Corrfunc: Blazing fast correlation functions with SIMD Intrinsics

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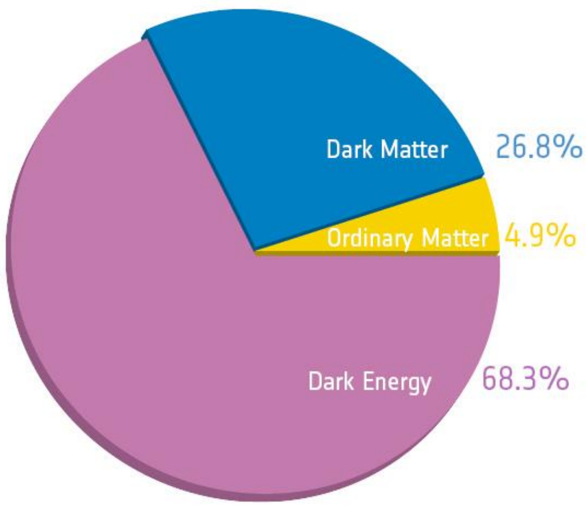
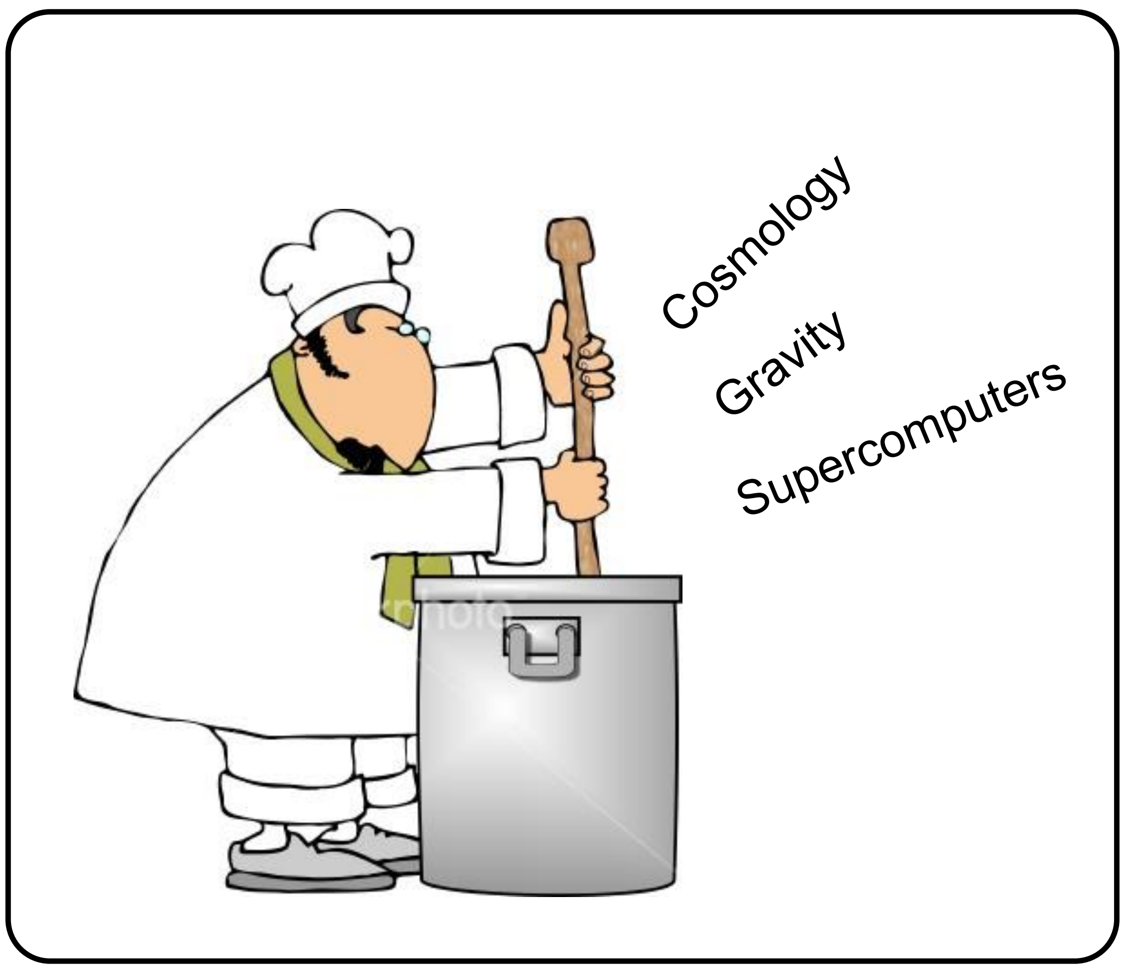
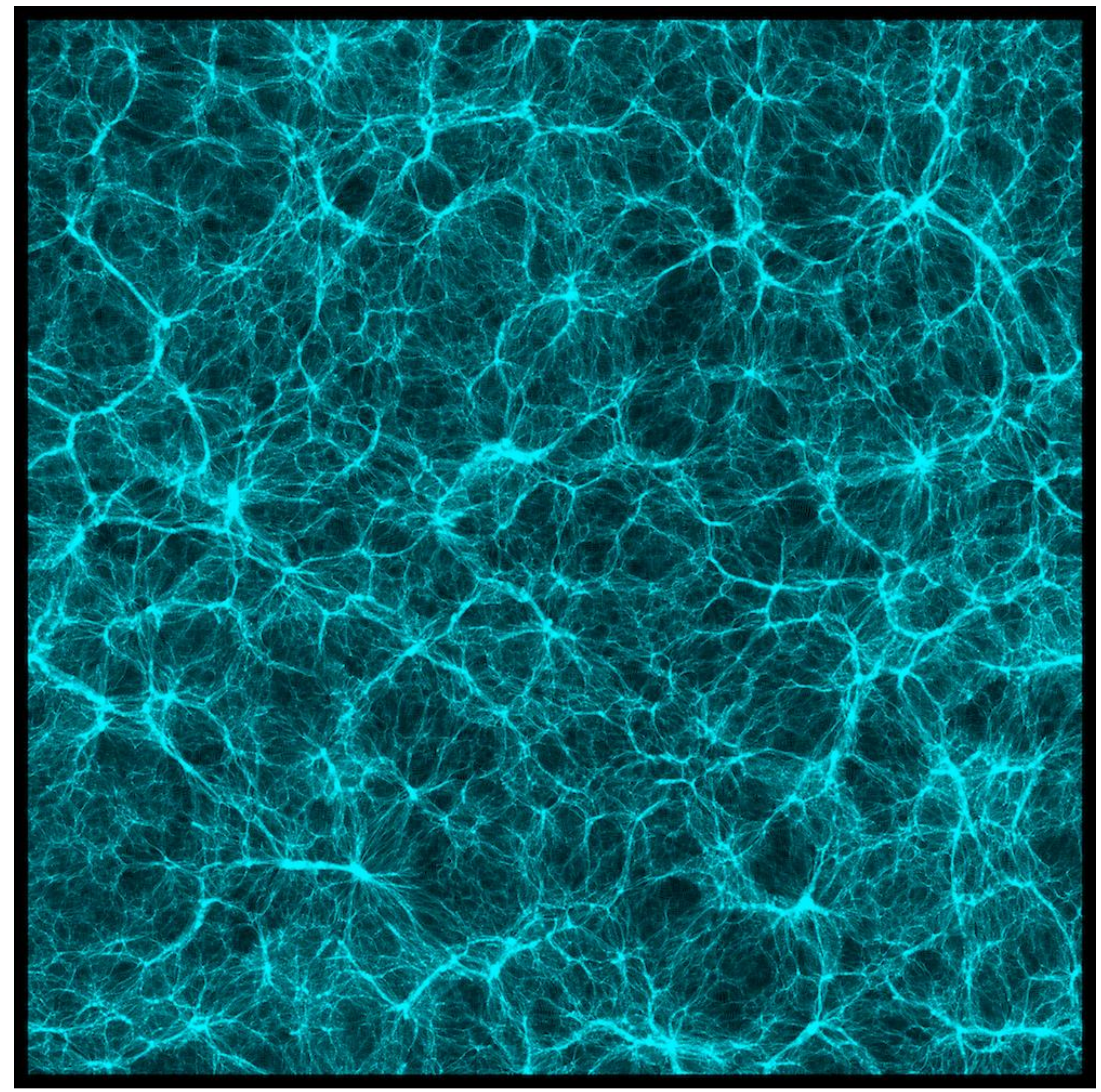
Repo: github.com/manodeep/Corrfunc/
Collaborators: Lehman Garrison
Contributors: Andrew Hearin, Nick Hand

