SWIFT: Task-based parallelism, hybrid shared/distributed-memory parallelism, and SPH simulations

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SECS/ICC, Durham University
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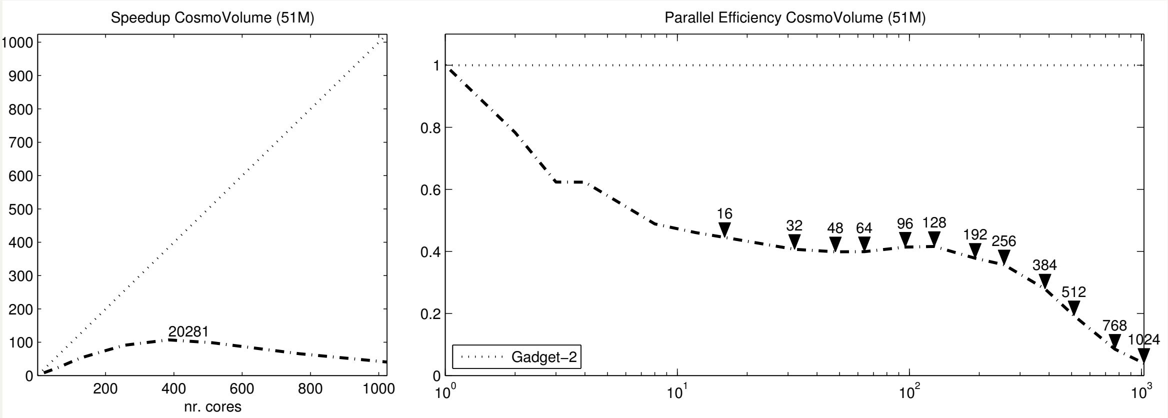
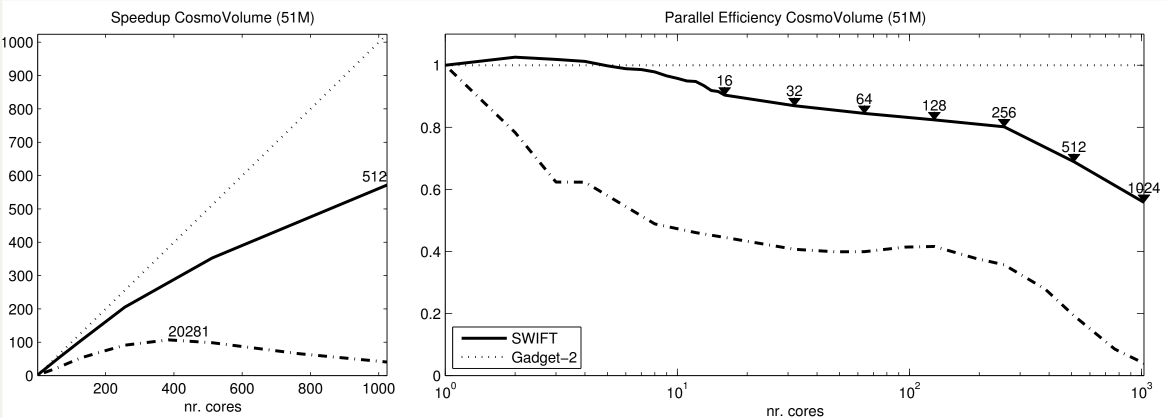
Introduction
This talk in a nutshell



- 51M particle EAGLE box ($z = 0.5$) SPH-only simulation on the COSMA5 cluster.



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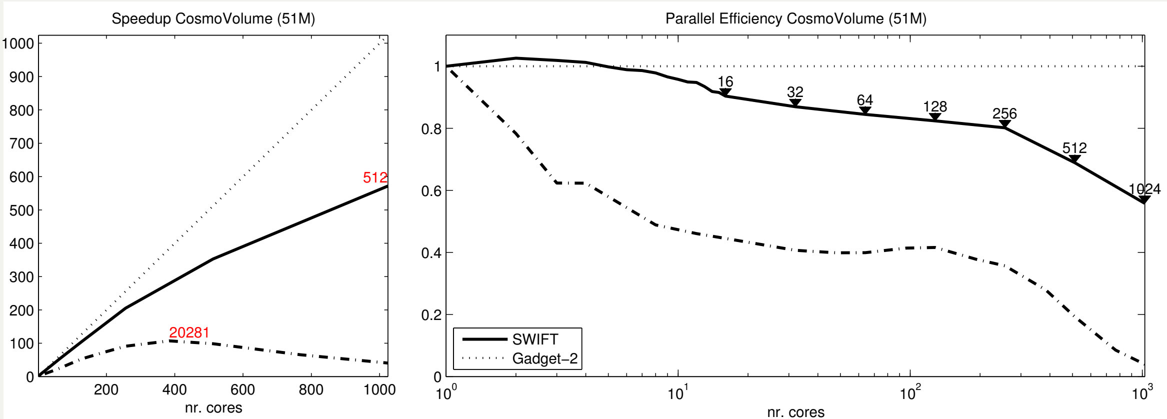

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- SWIFT: Strong scaling up to 1024 cores with 60% parallel efficiency.
- $\sim 40\times$ faster than GADGET.

