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Scaling Generalized N-Body Problems, a Case Study from Genomics

Presented by Marquita Ellis

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The University of California at Berkeley
Lawrence Berkeley National Laboratory

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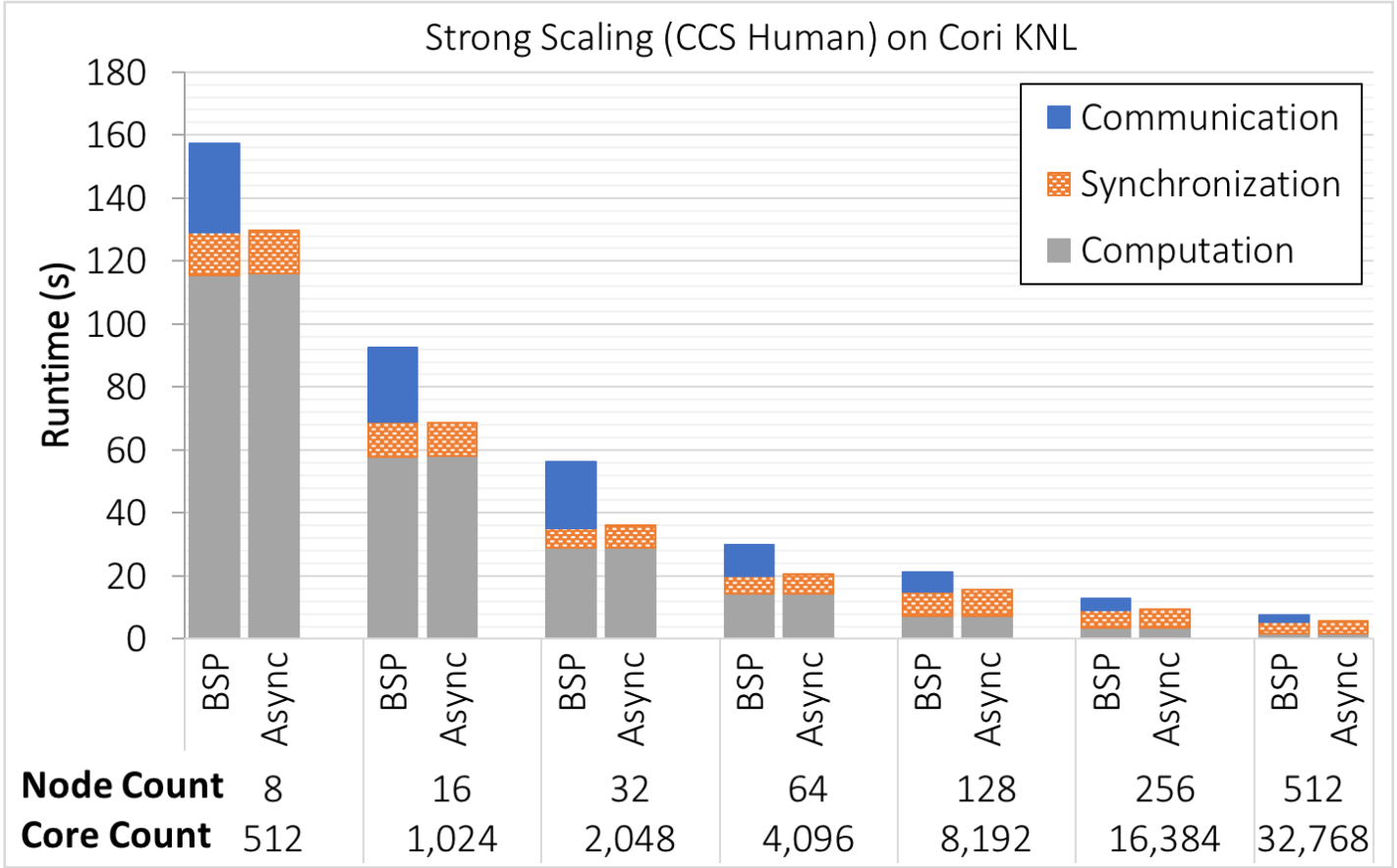

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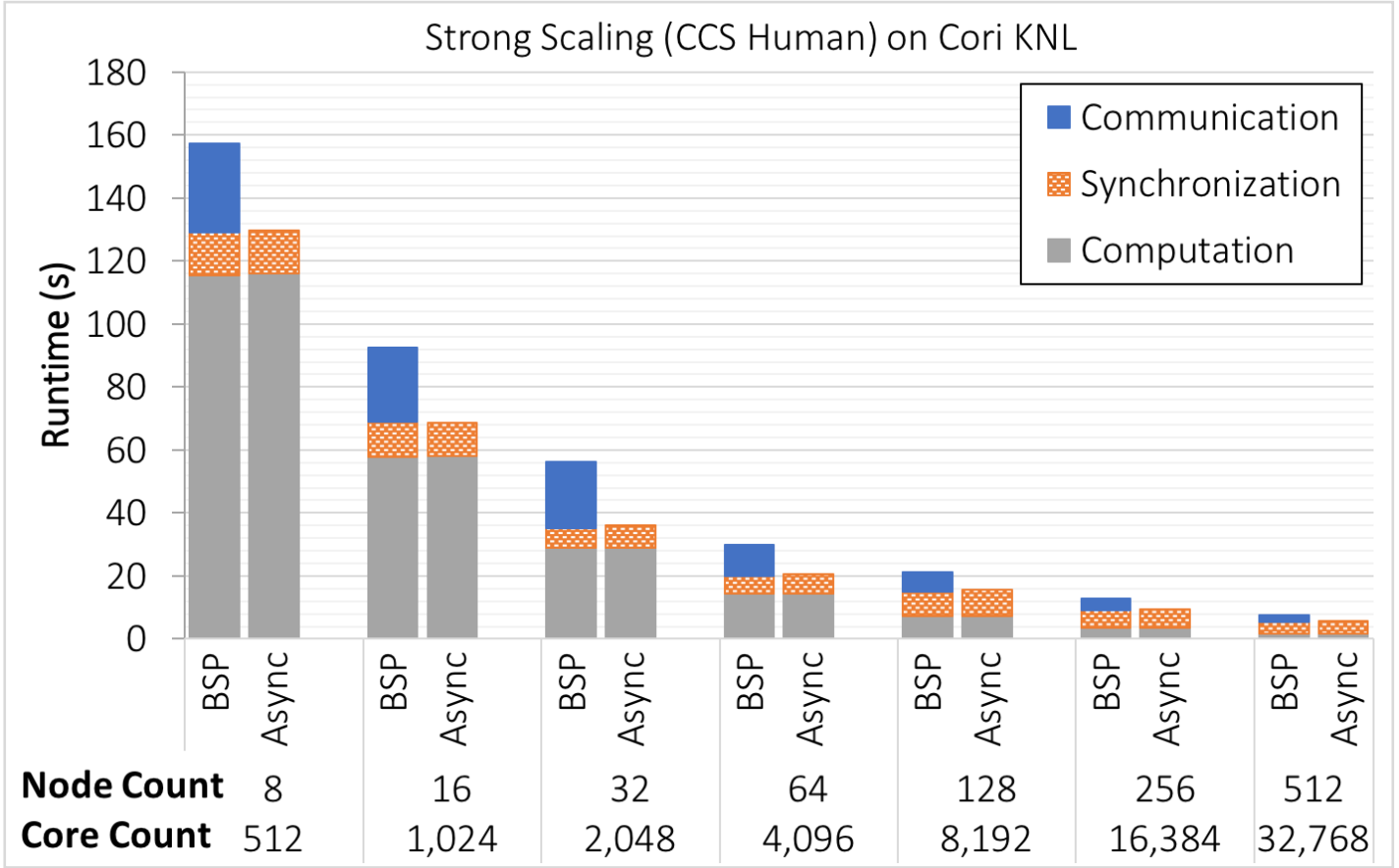

- At first glance, the communication-hiding approach seems trivially to be the right approach
- However, for this type of problem, there is a non-trivial balancing act between the communication, computation, and memory

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- Redundancy or *repeats* are also inherent in certain genomes, esp. plants, interesting for biofuel, medicine, food, etc.

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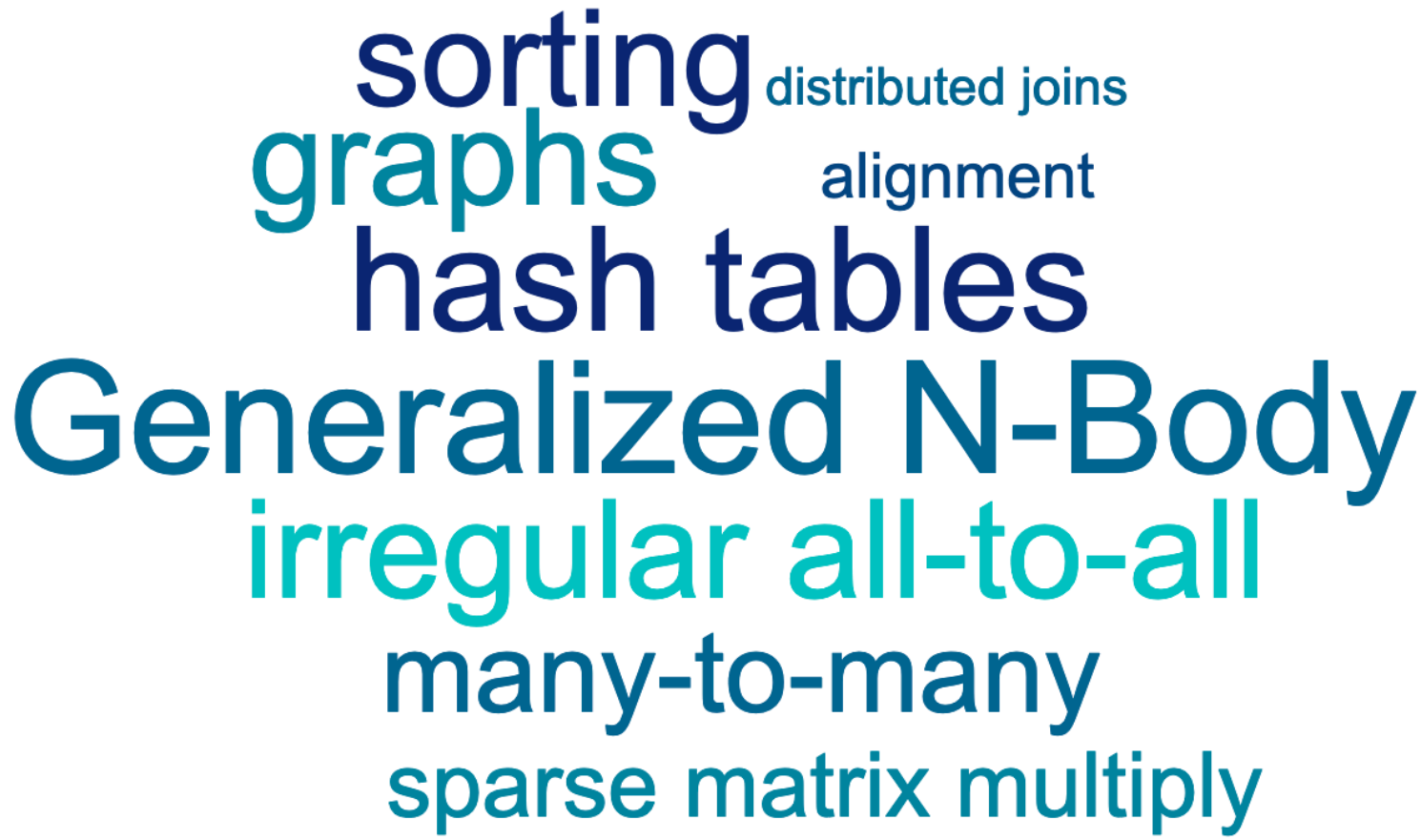
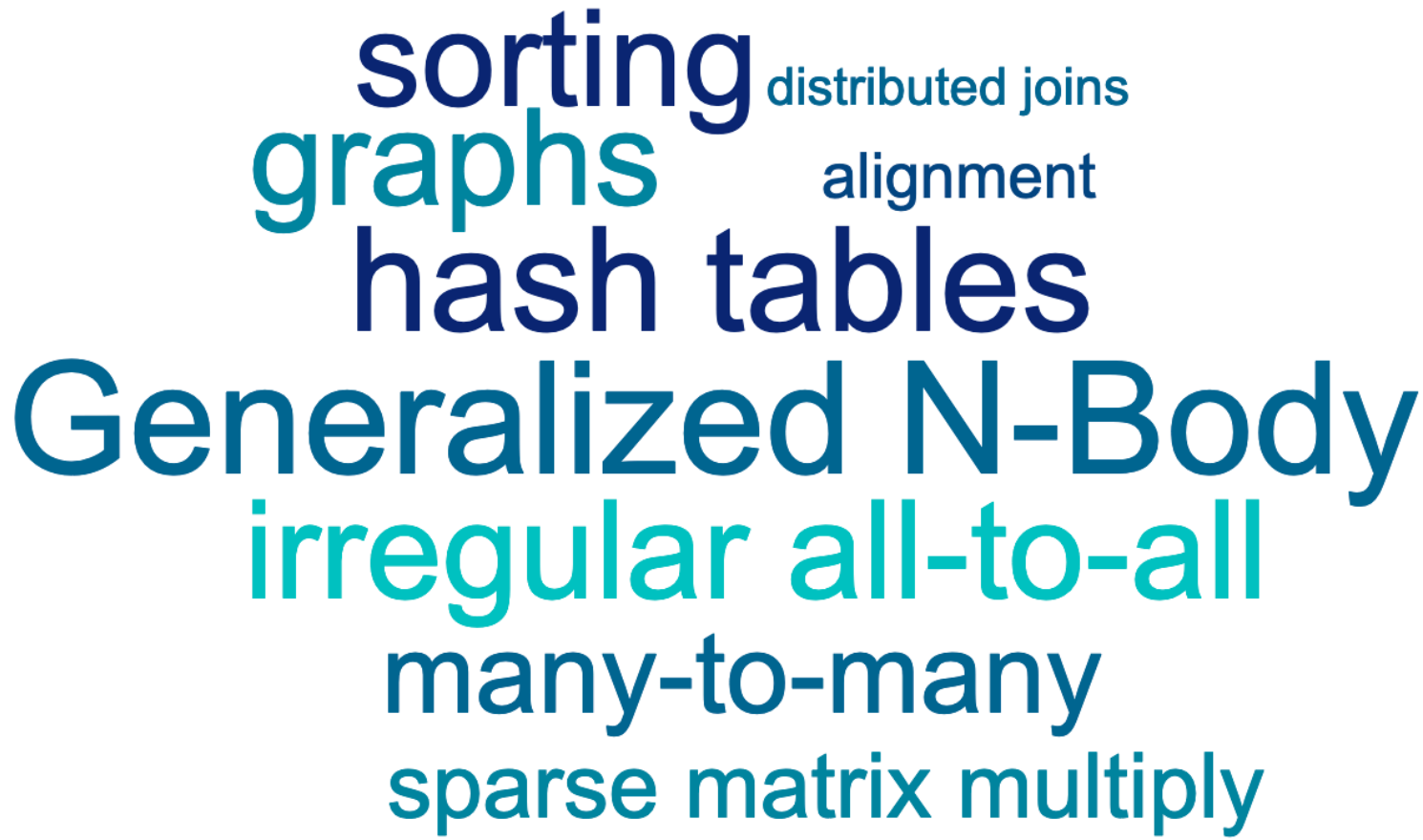
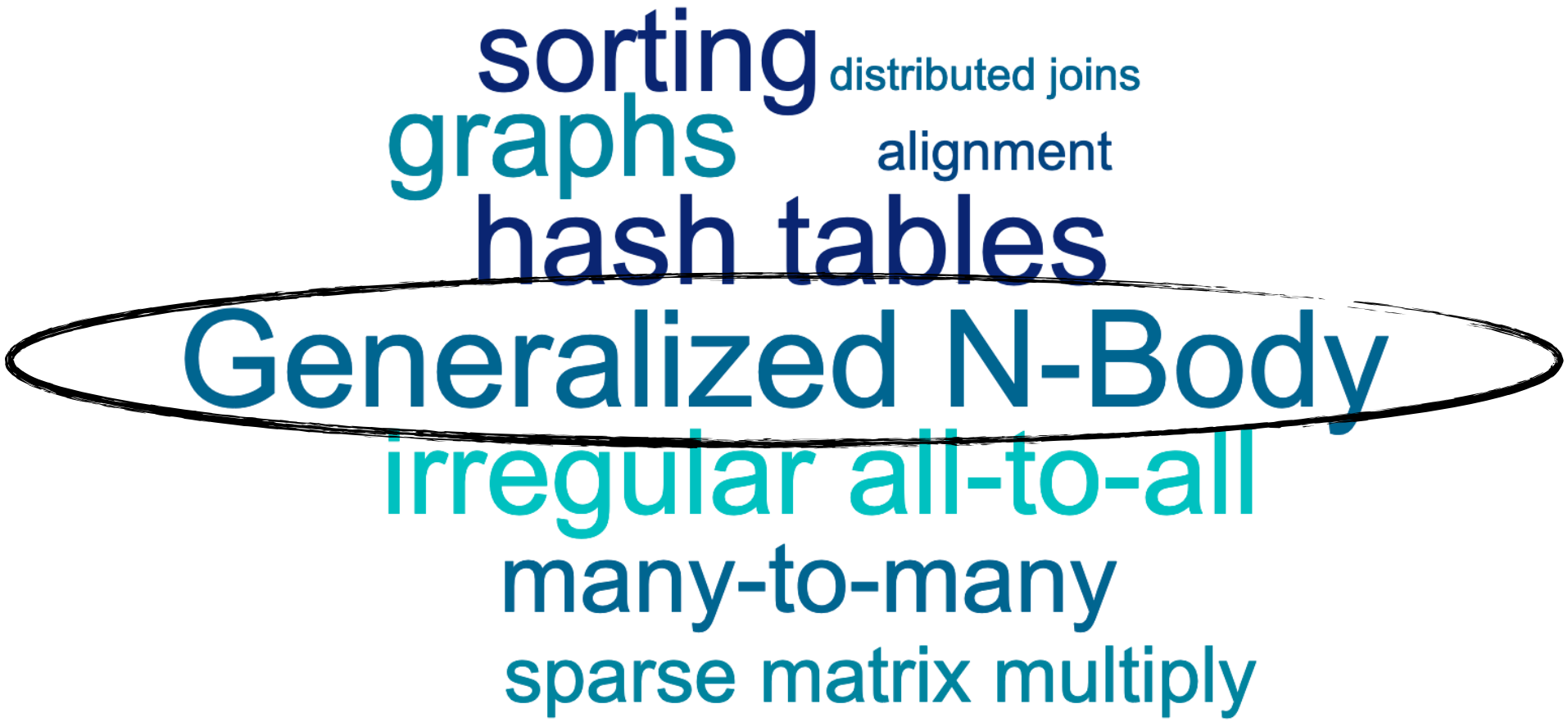
  - yields a sparse unstructured graph that is also very large, discovered at runtime
- Heuristic approaches to pairwise alignment can reduce the n^2 to average-case $O(n)$
  - their early termination leads to *more* irregularity in the computation at runtime


sorting
distributed joins
graphs
alignment
hash tables
Generalized N-Body
irregular all-to-all
many-to-many
sparse matrix multiply



See also Yelick et al., "The Parallelism Motifs of Genomic Analysis." In Philosophical Transactions of the Royal Society A 378, no. 2166 (2020): 20190394.

