SWIFT:

Task-based Calculation + Task-based MPI + Task-based I/O = Maximal Performance

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Durham University

This work is a collaboration between two departments at Durham University (UK):

- The Institute for Computational Cosmology,
- The School of Engineering and Computing Sciences,

with contributions from the astronomy group at the university of Ghent (Belgium), St-Andrews (UK), Lausanne (Switzerland)
as well as the DiRAC and STFC software team at Hartree (UK).

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Introduction

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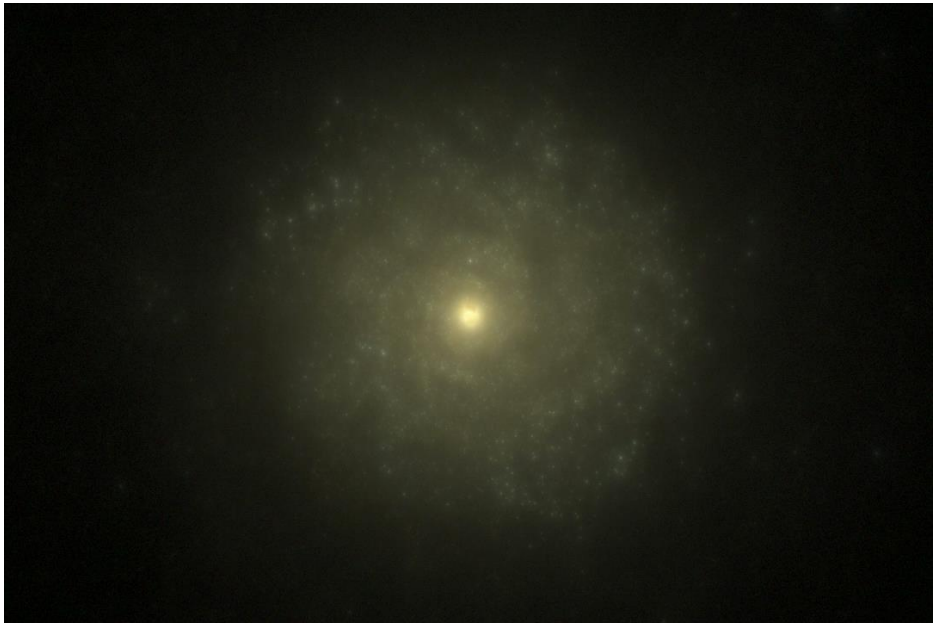
What we do and how we do it

- Cosmological simulations of the formation of galaxies.
- EAGLE project: 48 days of computing on 4096 cores, most cited astronomy paper of 2015.
- Simulate gravity and hydrodynamics with particles.
- Large dynamic range and >2M time-steps.



HPC Challenges in 2017

- Exploit all 3 levels of parallelism (MPI, threads, vector instructions).
- Decrease the CPI as much as possible (high FLOP / Byte read).
- Hide inter-node communications.
- Fast i/o on parallel file systems with many other users.

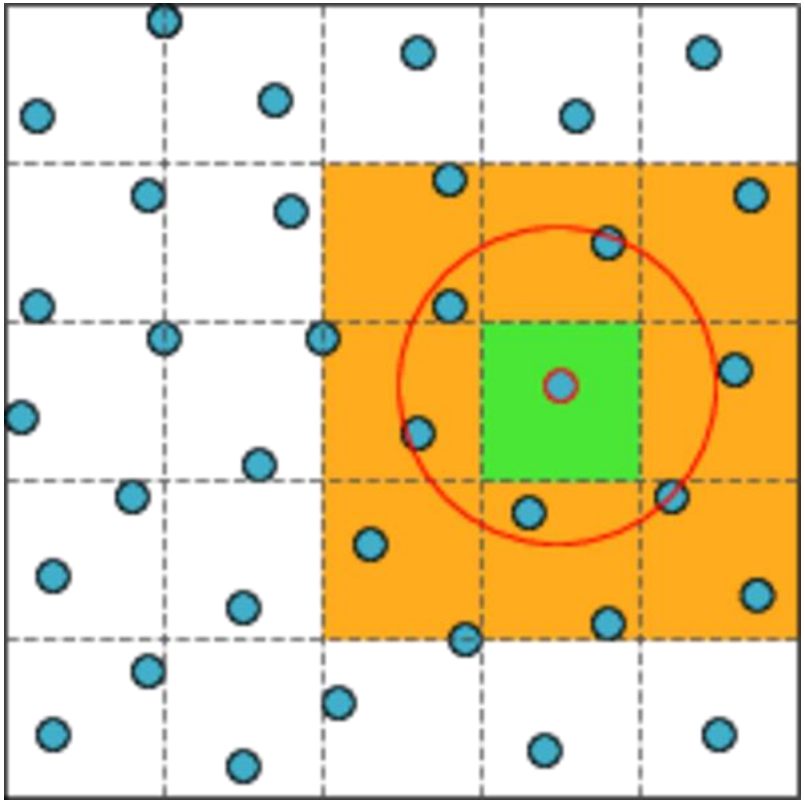
Challenges of our simulations

- Particles are unstructured in space.
  → No simple vectorizable pattern.
- Particles will move and the neighbours they interact with will change at every time-step.
  → No pre-computed list or mesh that can be re-used over and over.
- Particles have individual time-steps.
  → Hard to load balance steps with only a handful of particles.
- Interactions are computationally cheap.
  → Likely dominated by memory bandwidth.

SWIFT particle hydrodynamics

Lesson 1: Make things predictable.

- Neighbour search done using a grid with ~500 particles per cell.
- Cell size designed to match search radius.
- Particles only interact with same cell or 26 neighbouring cells.
- Can now list all interactions!