Introduction

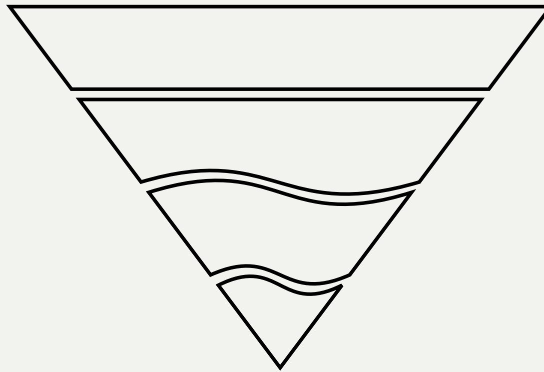
A hierarchy of contributions

Domain Science

Software

Algorithms

Paradigms



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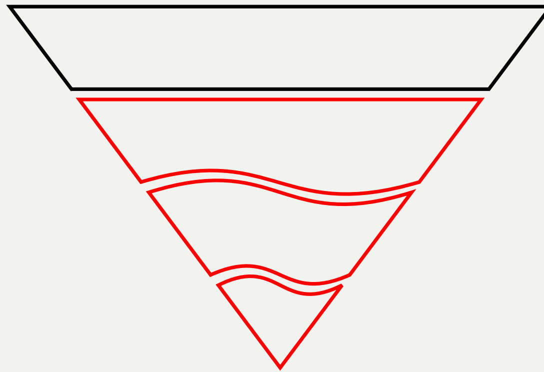

Task-based parallelism

Replacing the paradigm

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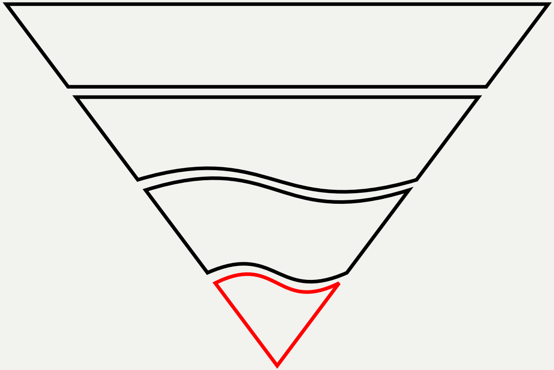
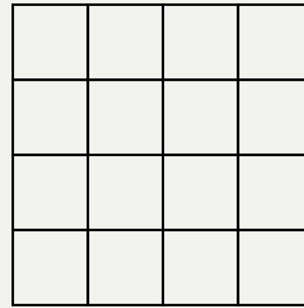


Task-based parallelism

The problem with distributed-memory parallelism

- Distributed-memory parallelism, e.g. using MPI, is based on data decomposition, i.e. each processor is assigned part of the problem to work on and communicates with its neighbours.
- Surface-to-volume ratio problem: As the number of cores increases, the amount of computation per core (volume) decreases while the relative amount of communication (surface) increases, eventually dominating the entire computation.
  $\longrightarrow$ We can always do larger simulations, but not smaller simulations faster.



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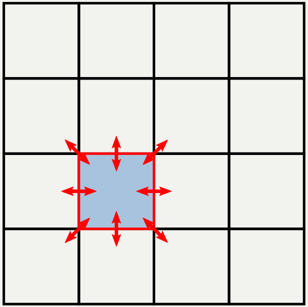

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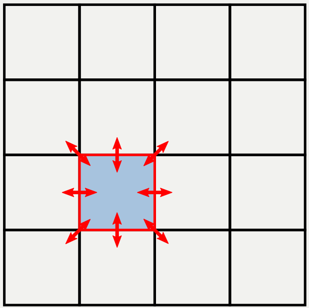

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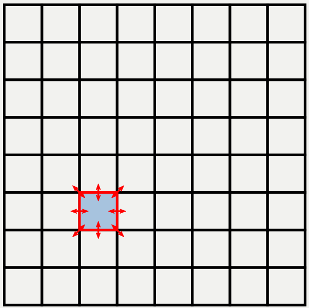

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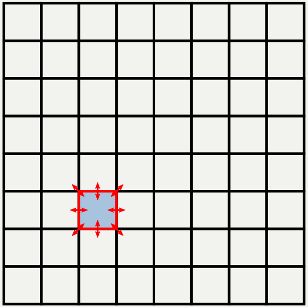

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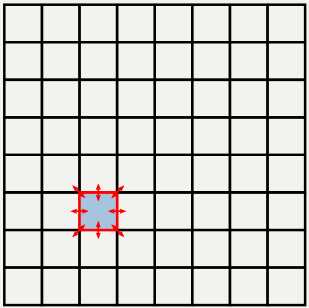

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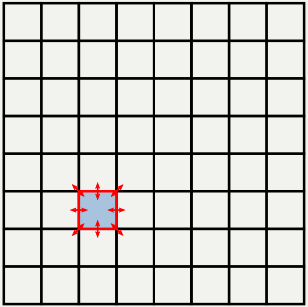

Task-based parallelism

The problem with OpenMP

- Shared-memory parallelism using OpenMP, i.e. annotating an inherently serial code, is often hampered by frequent synchronization.
- Concurrency problems need to be addressed explicitly, e.g. using barriers or atomic instructions.
- These overheads associated with these two problems only get worse as the number of cores increases.

