Title: Scientific Computing and Computational Science

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Abstract:

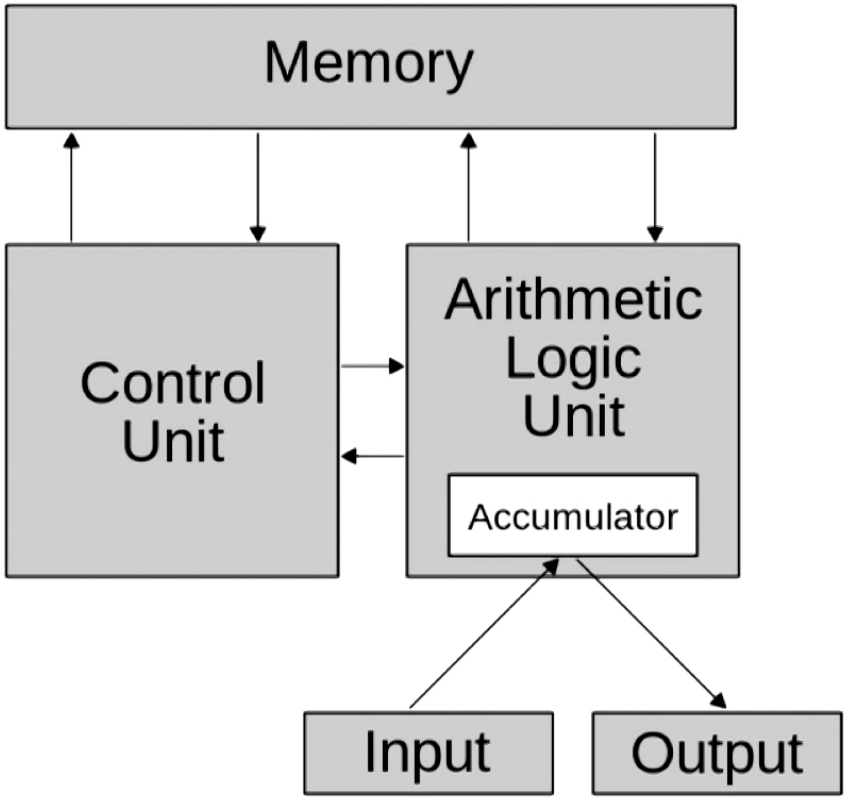
Scientific Computing and Computational Science

Erik Schnetter, Perimeter Institute

Making Quantum Gravity Computable, 2017-05-19

- What is a Computer?
- How do I program it?

Von Neumann Architecture



Sequential Execution:

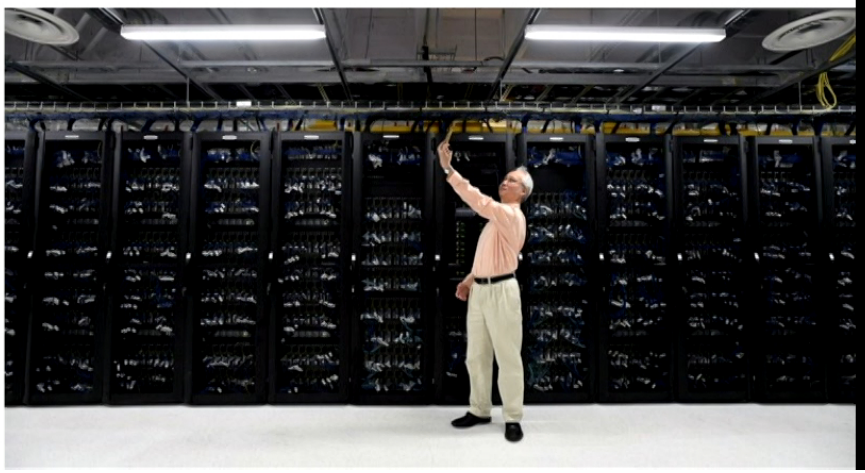
x := a + b

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

[Wikipedia]