SWIFT particle hydrodynamics

```
for (int ci=0; ci < nr_cells; ++ci) {    // loop over all cells (>1 000 000)
   for(int cj=0; cj < 27; ++cj) {        // loop over all 27 cells neighbouring
cell ci

      const int count_i = cells[ci].count;  // Around 400-500
      const int count_j = cells[cj].count;

      for(int i = 0; i < count_i; ++i) {
         for(int j = 0; j < count_j; ++j) {

            struct part *pi = &parts[i];
            struct part *pj = &parts[j];

           INTERACT(pi, pj);   // symmetric interaction (low FLOPS)
} } } }
```

SWIFT particle hydrodynamics

```
for (int ci=0; ci < nr_cells; ++ci) {
   for(int cj=0; cj < 27; ++cj) {
```

Threads + MPI

```
      const int count_i = cells[ci].count;  // Around 400-500
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      for(int i = 0; i < count_i; ++i) {
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            struct part *pi = &parts[i];
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} } } }
```

Vectorization

Single-node parallelisation

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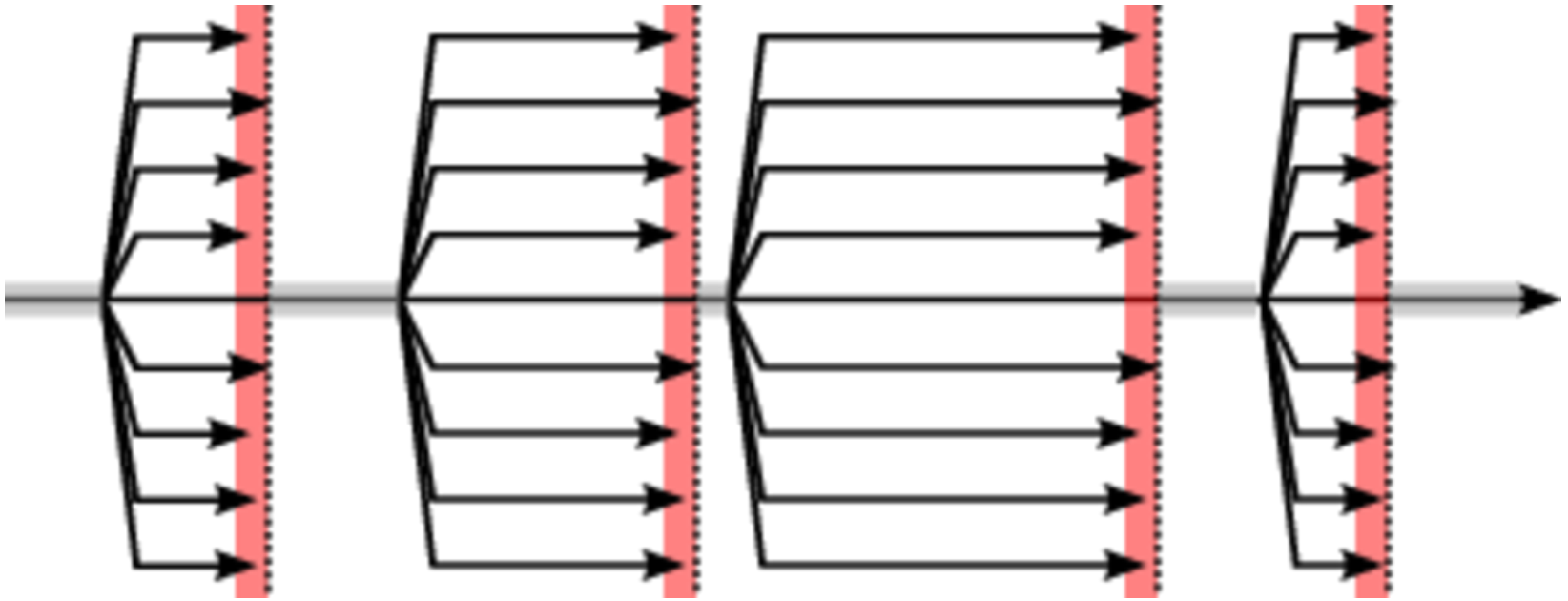
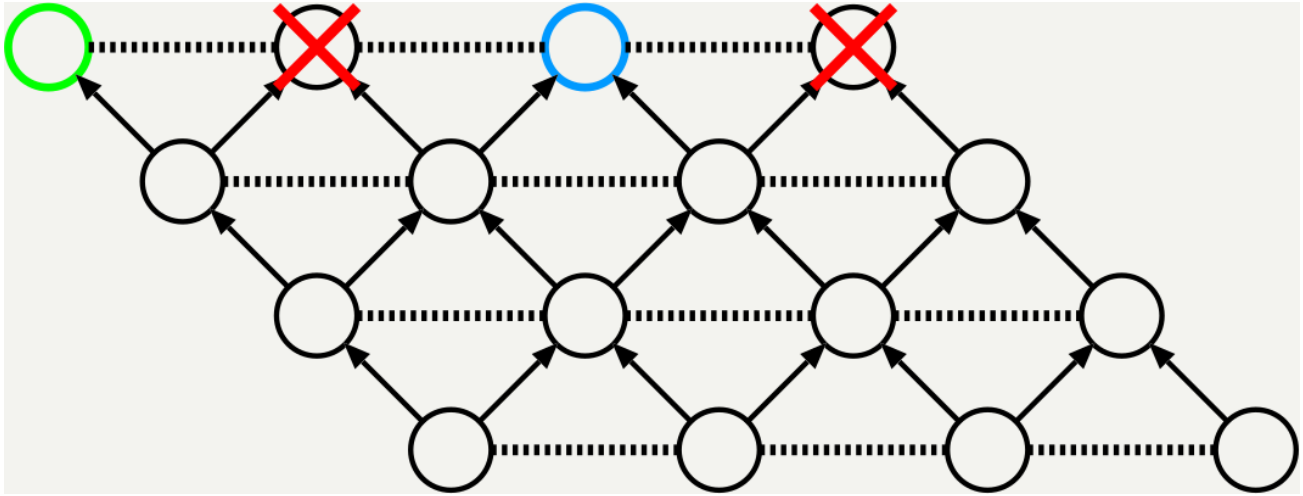
Traditional parallelisation pattern