ΛCDM Picture: Galaxies live in Halos

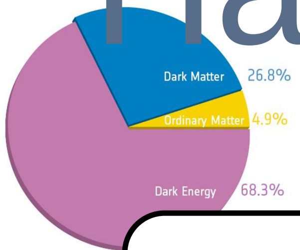


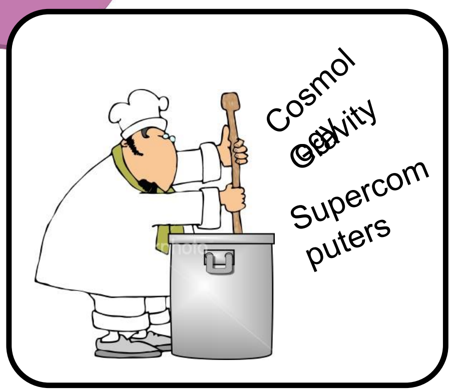


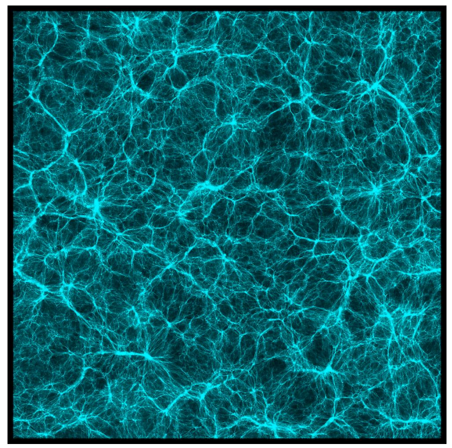


LasDamas Simulations, XSEDE/TACC

ΛCDM Picture: Galaxies live in Halos

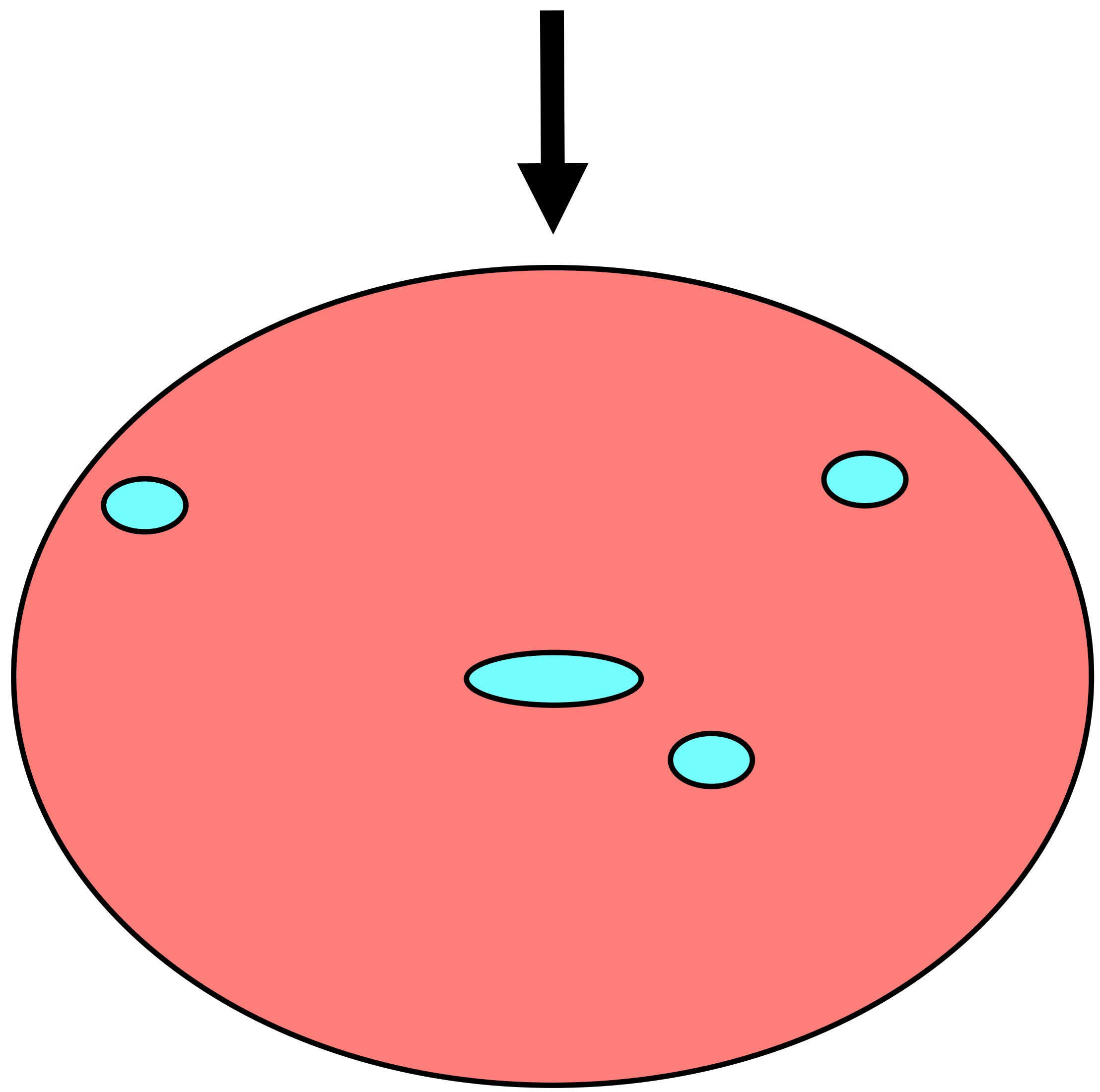




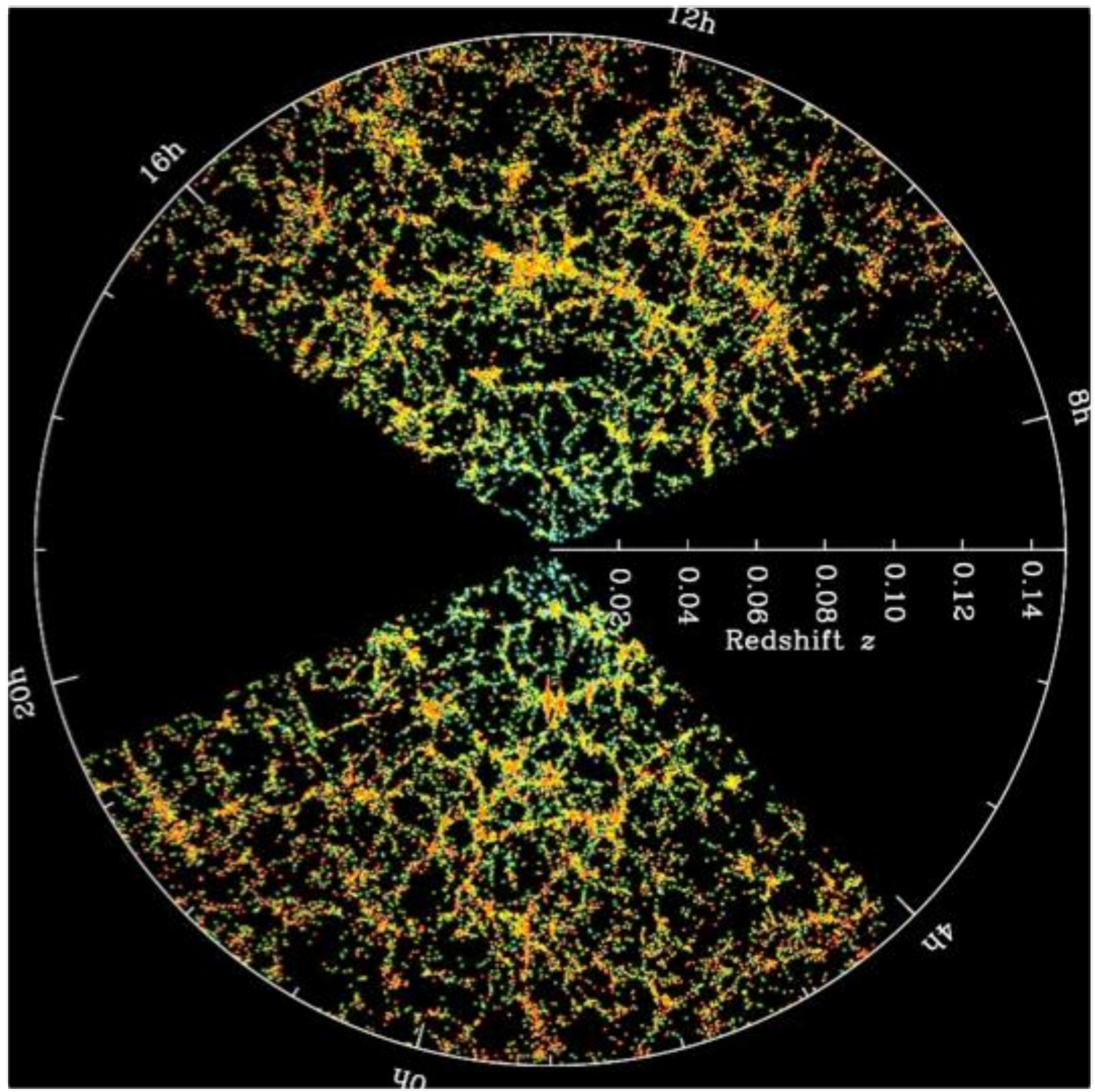


+

Baryon Physics (messy)



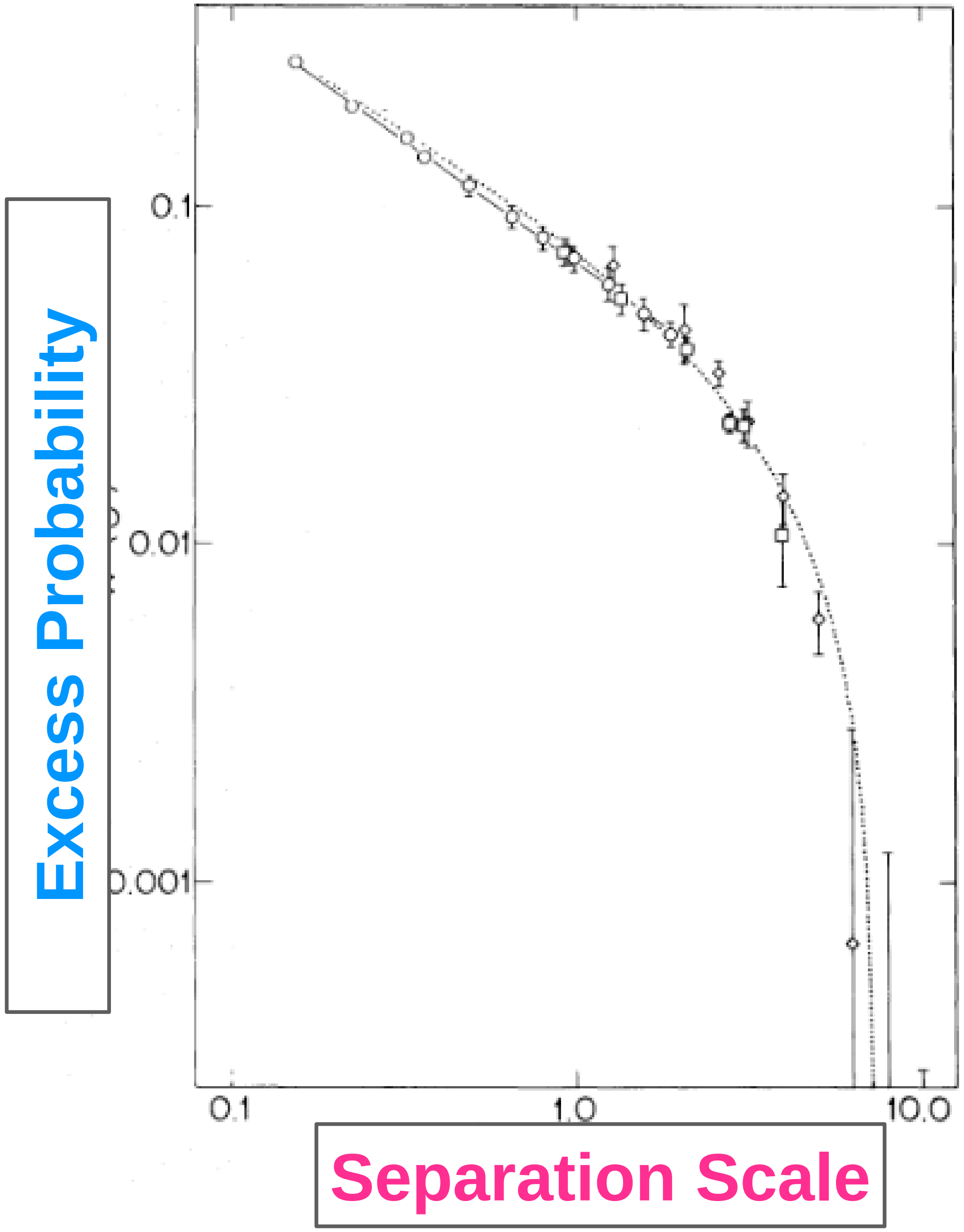
Quantifying the Galaxy Distribution



What is a Correlation Function?

- Measures the excess probability of finding a pair at some separation.

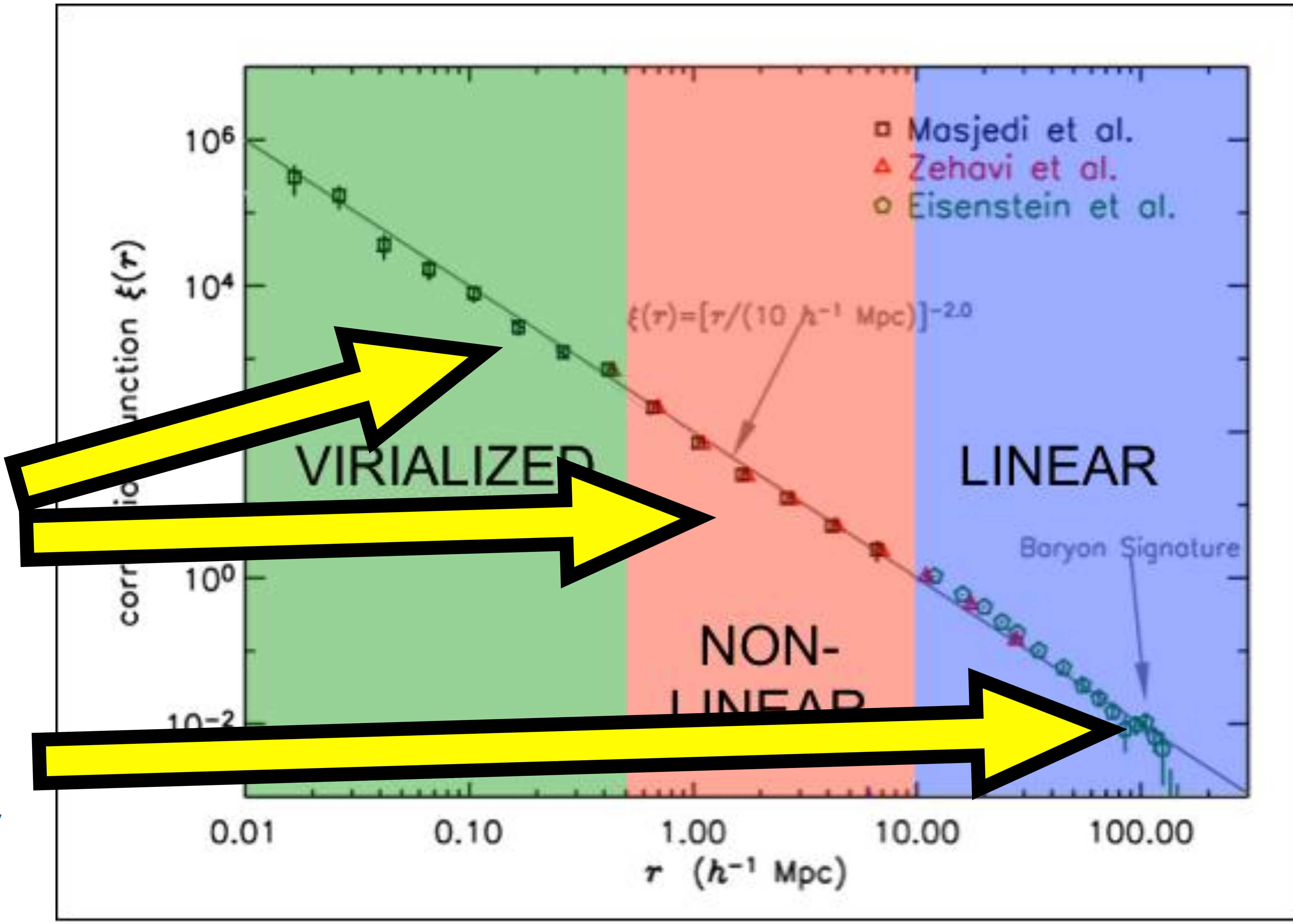
Groth & Peebles, 1977



Galaxy Clustering on different scales

Galaxy formation physics

Gravity + Cosmology



Masjedi et al. (2006)

Correlation functions are fundamental to understand how galaxies populate halos

Code for a Correlation Function

```
for(int i=0;i<N1;i++) {
  for(int j=0;j<N2;j++) {
    double dist = @distance_metric@(point[i], point[j]);
    if(dist < mindist || dist >= maxdist) {
      continue;
    }

    int ibin = @dist_to_bin_index@(dist);
    numpairs[ibin]++;
  }
}
```

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}
```

Simple Code is … simple

- Ignores domain knowledge

  (maxdist << L)

- Not optimal for hardware*****

- Can not be vectorized by

  compiler

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for(int i=0;i<N1;i++) {
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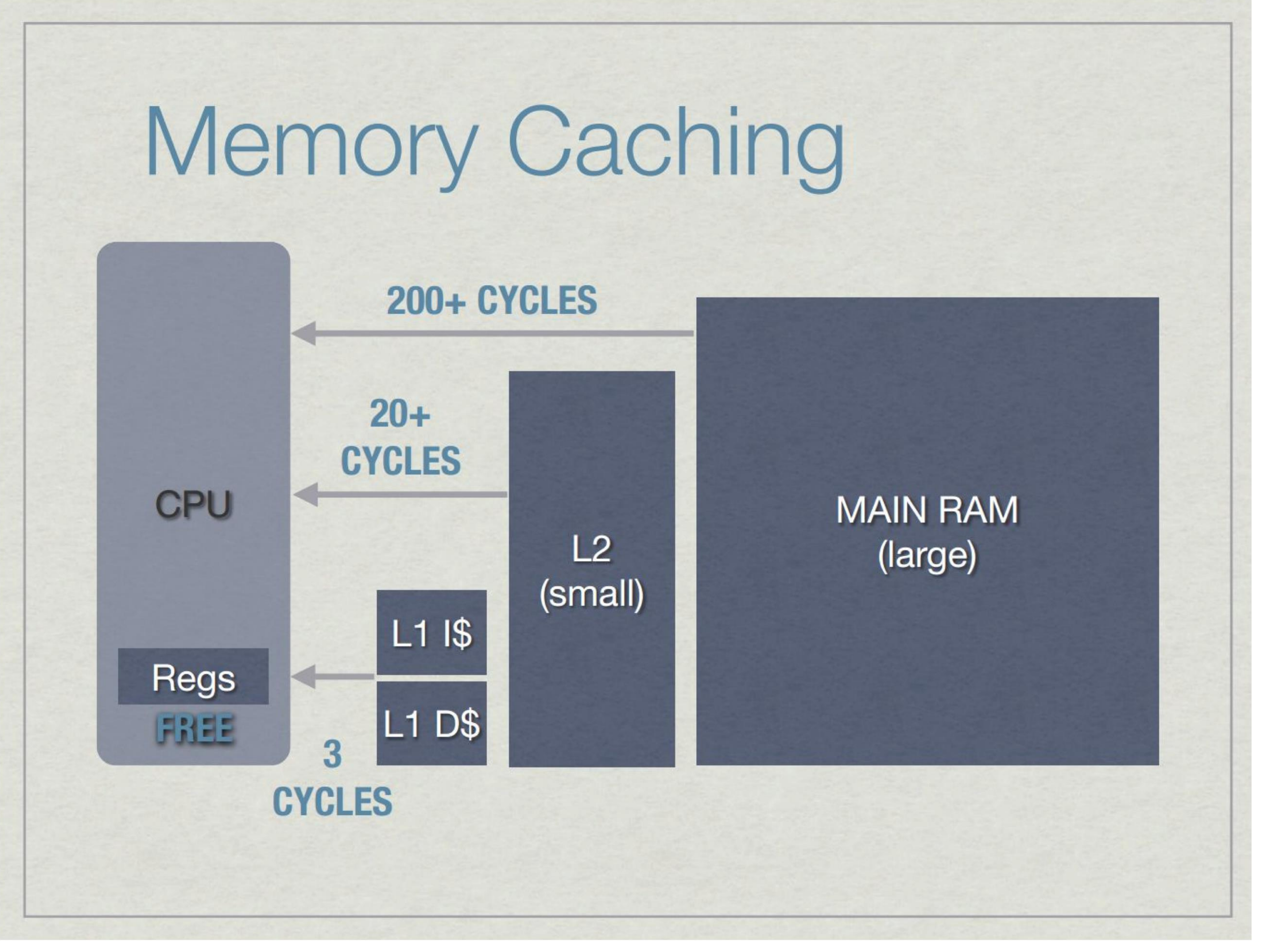
}
```