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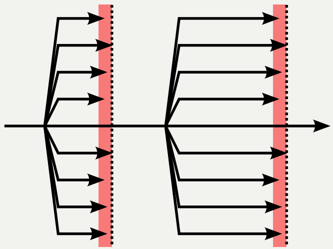

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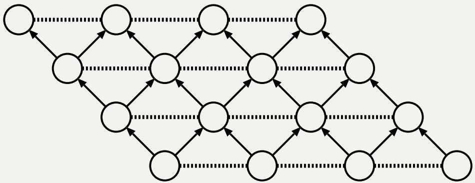

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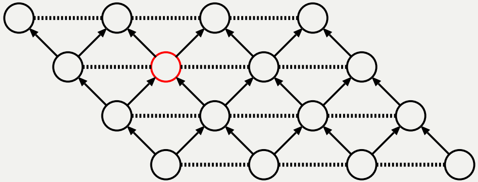

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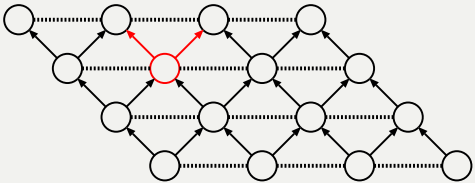

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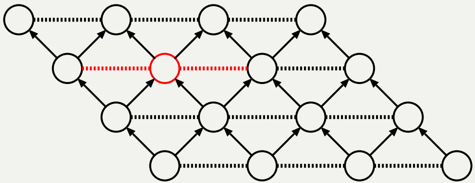

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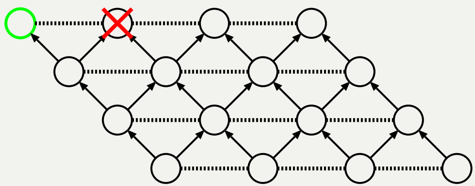

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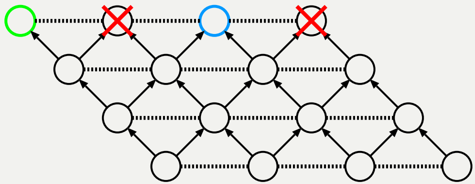

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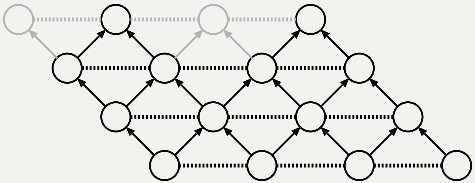

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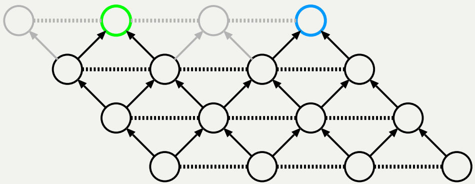

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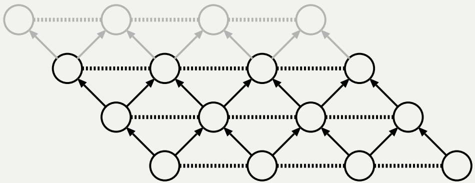

Task-based parallelism

Main advantages

- The order in which the tasks are processed is highly dynamic and adapts automatically to load imbalances.
- If the dependencies and conflicts are specified correctly, we do not have to worry about concurrency at the level of the individual tasks.
  $\longrightarrow$ No need for expensive explicit locking, synchronization, or atomic operations.
- The same approach can be applied to more unconventional many-core systems such as GPUs or the Intel Phi.
- However, this usually means that we have to completely re-think our entire computation, e.g. redesign it from scratch to make it task-based.

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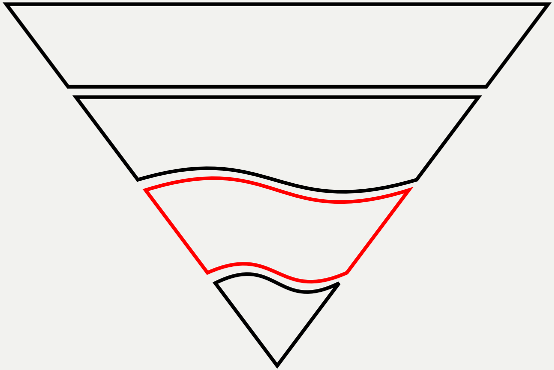

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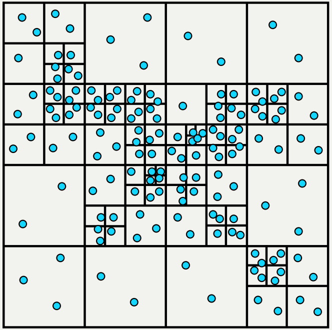
- Neighbour-finding up and down the tree is simple, but has some problems:
  - Worst-case cost in $\mathcal{O}(N^{2/3})$ per particle.
  - Low cache efficiency due to scattered memory access.
  - Symmetries cannot be exploited, i.e. each particle pair is found twice.
- Parallelization is trivial, but only because symmetries are not exploited.