Our case study is a representative Generalized N-Body problem from Genomics



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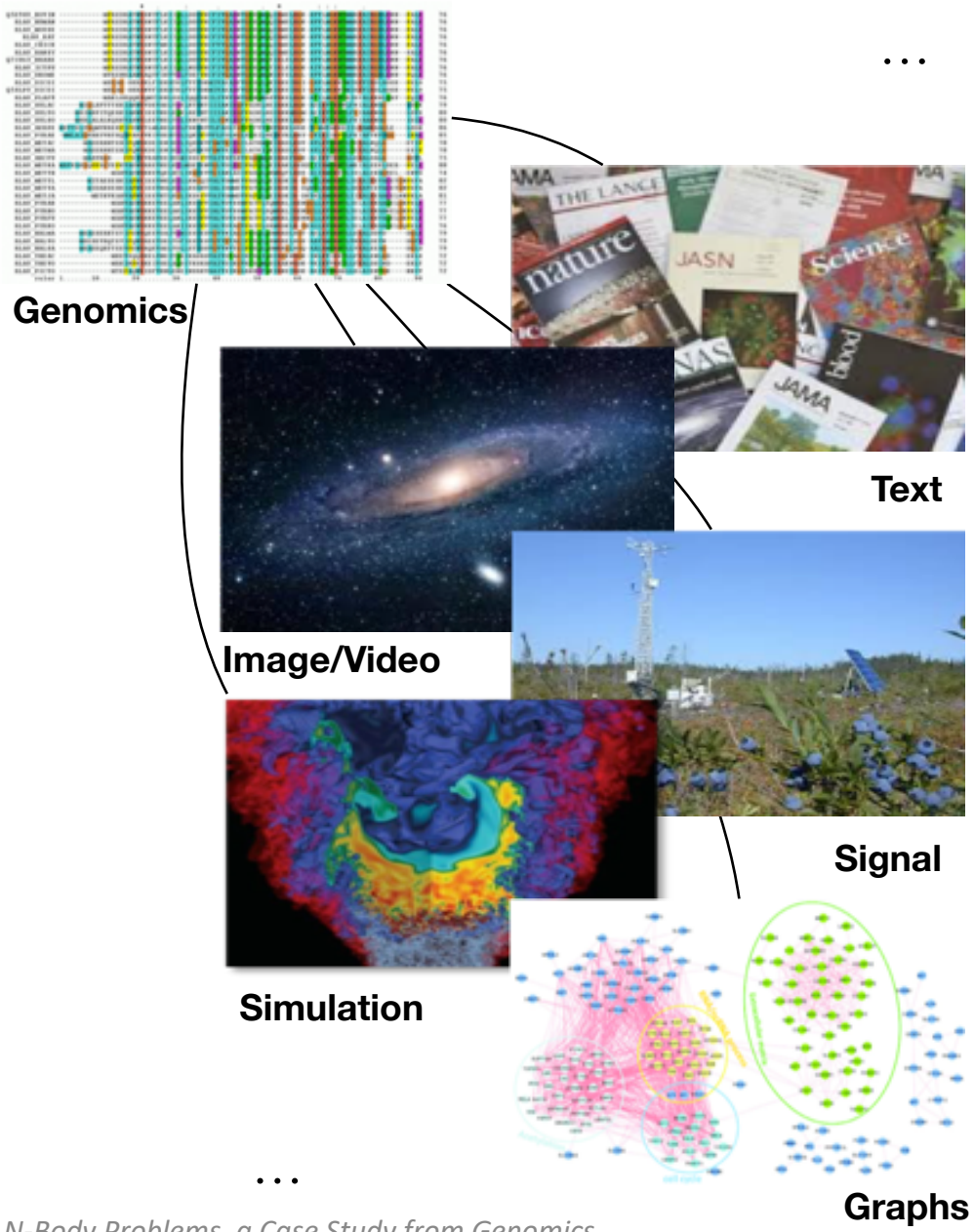
- Our Generalized N-Body instance is a many-to-many comparison of long, variable length strings (bodies) via pairwise alignment (similarity metric)
- with significant similarities to other Generalized N-Body problems in Bioinformatics
  - pangenomics, similarity across genomes
  - metagenomics, clustering DNA fragments from different species in the same sample
  - proteomics, similarity searches in massive protein data sets
  - informatics, more general text and document analysis

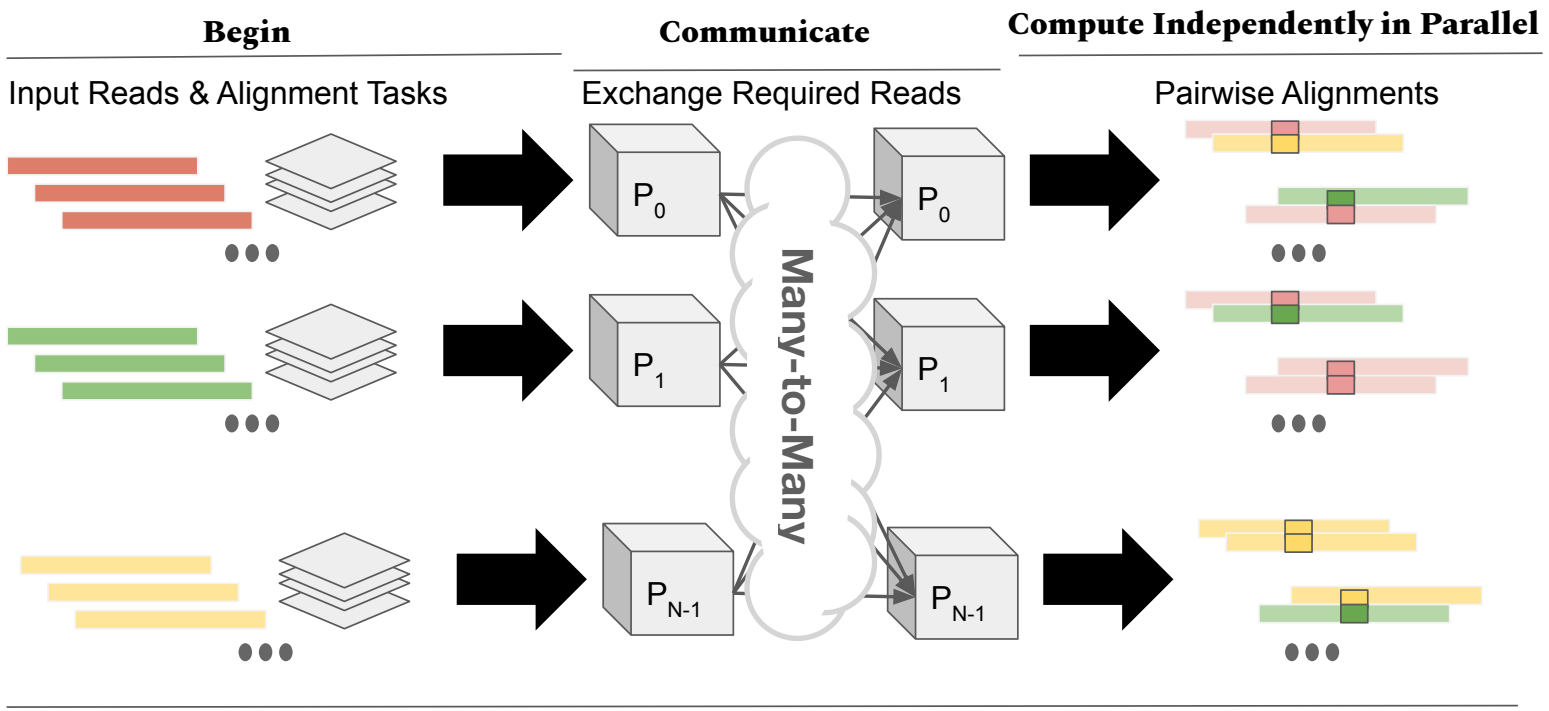
Big Picture Goals

- Develop scalable software for scientific discovery
  - build “wet” science - computer science bridges
  - in collaboration with JGI, UCB, MCB@UCB
  - Exascale Computing Project
- Generalize and generate insights for scaling other irregular big data applications



Big Data

Data-Independent Approach (1/2), Bulk-Synchronous Parallel (BSP)



End: output alignments exceeding minimum scoring threshold in parallel

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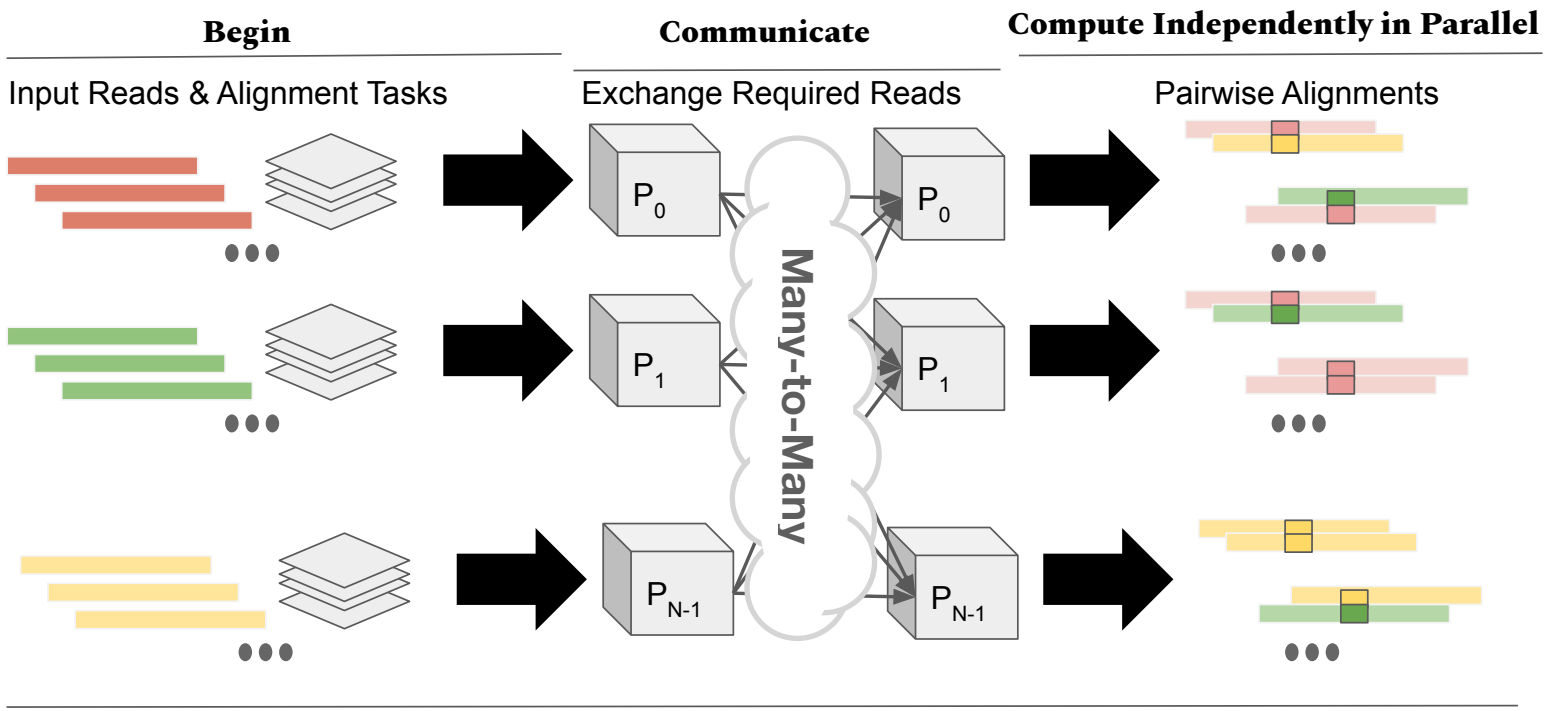

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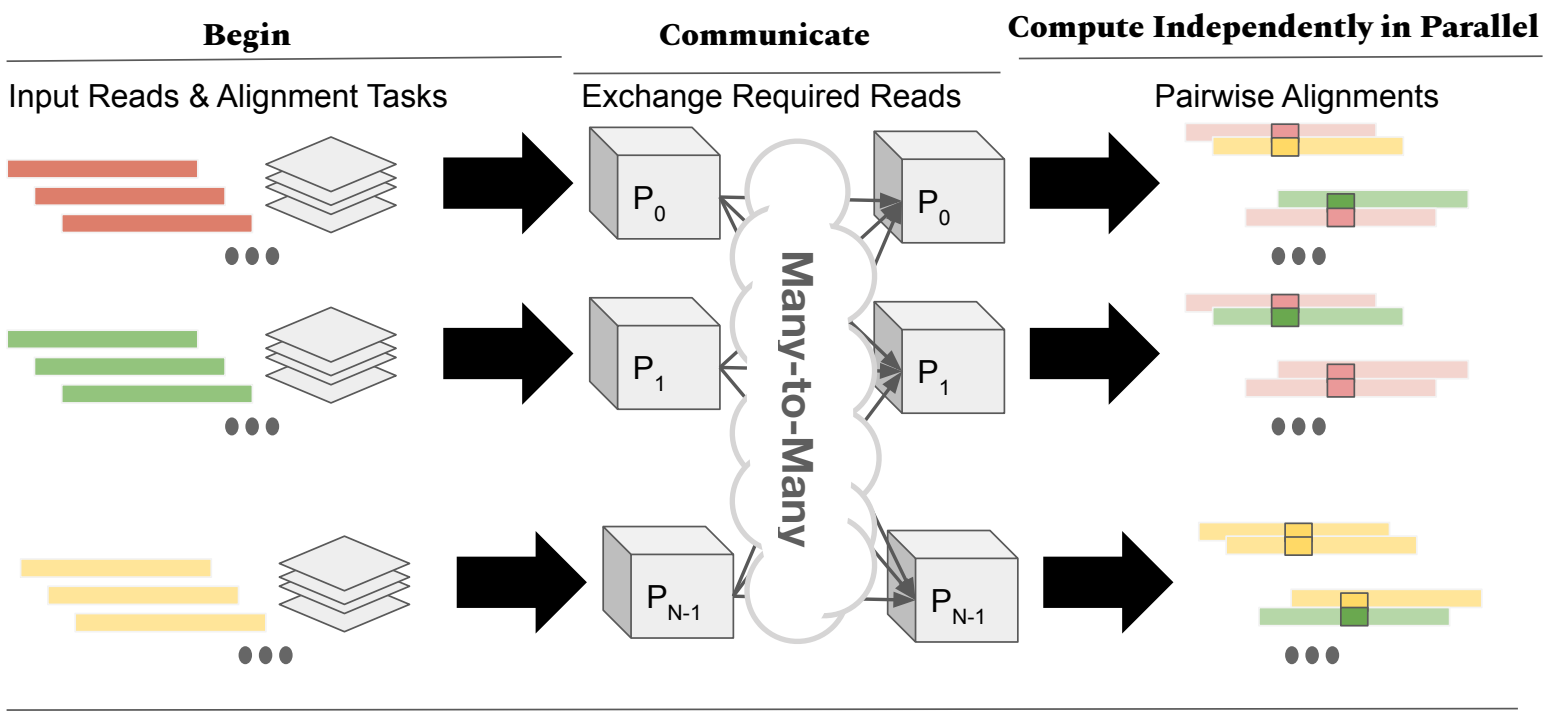