Hardware Detour

Memory access is slow



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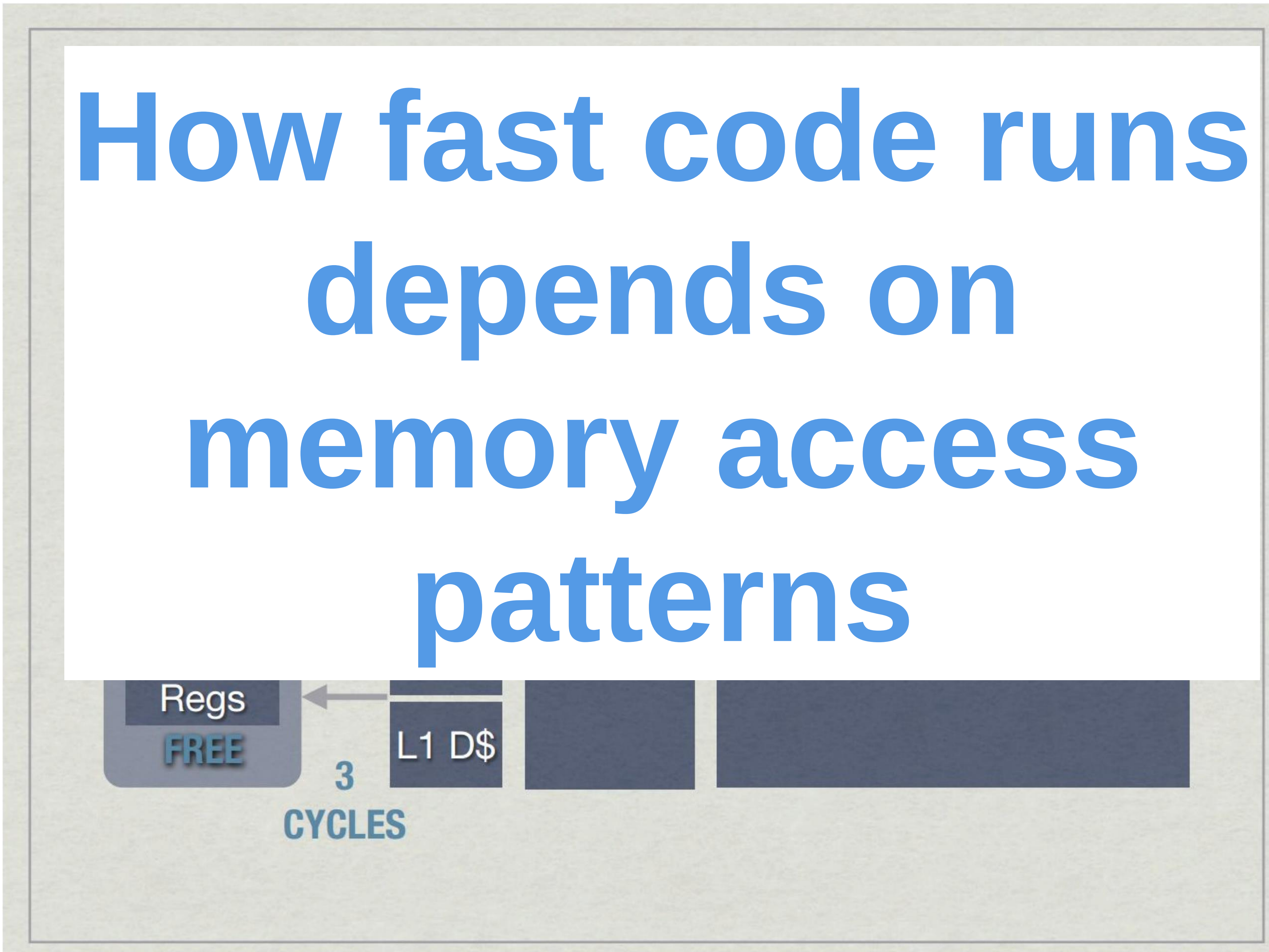
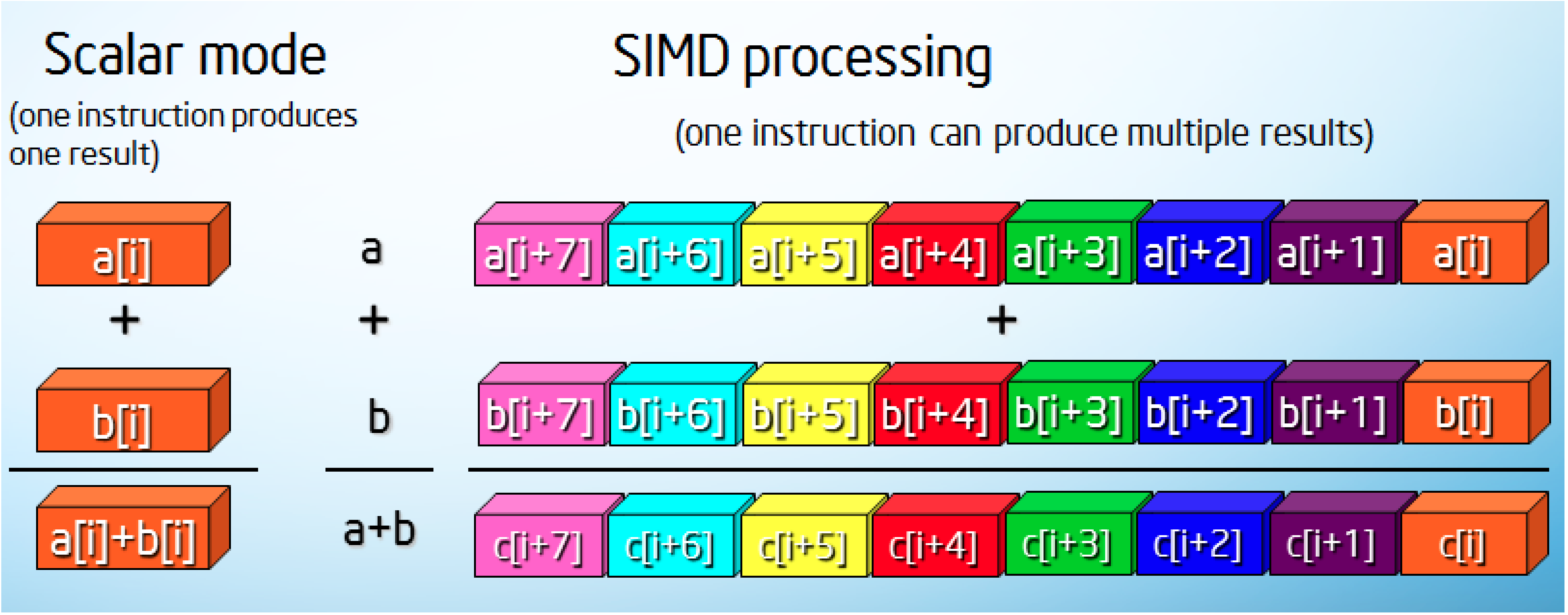


How fast code runs depends on memory access patterns

Vector Instructions (SIMD)



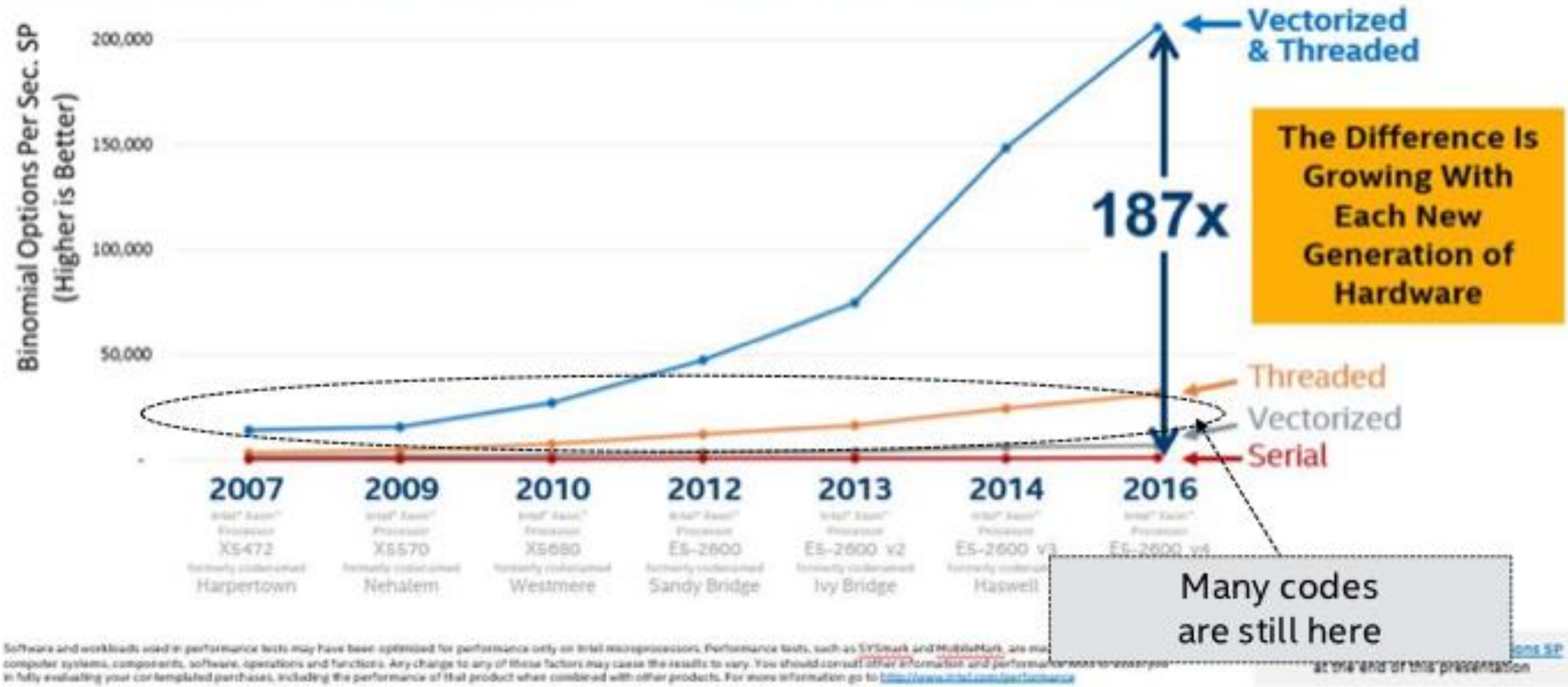
Untapped Potential Can Be Huge!