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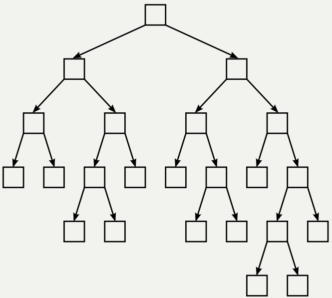

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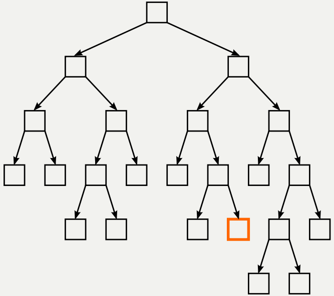

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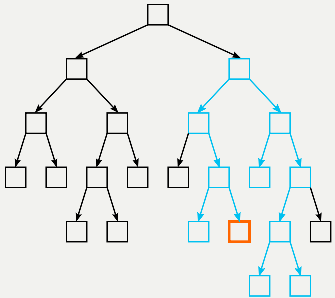

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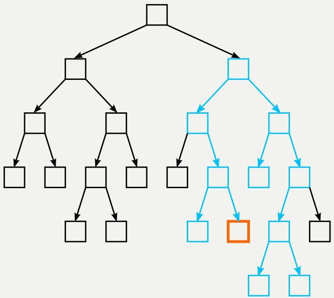

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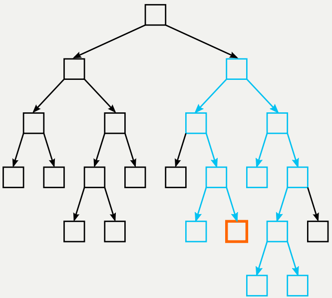

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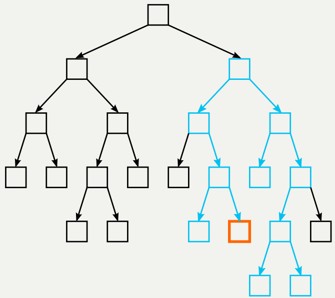

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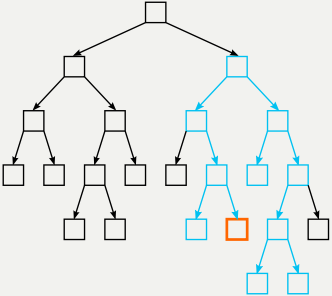
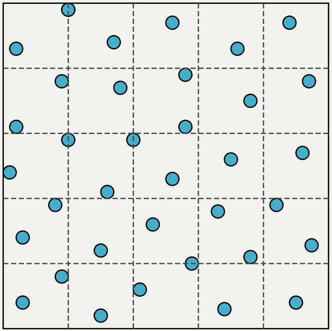


Algorithms for SPH

Hierarchical cell pairs

- We start by splitting the simulation domain into rectangular cells of edge length at least h_{max}.
- All interacting particle pairs are then in either in the same cell, or in a pair of neighbouring cells.
- Finding all neighbours within each cell or between each pair of cells can be used as a task.
- If the particles in the cell or cell pair are sufficiently small, the task can be split.
- Finally, the particles in each cell pair are first sorted along the cell pair axis to speed-up neighbour-finding.



- We start by splitting the simulation domain into rectangular cells of edge length at least $h_{\max}$.
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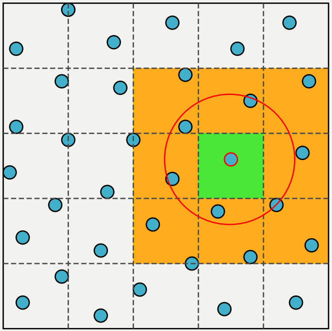

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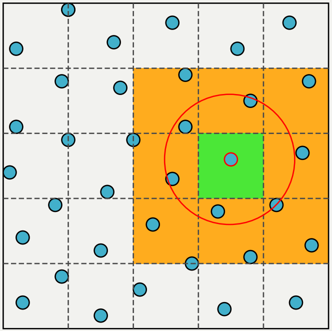

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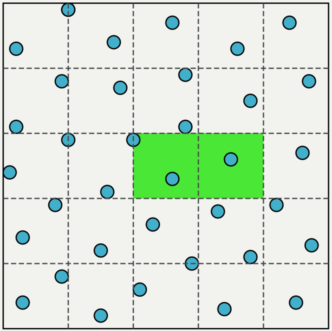