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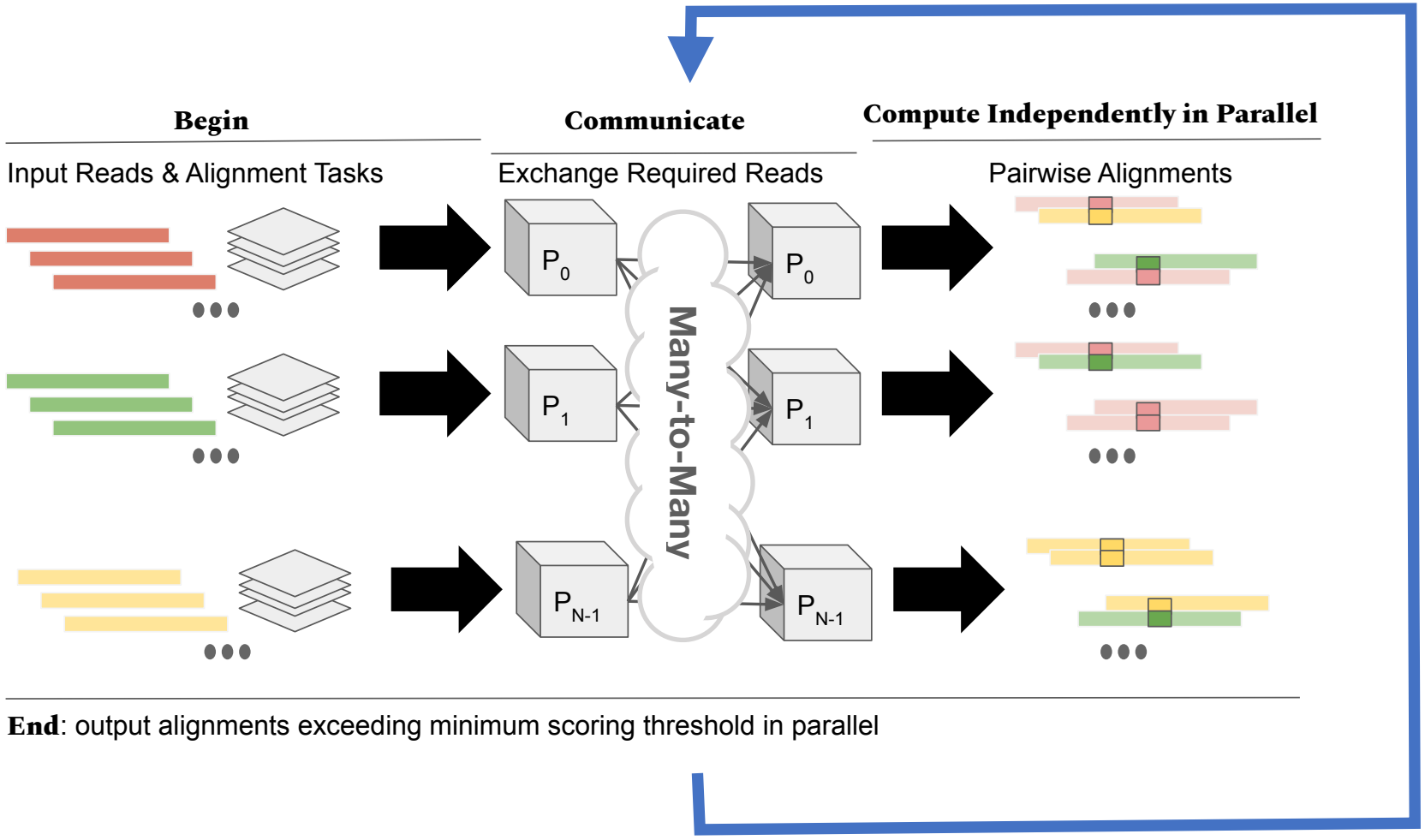

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In practice, communicating in multiple memory-limited exchanges may be necessary

Data-Independent Approach (2/2), Asynchronous (Async)

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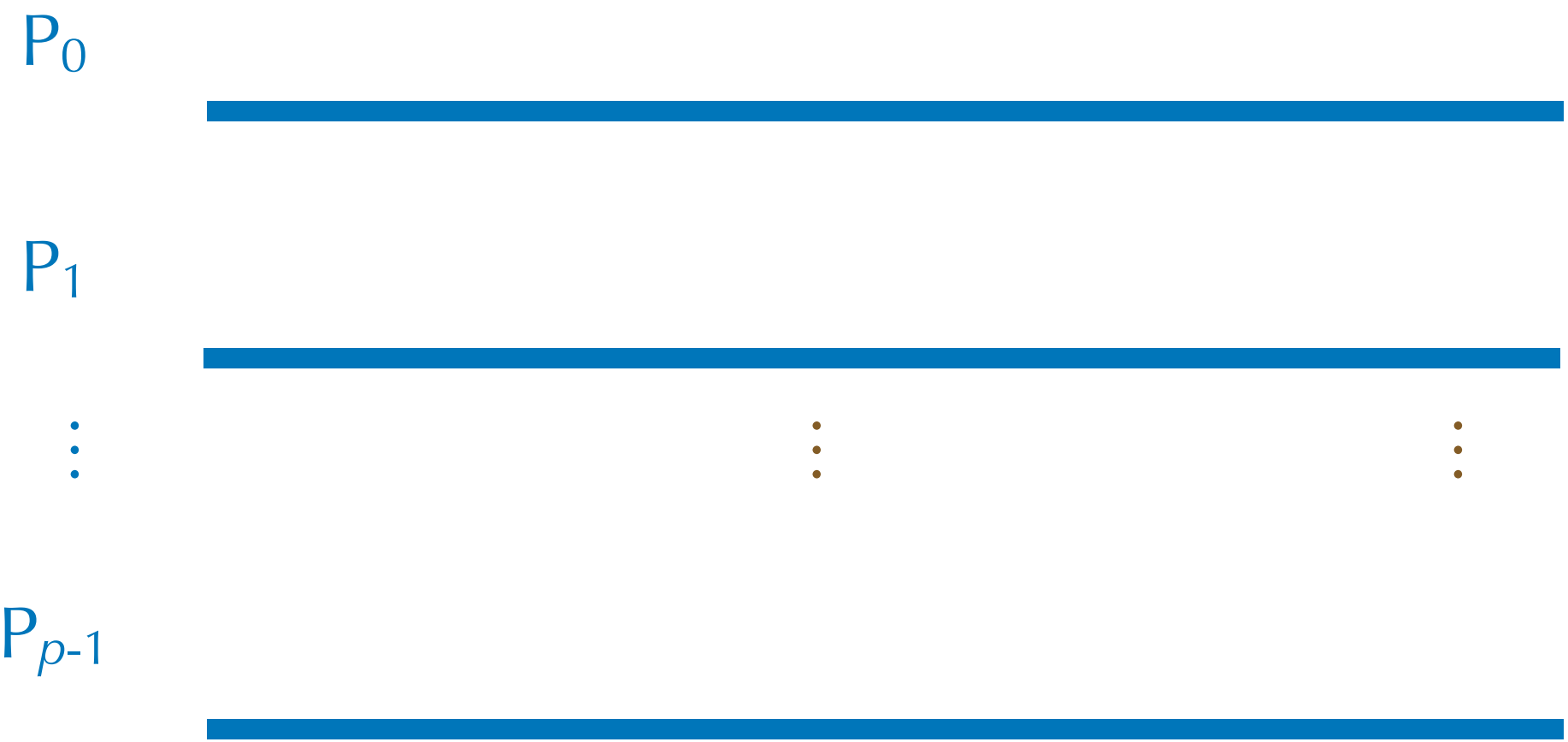
- Each remote string is retrieved one at a time, asynchronously (as necessary)

Data-Independent Approach (2/2), Asynchronous (Async)

High-Level Illustration (SPMD)



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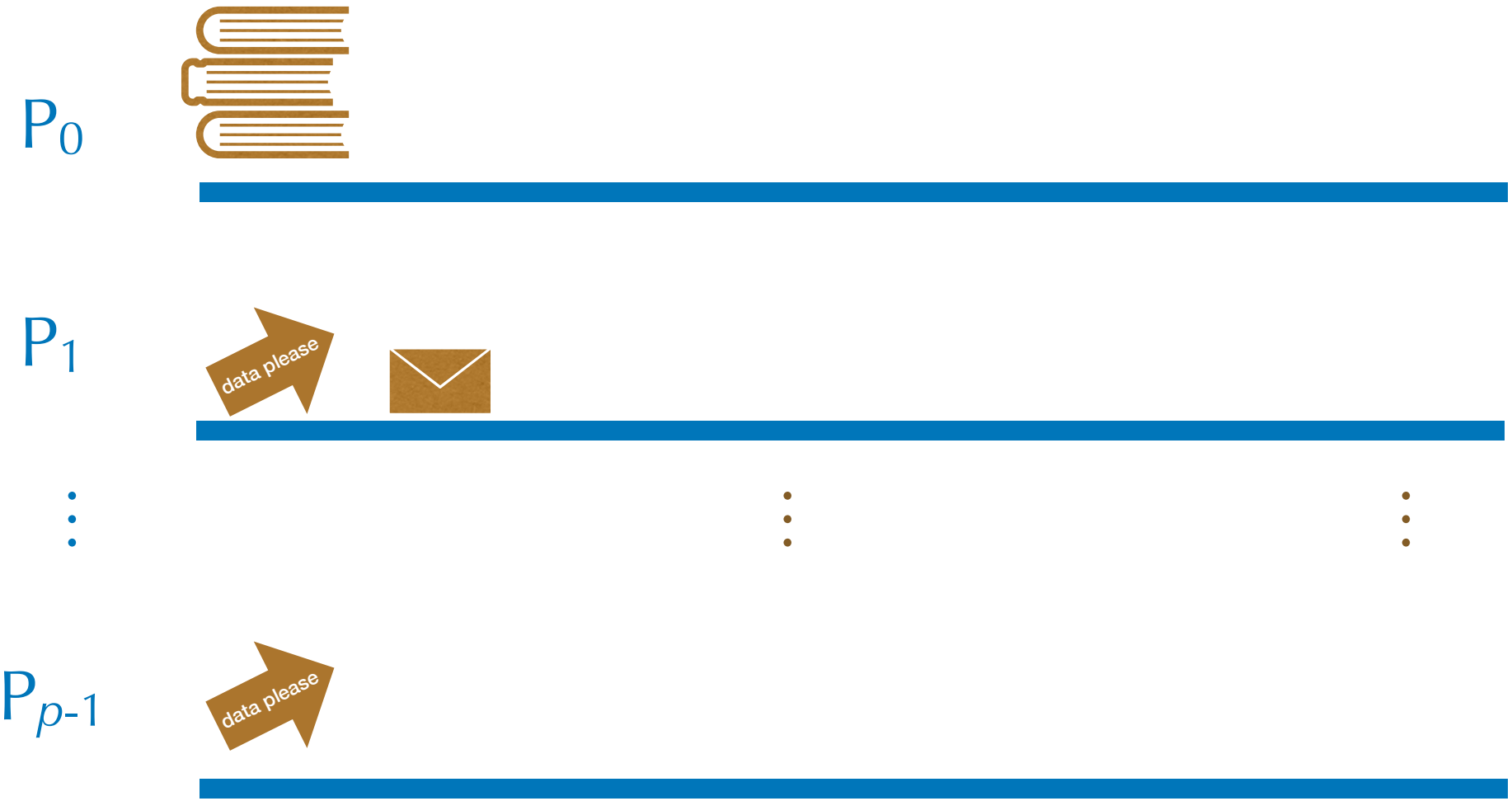

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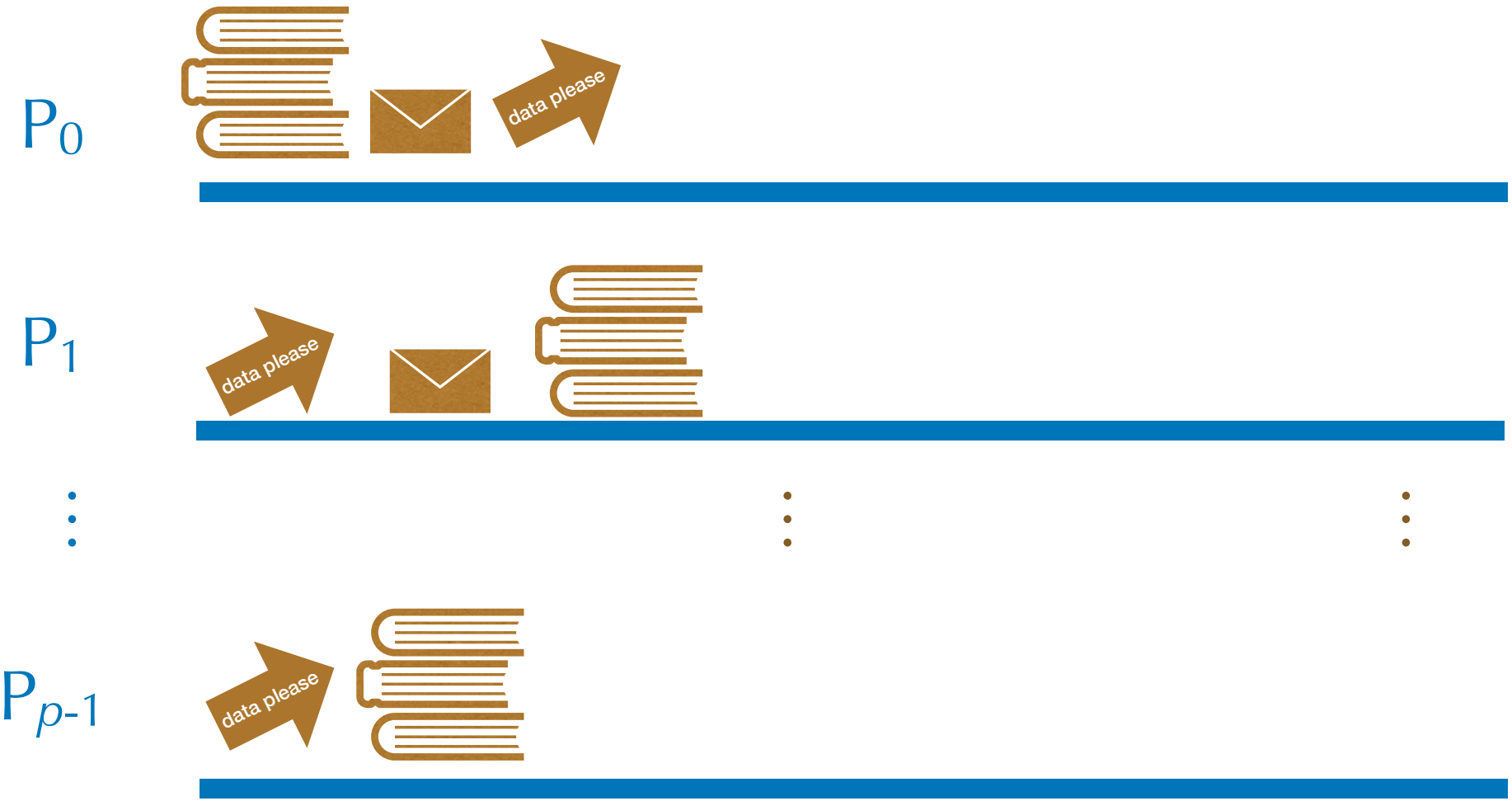

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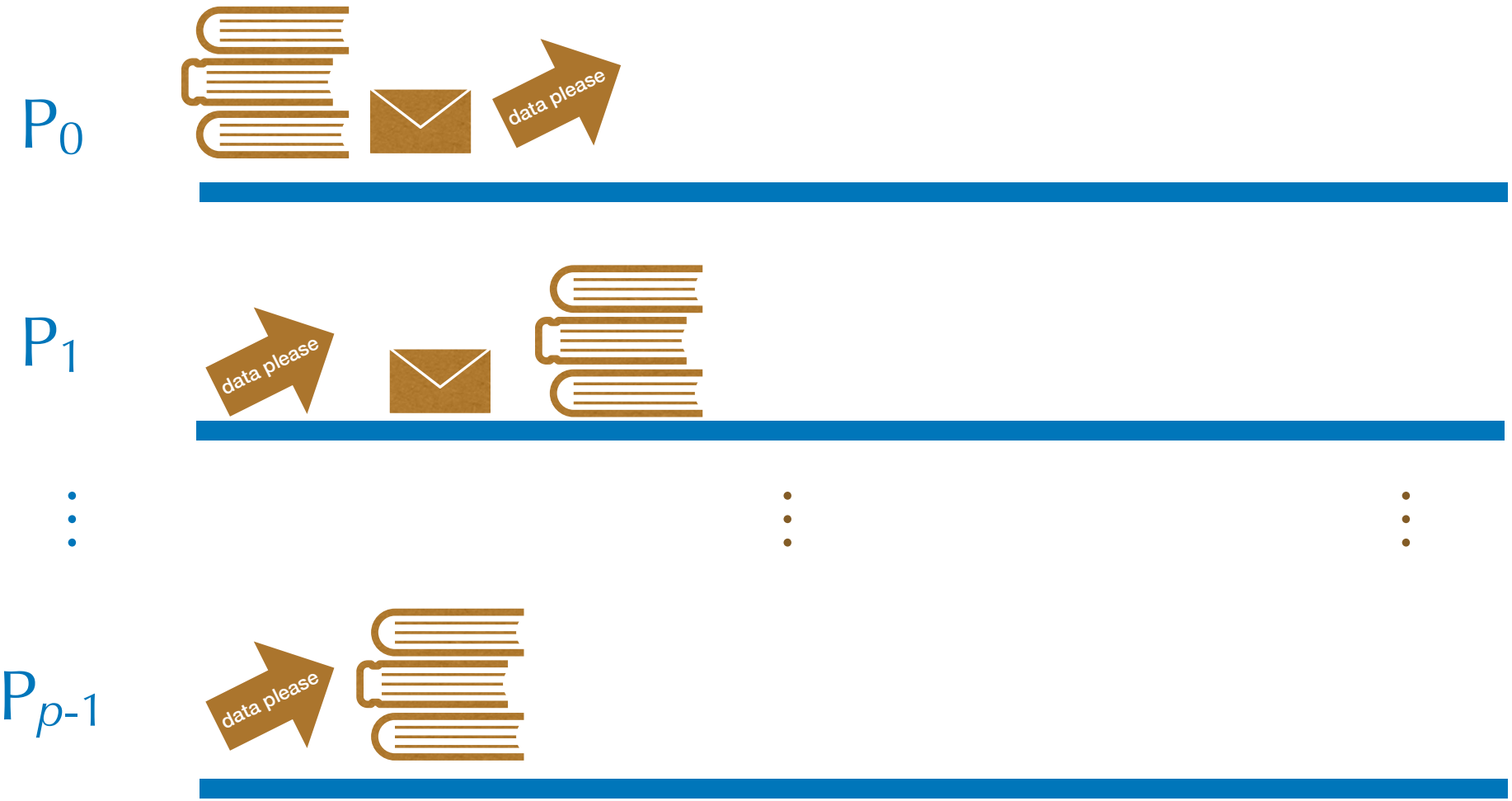