Configurations for Binomial Options SP at the end of this presentation

K. O'Leary, Intel

Vectorize & Thread or Performance Dies

Threaded + Vectorized can be much faster than either one alone

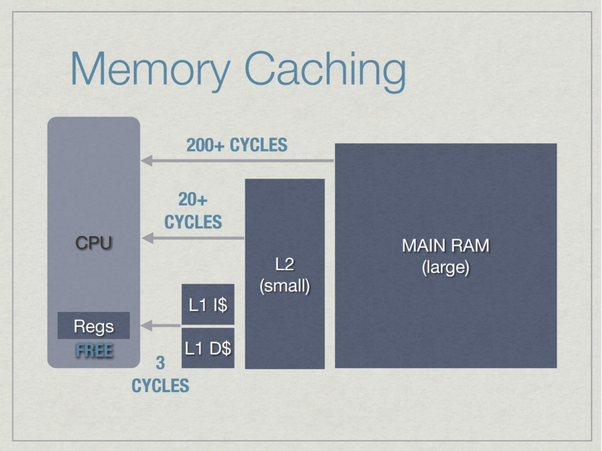


Software and workloads used in performance tests may have been optimized for performance only on Intel microprocessors. Performance tests, such as SYSmark and MobileMark, are measured using specific computer systems, components, software, operations and functions. Any change to any of those factors may cause the results to vary. You should consult other information and performance tests to assist you in fully evaluating your contemplated purchases, including the performance of that product when combined with other products. For more information go to http://www.intel.com/performance

Optimization Notice

SCEC, Dec 2018

Hardware —> Performance



- Power scales as freq^3
  - Multi-cores at lower clock (instead of one core with a 3GHz clock, 2 cores with 2.1 GHz provides 1.4x op/s @ 70% power)
- Memory access is slow
  - Layers of (smaller, faster, dedicated) -> (larger, slower, shared) caches
- Only one instruction per clock cycle
  - but, clock speeds have stalled
    - More calculations per clock tick (SIMD/vectorization)

Vectorized operations with efficient memory access within independent kernels

Back to Corrfunc

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  (maxdist << L)