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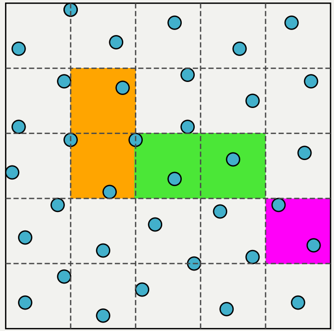

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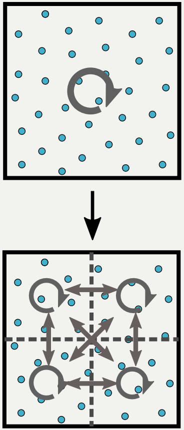

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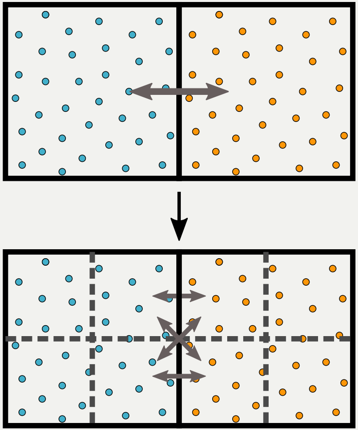

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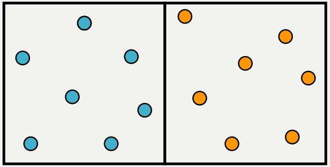

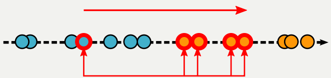

Algorithms for SPH

Task hierarchy

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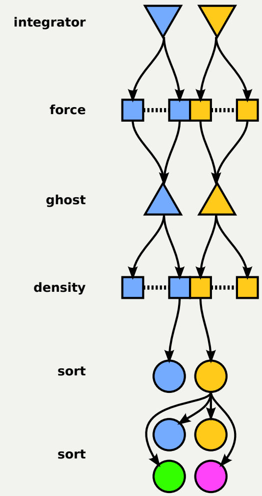

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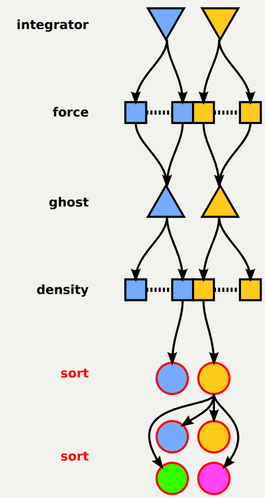

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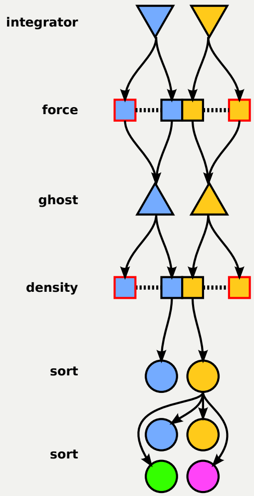

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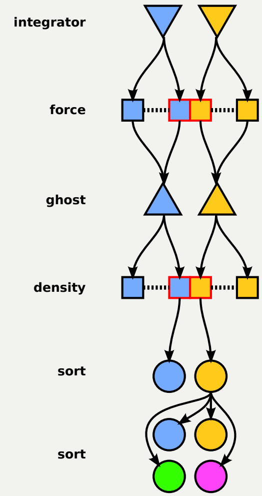

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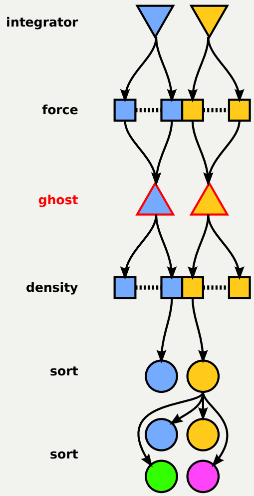

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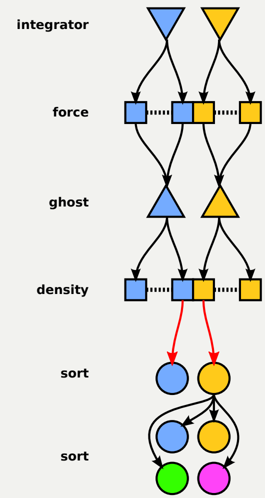

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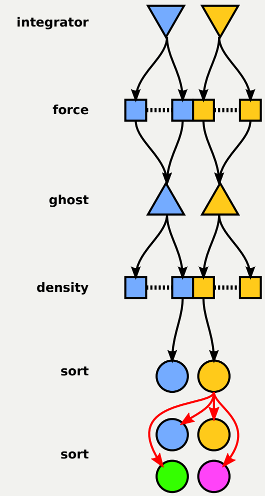