"fork + join" model



Task-based parallelism

"Shared-memory parallel programming paradigm in which the computation is formulated in an implicitly parallelizable way that automatically avoids most of the problems associated with concurrency and load-balancing."



We use our own (problem agnostic !) Open-source library *QuickShed*.

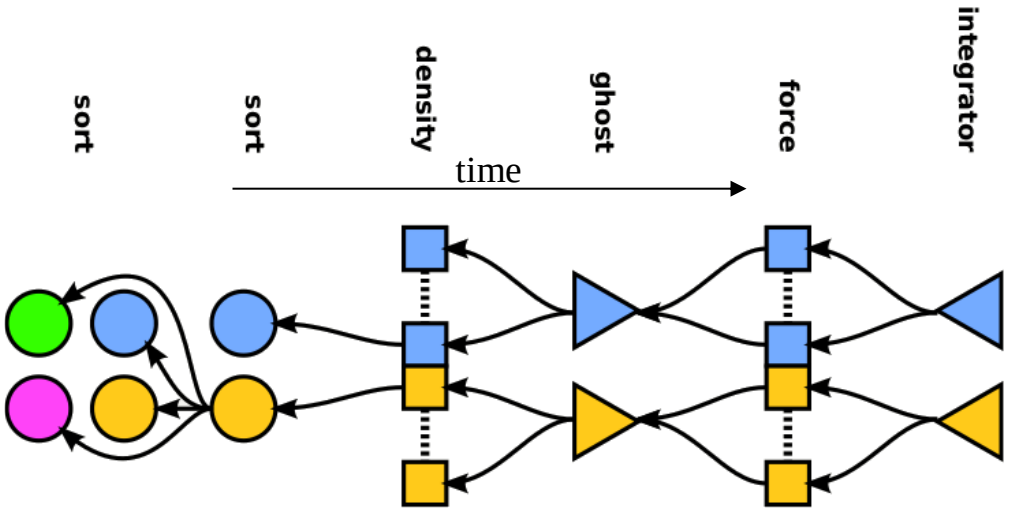
arxiv:1601.05384

Task-based parallelism

- Many libraries out there:
  - HPX
  - Charm++
  - HiHat
  - OmpSS
  - …
- Quickshed is a simple (3000 lines) C library which handles conflicts and dependencies, MPI communications and accelerators offloading.
- arxiv:1601.05384

Task-based parallelism

- Requires to re-write the software and not “just” add pragmas.
- Allows for simple (application scientist friendly!) code within tasks.
- Express the underlying algorithm as a graph.



Single node parallel performance

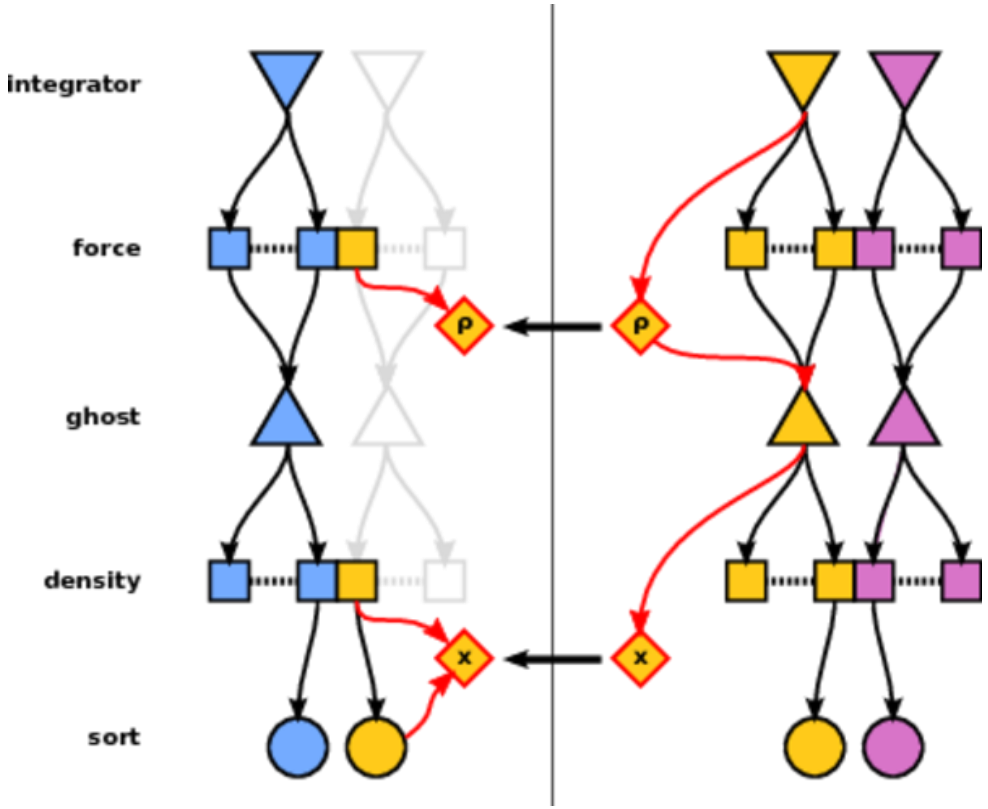
Almost perfect load-balancing on 16 cores.