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      continue;
    }

    int ibin = @dist_to_bin_index@(dist);
    numpairs[ibin]++;
  }
}
```

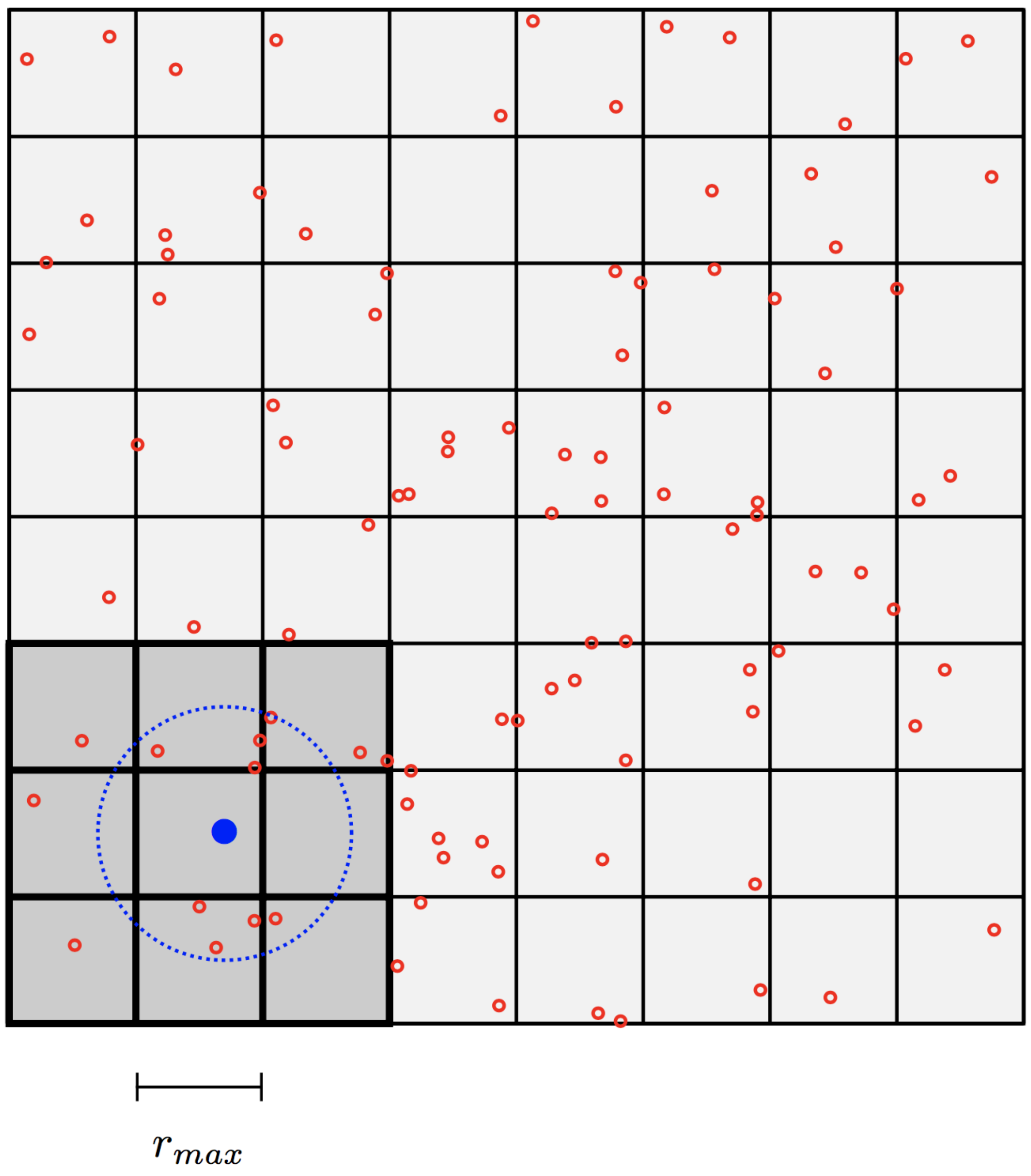
How Corrfunc works

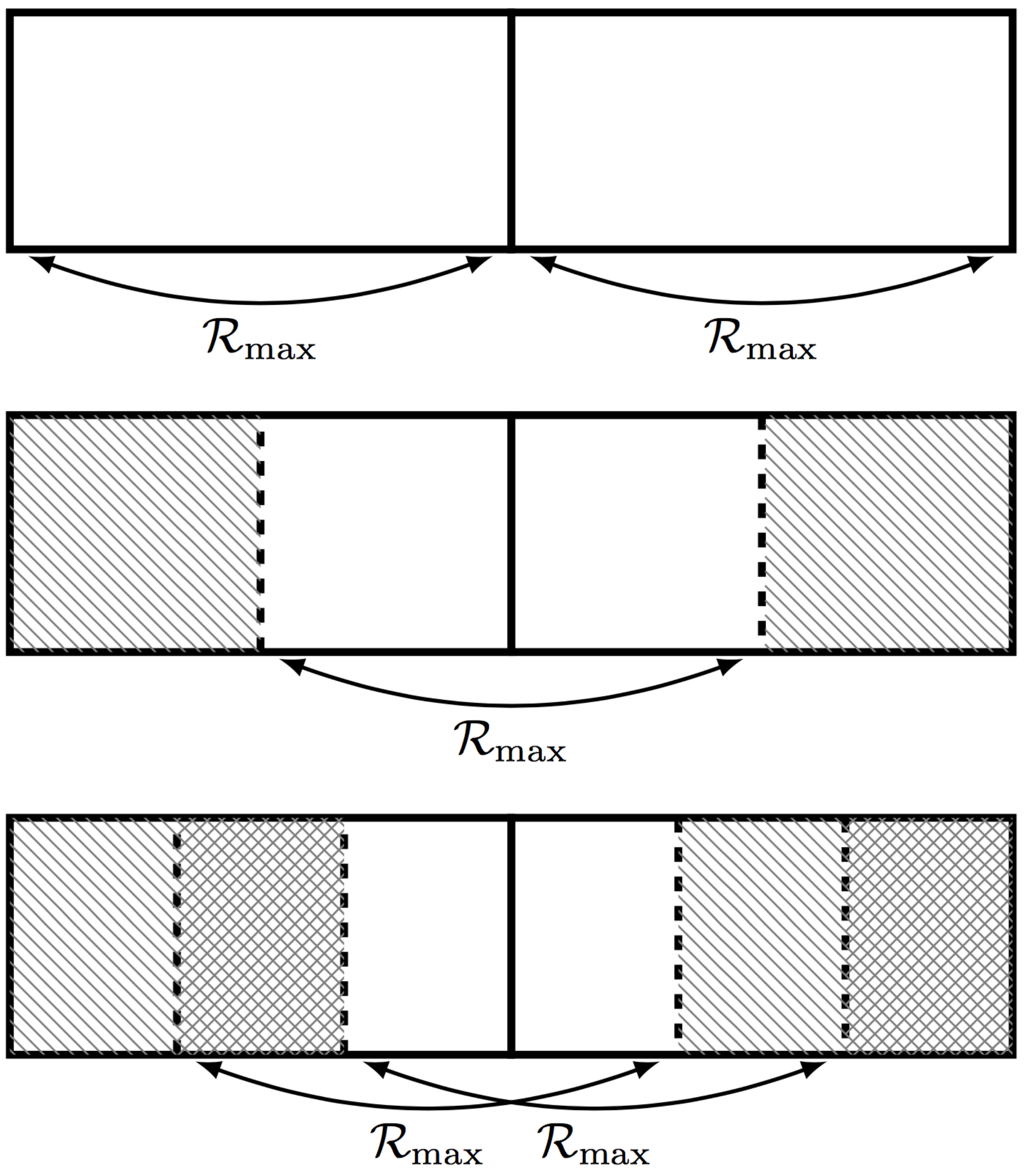
- Grids the particle distribution into 3D cells of size ~Rmax
- Stores particles contiguously within each cell
- Sorts particles within a cell in z
- Only associates pairs of cells that **may** contain pairs
- Uses vectorised kernels on cell-pairs
- Outer OpenMP loop over cell-pairs

Why Corrfunc is FAST

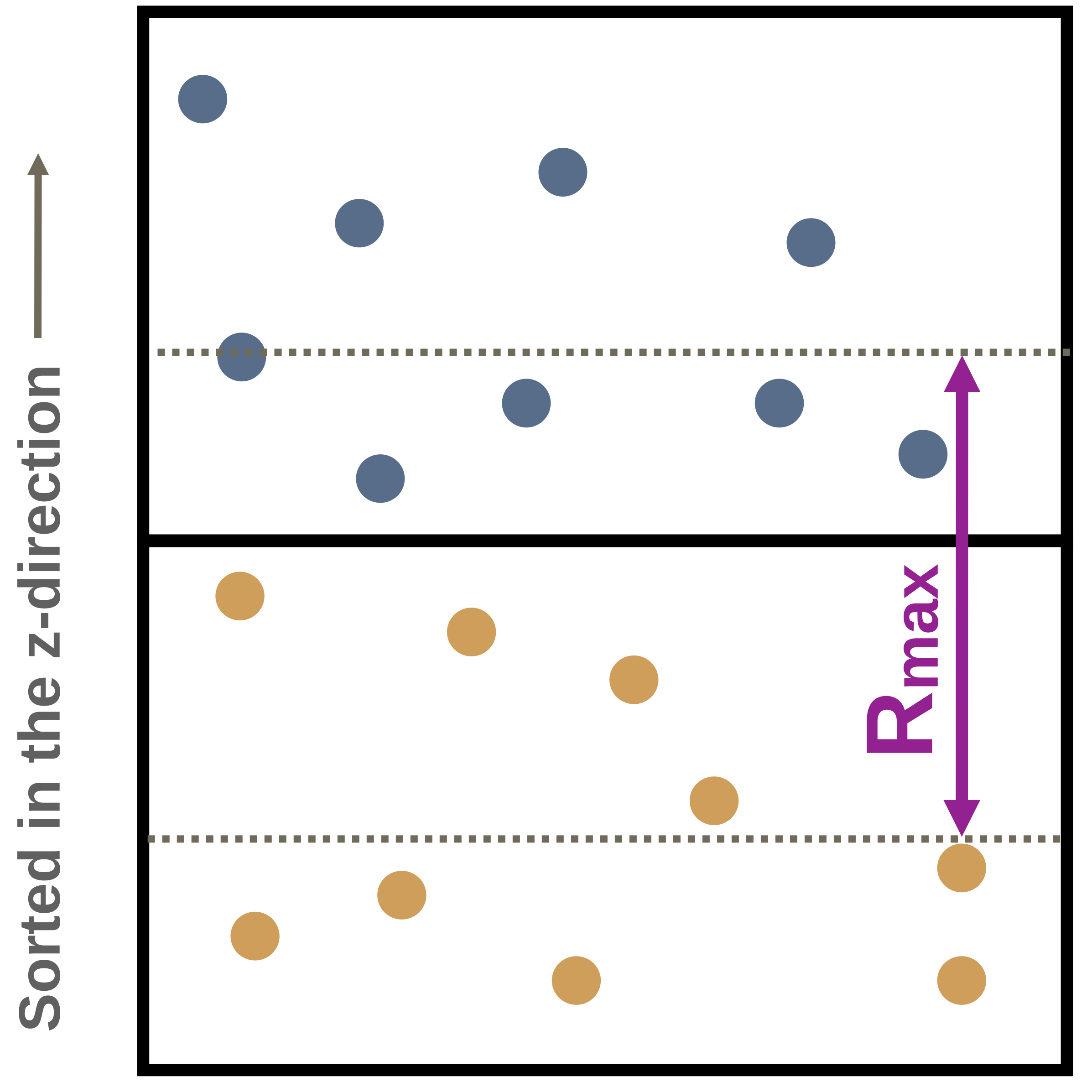
- Grids extent with cells of Rmax (**domain knowledge**)
- Stores particles contiguously within each cell (**memory access**)
- Uses sorting to prune (**algorithmic complexity**)
- Uses vector intrinsics (**vectorization**)
- Uses OpenMP (**multi-core**)

Why Corrfunc is FAST: 3D Grid

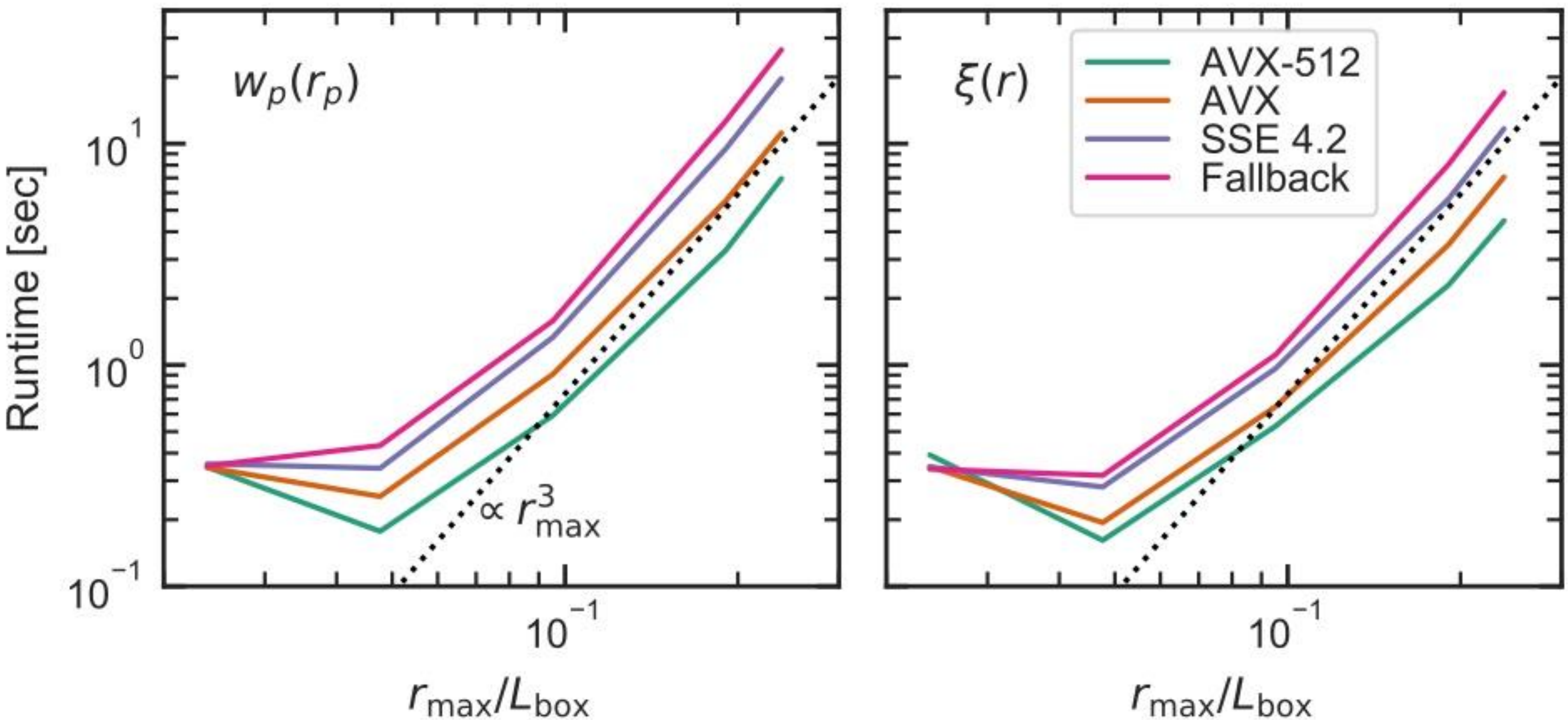




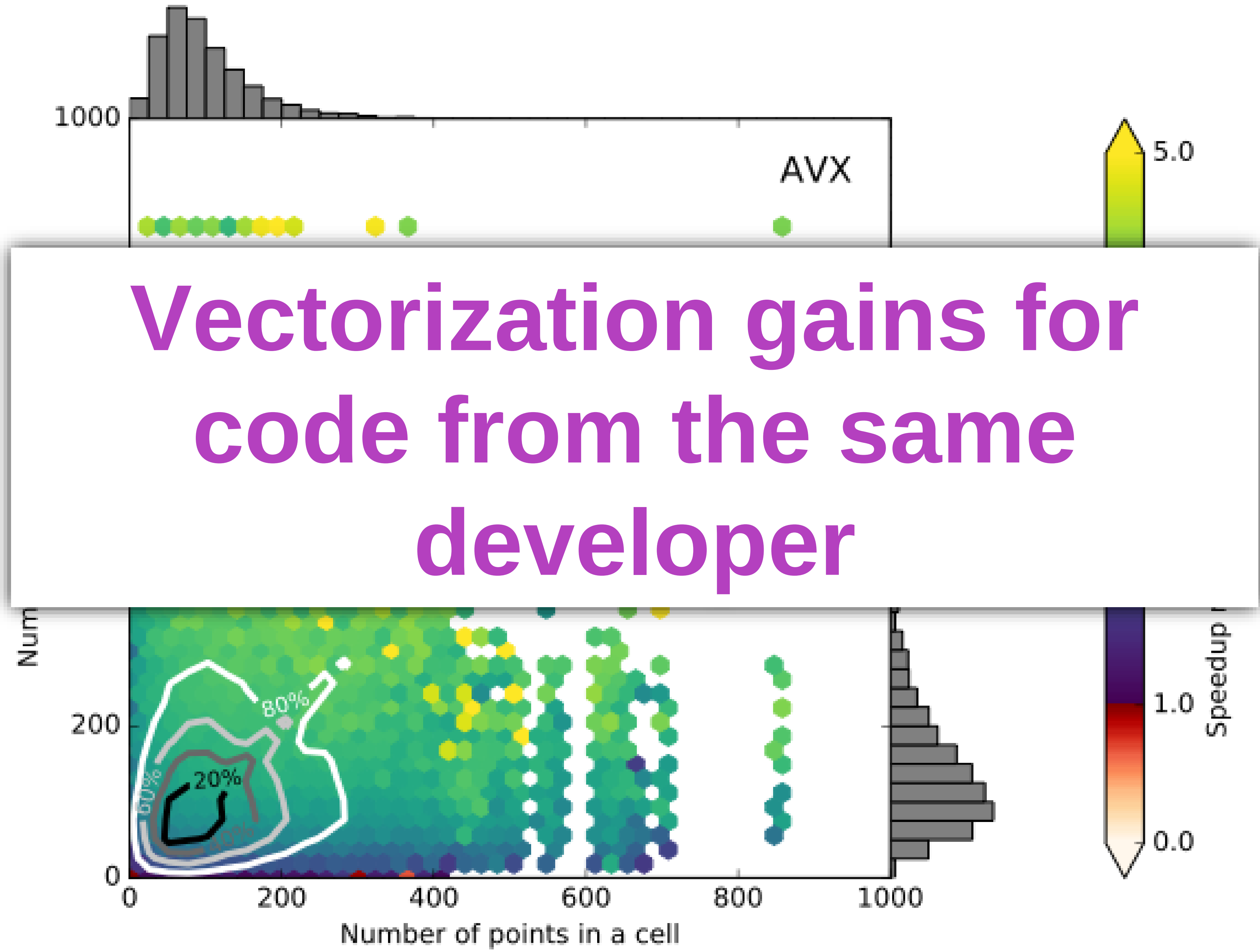
Why Corrfunc is FAST: Sorting



Performance of SIMD Kernels

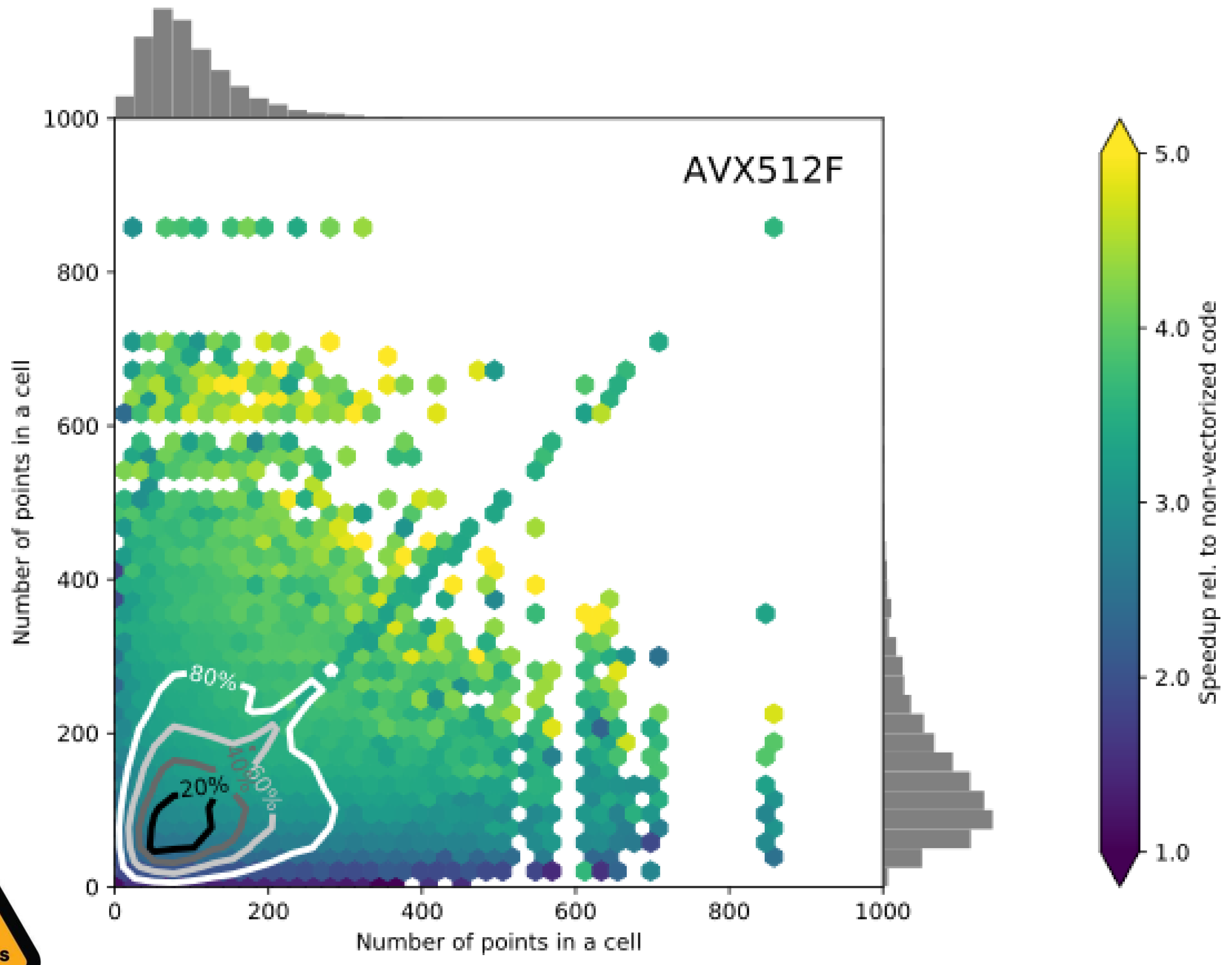


Speedup from Vectorization (AVX)



Vectorization gains for code from the same developer

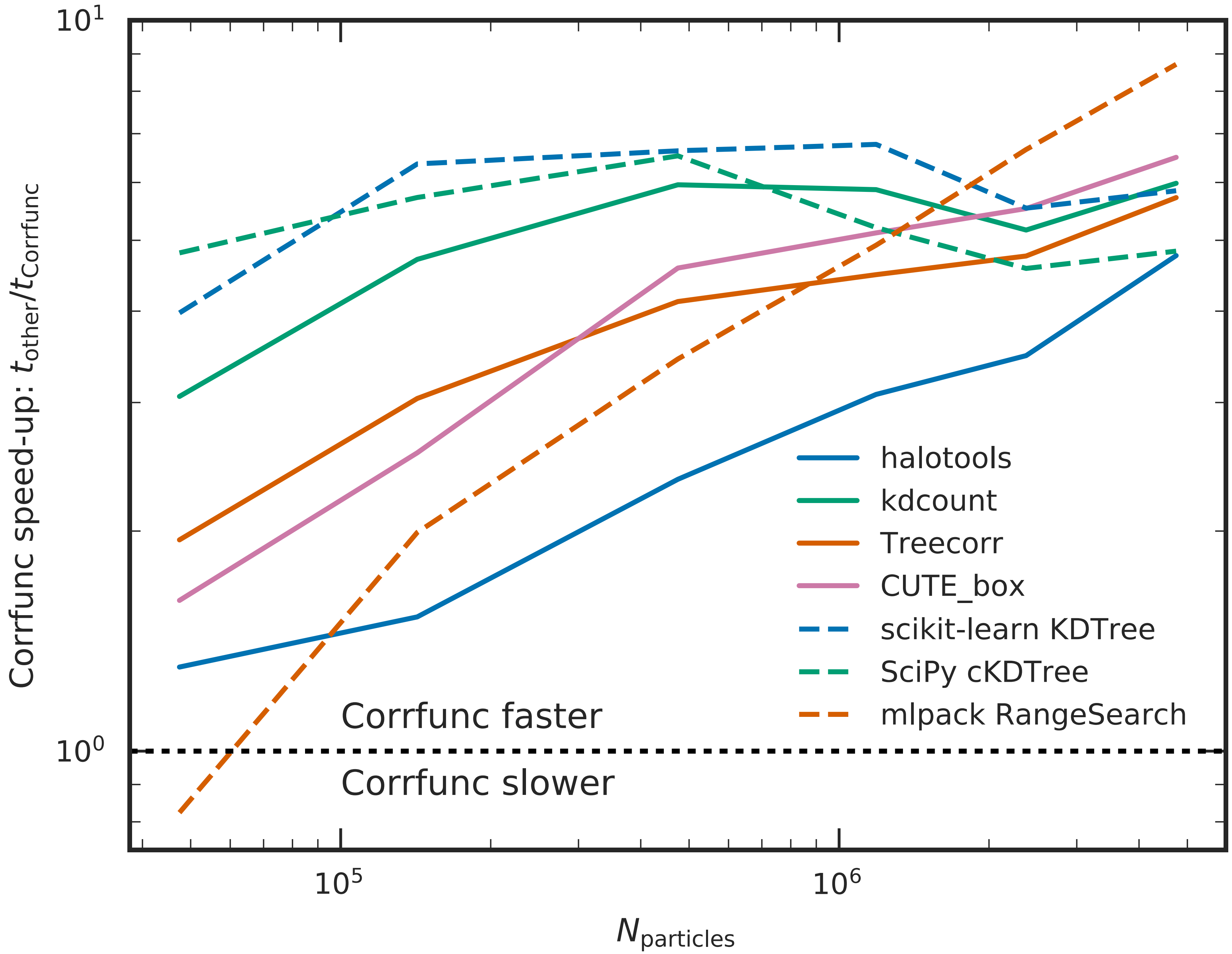
Speedup from Vectorization (AVX512)



OzSTAR Supercomputing

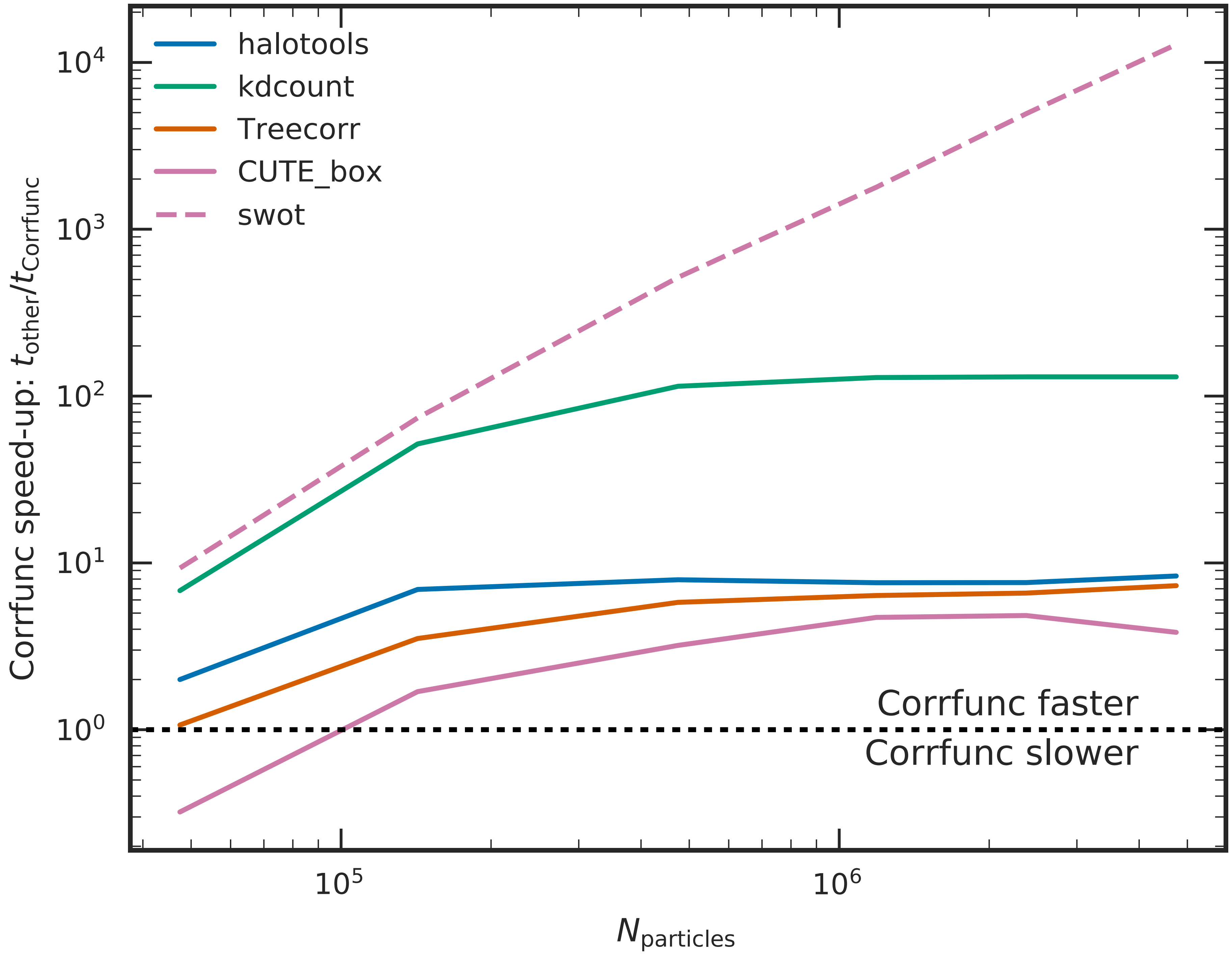
Corrfunc Performance: Single-core

on github:
paper/scripts/generate_code_comparison.py



Corrfunc Performance: Multi-core

on github:
paper/scripts/generate_code_comparison.py



Why I wrote open-sourced Corrfunc

- Inherited codes took ~5 mins. MCMC would have exceeded the funding duration.
  - fast private version for my specific use-case
- Created custom code for experts with 6000x speedup (took < 24 hrs to create)
- Demonstrated the need for a fast, flexible, open-source package