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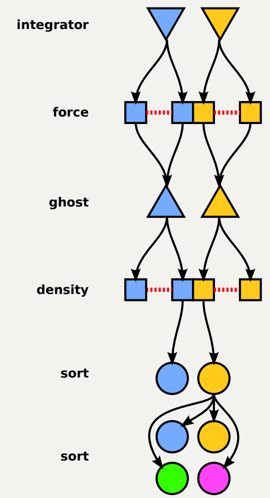

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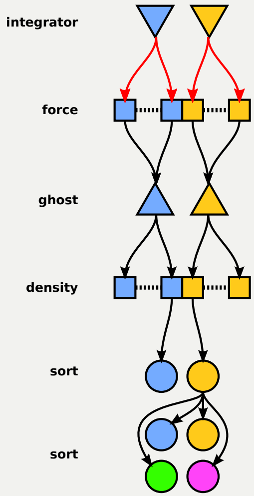

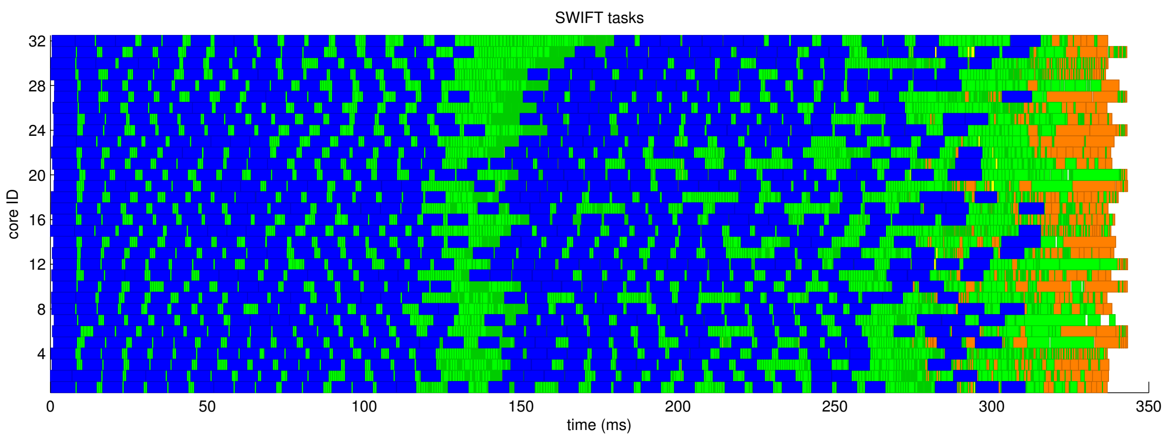

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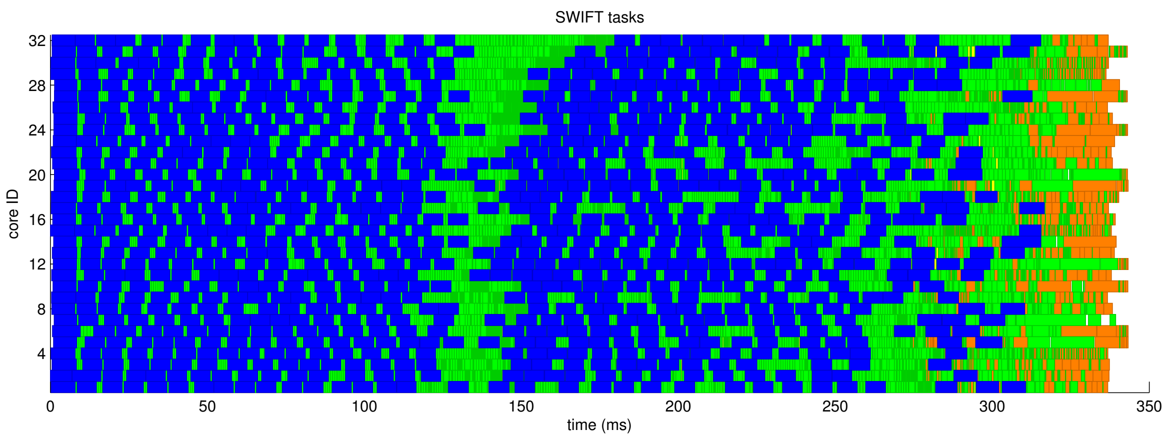
Algorithms for SPH
Dynamic task allocation



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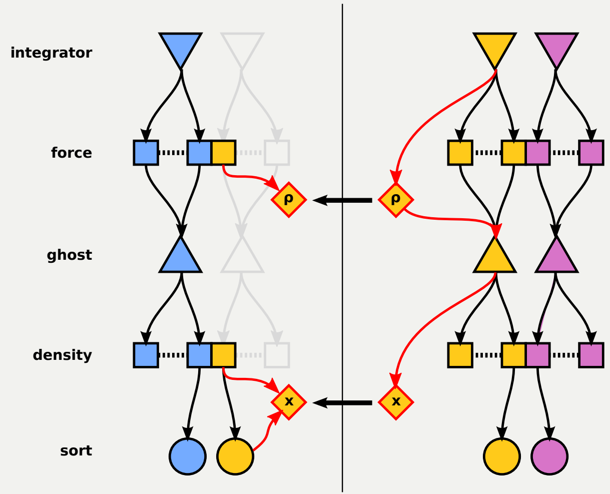
Algorithms for SPH

Hybrid shared/distributed-memory parallelism

- Domain decomposition between multi-core nodes, task-based parallelism within each node.
- Each cell is owned by one node alone, and tasks involving foreign nodes are made dependent on communication tasks.
- Communication tasks execute dynamically and asynchronously, overlapping with computation.