Multi-node parallelism

Multi-node parallelism

- Can’t afford the usual “send then compute” pattern.
- Need the same flexibility as on one rank as tasks are executed in random order.
- Send small parts of the data within the tasking system.
  → Requires library that correctly implements `MPI_THREAD_MULTIPLE`.
  → Many experienced users and textbooks advise against this.
- If problem big enough, no need to care about latency or bandwidth!
- Very efficient use of the machine (network and FPUs at the same time!).

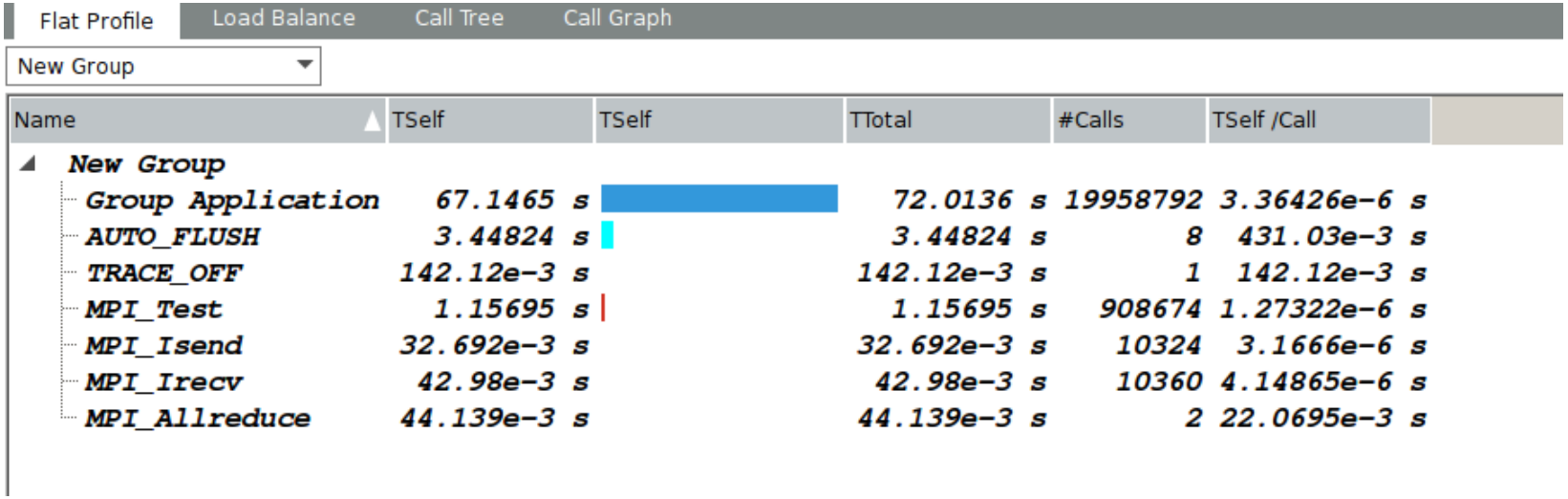
Multi-node parallelism



Some details

- Communication tasks do not perform any computation:
  - Call `MPI_Issend()` and `MPI_Irecv()` when enqueued.
  - Check communications have arrived with `MPI_Test()`.
- Maximal performance: increase `I_MPI_EAGER_THRESHOLD` to allow for most messages to be sent directly.
- Start the purely local tasks first, then the ones that depend on MPI data.

Multi-node parallelism



Name	TSelf	TSelf	TTotal	#Calls	TSelf /Call
New Group					
Group Application	67.1465 s		72.0136 s	19958792	3.36426e-6 s
AUTO_FLUSH	3.44824 s		3.44824 s	8	431.03e-3 s
TRACE_OFF	142.12e-3 s		142.12e-3 s	1	142.12e-3 s
MPI_Test	1.15695 s		1.15695 s	908674	1.27322e-6 s
MPI_Isend	32.692e-3 s		32.692e-3 s	10324	3.1666e-6 s
MPI_Irecv	42.98e-3 s		42.98e-3 s	10360	4.14865e-6 s
MPI_Allreduce	44.139e-3 s		44.139e-3 s	2	22.0695e-3 s

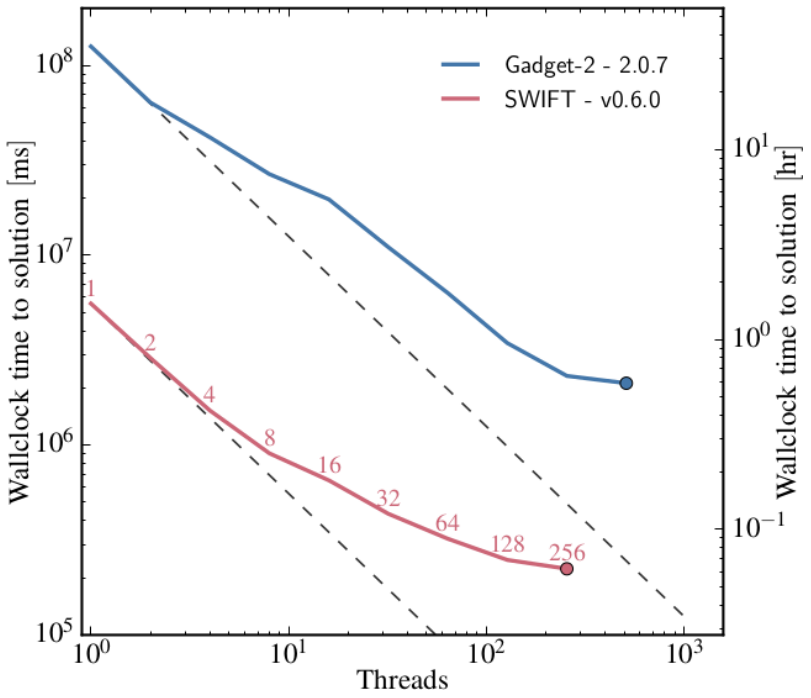
Intel ITAC output from two 36 cores Broadwell nodes.
→ More than 10’000 point-to-point communications over this time-step!
→ Almost 1’000’000 calls to `MPI_Test()`.

