256-bit VALU VBlend
256-bit FShuffle FBlend
ALU Branch Shift
Store Data
2x32B
32B
L2 TLB
L1 DTLB
32KB L1 D-Cache (8 way)

Sequential vs. Parallel

- Modern CPUs are highly parallel
  - Many cores (20)
  - Each core is superscalar (10…100)
  - Vector ("SIMD") operations (4)
  - FMA (a*b+c) (2)

- Algorithms need to be parallel (many independent steps), not sequential (each step depending on the previous)
  - Bad: Update a structure element-by-element
  - Good: Create a new structure from an existing one


System Interface
L2 Cache
Memory Control
L1 Cache
Int Exec
Sched
Decode
Trace Cache
FP Exec
Out of Order Control
UCode
[edwardbosworth.com]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Performance Measures

- *Theoretical Peak Performance*
  1. Computing: Floating point operations per second (Flop/sec)
  2. Data access: Bytes per second (Byte/s)

- Typical numbers for a modern workstation:
  - 1,000 GFlop/sec (Giga, 10^9)
  - 100 GByte/sec
  - Ratio: 0.1 Byte/Flop

- Memory (RAM): 100 GByte

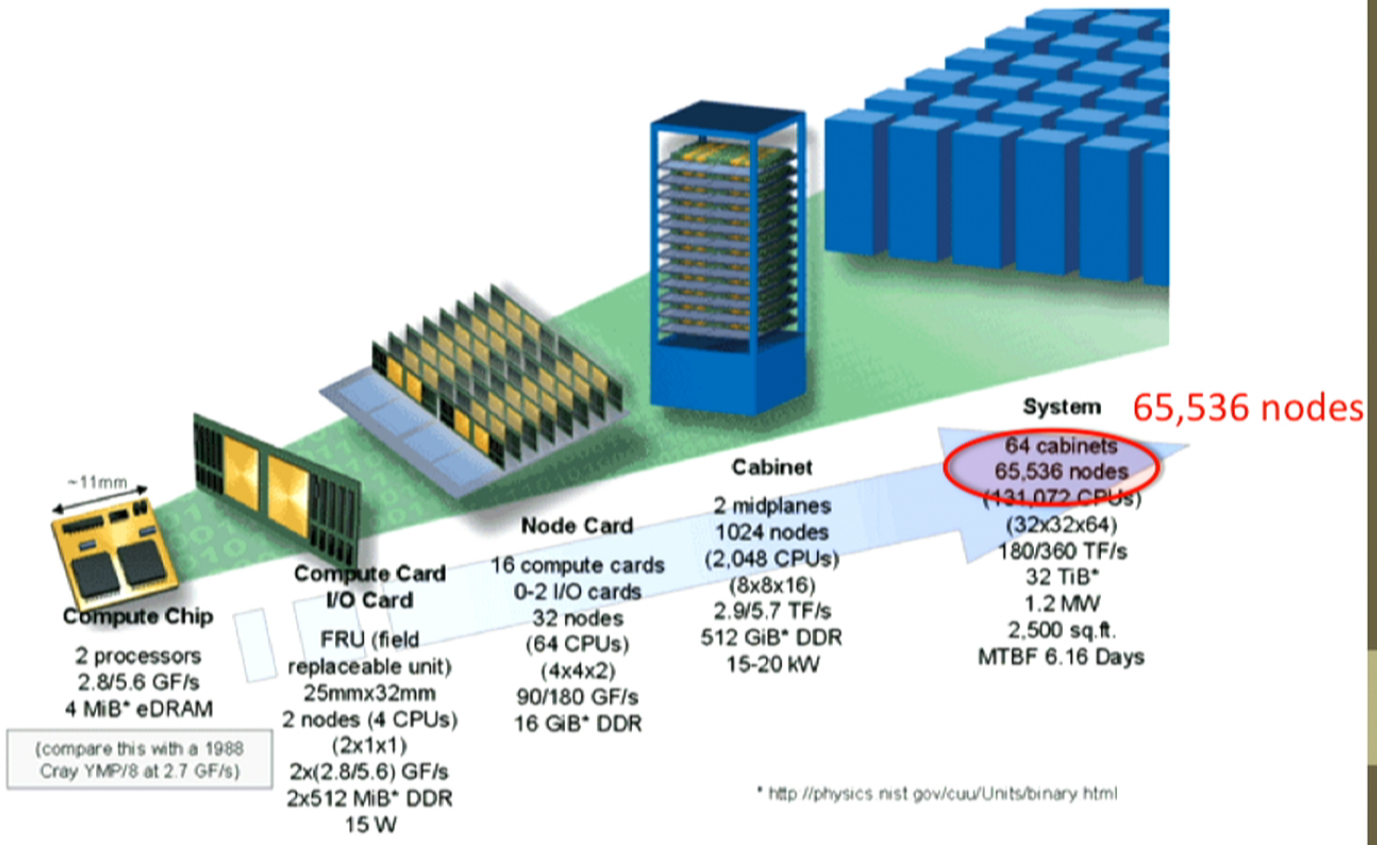
Algorithm characteristics

- Algorithms can be characterized by the number of calculations they perform (Flop) and amount of data they process (Byte)

- Matrix multiplication (n*n matrices, 8 Byte per number):
  - $2n^3$ Flop
  - $24n^2$ Byte
  - 12/n Byte/Flop
  - Thus: compute bound even for moderate n