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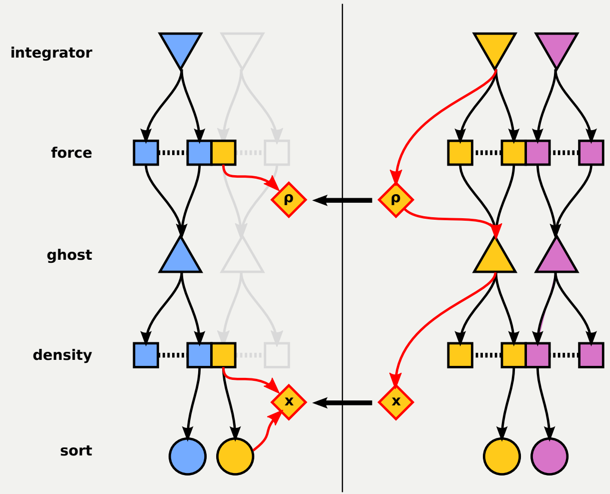

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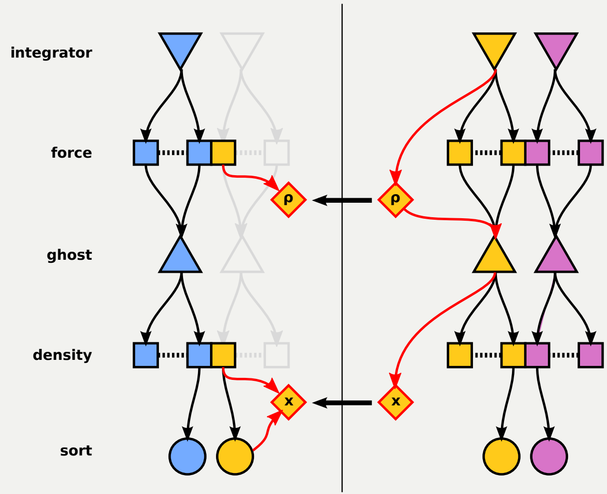

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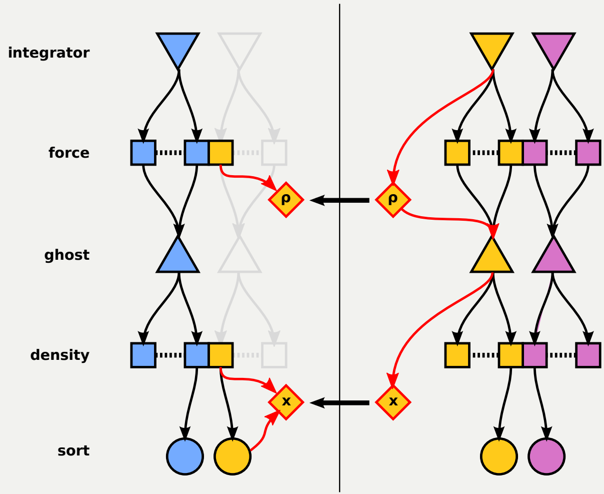

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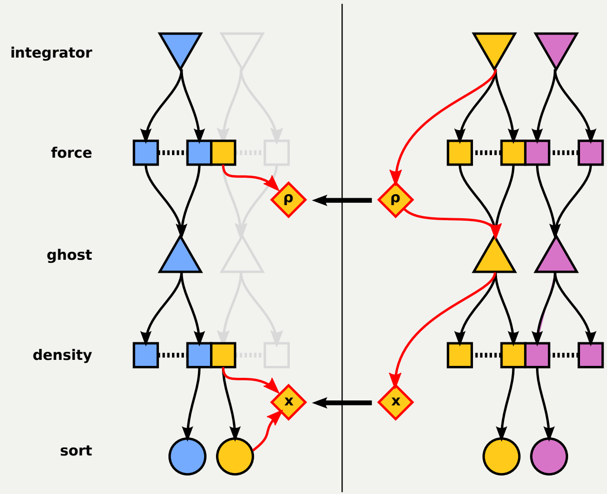