Performance vs. Gadget-2

- Strong scaling of realistic problem.

- Same accuracy.
- Same hardware.
- Same compiler.
- Same solution.

- 30.4x speed-up on 1 node!
- Code keeps scaling beyond 512 cores.



Quick I/O sneak-peak

Task-based i/o

- i/o is another bottleneck where the run halts and under-uses the cluster.
- Traditional pattern is to stop and dump everything.
- Huge load on the filesystem and network!
- Very inefficient! Very hard to achieve theoretical peak i/o especially on crowded systems.

Task-based i/o

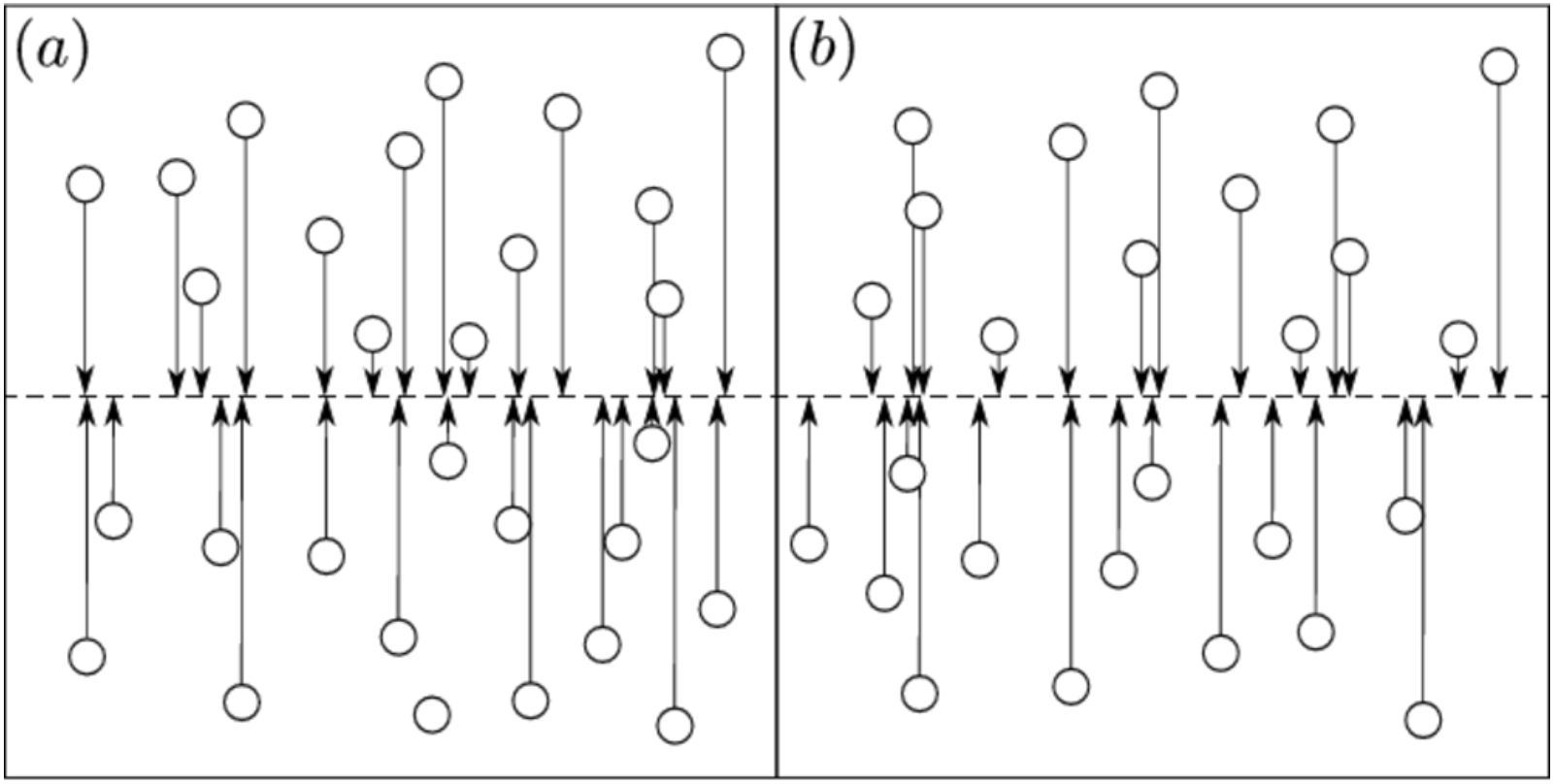
- Take advantage of the time-step hierarchy.
- Dump only parts of the data that vary rapidly (i.e. has changed a lot since last dump).
- Work on a cell-by-cell basis.
- Do this within the tasking system while the rest is happening.
  → No “stop and dump” pattern.
- Use memory-mapped files for maximal efficiency.