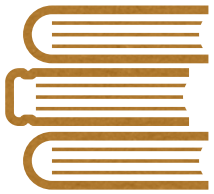

Potentially long-running pairwise alignment tasks

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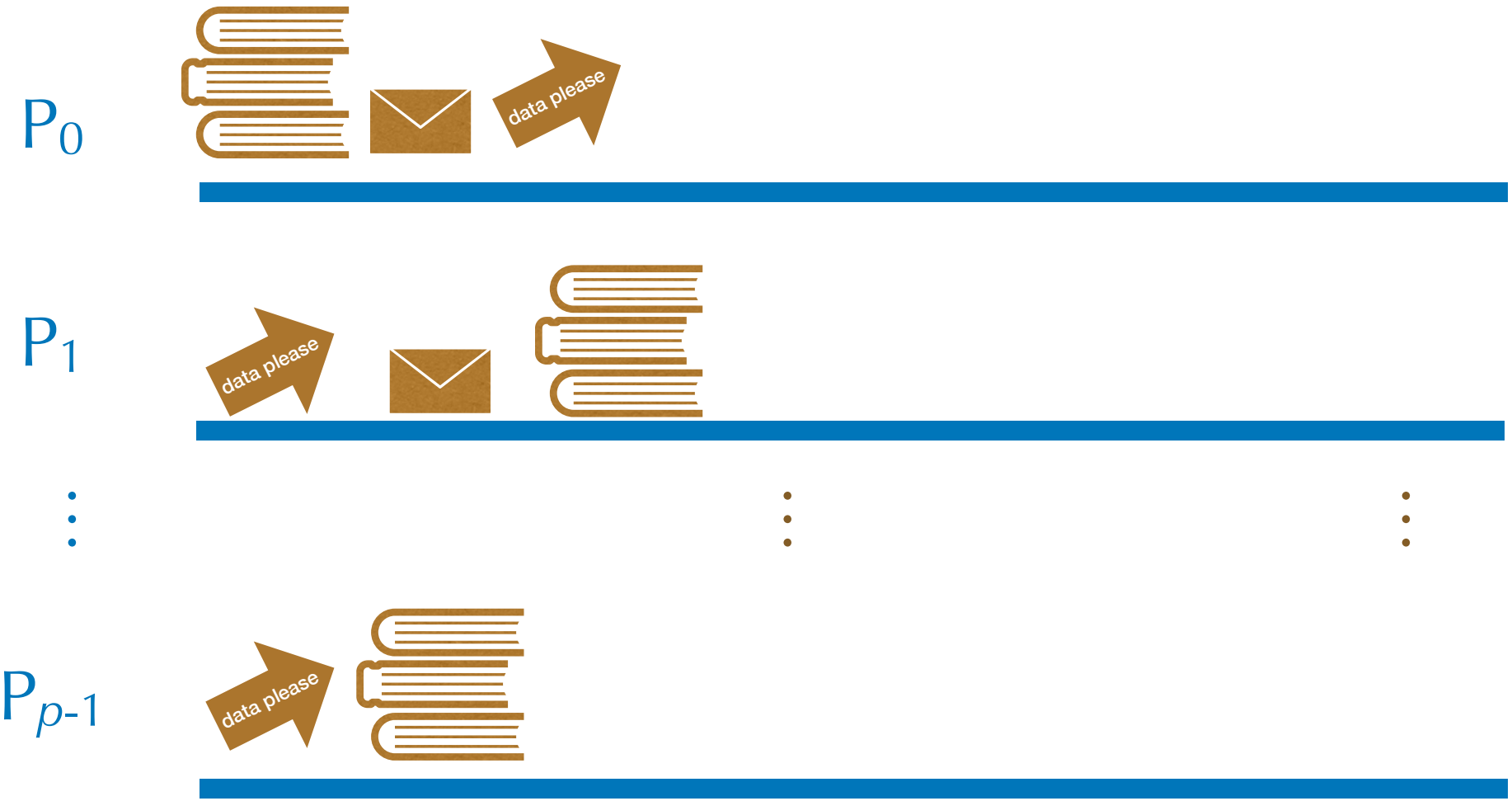

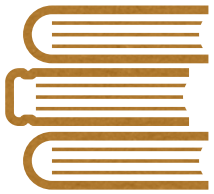

Potentially long-running pairwise alignment tasks

Nonblocking request for remote data

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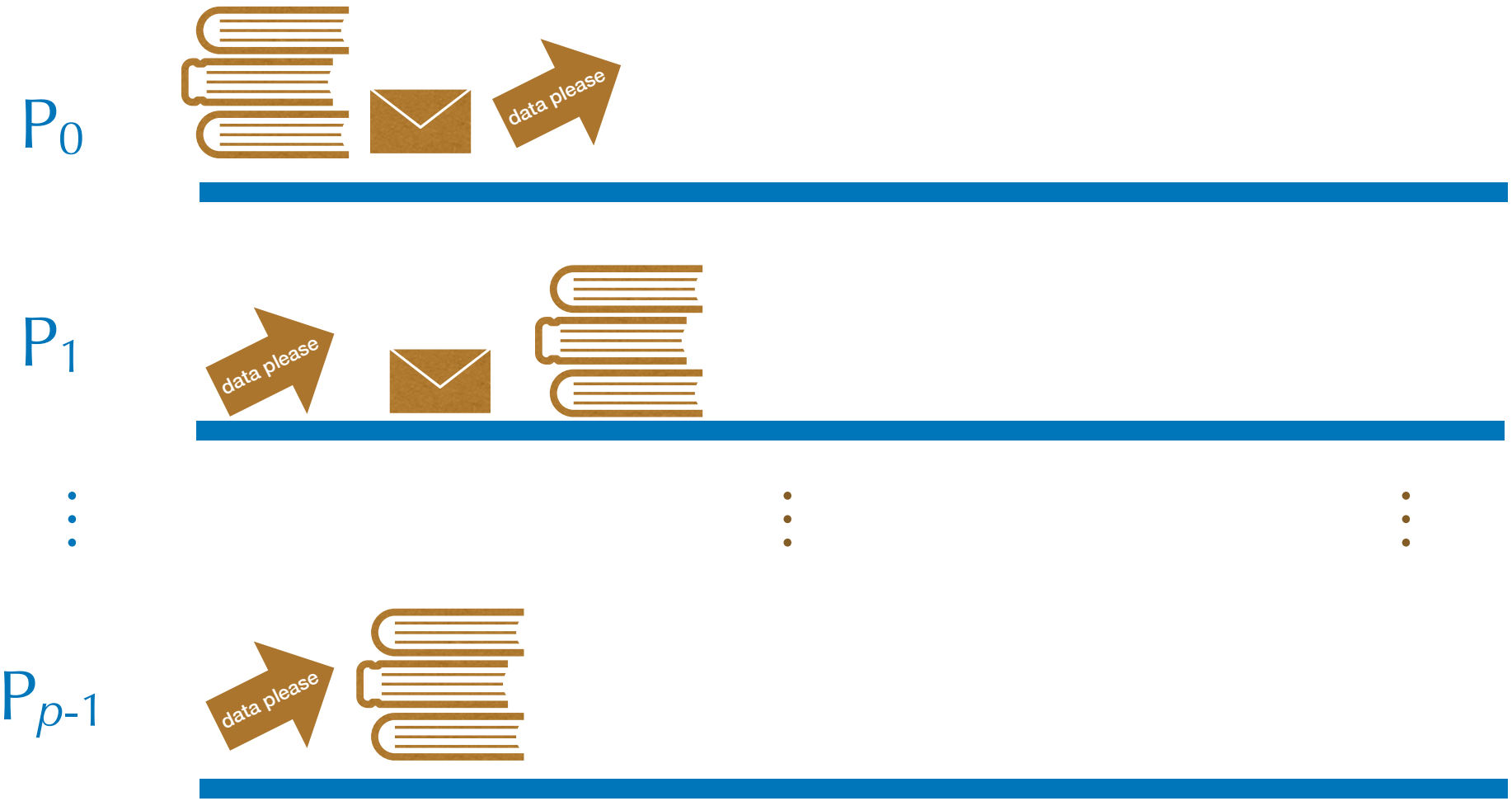

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data please

Nonblocking request for remote data

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Unclear how well the *Async* approach will perform in practice

Potential Advantages

- ~maximizes injection speed
- ~minimizes memory footprint
- communication-computation hiding

…

Potential Disadvantages

- ~maximizes number of messages
- pays round-trip cost for each remote read (datum) as needed
- exacerbated load imbalance

…

How do these approaches perform with real workloads?

Experimental Setup

Intra-node strong scaling

1 - 128 node strong scaling

8 - 512 node strong scaling

Short Name	Species	Reads	Tasks
E. coli 30×	*Escherichia coli*	16,890	2,270,260
E. coli 100×	*Escherichia coli*	91,394	24,869,171
Human CCS	*Homo sapiens*	1,148,839	87,621,409

Cray XC40, “Cori KNL” (KNL partition)
Cray Aries, Dragonfly Topology
Node architecture:

- Single socket
- Intel Xeon Phi Knights Landing processor
- 68 cores @1.4 GHz
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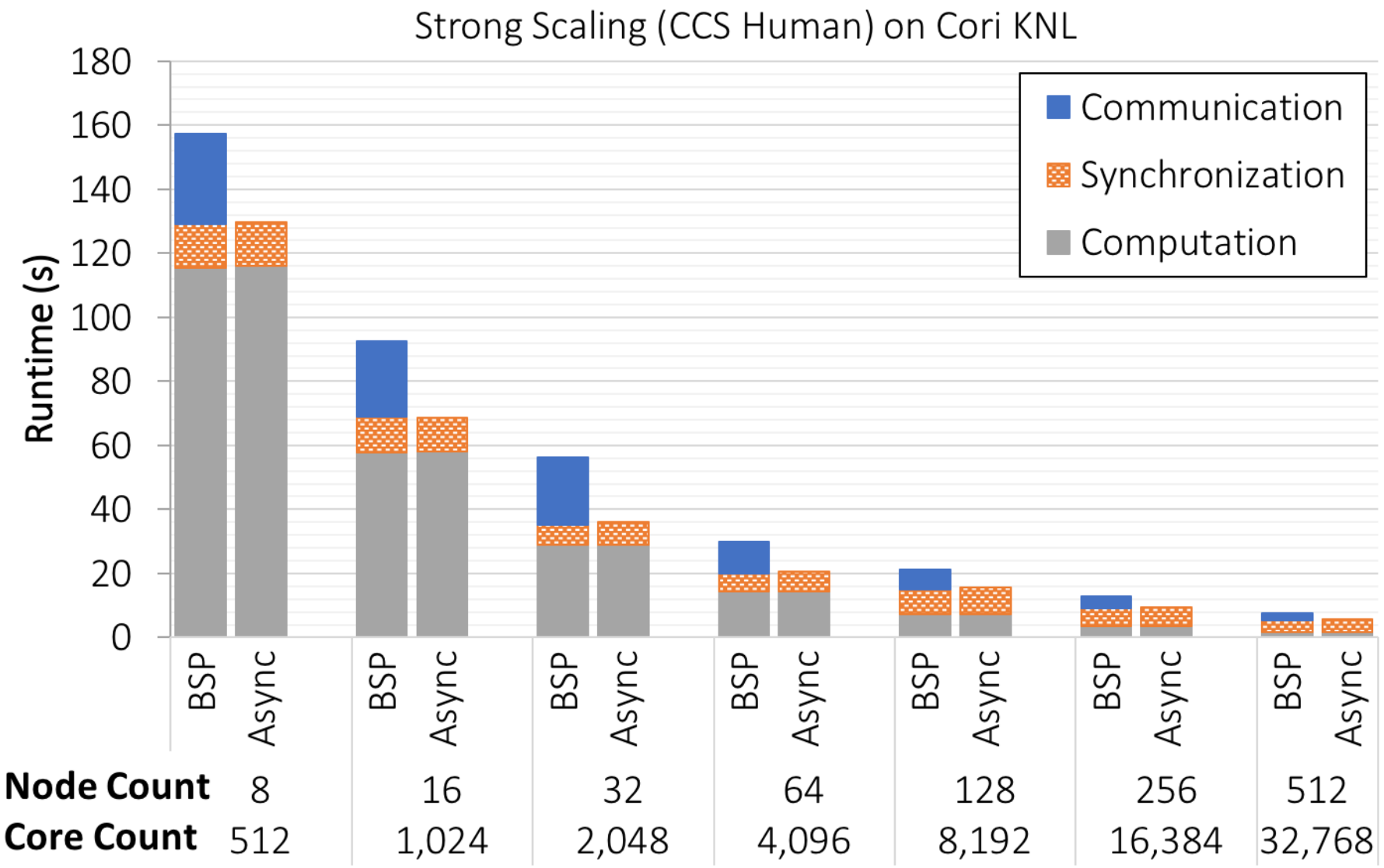
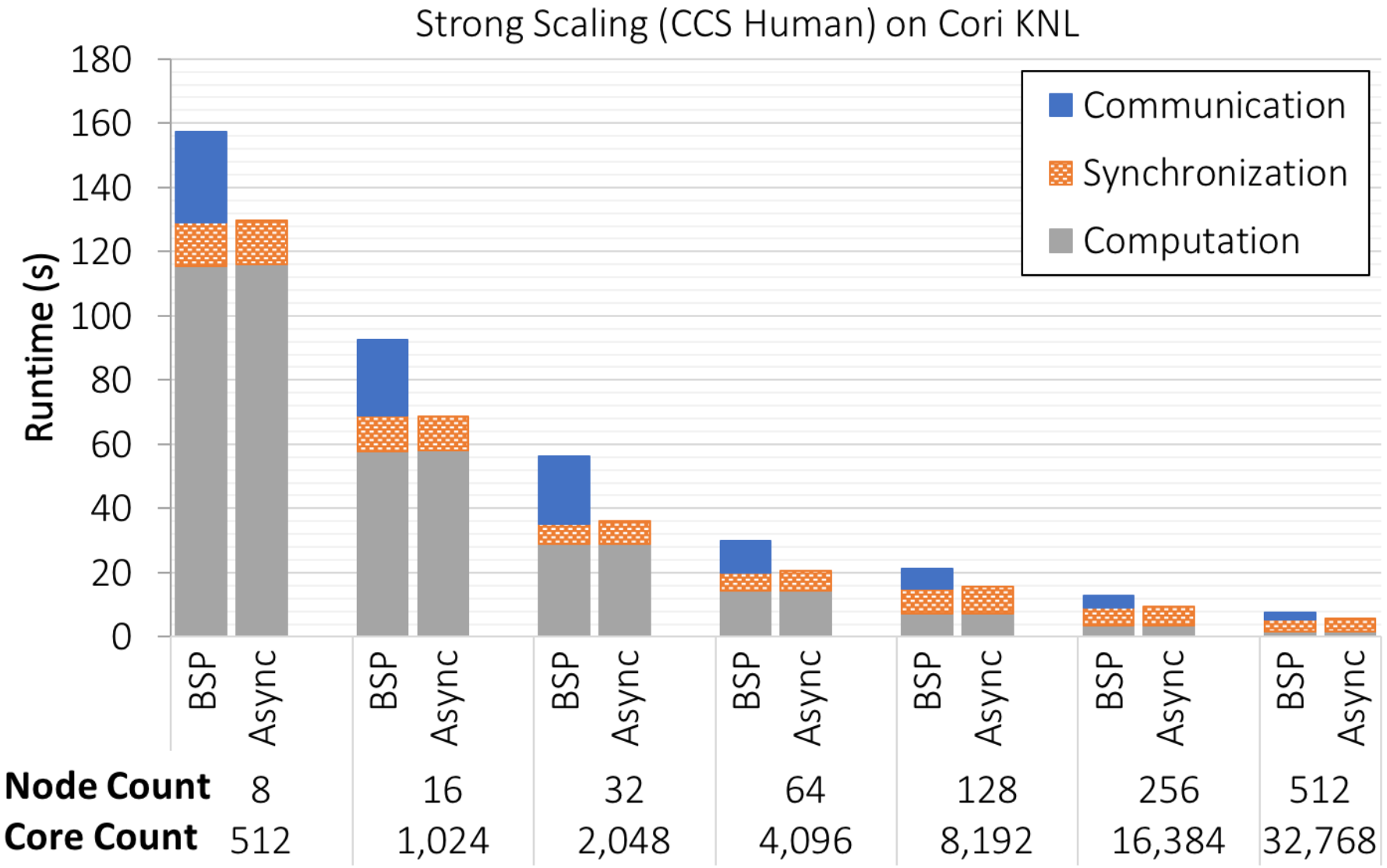

Strong Scaling (CCS Human) on Cori KNL
Runtime (s)
180
160
140
120
100
80
60
40
20
0
Communication
Synchronization
Computation
BSP
Async
Node Count
8
16
32
64
128
256
512
Core Count
512
1,024
2,048
4,096
8,192
16,384
32,768