- Matrix addition:
  - n^2 Flop
  - $24n^2$ Byte
  - Ratio: 24 Byte/Flop
  - Thus: memory bound

Supercomputer architecture

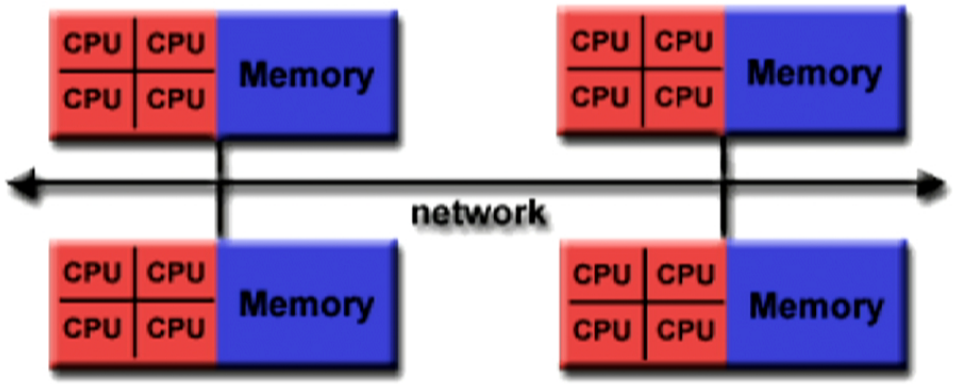


Supercomputer?

Top500

[top500.org]

Distributed Memory



[computing.llnl.gov]

- Need to *partition* data structures
- Need to *exchange information* at (artificial) inter-node boundaries
- Permeates the whole program, quite difficult in practice

Software Architecture

- Every decade or two, there is a paradigm shift in software architecture
  - 1980s: modular programming ("information hiding" / programs form a group)
  - 1990s: object oriented programming
  - 2000s: parallel programming (multi-threading)
  - 2010s: (?) functional (declarative) programming

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Parallel Programming Algebra

- Problems: Access conflicts, deadlocks
  - Naively parallel programs do not form a group
- Relatively recent solution, found today e.g. in C++, Python:
  - *Future*: "black box" holding the result of a calculation that is not yet finished
  - Accessing a future automatically waits until the result is ready
  - *Async*: (asynchronous execution): "function call" returning a future, without waiting for the result
  - C++: Future is a "container" (or could be)
  - Category theory: Future is a monad