Vectorization

Vectorization

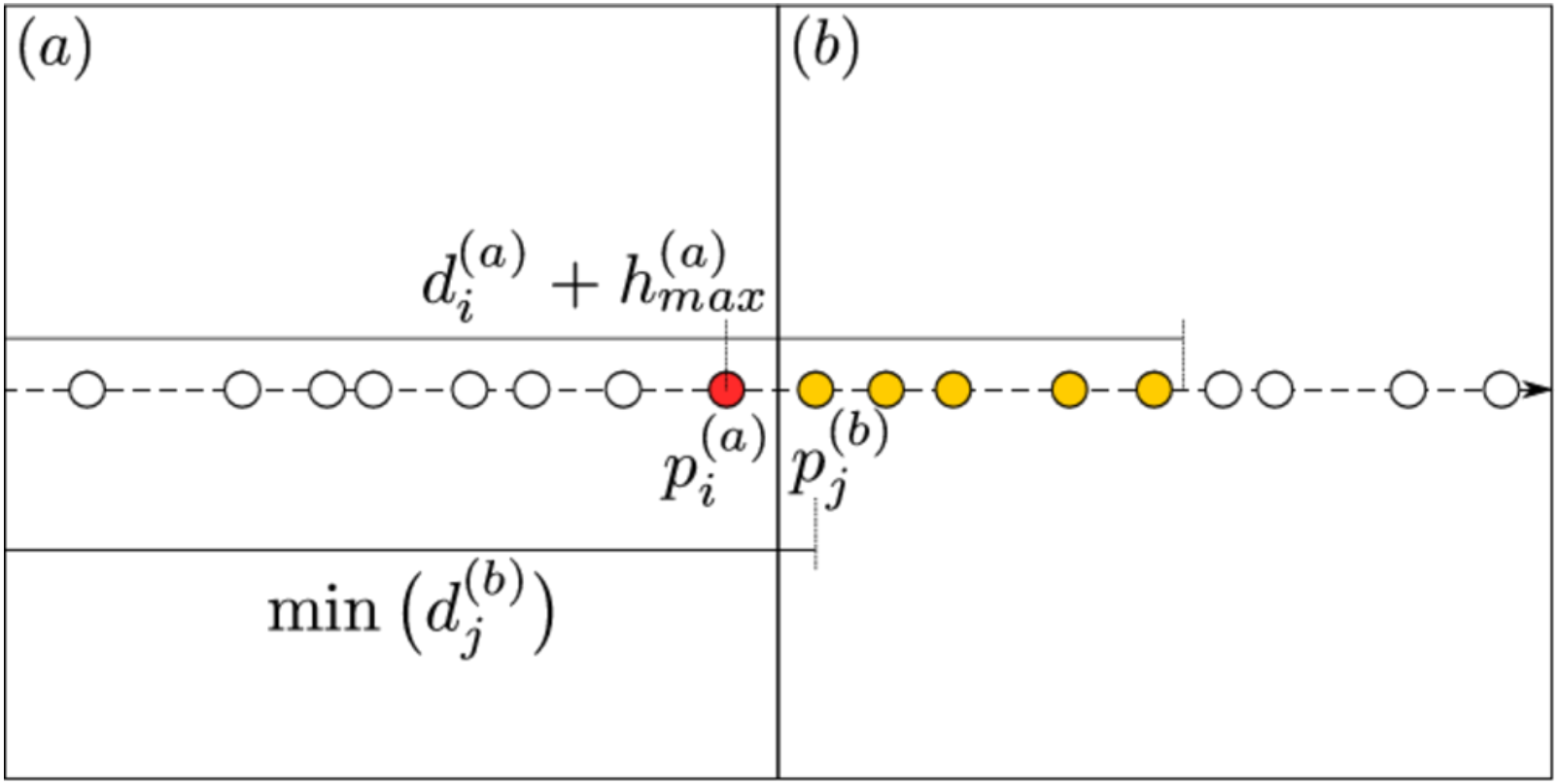
- Interact particles in one cell with particles in another cell.
- → naively N^2 algorithm.
-
- Need to construct local SoA cache for higher efficiency.
-
- Pre-sort particles on axis linking cells.
-
- Allows to only probe part of the interactions.
- → Reduce the number of false-positives!
-
- Need to use intrinsics as pattern too complex for auto-vectorizers.