- That initial 5 min calc. now takes ~5 secs with **Corrfunc**

Writing Portable and Fast Software is Difficult

- Python removes the portability issue
    - but not fast
- Compiled extensions use very basic compiler options (defaults options are the ones used for compiling python)
- Compile with the highest compiler-supported ISA
    - Check ISA at runtime

Usability/Sustainability trumps everything

Conclusions

- **Corrfunc** is optimised using domain knowledge, good memory access pattern, vectorization and OpenMP
- **Corrfunc** is “blazing fast” and
  - modular, user-friendly, documented, tested, OpenMP parallel, flexible API access, …
  - GPU version coming - thanks to ADACS
- my highest cited bib-entry for last year (ascl.net/1703.003)

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Title:	Corrfunc: Blazing fast correlation functions on the CPU
Authors:	Sinha, Manodeep; Garrison, Lehman
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Publication Date:	03/2017
Origin:	ASCL
Keywords:	Software
Bibliographic Code:	2017ascl.soft03003S

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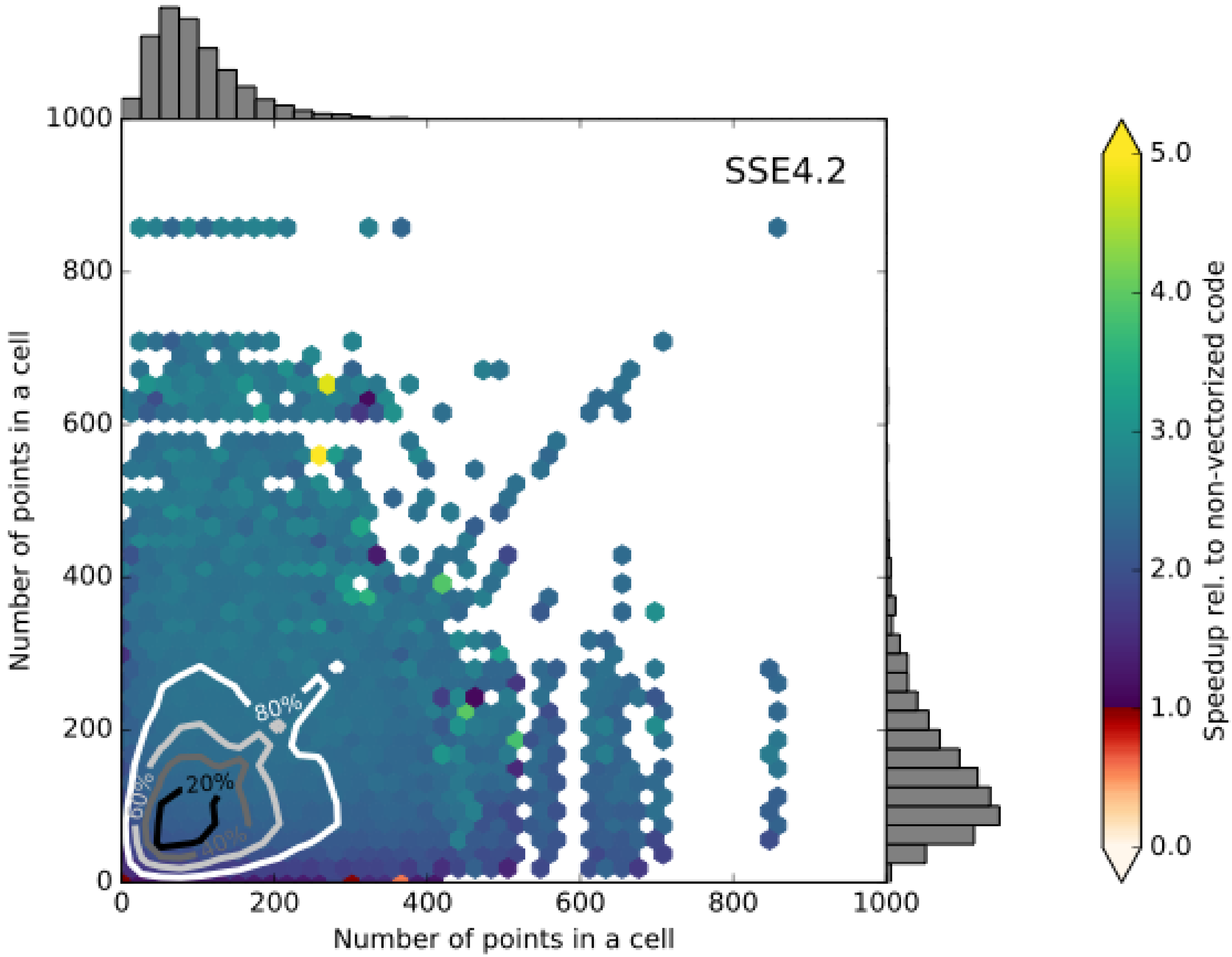
```c
for(int64_t i=0;i<N0;i++) {
    const AVX512_FLOATS m_xpos  = AVX512_SET_FLOAT(*x0++);
    const AVX512_FLOATS m_ypos  = AVX512_SET_FLOAT(*y0++);
    const AVX512_FLOATS m_zpos  = AVX512_SET_FLOAT(*z0++);
    DOUBLE *localx1 = x1, *localy1 = y1, *localz1 = z1;
    for(int64_t j=0;j<N1;j++) {
        AVX512_MASK m_mask_left = (N1 - j) >= AVX512_NVEC ? ~0:masks_per_misalignment_value_DOUBLE[N1-j];
        const AVX512_FLOATS m_x1 = AVX512_MASKZ_LOAD_FLOATS_UNALIGNED(m_mask_left, localx1);
        const AVX512_FLOATS m_y1 = AVX512_MASKZ_LOAD_FLOATS_UNALIGNED(m_mask_left, localy1);
        const AVX512_FLOATS m_z1 = AVX512_MASKZ_LOAD_FLOATS_UNALIGNED(m_mask_left, localz1);