Functional Programming

- Dichotomy between mathematics and programming:
  1. Math is about eternal truths (there is no "time" in a proof)
  2. Programs execute sequentially
- How can one prove statements about programs?
  - (1990s: Programs are monads…)

- Functional programming:
  - Design programs to be order-independent (as much as possible)
  - Remove distinction between data and functions

```
let x = 1
  in sin(x)
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let f = sin
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Programming Languages

- For non-trivial projects, need these properties from a programming language:
  1. Dynamic user interface (e.g. Mathematica's notebooks)
  2. Modularity (collaborative programming), i.e. safety features, abstractions (C++)
  3. High efficiency where needed (e.g. matrix multiplication)
- There are many languages (Fortran, C++, Python, Matlab, Mathematica, …)
- Few languages offer all features; most projects use multiple languages

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- From juliacode.org:
  - high-level, high-performance dynamic programming language for technical computing
  - sophisticated compiler
  - distributed parallel execution
  - numerical accuracy
  - extensive mathematical function library
  - mature, best-of-breed open source C and Fortran libraries for linear algebra, random number generation, …
  - powerful browser-based graphical notebook interface
- But: only few years old, still immature

Numerical Analysis

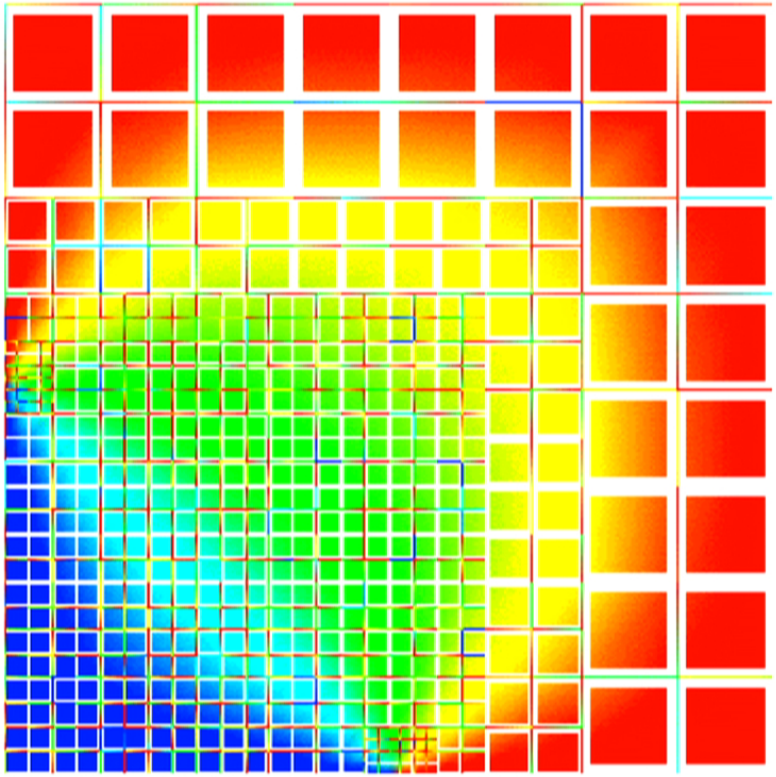
- How to solve a PDE on a computer
  - How to approximate fields via finite-dimensional spaces: discretization

- Obvious superficial similarities between *discretization* and *quantization*
  - Can some interesting ideas be transferred?

PDE Discretization

- Given: A PDE *L*, acting on a set of fields *U*:
  - L(U) = 0
- Choose a sequence of bases B_n for U
  - Different *resolutions*, indexed by n
- Choose discrete approximate operators L_n
  - Yes, this is a choice
- Solve $L_n(U_n) = 0$ for several n
- Extrapolate to find U (*Richardson extrapolation*)