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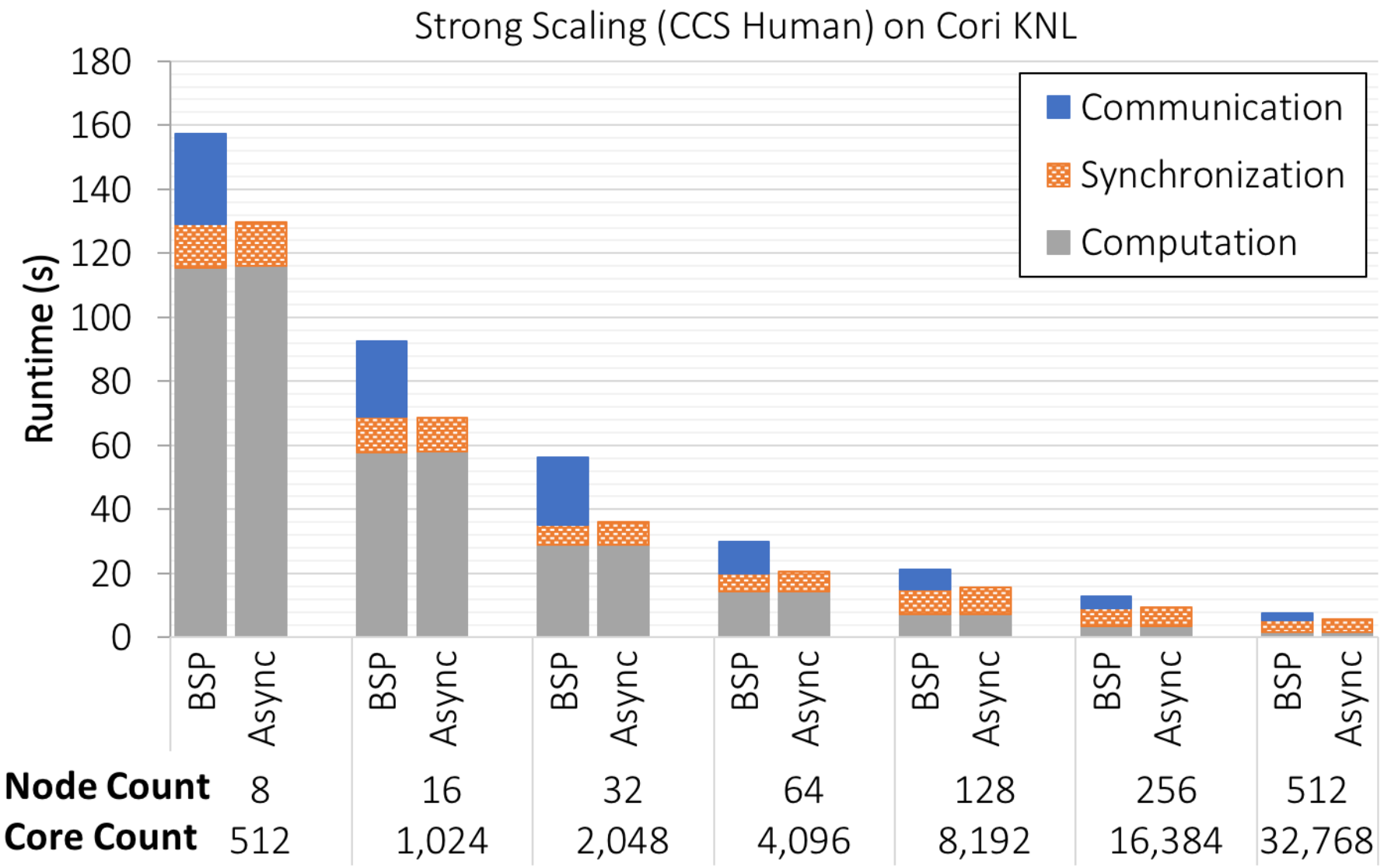

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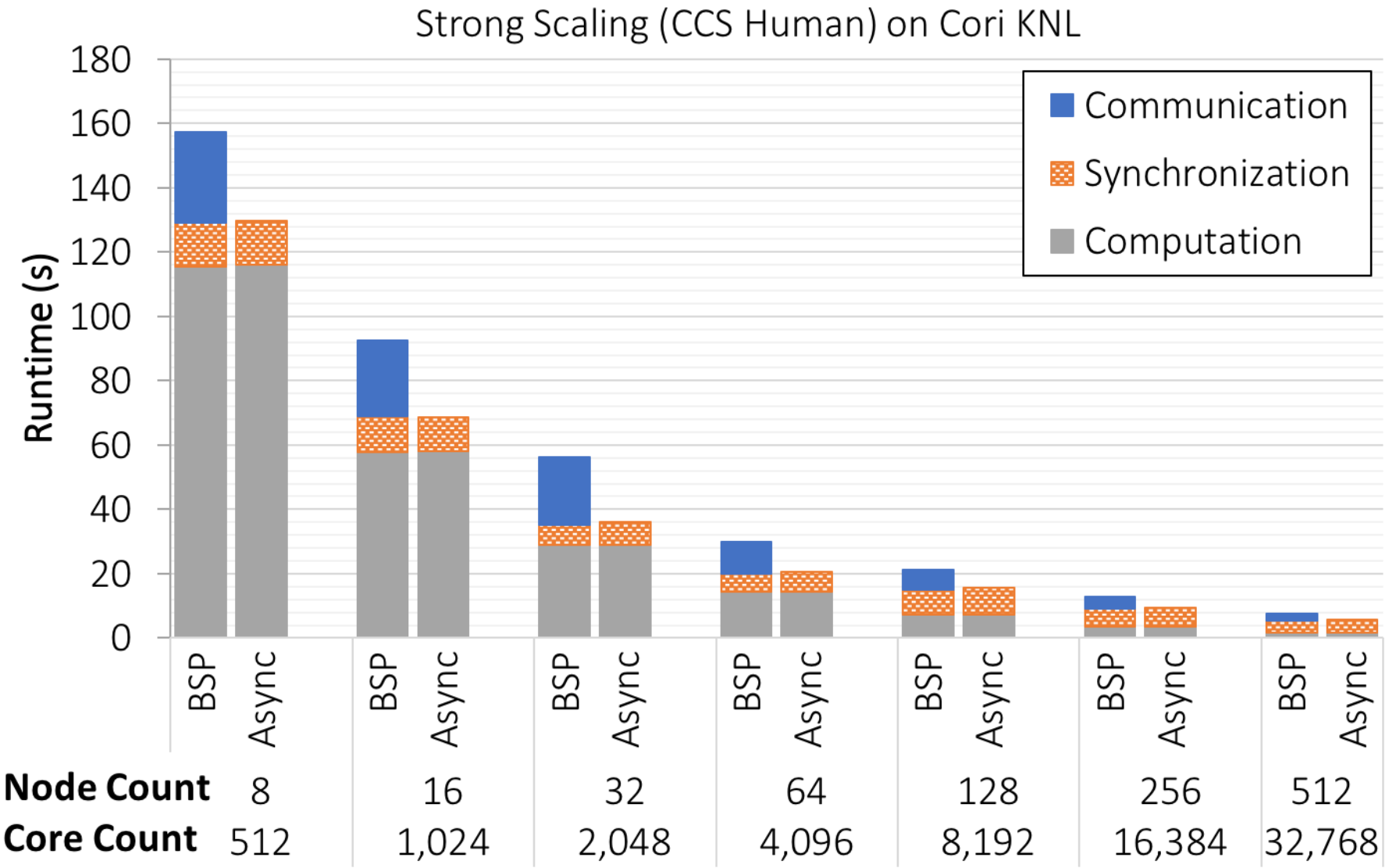

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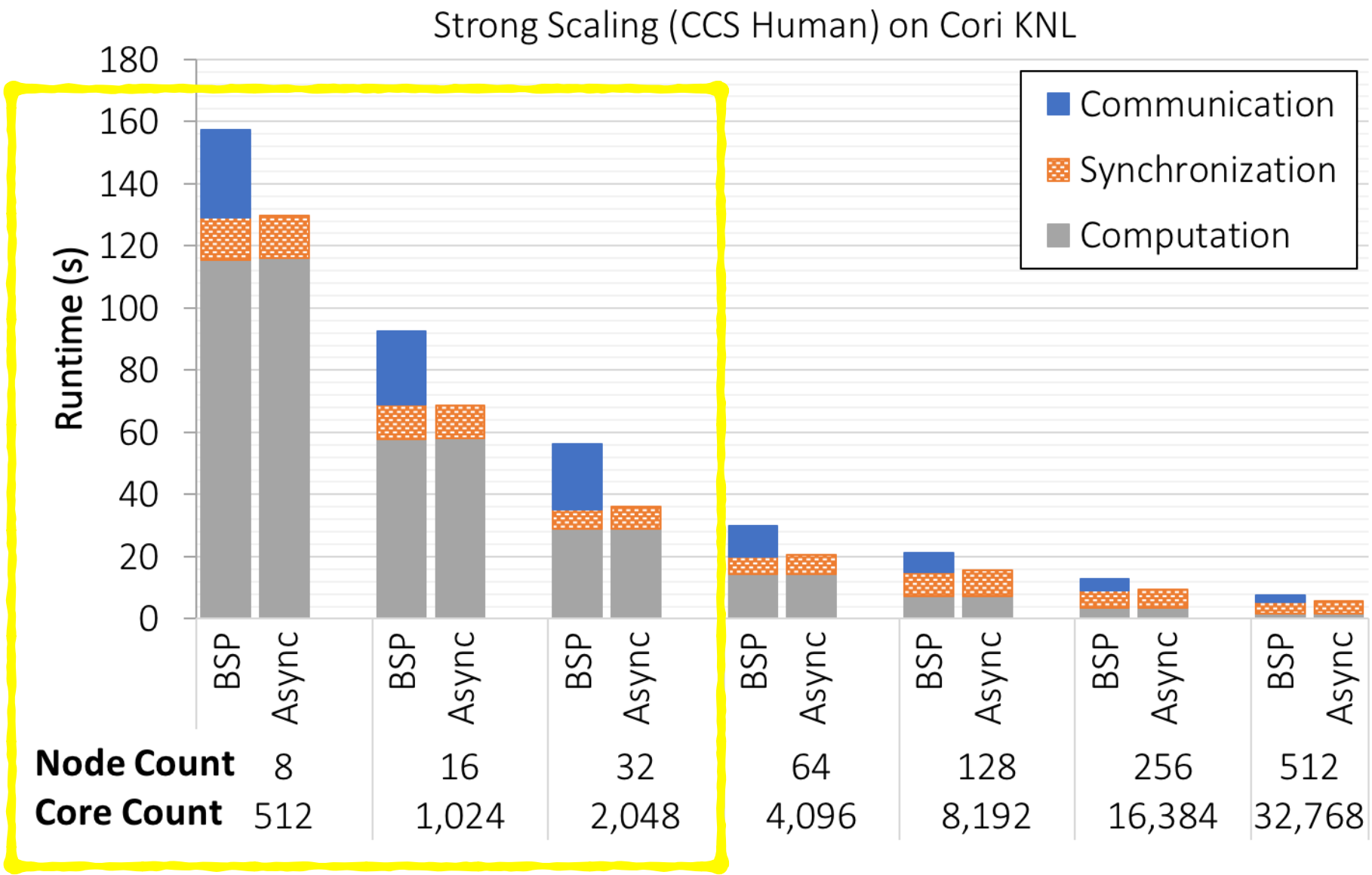
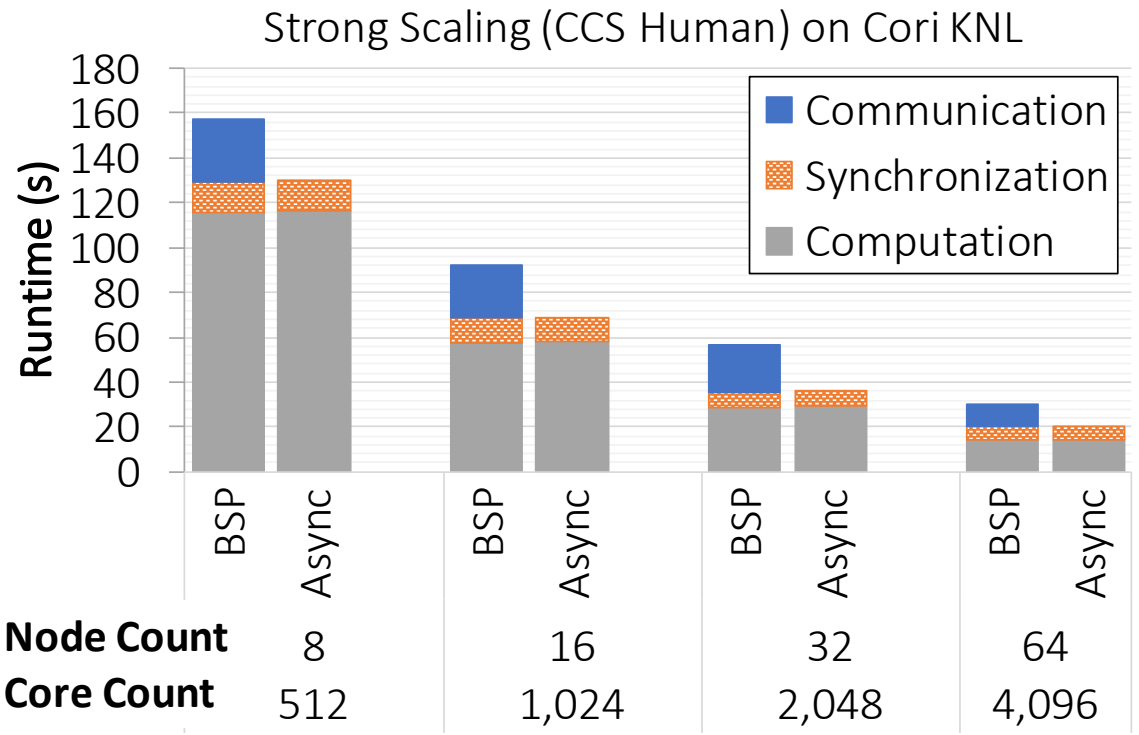
- focus now: communication time (blue, top bars)



- **8-32** nodes, BSP communication overhead is **18-37%**
- Async is up to 20% more efficient with effective communication hiding

8-32 nodes, memory limits necessitate multiple BSP exchanges, increasing overall communication overhead



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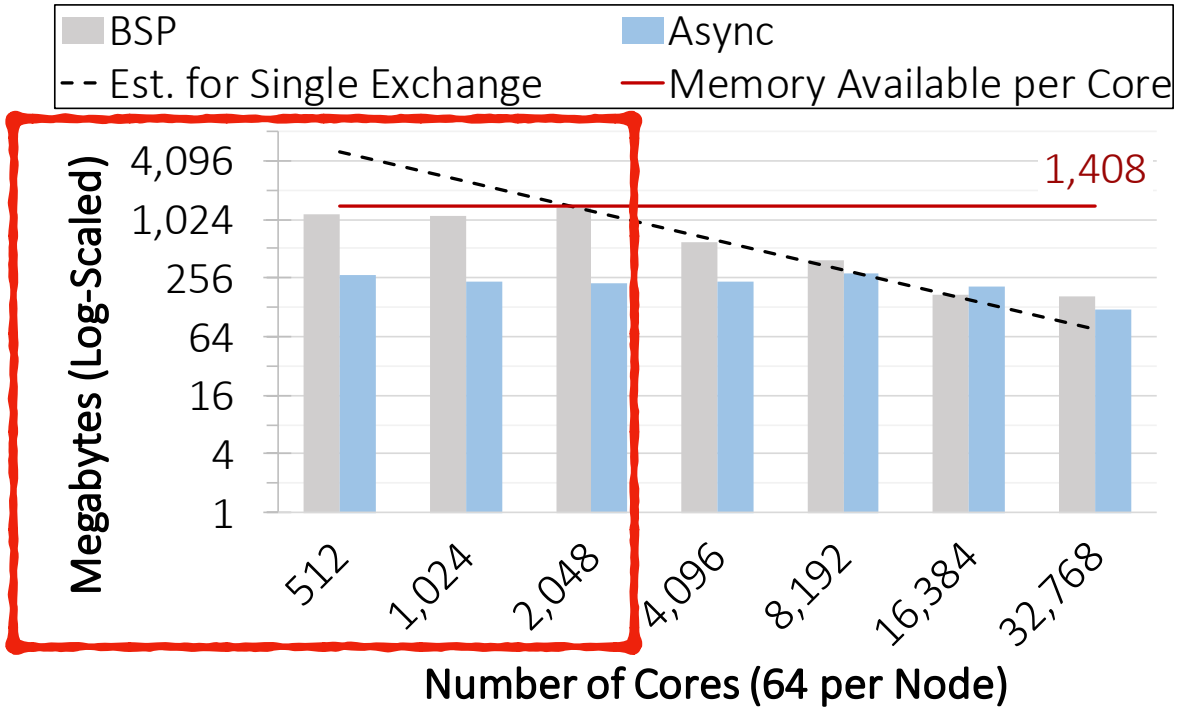
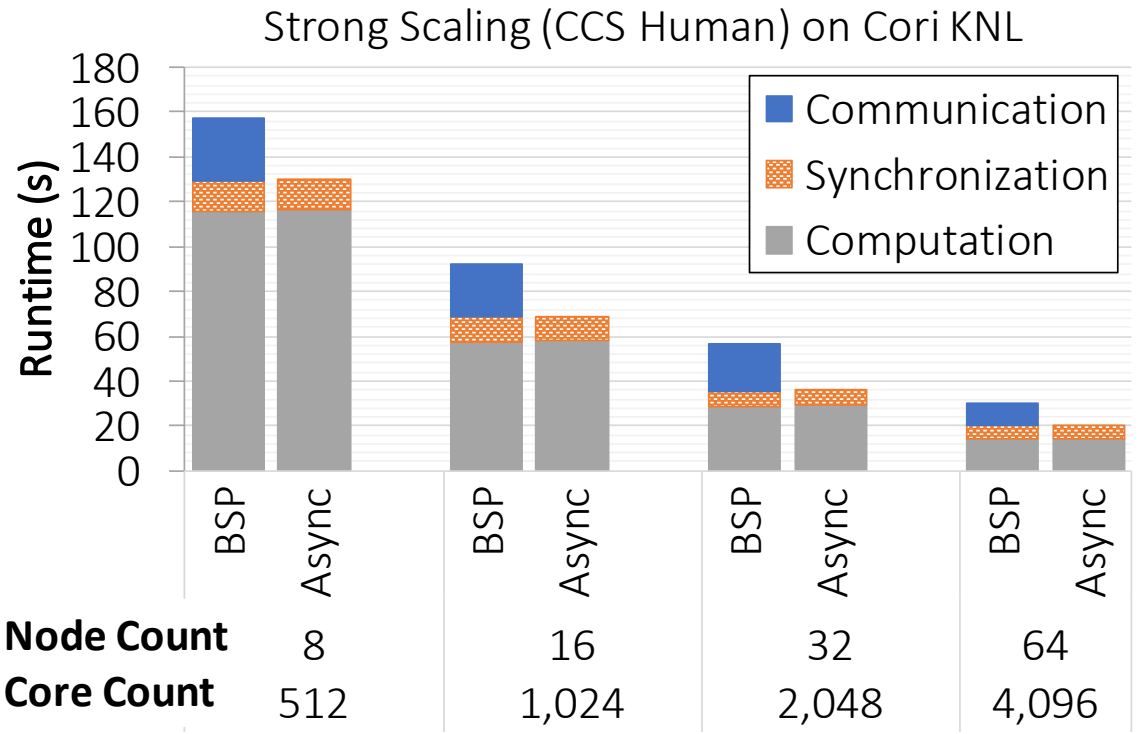
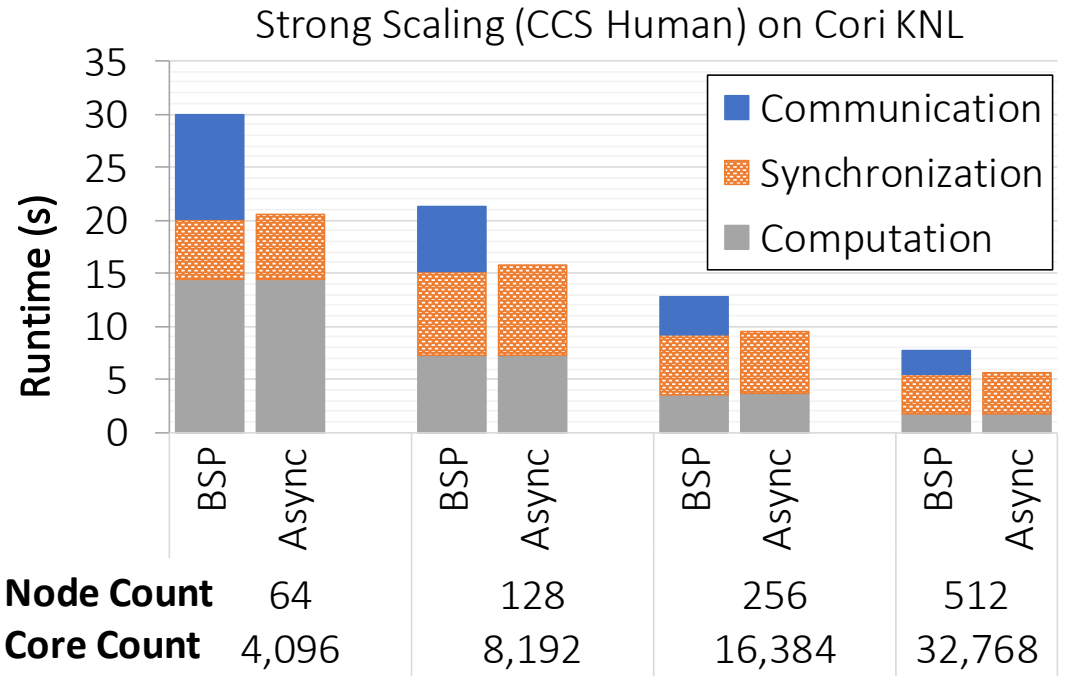