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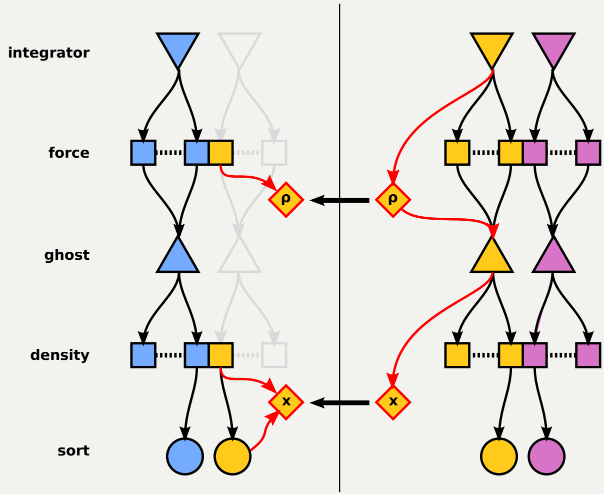

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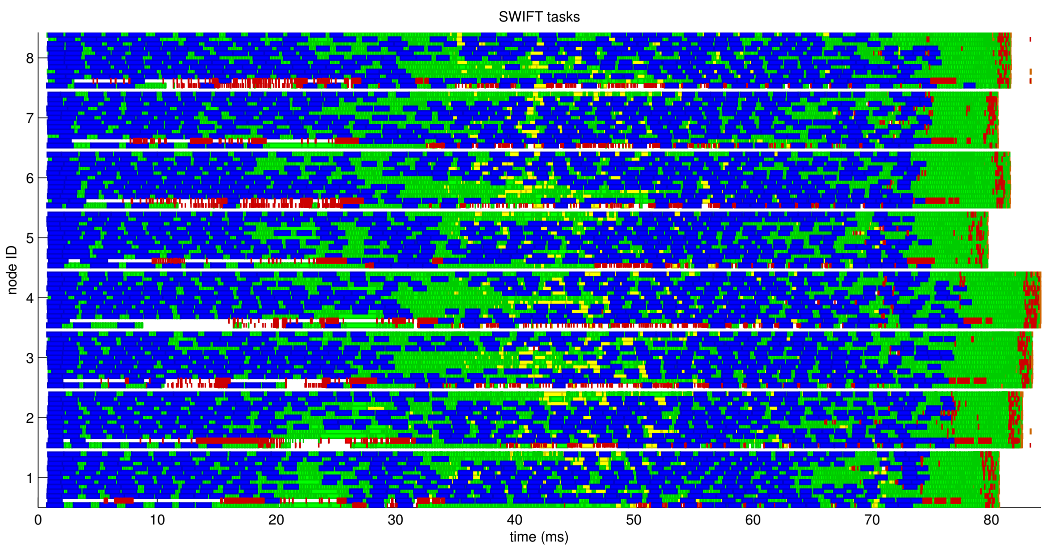

- This approach still suffers the same surface-to-volume ratio problem as other distributed-memory computations, but at a much smaller scale.
  $\longrightarrow$ Only one MPI-node per physical node.
- Future increases in the number of cores per node will not affect distributed-memory parallel scalability.
- The domain decomposition can be computed along the task graph with standard graph partitioning, e.g. METIS.
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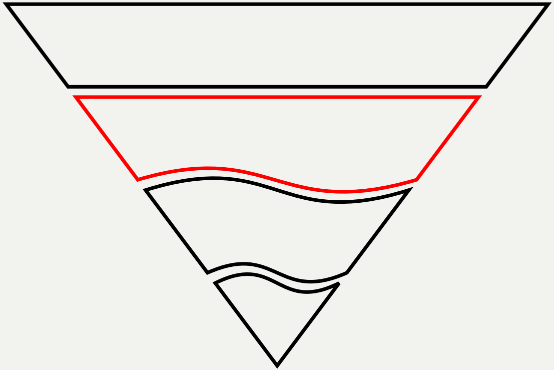
Domain Science

Software

Algorithms

Paradigms



- Close collaboration with the Institute for Computational Cosmology (ICC) at Durham University.
  $\longrightarrow$ Make sure we're building a software that can actually be used.
- Main goal is to replace GADGET, the most popular Open-Source cosmological simulation code.
- Massively multi-scale problems, with millions to billions of particles, run on both desktops and supercomputers.
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- Mixed-precision arithmetic for better performance and vectorization, lower memory requirements.
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SWIFT

Main features

- 15'000 lines of C written by *Computer Scientists*, using `pthreads` and MPI, fully Open-Source.
- Explicit vectorization (switched off in the benchmarks here for fairness).
- Mixed-precision arithmetic for better performance and vectorization, lower memory requirements.
- Currently porting to CUDA-based GPUs and the Intel Phi.
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Conclusions

Our contributions

- Extended task-based parallelism conceptually to include *task conflicts*.
  $\longrightarrow$ Scheduling is trickier, but much more flexible.
- Faster and more cache-efficient algorithms for *neighbour-finding* in multi-scale particle systems.
  $\longrightarrow$ More than $7\times$ faster than GADGET-2 on a single core.
- Fully data-driven, asynchronous, and dynamic *hybrid shared/distributed-memory parallel model*.
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  $\longrightarrow$ Continue developing the task-based paradigm.

Thank you for your attention!