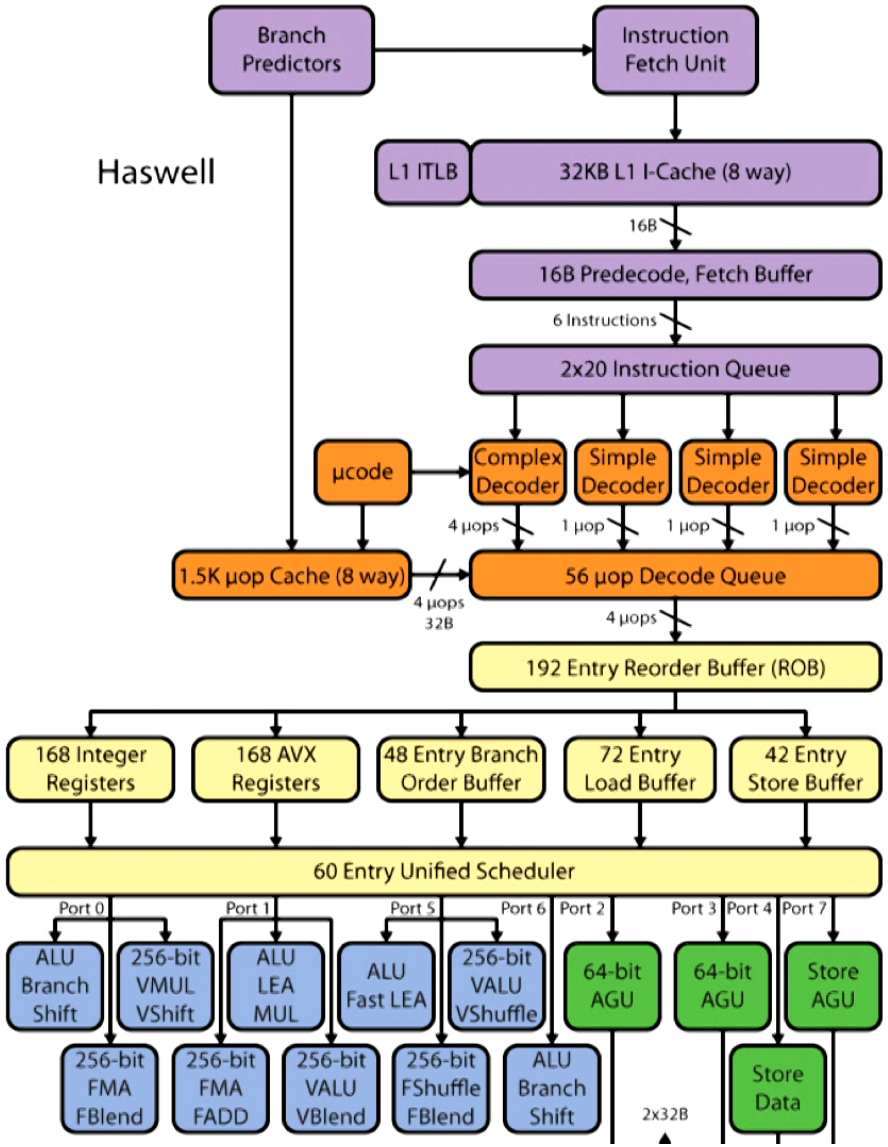
C64 (1984)

Graham (UW, 2017) [The Record]