With sufficient memory for a single BSP exchange, 64-512 nodes, efficiency gap decreases to 4-13%



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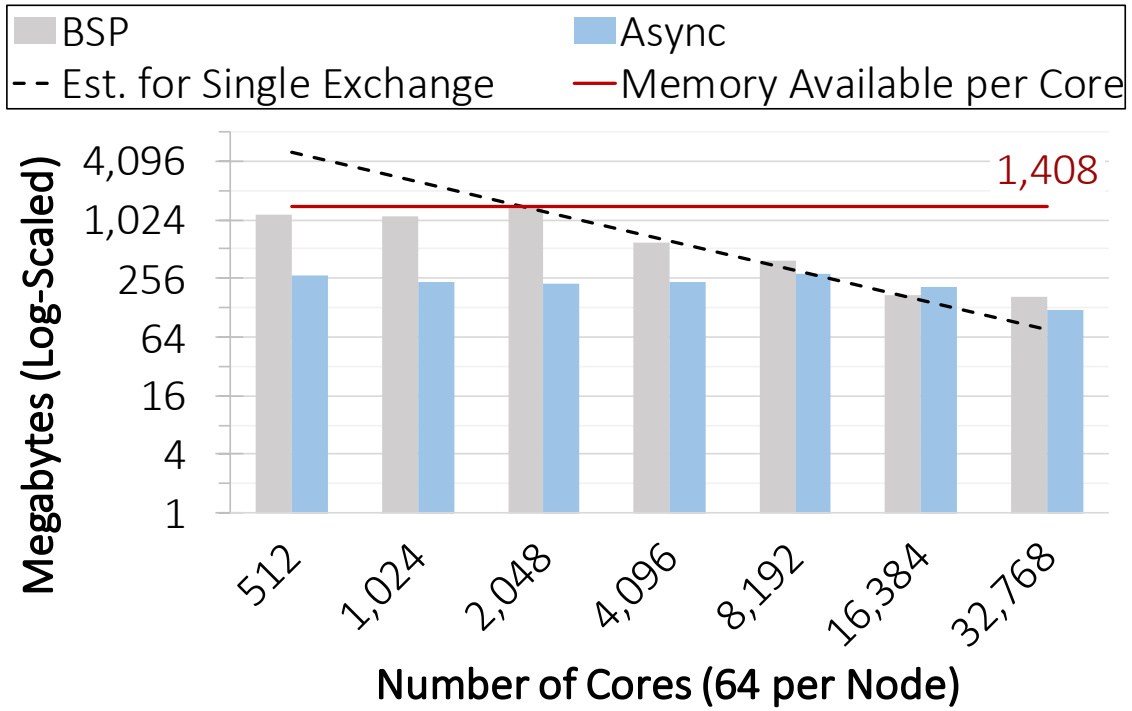

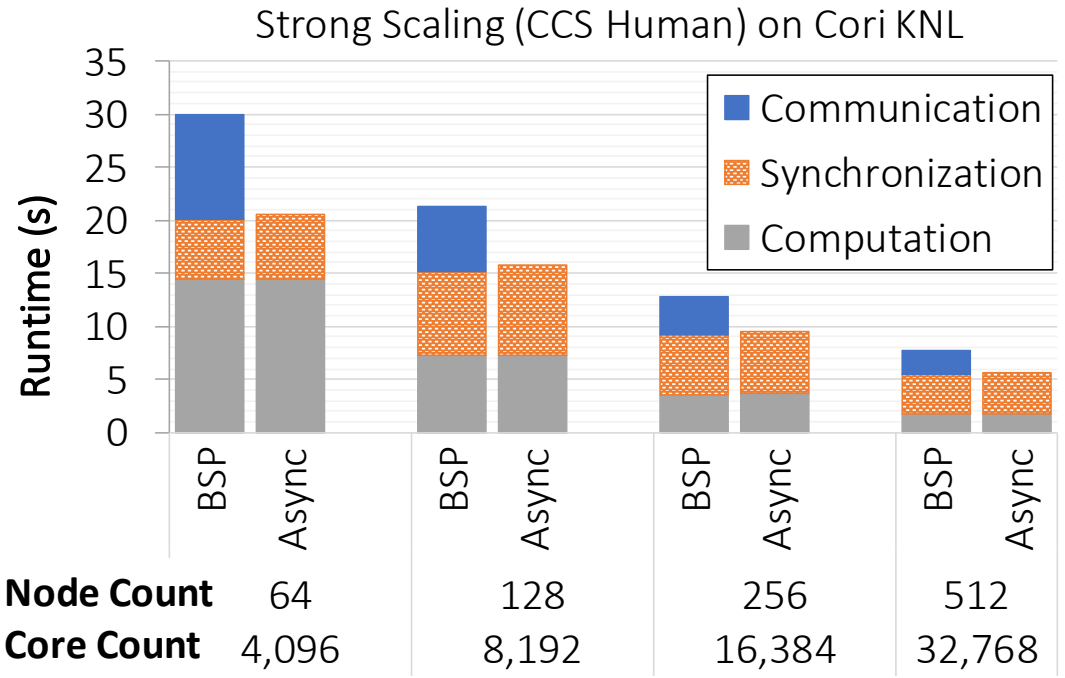

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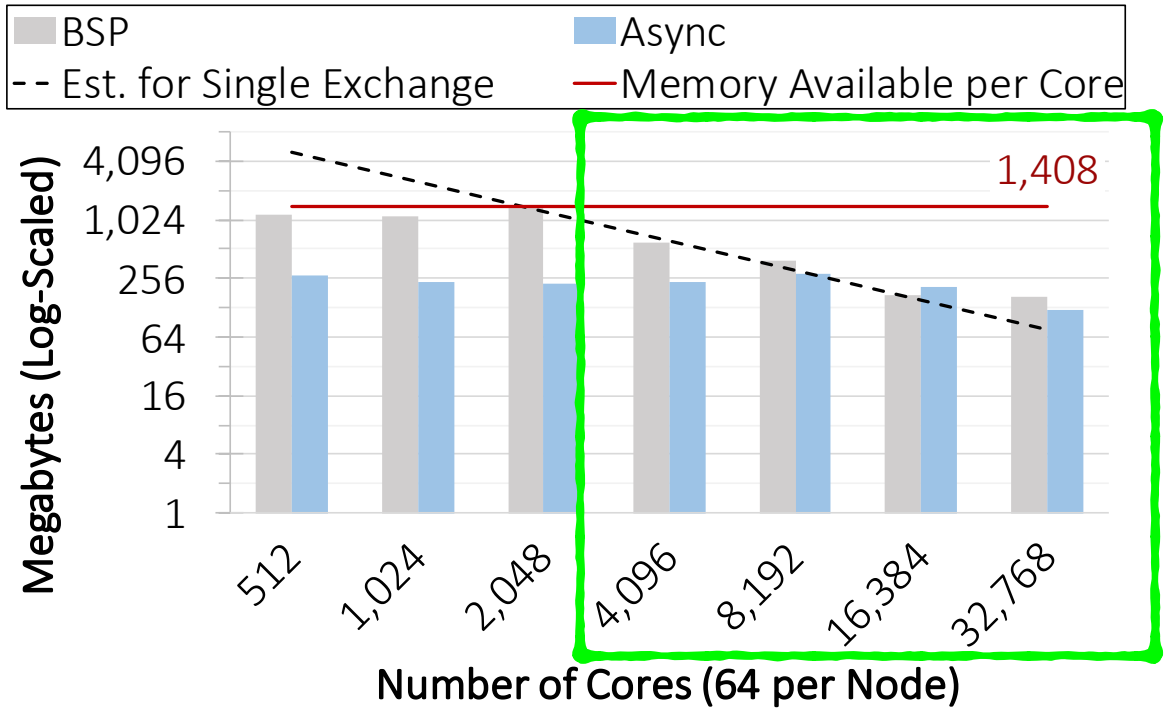

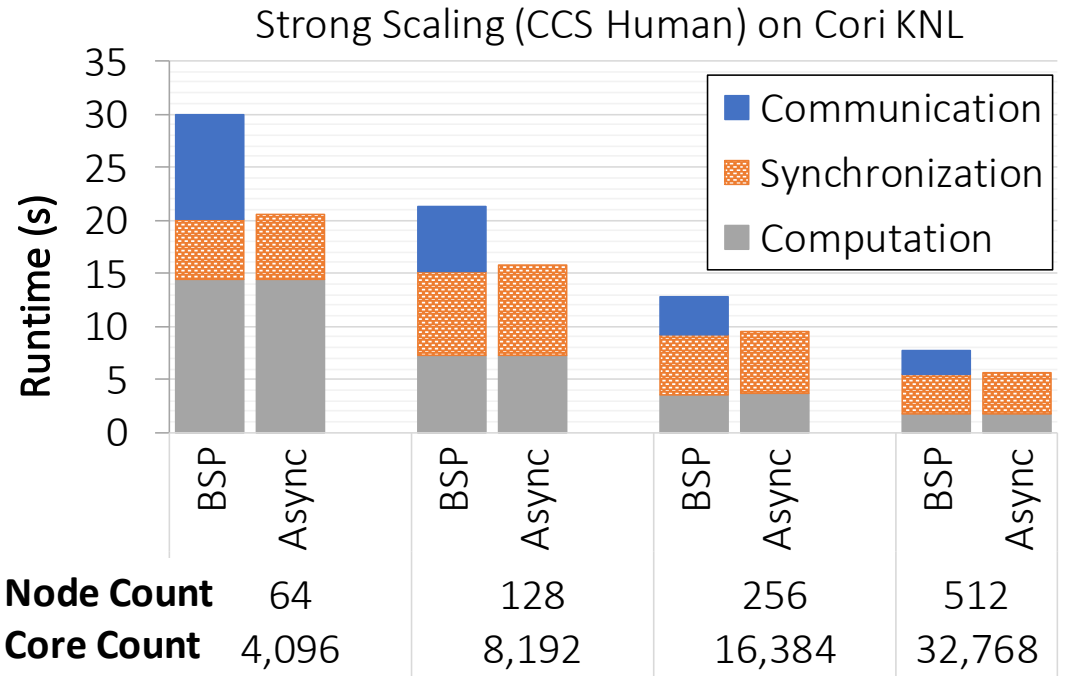

^ note, **y-axis s**cale adjustment of 6x

What are the relative unhidden communication costs?

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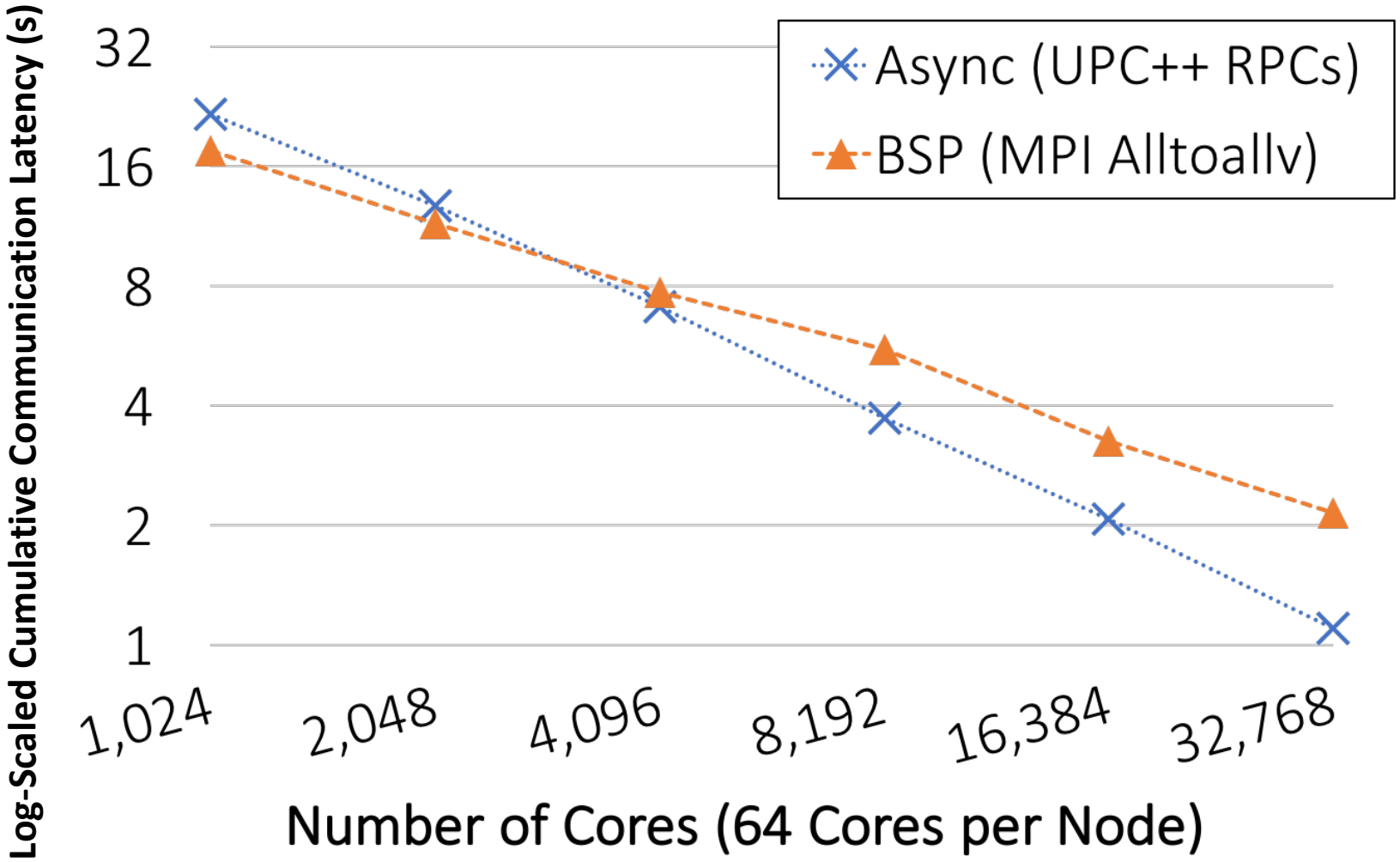
- Measured/validated using a mode that skips the computation
- Async sends many more messages with variable round-trip latency
- Number of messages scale inversely with the number of parallel processors
- In aggregate, Async communication-computation overlap balance out



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- Keys for effective communication-computation overlap for data-intensive Generalized N-Body problems like these
  - **balance** of round-trip or one-sided **message latencies** to **pairwise/tuple-wise computations** on average
  - one example implication: optimizing the computation (pairwise alignment) in this case is only independent from communication optimization up to a point…

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- Other opportunities and optimization suggestions are highlighted in the full text
  - also more depth on both the computational and communication load imbalance…

Final Remarks

- The code is available on SourceForge (DiBELLA)
- for use with general DNA inputs for *read to read overlap and alignment*
  - and for other bioinformatics problems, e.g. proteomics, with reasonable refactoring effort
- for performance-focused studies and benchmarking as demonstrated

Acknowledgements

This research was supported in part by the **Exascale Computing Project** (17-SC-20-SC), a collaborative effort of the **U.S. Department of Energy Office of Science** and the **National Nuclear Security Administration** and by the **National Science Foundation** as part of the SPX program under Award number 1823034. This research used resources of the **National Energy Research Scientific Computing Center (NERSC)**, a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231.