Vectorization



Willis et al., Parco, 2017

Vectorization



Willis et al., Parco, 2017

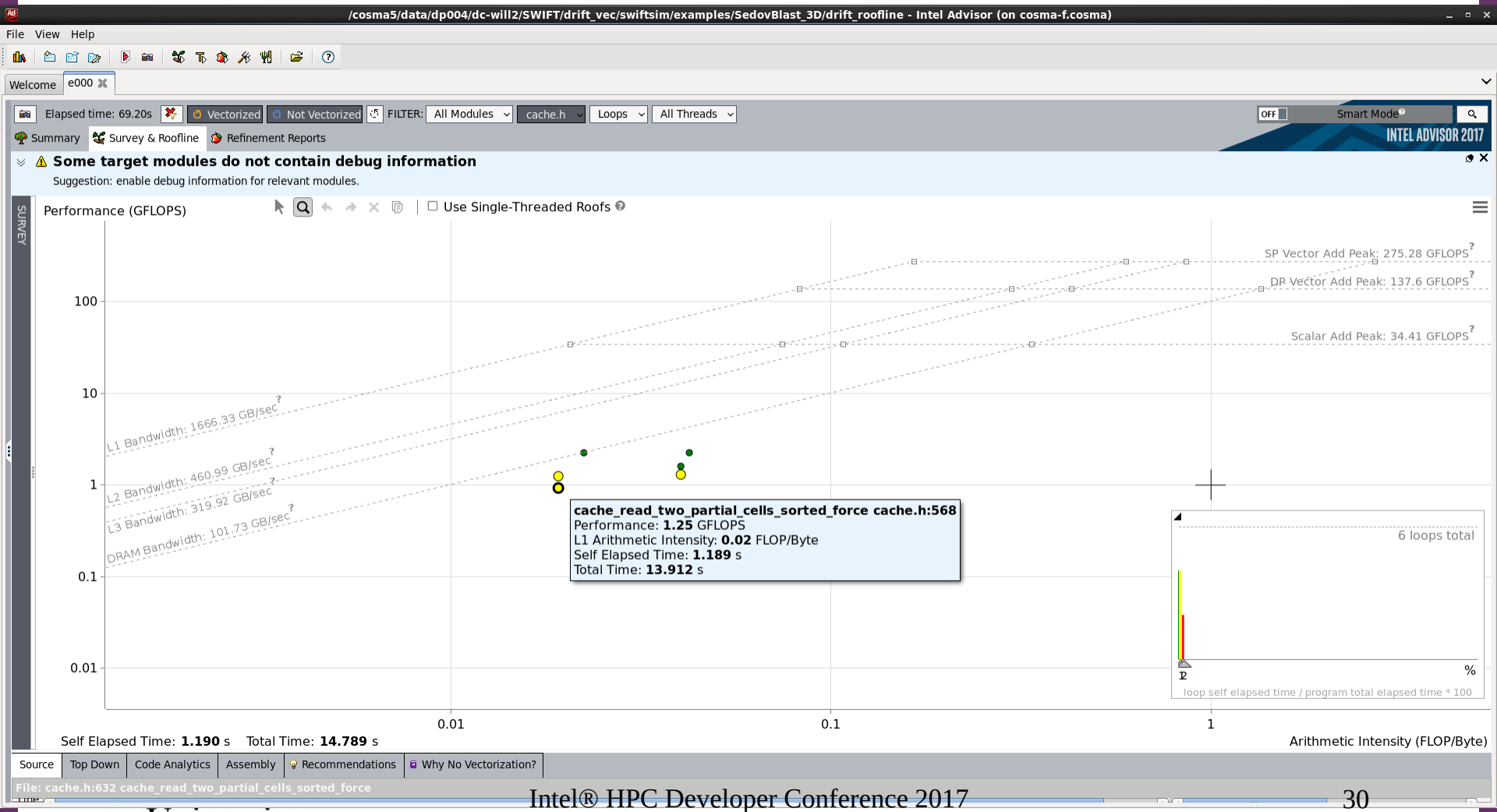
Vectorization

Machine Name	CFLAGS	Scalar Time [ms] (`-no-vec -no-simd`)	Vectorised Time [ms]	Speed-up
COSMA-5	`-xAVX`	0.56	0.25	2.24x
Hamilton	`-xCORE-AVX2`	0.49	0.20	2.43x
Kyll	`-xMIC-AVX512`	1.98	0.49	4.07x

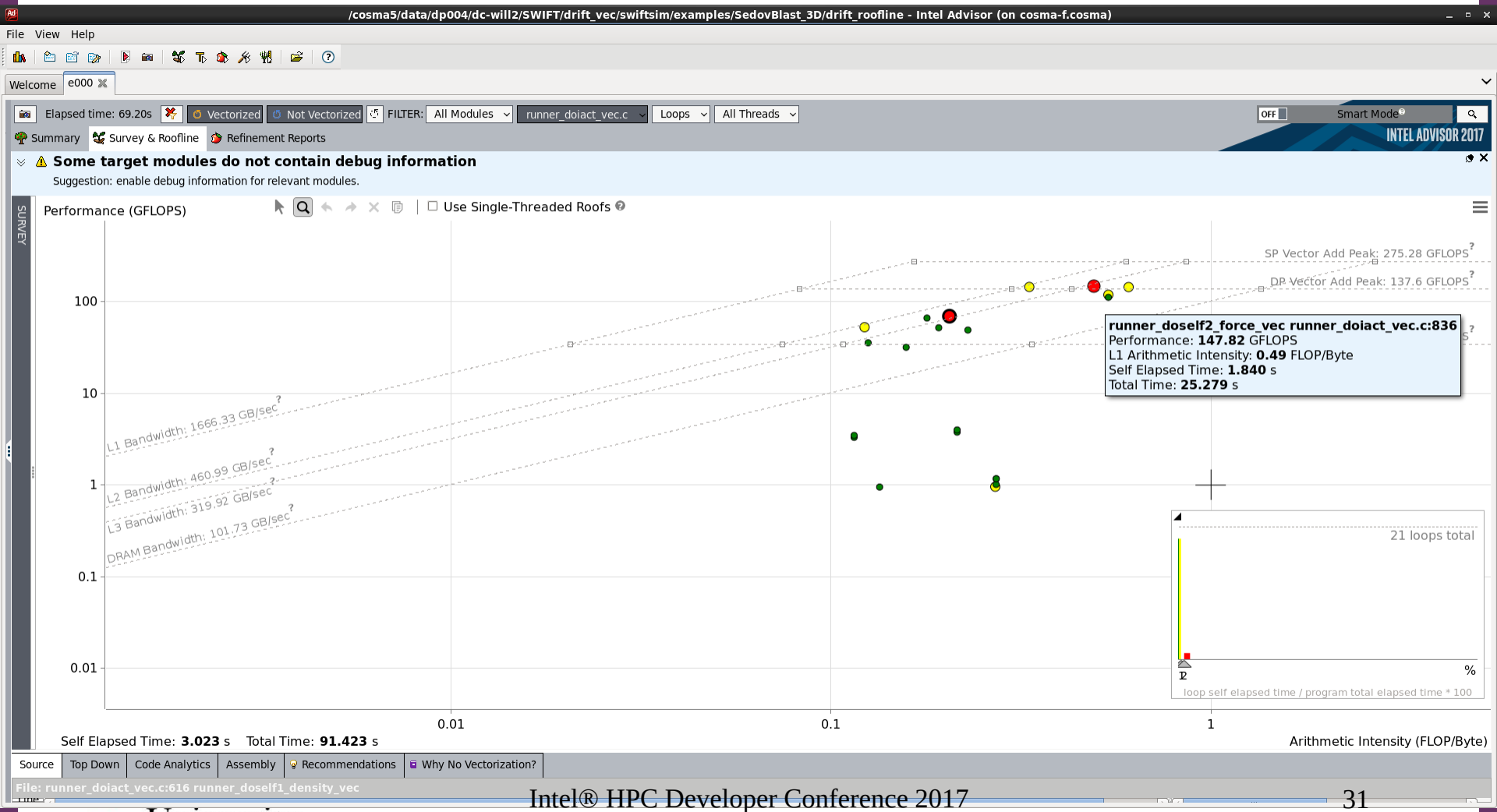
More than 12x faster than a “perfect” naive implementation.