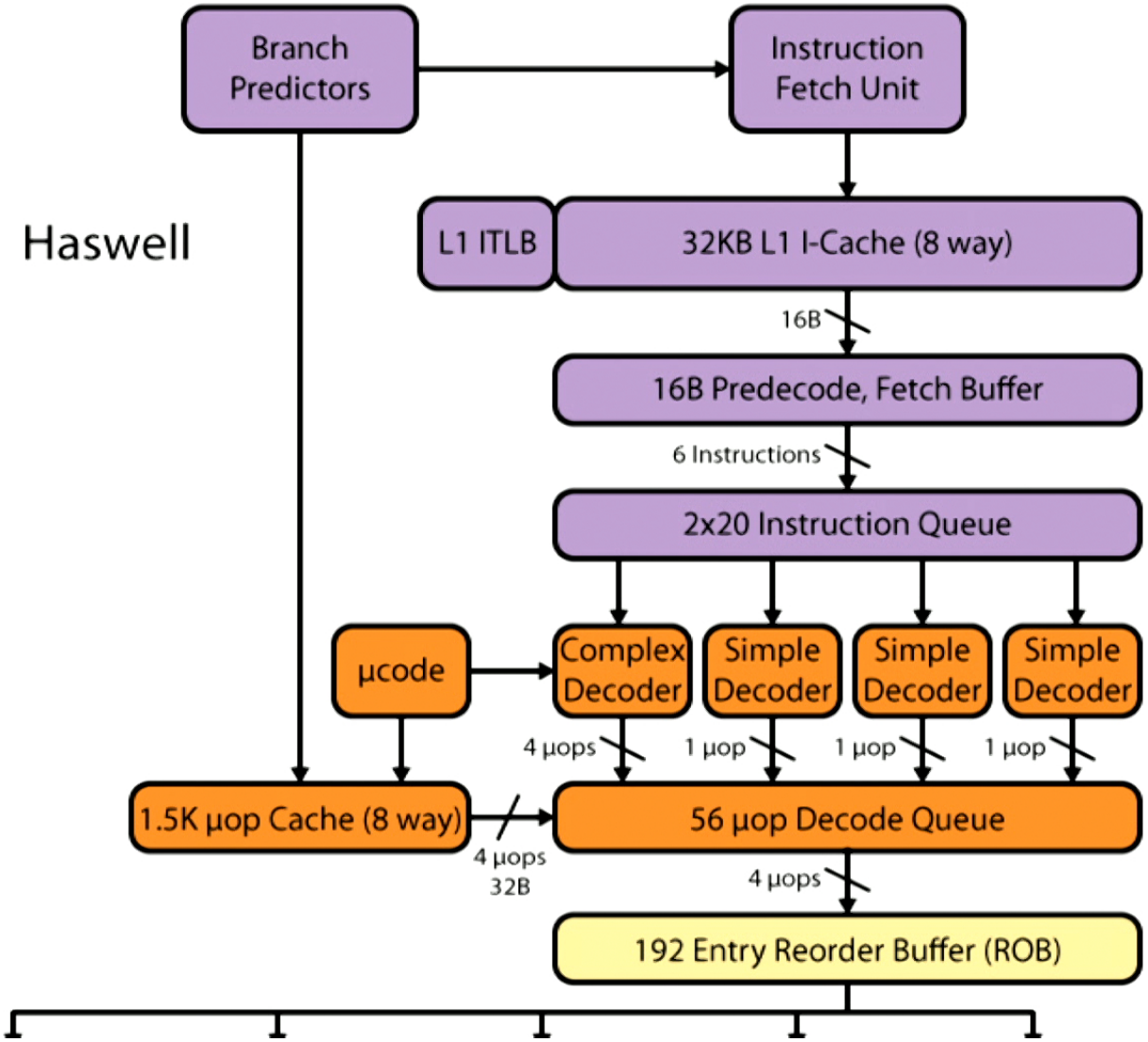
Algorithm Development

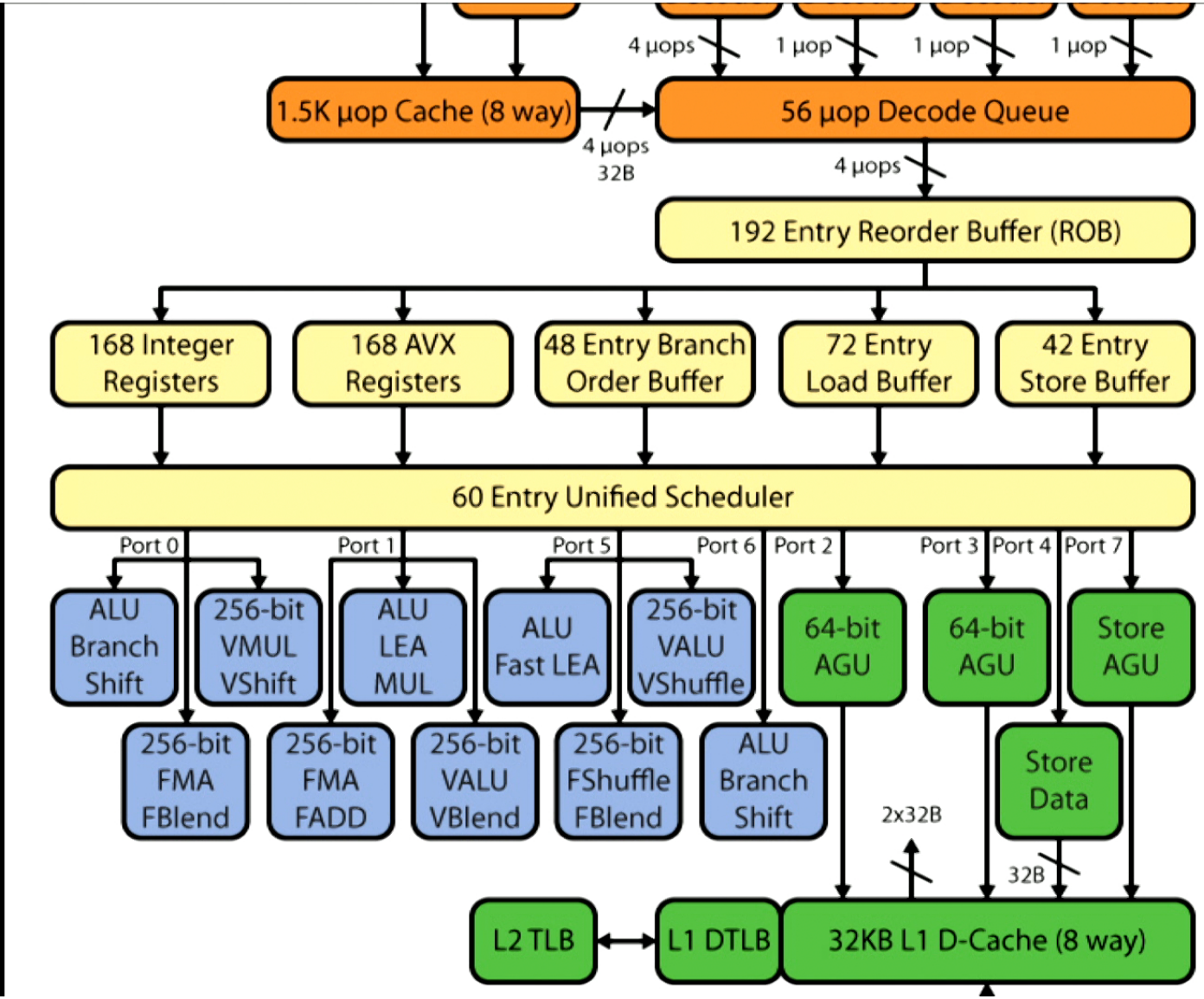
- Naïve idea:
  - Von Neumann (and others) developed a theoretical model of computing
  - Take an algorithm (i.e. constructive proof), map it to this model, implement it in a computer language
- In practice:
  - What is possible (and what is efficient) is not determined by an abstract model, but by current-day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



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)