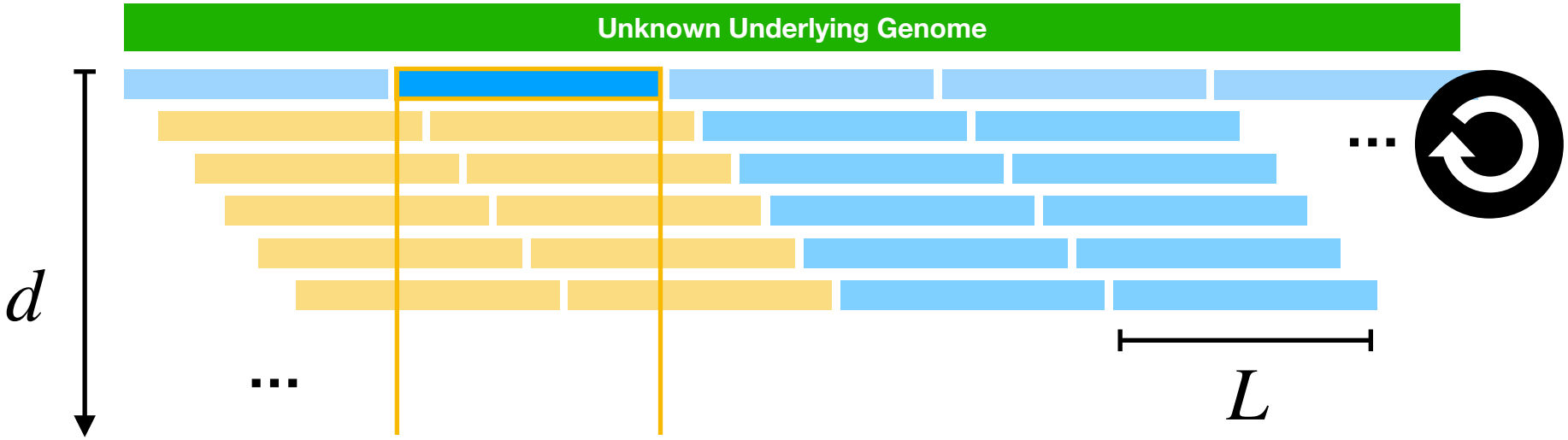
We thank our **5 anonymous reviewers** for their **invaluable feedback**!

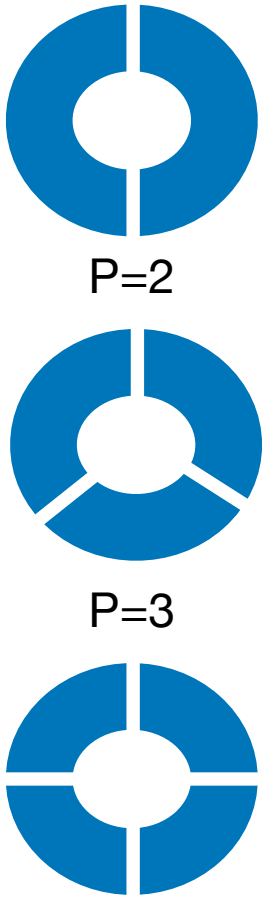
Questions

Appendix

Lemma: (in general) any partitioning of the reads will cut hyperedges due to the underlying sequencing methodology

Perfect world: no errors, uniform read lengths, perfectly uniform coverage, no *repeats*, "circular" genome





- Each **read** overlaps with **2(*d*-1) other reads**
- Partitioning cannot cut fewer than (*P* x *d*) hyperedges, P > 1

Reality: the hypergraphs are sparse

*** we expect this from k-mer filtering among other reasons**

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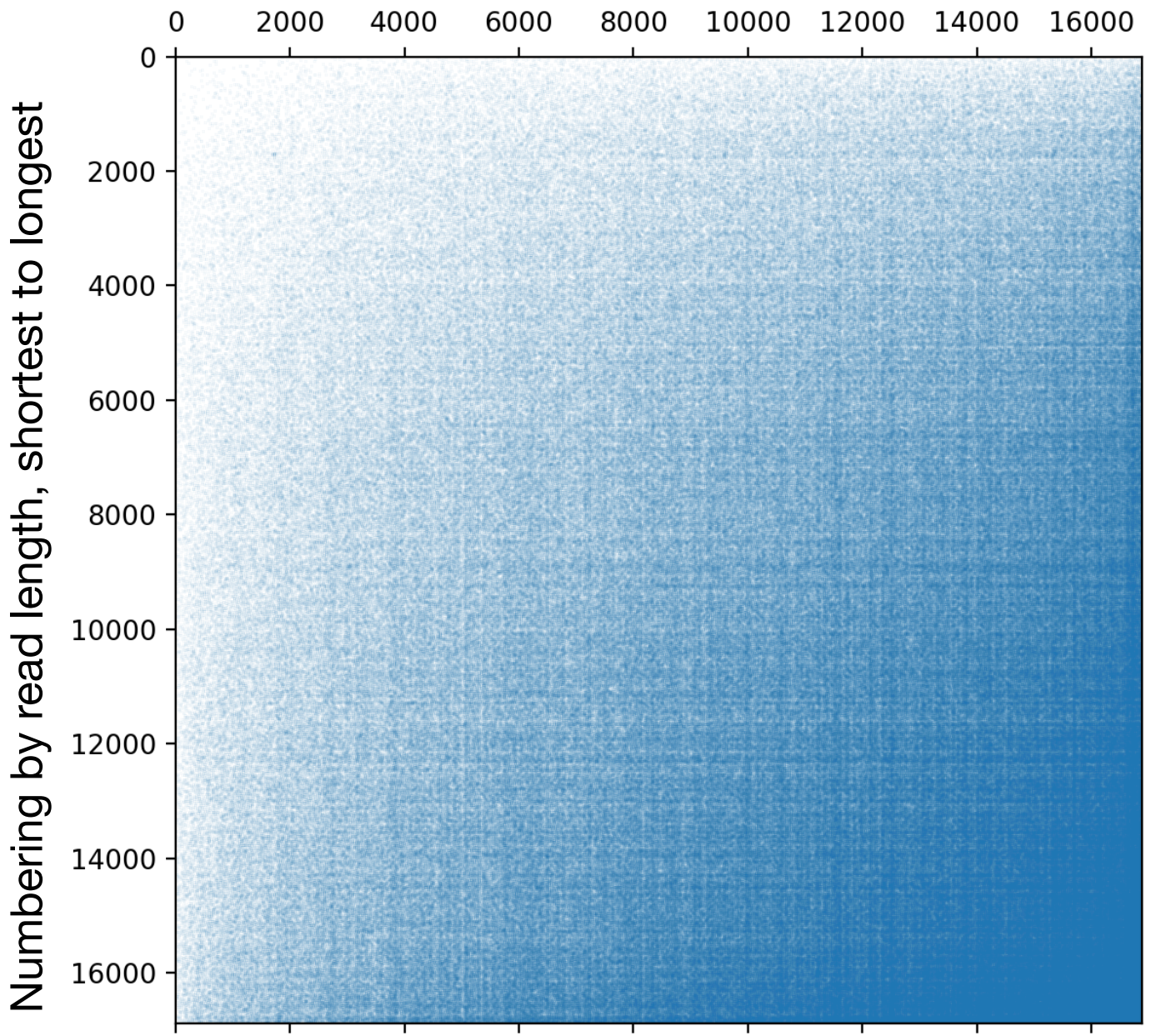
Plotted as Read by Read Matrix



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Looks dense but is very sparse!

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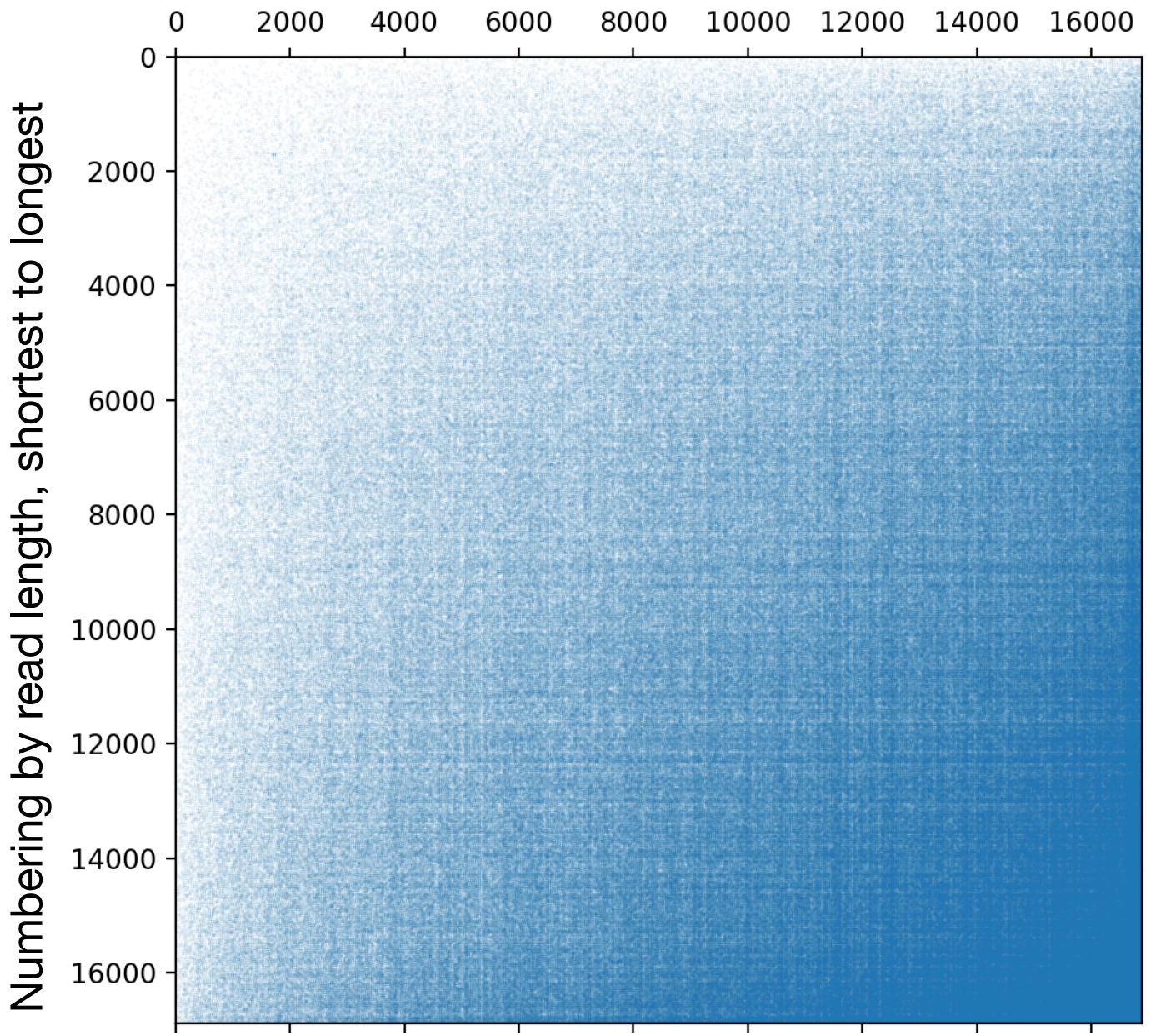

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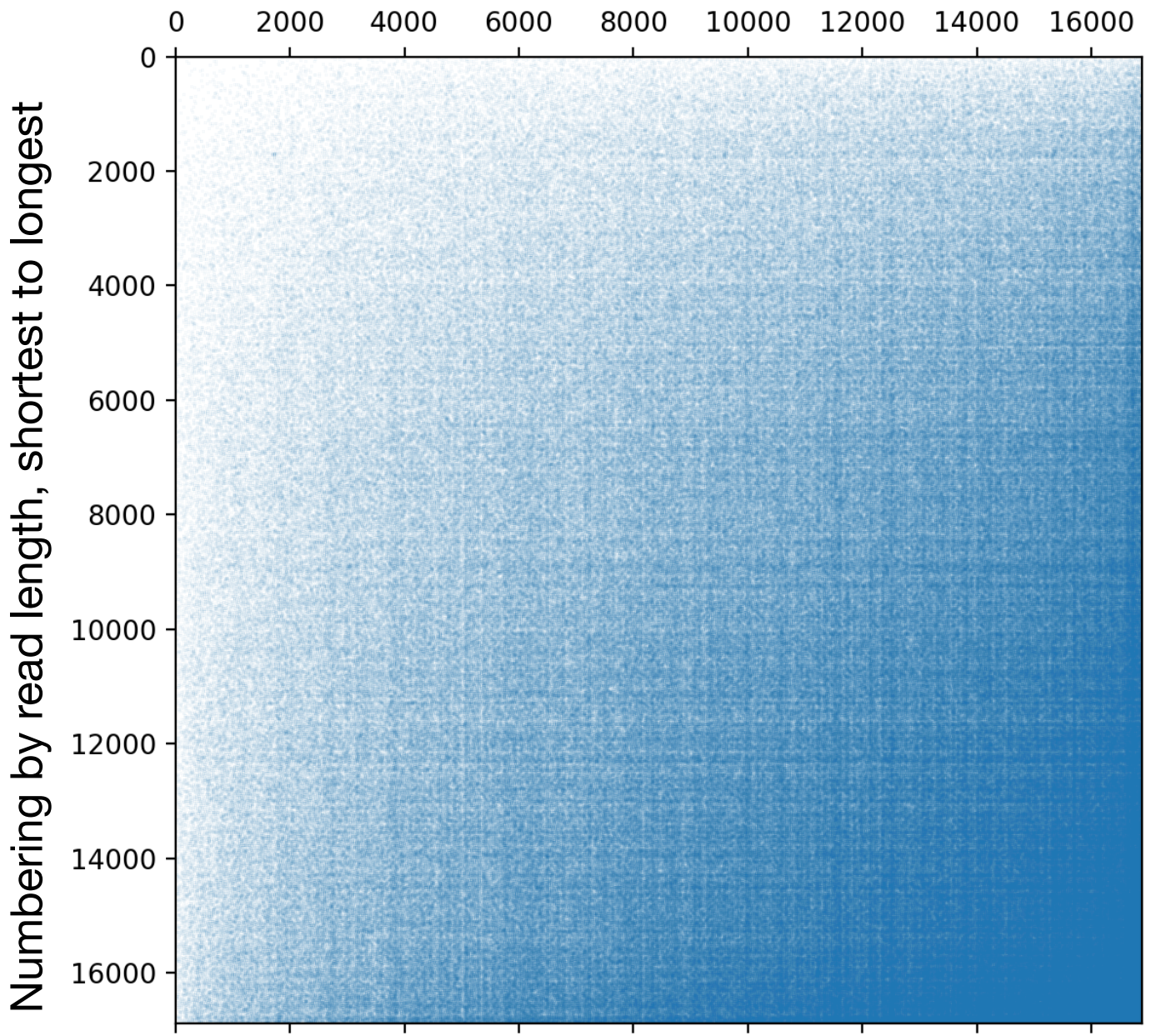

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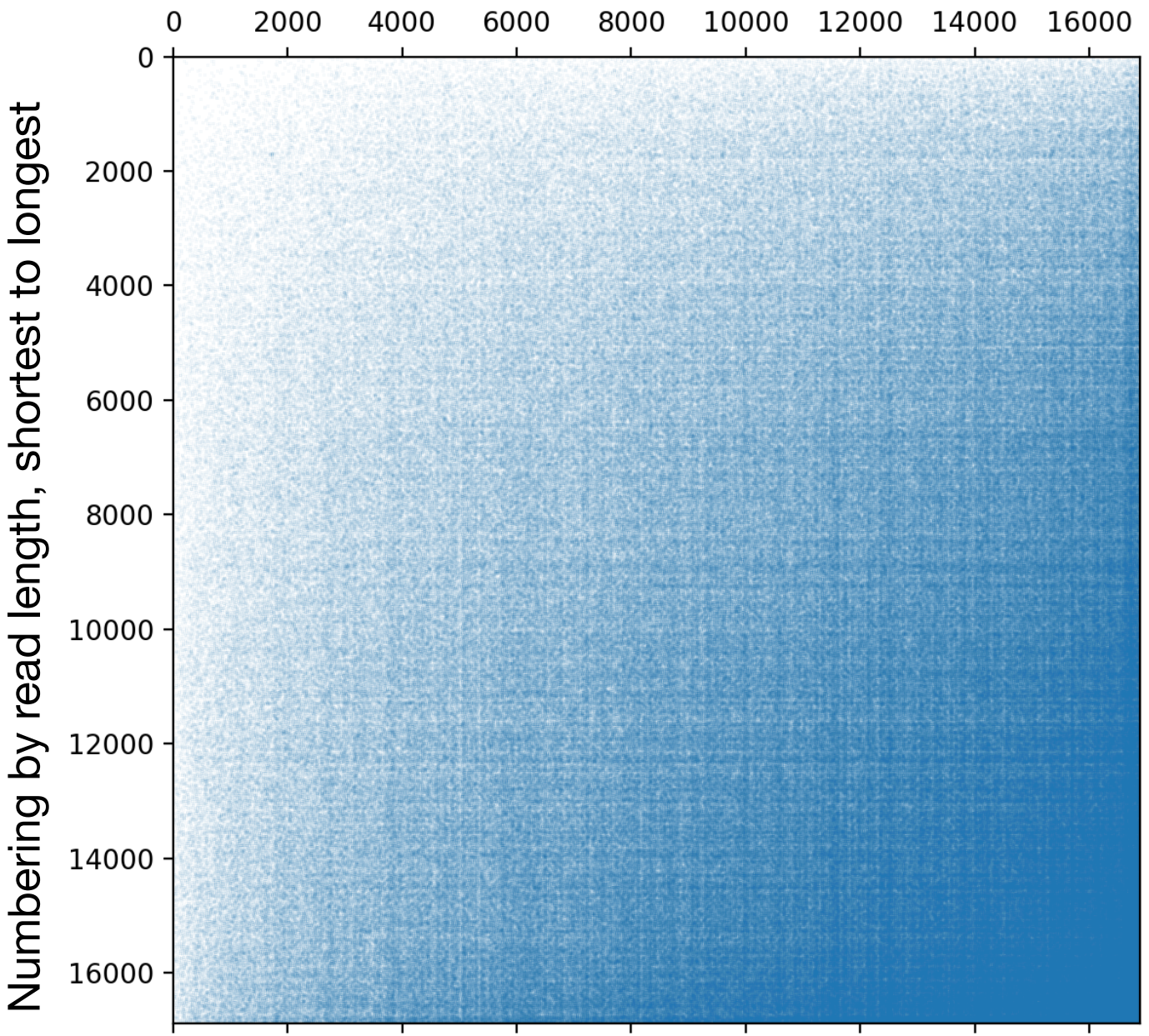