        /* this might actually exceed the allocated range but we will never dereference that */
        localx1 += AVX512_NVEC;
        localy1 += AVX512_NVEC;
        localz1 += AVX512_NVEC;

        const AVX512_FLOATS m_xdiff = AVX512_SUBTRACT_FLOATS(m_x1, m_xpos);  /* (x[j:j+NVEC-1] - x0) */
        const AVX512_FLOATS m_ydiff = AVX512_SUBTRACT_FLOATS(m_y1, m_ypos);  /* (y[j:j+NVEC-1] - y0) */
        const AVX512_FLOATS m_zdiff = AVX512_SUBTRACT_FLOATS(m_z1, m_zpos);  /* z2[j:j+NVEC-1] - z1 */

        const AVX512_FLOATS m_sqr_xdiff = AVX512_SQUARE_FLOAT(m_xdiff);  /* (x0 - x[j])^2 */
        const AVX512_FLOATS x2py2  = AVX512_FMA_ADD_FLOATS(m_ydiff, m_ydiff, m_sqr_xdiff);/* dy*dy + dx^2*/
        const AVX512_FLOATS r2 = AVX512_FMA_ADD_FLOATS(m_zdiff, m_zdiff, x2py2);/* dz*dz + (dy^2 + dx^2)*/
        const AVX512_MASK m_rpmax_mask = AVX512_MASK_COMPARE_FLOATS(m_mask_pimax, r2, m_sqr_rpmax, _CMP_LT_OQ);
        /* Create a combined mask */
        /* This gives us the mask for all sqr_rpmin <= r2 < sqr_rpmax */
        m_mask_left = AVX512_MASK_COMPARE_FLOATS(m_rpmax_mask, r2, m_sqr_rpmin, _CMP_GE_OQ);
        if(m_mask_left == 0) {
            continue;
        }
        /* Loop backwards through nbins. m_mask_left contains all the points that */
        /* are less than rpmax at the beginning of the loop. */
        for(int kbin=nbin-1;kbin>=1;kbin--) {
            const AVX512_MASK m_bin_mask = AVX512_MASK_COMPARE_FLOATS(m_mask_left, r2,m_rupp_sqr[kbin-1],_CMP_GE_OS);
            npairs[kbin] += bits_set_in_avx512_mask_DOUBLE[m_bin_mask];
            /* ANDNOT(X, Y) -> NOT X AND Y */
            m_mask_left = AVX512_MASK_BITWISE_AND_NOT(m_bin_mask, m_mask_left);
            if(m_mask_left == 0) {
                break;
            }
        }
    }
}
```

Corrfunc Kernel

https://gist.github.com/manodeep/ffdc60024fd6df8b5264657f0be2f967

Speedup from Vectorization (SSE4.2)



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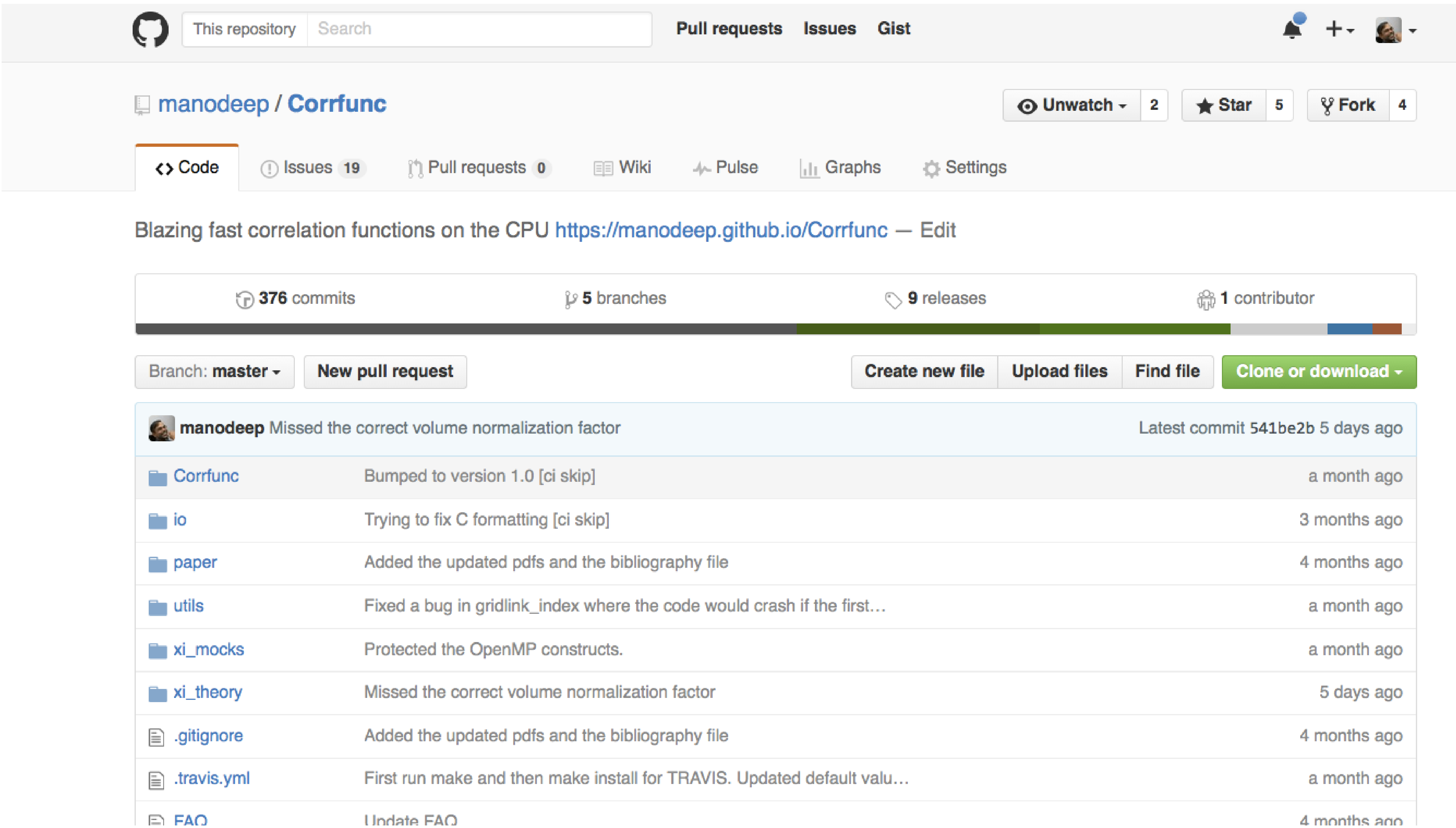
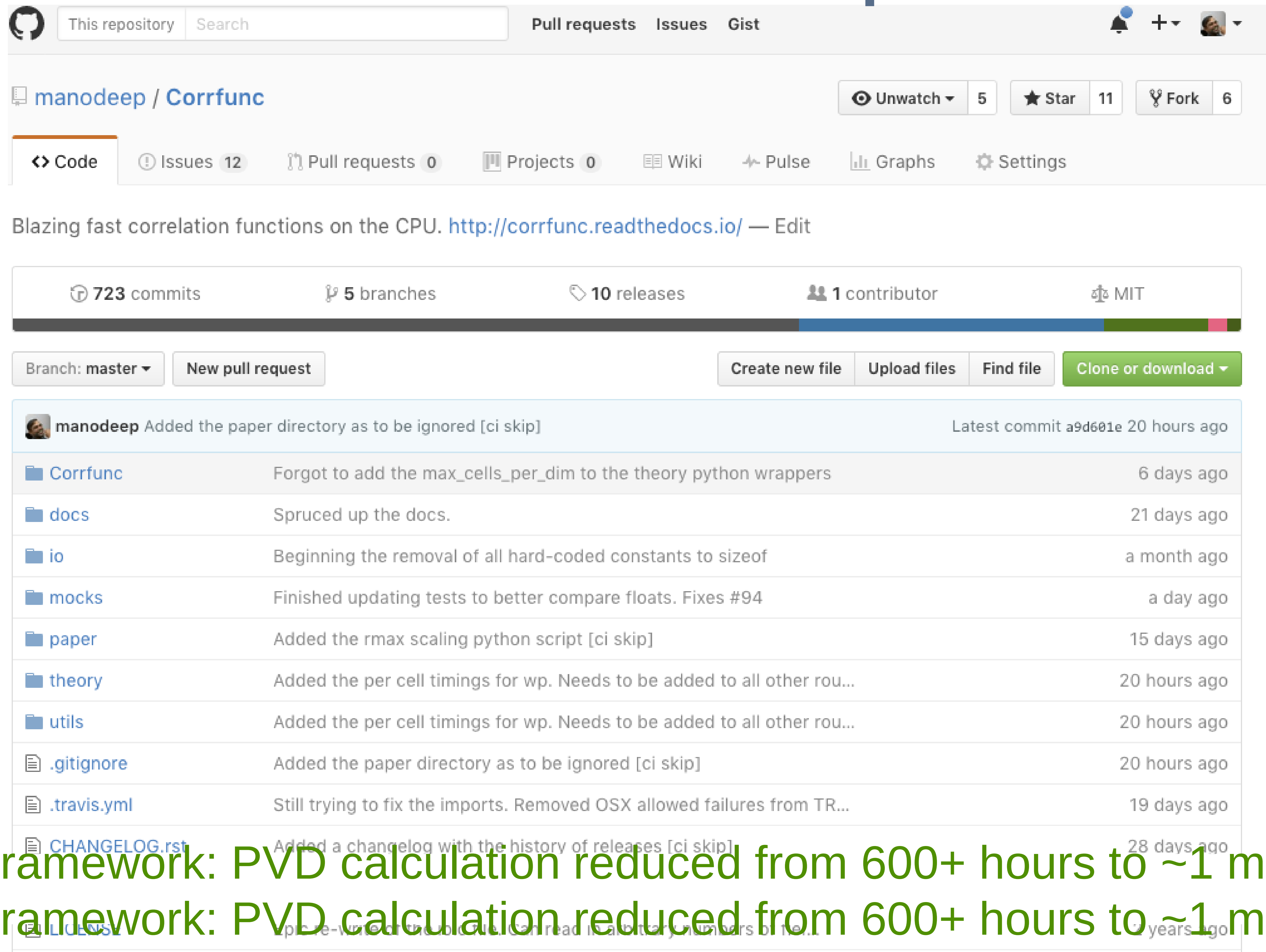
github.com/manodeep/Corrfunc/



Framework: PVD calculation reduced from 600+ hours to ~1 min