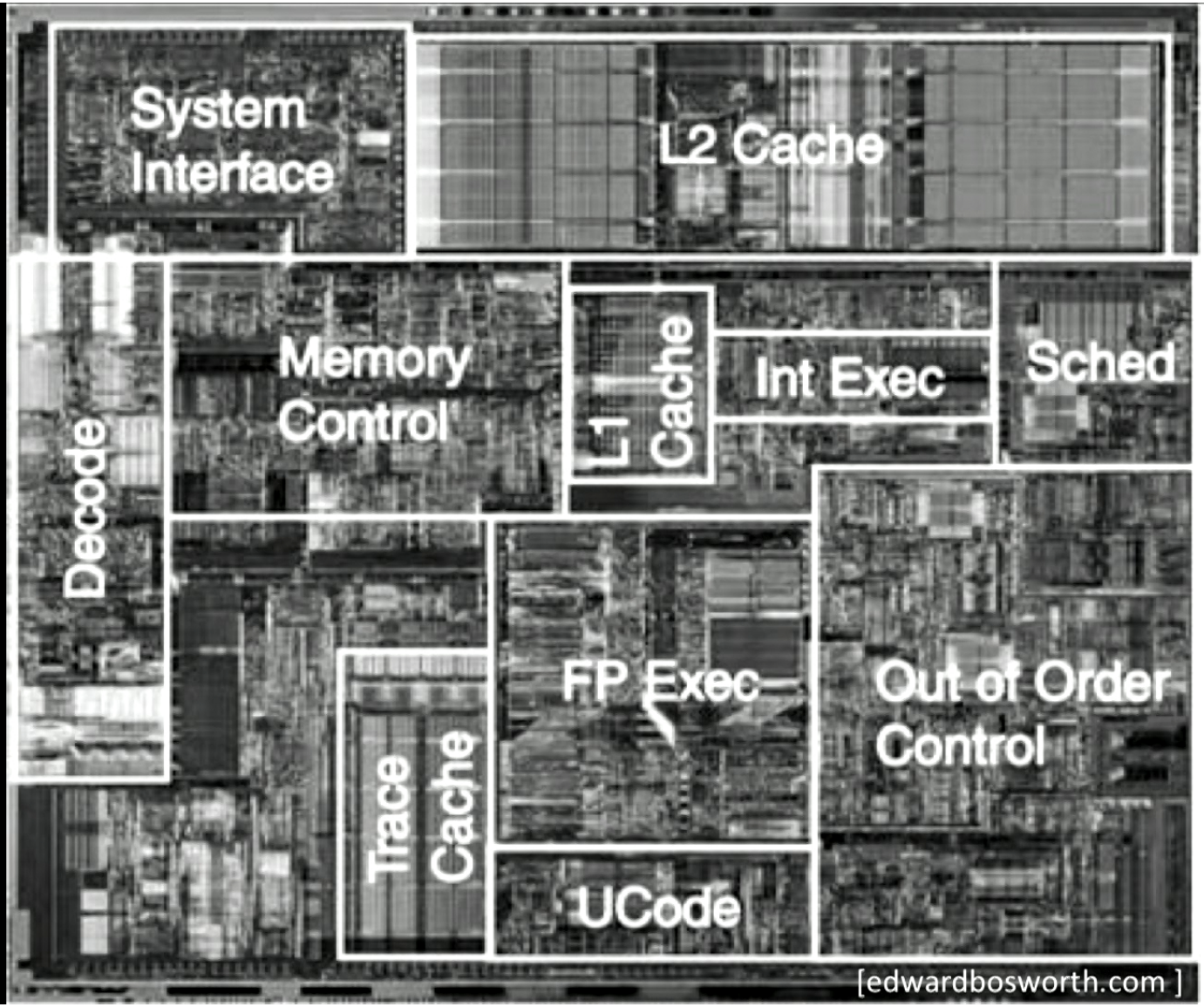

4 µops
1 µop
1 µop
1 µop
1.5K µop Cache (8 way)
4 µops
32B
56 µop Decode Queue
4 µops
192 Entry Reorder Buffer (ROB)
168 Integer Registers
168 AVX Registers
48 Entry Branch Order Buffer
72 Entry Load Buffer
42 Entry Store Buffer
60 Entry Unified Scheduler
Port 0
Port 1
Port 5
Port 6
Port 2
Port 3
Port 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)