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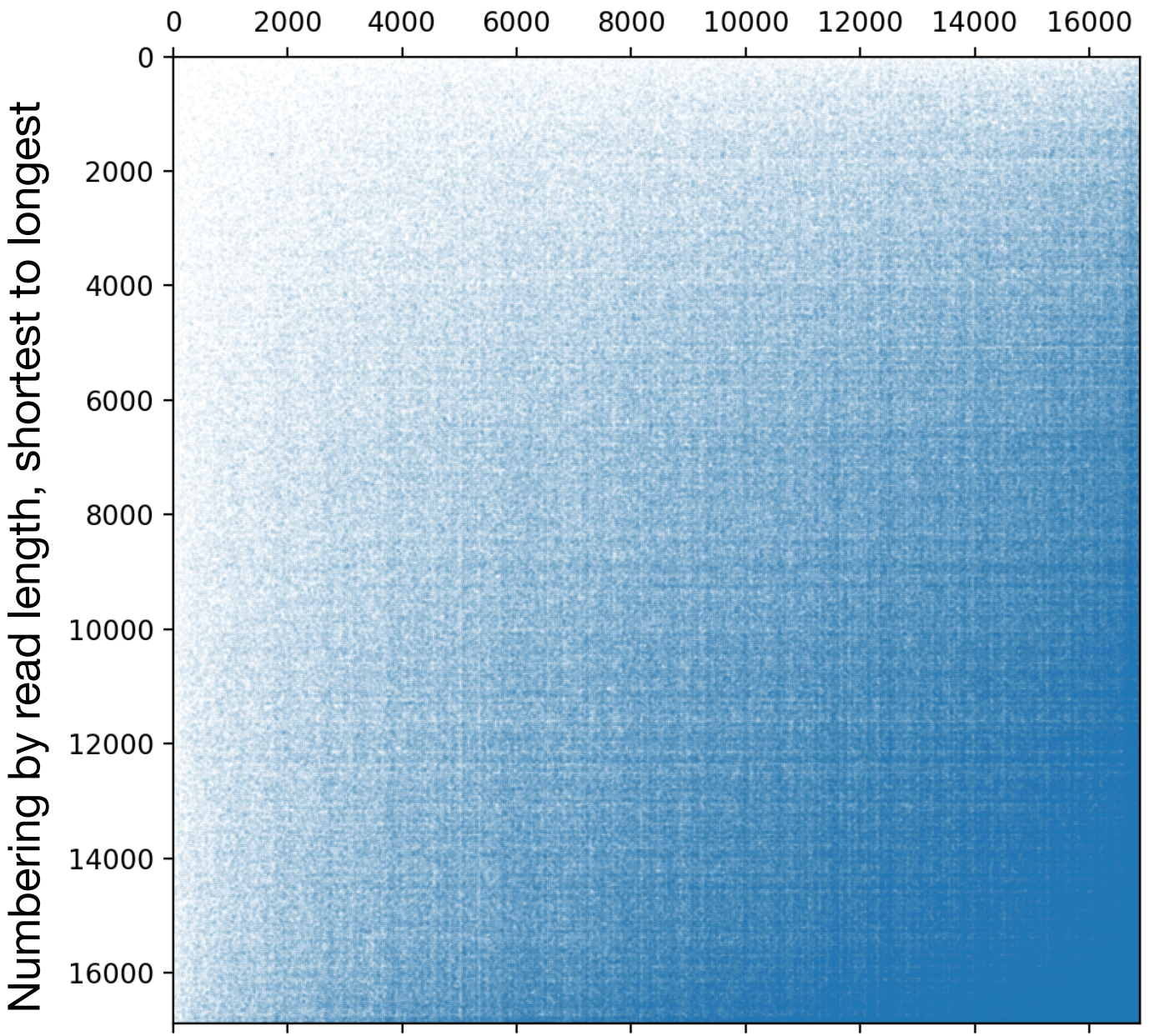

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- making the non-zeros visible in the plot, makes the matrix look dense

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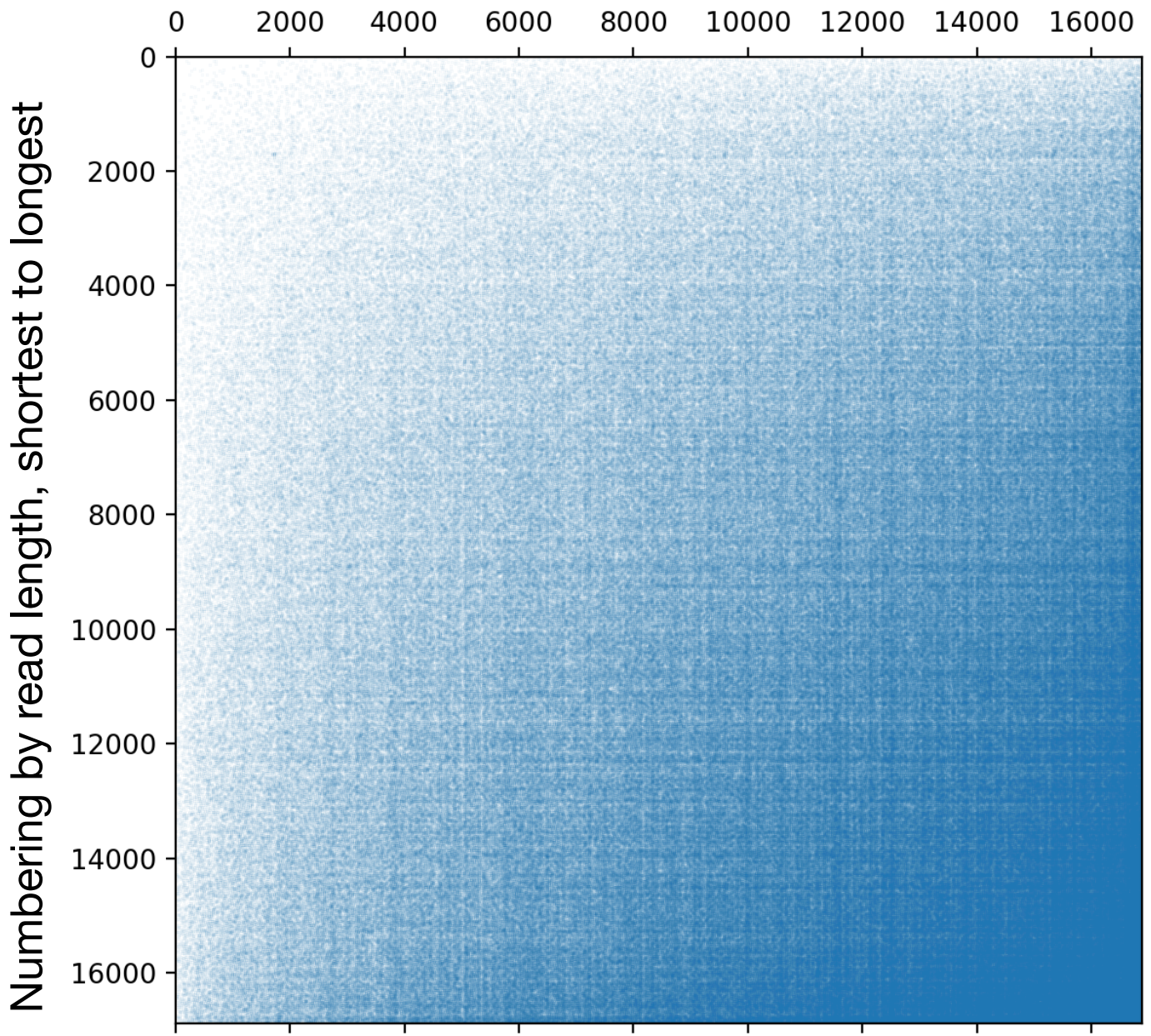
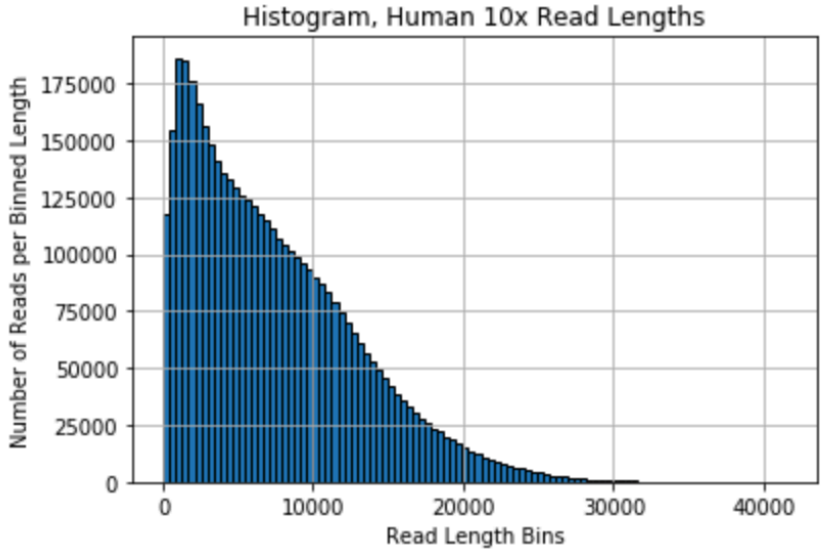
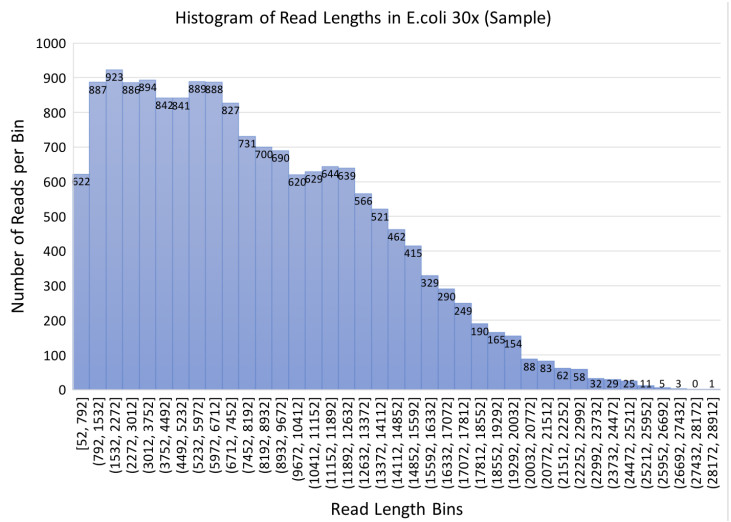
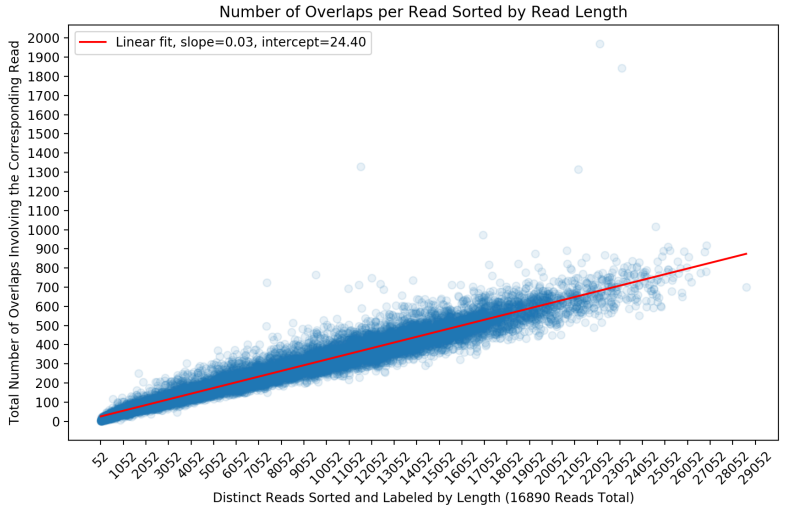


Large sparse unstructured hypergraph







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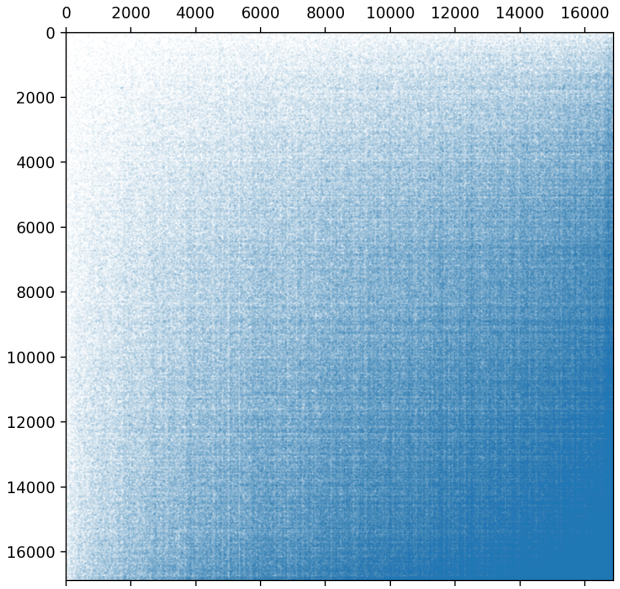

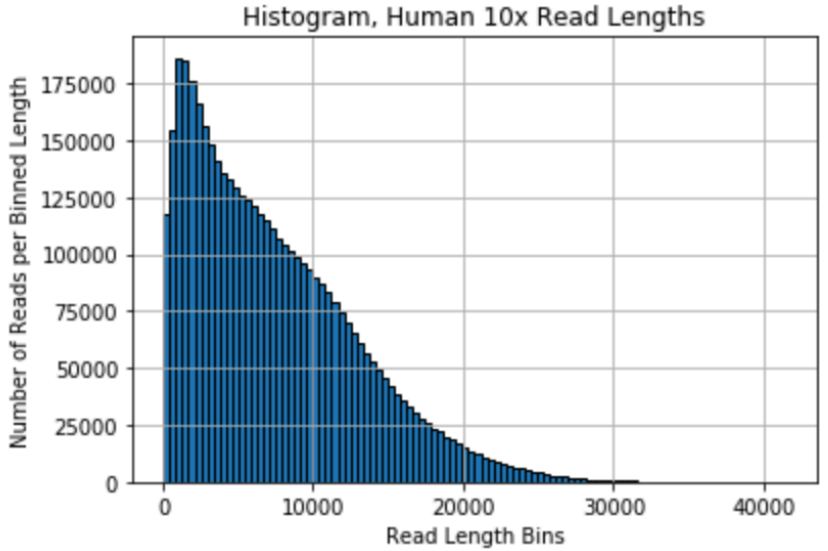

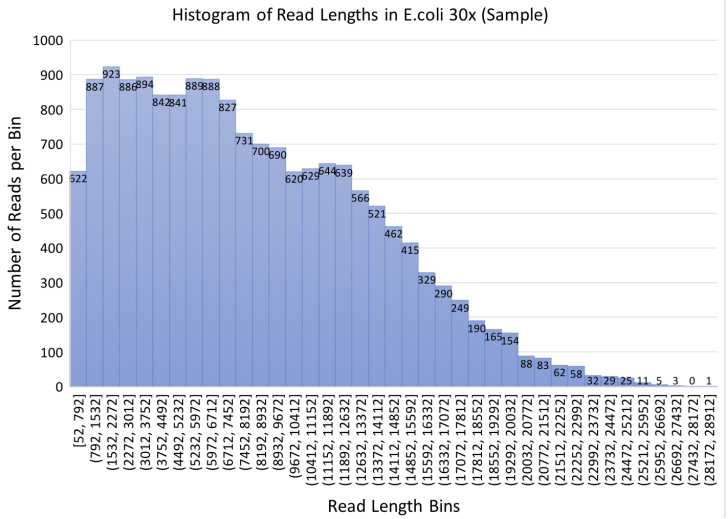

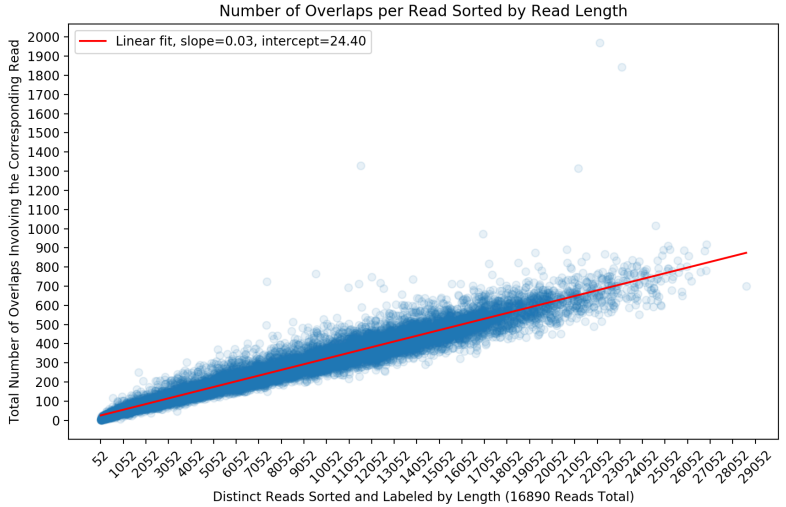

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