github.com/manodeep/Corrfunc/



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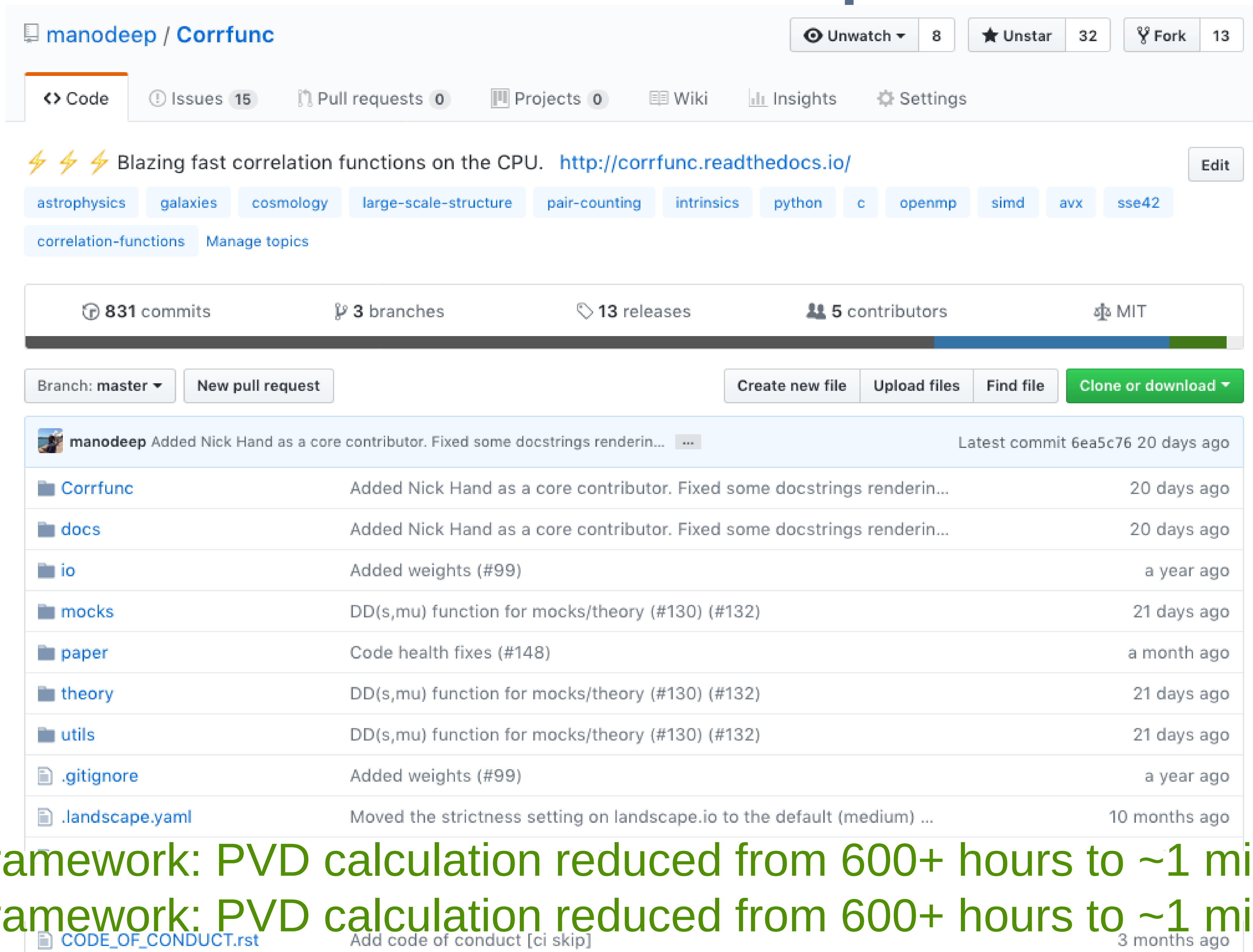

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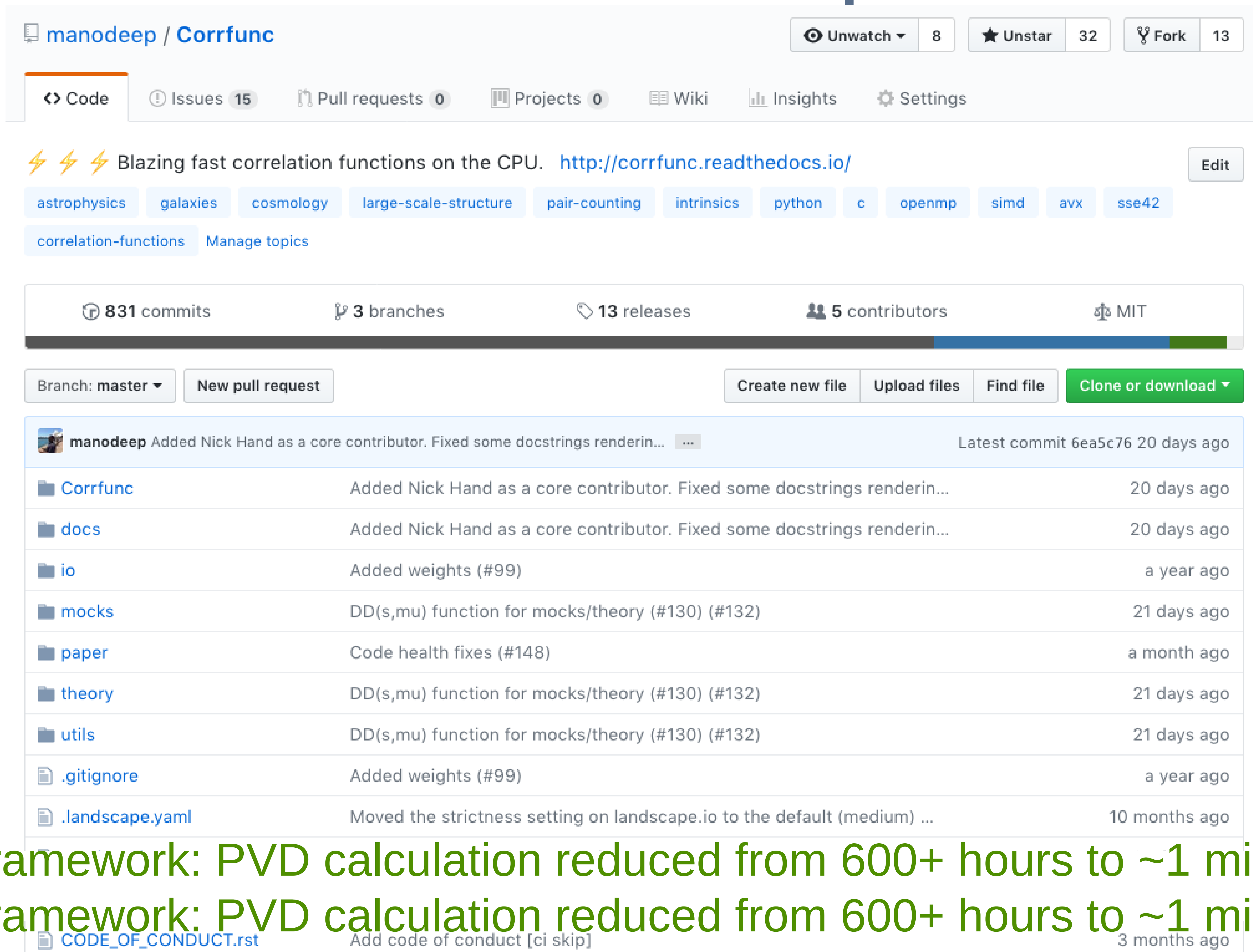

Framework: PVD calculation reduced from 600+ hours to ~1 min

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Memory access is slow

- Speed of light limitations (30 cm/ns)
  - For a 3 GHz clock, light only travels 10 cm
- Many hardware layers between requesting memory and getting data
- CPUs need to perform many calculations simultaneously

Bottlenecks in computing

How fast code runs depends on memory access patterns

https://blog.codinghorror.com/the-infinite-space-between-words/

How fast code runs depends on memory access patterns

How a CPU keeps busy (also why we got “Meltdown”)

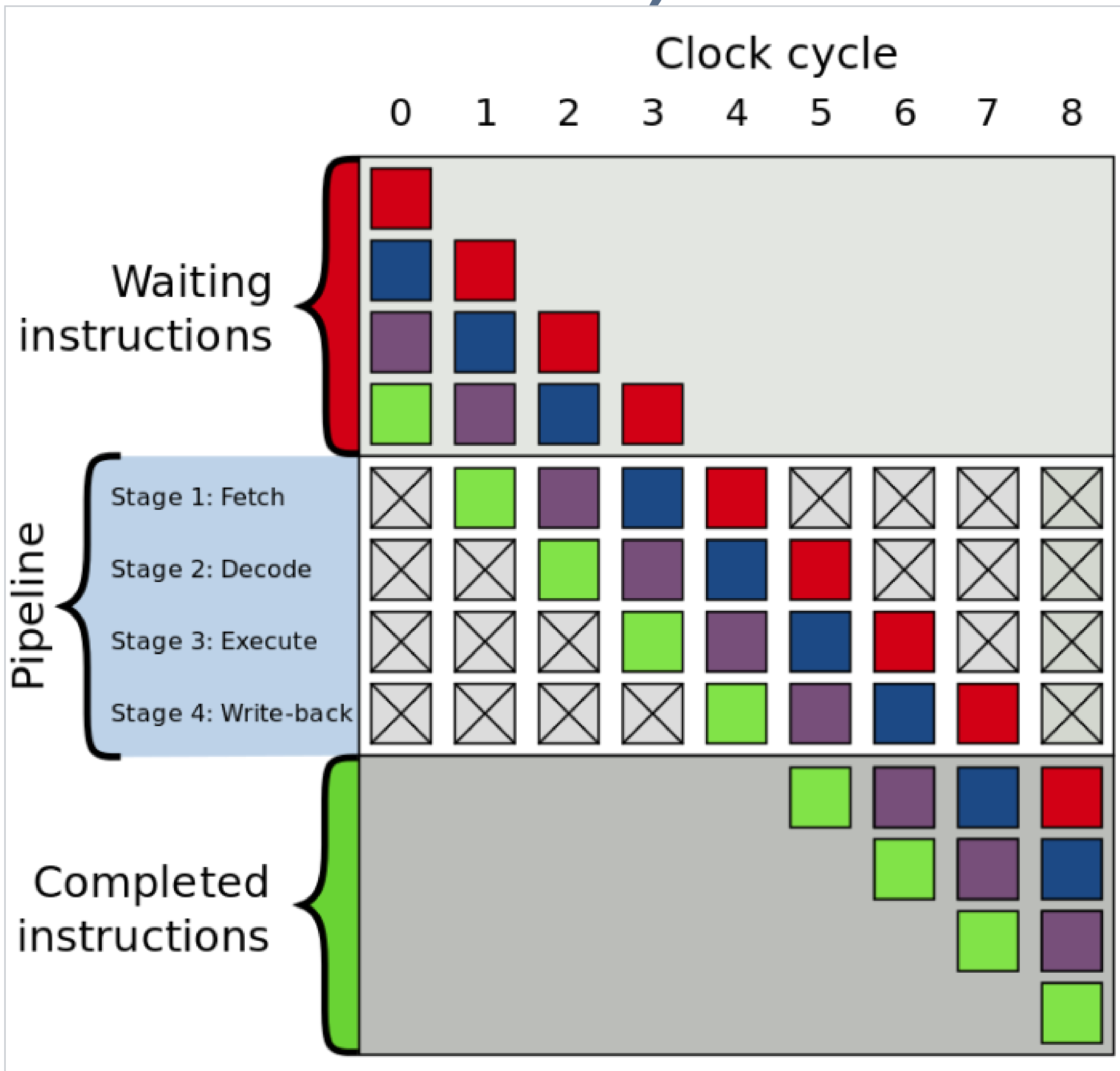
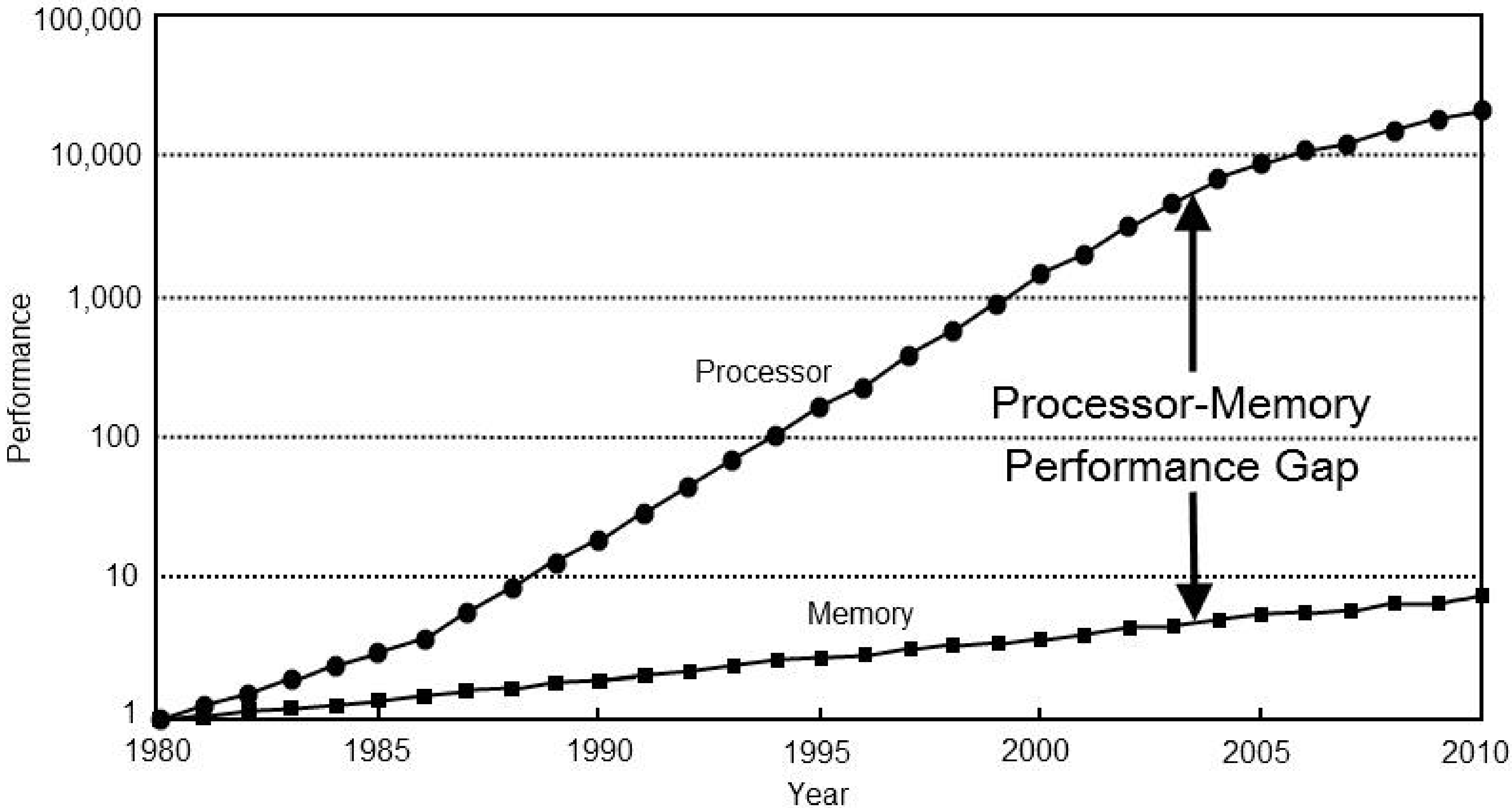


Figure 1: Example of 4-stage pipeline. The colored boxes represent instructions independent of each other

CPU Performance Bottlenecks



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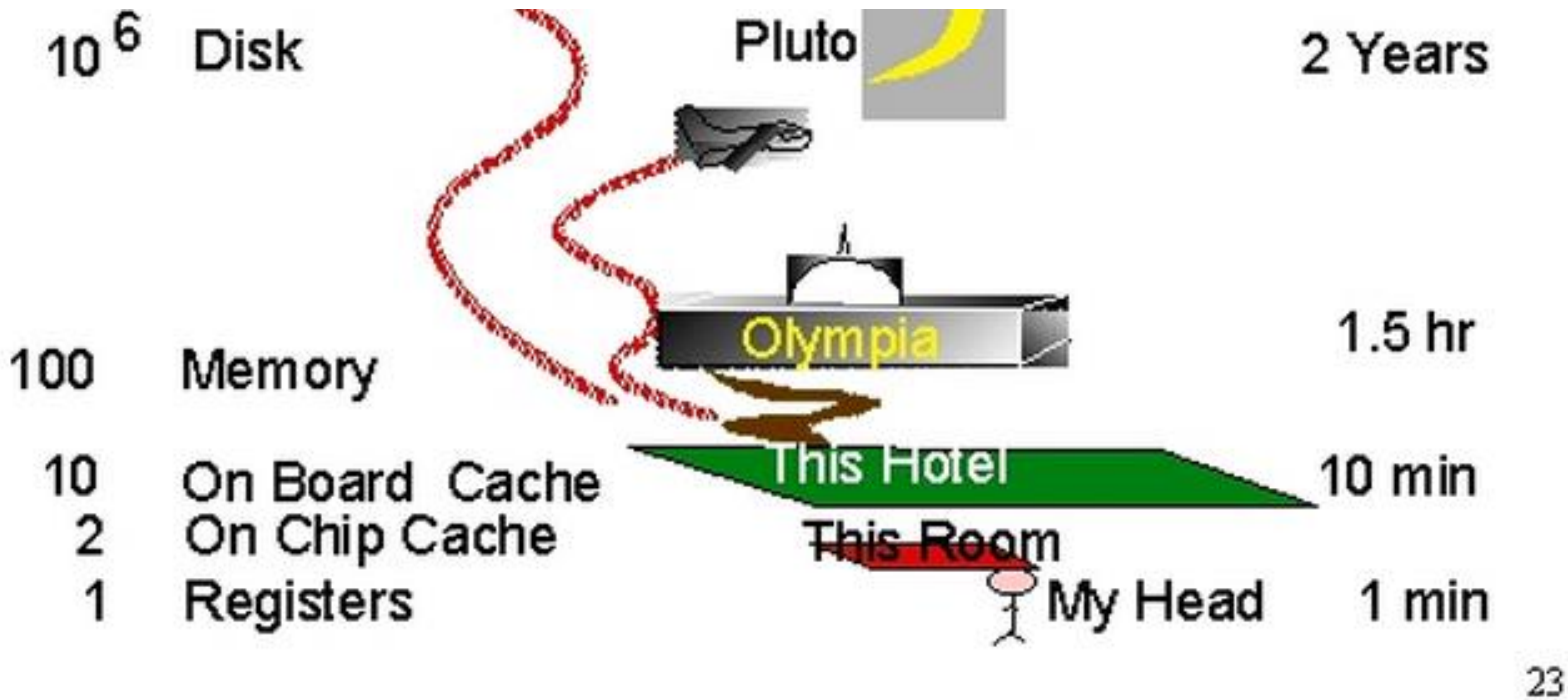

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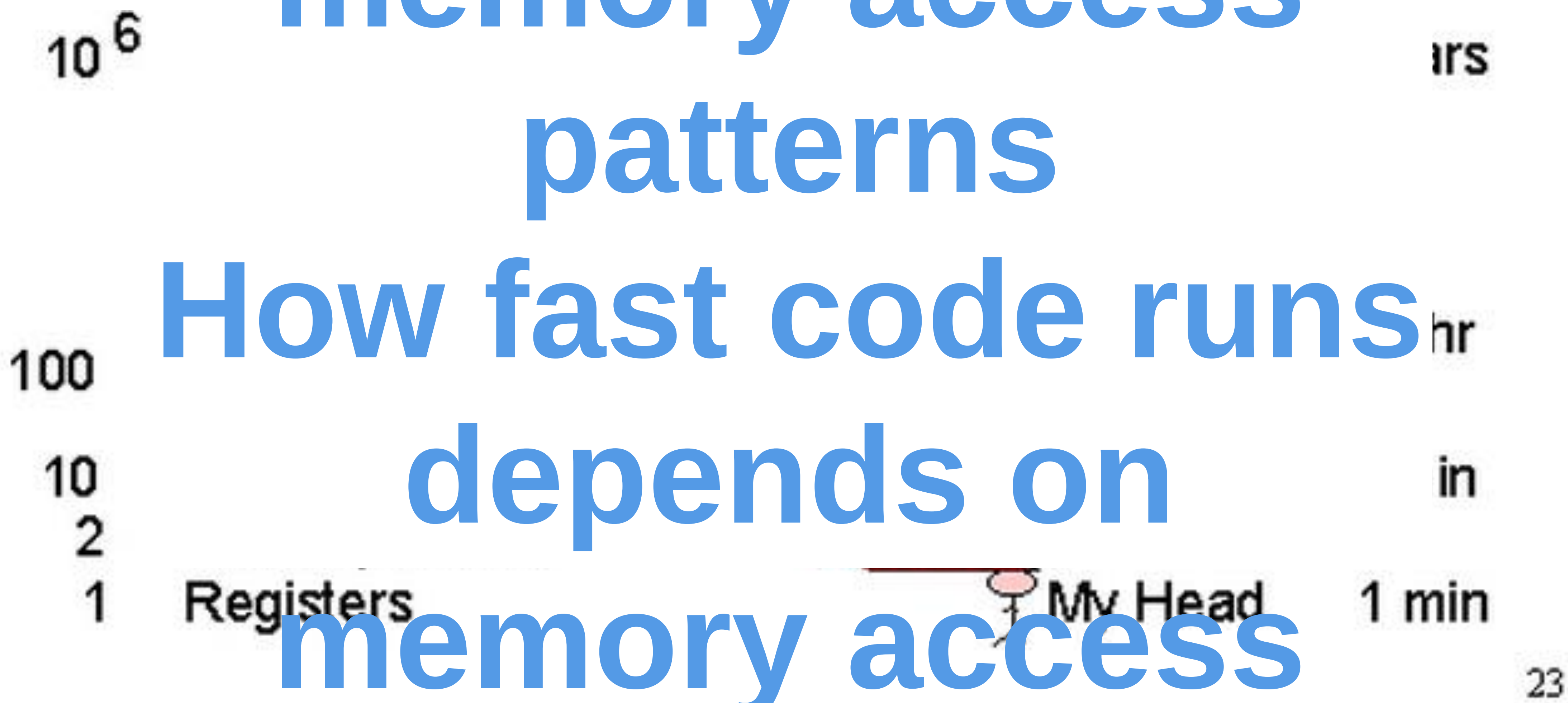

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How fast code runs depends on memory access patterns

Not all operations are equal

- Modern cpus are extremely complex and try to predict data access patterns (hence, MELTDOWN, SPECTRE hardware bugs)
  - avoid if conditions (use `?' for the ternary operator)
- Divisions are 5 times more time-consuming than multiplication
  - Beware of trigonometric functions (use trig. identities, if possible)
- Profile your code. I am wrong > 50% of the time

Users vs CPU vendor

- User: Fastest time to solution is better
- Vendor: Lowest power consumption for a fixed problem size while maintaining/improving time to solution
- These two metrics are not the same

User wishlist vs CPU Features

- User: Faster CPU clocks (write old-style code)
- Physics is a buzzkill
- Vendor: Slower and many more individual cores per cpu (think GPUs) with wider vector widths (more calculations per clock tick)