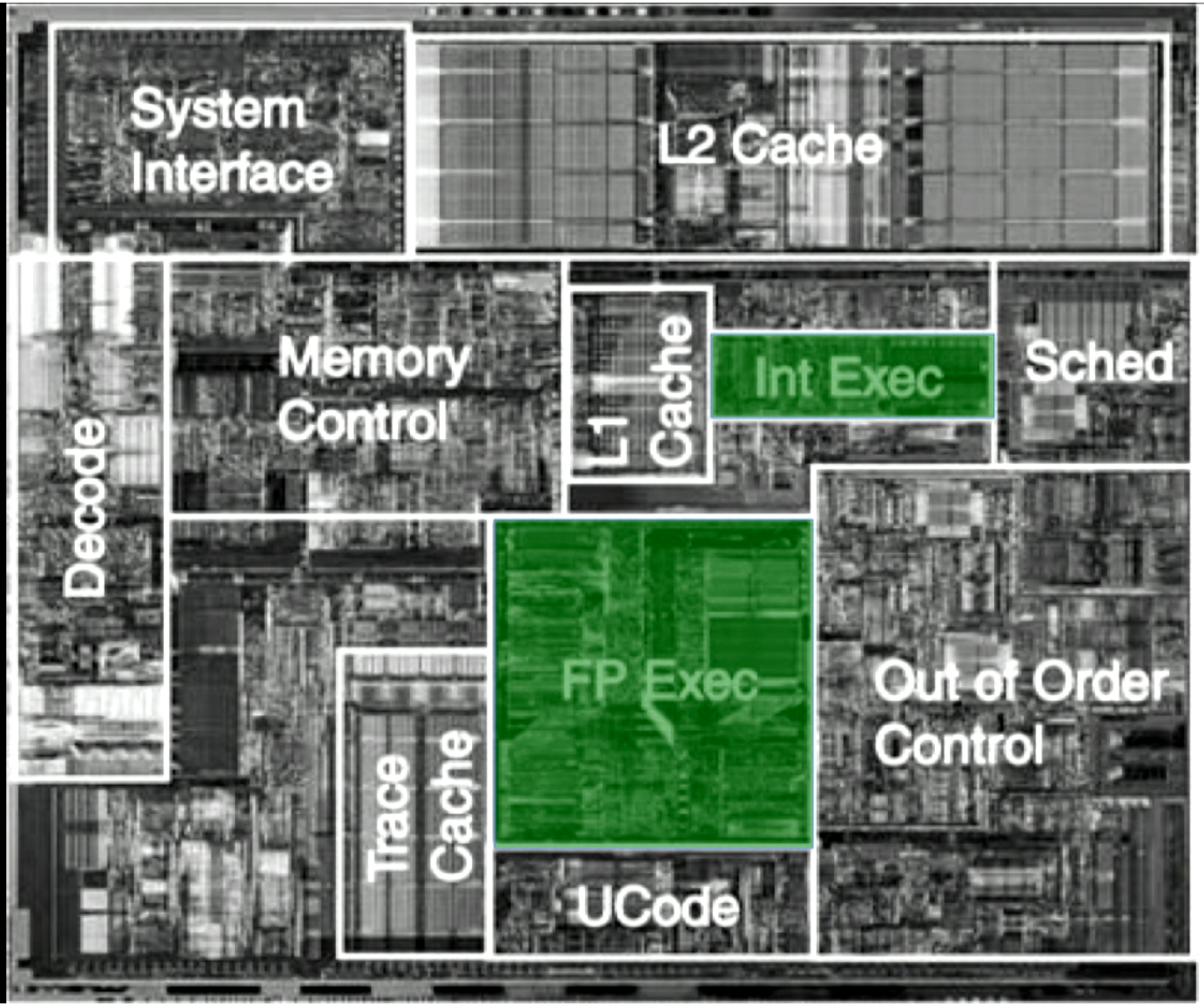
Sequential vs. Parallel

- Modern CPUs are highly parallel:
  - Time for one add operation: 10^{-9} sec
  - Peak performance: 10^{12} Flop/sec
- Efficient algorithms need to be parallel, not sequential
  - Operations need to be *local* and *independent*

Causality

- Newtonian: Events have a unique global order