Discretization



[wissrech.iam.uni-bonn.de]

Common Discretization Methods

- Finite Differences:
  - Sample solution at grid points, interpolate to define continuum
- Finite Elements:
  - Define elements with vertices, edges, faces, …; often used with differential forms
- Finite Volumes:
  - Split domain into cells; define fluxes through faces; commonly used for conservation laws
- Particle methods (*Lagrangian methods*):
  - Split matter/charges into "particles" that move and interact with neighbours; often used for conserved quantities with irregular distributions

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Mimetic Discretizations

- Some continuum properties may/will not hold in the discrete, e.g.:
  - Conservation
  - Integration by parts
  - Constraints
  - Sharp discontinuities
- Typically: Need to choose which properties are important for a system, represent these faithfully ("mimetic"), drop others
  - E.g. integration by parts: can be recovered by careful choice of derivative operators, integration weights, boundary definition

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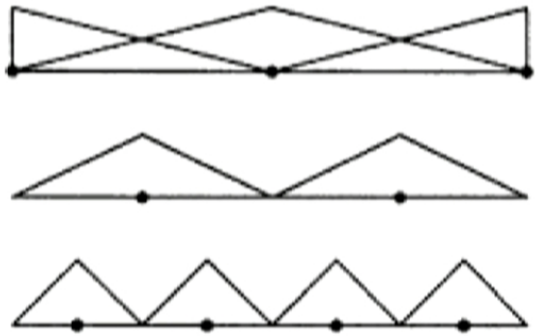
Hierarchical Basis



(a)

Finite Differencing

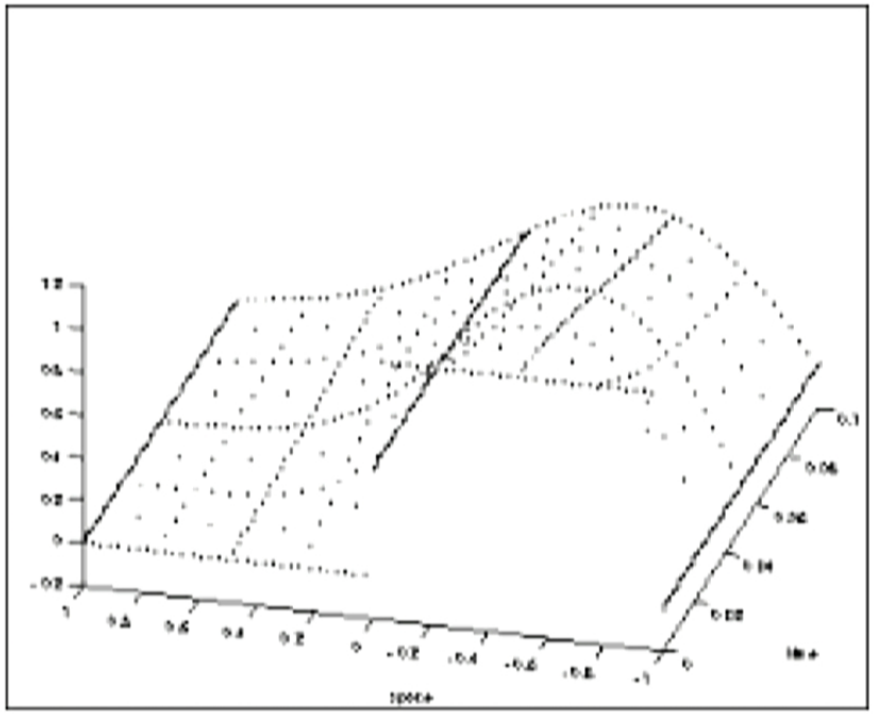
(b)

[www.nap.edu]

Sparse grids

Can represent
D-dimensional domain
with $O(2^D N)$ coefficients

Adapt grid to PDE



[wissrech.iam.uni-bonn.de]

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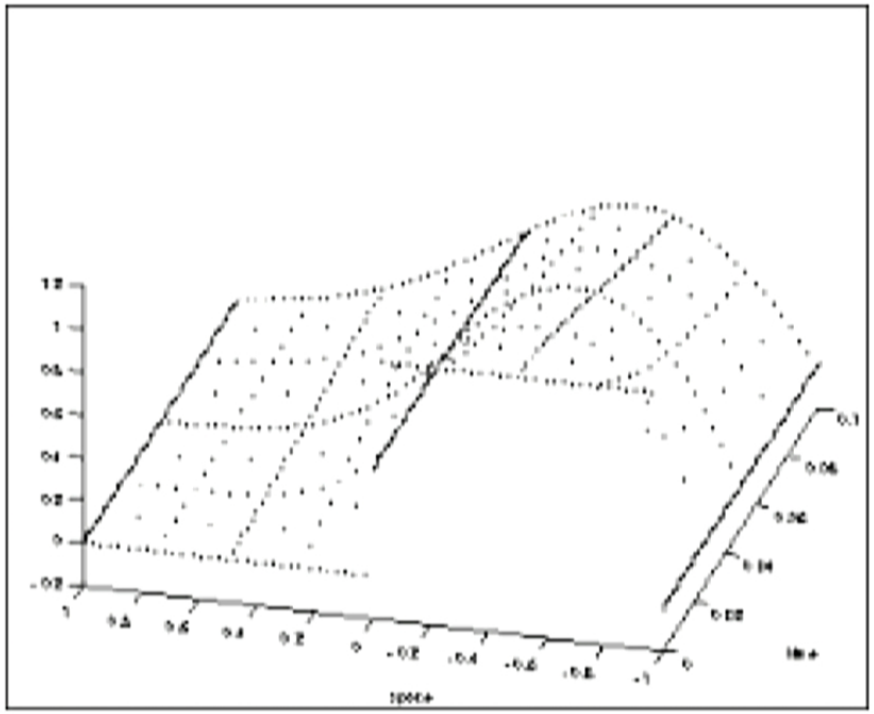
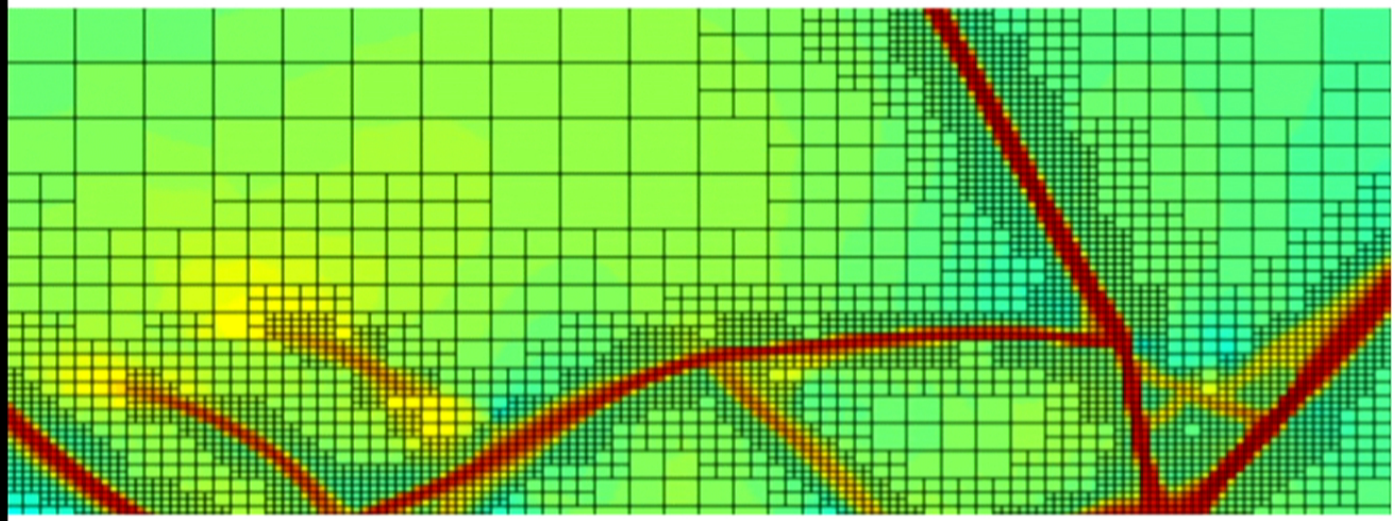


[wissrech.iam.uni-bonn.de]

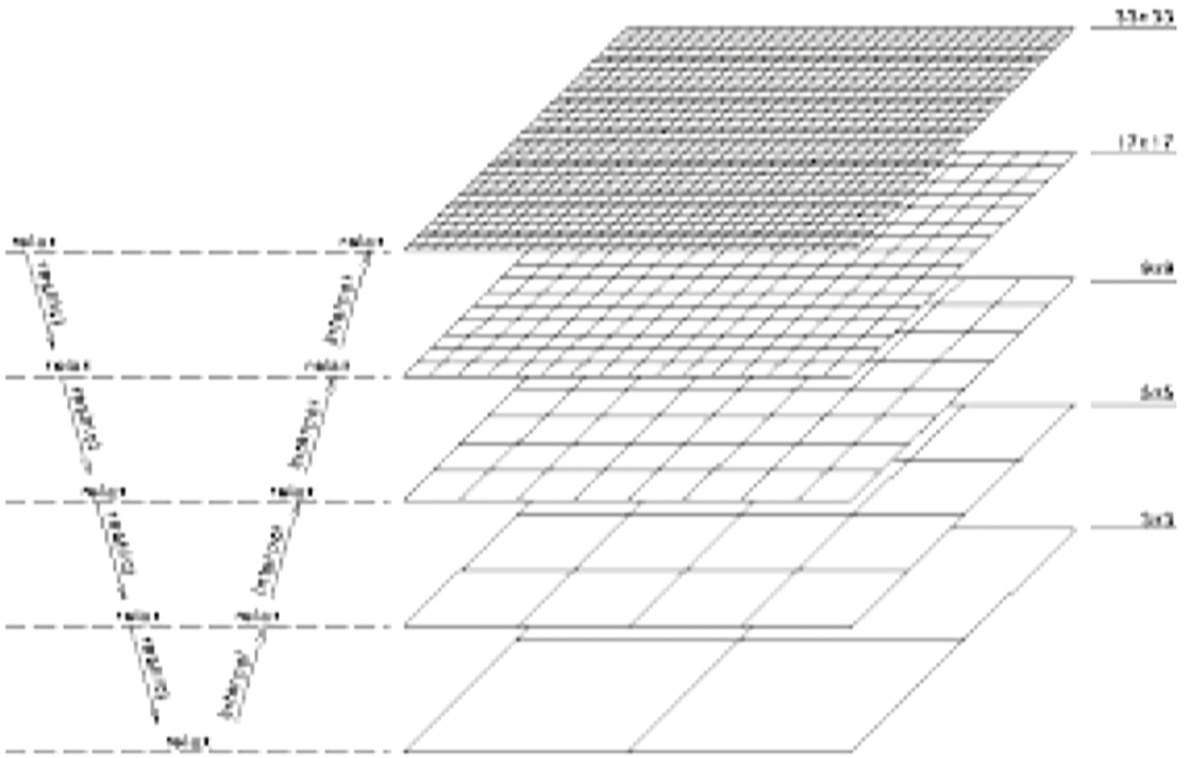
Adaptive Mesh Refinement

Dynamically adapt mesh to solution U



[jupiter.ethz.ch]

Multigrid Methods



[mgnet.org]

Summary

- Efficiency of algorithms depends on available computing architecture
  - Parallelism (independent operations, not sequential)
  - Data locality (operate on “neighbouring” data)
- Large problems require distributed memory
  - Partition data structure
- Modern software engineering:
  - Powerful concepts from group theory, category theory, e.g. future, async