Willis et al., Parco, 2017

Limitations – Memory bandwidth



Limitations – Memory bandwidth



Conclusions & Take-home messages

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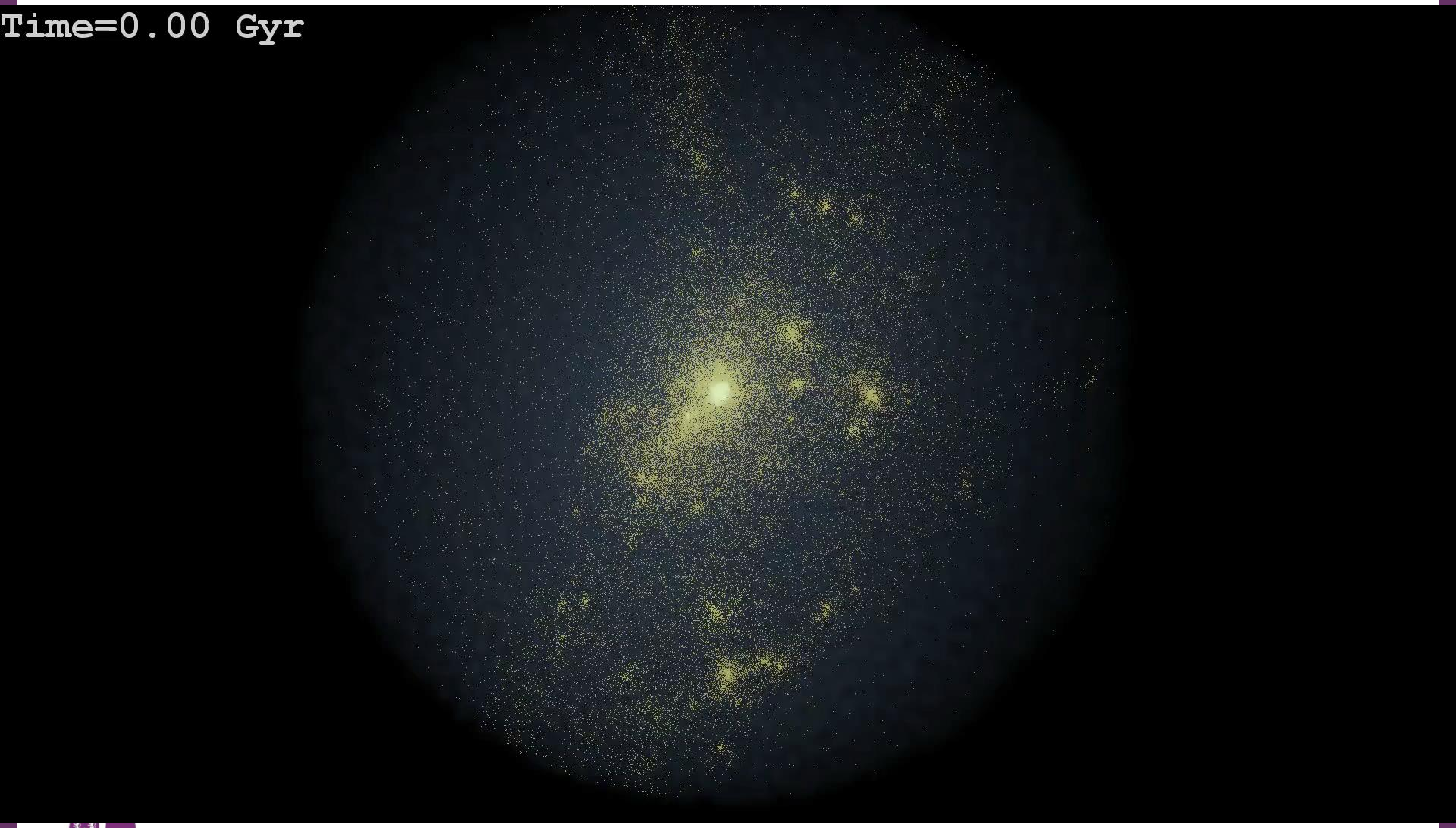
Conclusions

- New ideas can challenge pre-existing paradigms.
- Try new things.
- Clever algorithms are often better than vectorized naive code.
- Hiding communications, hiding i/o and a flexible scheduler are key to high performance on modern systems.



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