- (speed of light) times (0.33 ns) = 10 cm
  - Smaller than a laptop
- Relativistic: Events can have spacelike relation
  - "Statements can be reordered by the system"
  - aka "memory model", "cache coherency"


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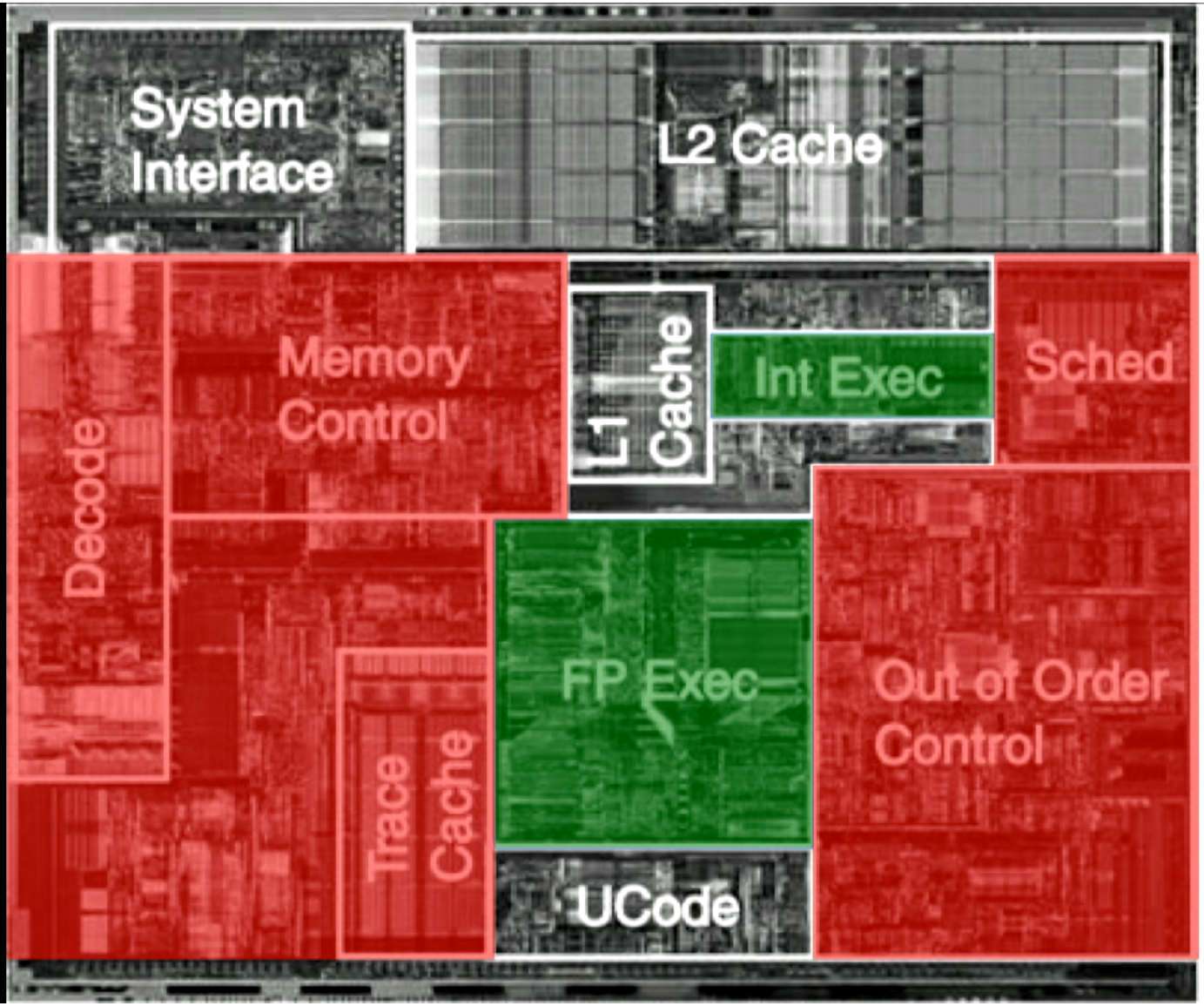
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UCode

Causality

- Newtonian causality:
  - A convenient fiction supported by hardware and standard programming languages
- Relativistic causality:
  - Reality; significantly faster, but amazingly difficult to use correctly
  - See also accelerators, GPUs

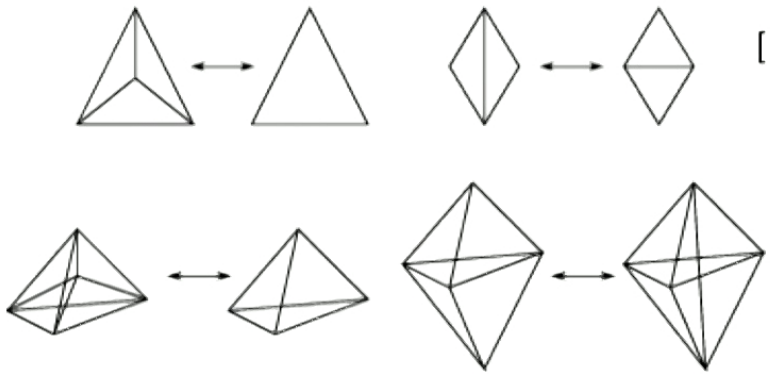
Energy Consumption

- Some well-known laws:
  - $Q = t \cdot I$ (parasitic capacity)
  - $U = R \cdot I$
  - $P = U \cdot I$
- Typical desktop CPU power and area:

  $50\ W / 200\ mm^2 = 2.5\ kW/m^2$
- Stovetop: $1.5\ kW / 750\ cm^2 = 0.2\ kW/m^2$

Supercomputer?

Are Pachner moves local? (Can they be parallelized?)



[Hellman, arXiv:1102.1688]

- Answer:
  - They are not local (only "almost local")
  - Need to form a monoid (or lattice?) for efficient parallelization

Object-Oriented Programming

- Current main-stream paradigm for large programs
- Objects:
  - Have a unique identity
  - Can model (classical) real-world items
  - Have a state that can change
- Problem:
  - Doesn't make sense for mathematical operations

Functional Programming

- "Functional" because there is an algebra of functions (e.g. composition)
- Usually:
  - Value semantics (no identities)
  - Referential transparency (immutability)
- Ideal for mathematical expressions, and for parallel programming
- (Surprisingly, can define object identities on top of this)

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?

- Functional programming:
  - Design programs to be order-independent
  - Remove distinction between data and functions

```
let x = 1
  sin(x)
end
```

```
let f = sin
   f(1)
end
```

- 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

- Note: only few years old, still immature

Summary

- Causality in computers is relativistic
  - Newtonian causality is an expensive fiction
- Computers are highly parallel machines
  - Even laptops and cell phones
- Object-oriented programming doesn't help with mathematical modeling
  - Mathematical entities do not have an identity (functional programming!)