Individual time-stepping in cosmological simulations: A challenge for strong scaling and domain decomposition algorithms

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with

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This work started as 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 groups at the university of St-Andrews (UK), Perth (Australia), Leiden (Netherlands), Lausanne (Switzerland) as well as the DiRAC and CSCS software teams.

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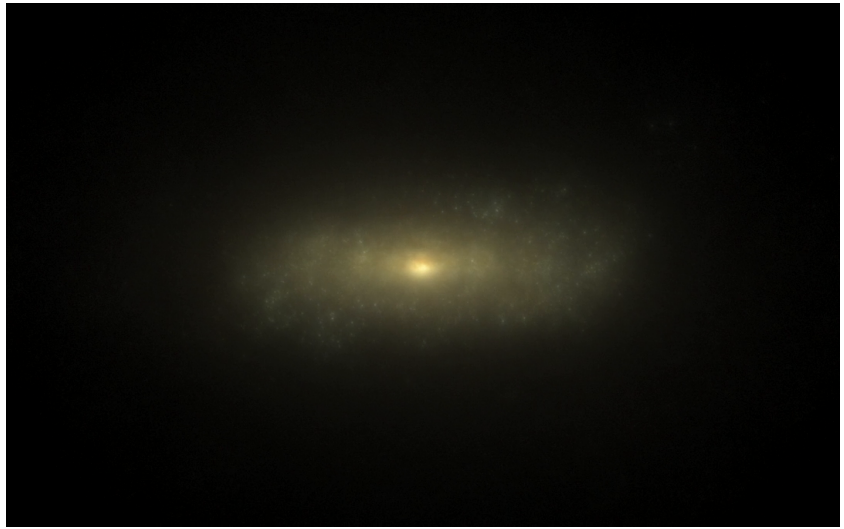
Our software is part of the benchmarking challenge for new DiRAC (UK) systems.

What we do and how we do it

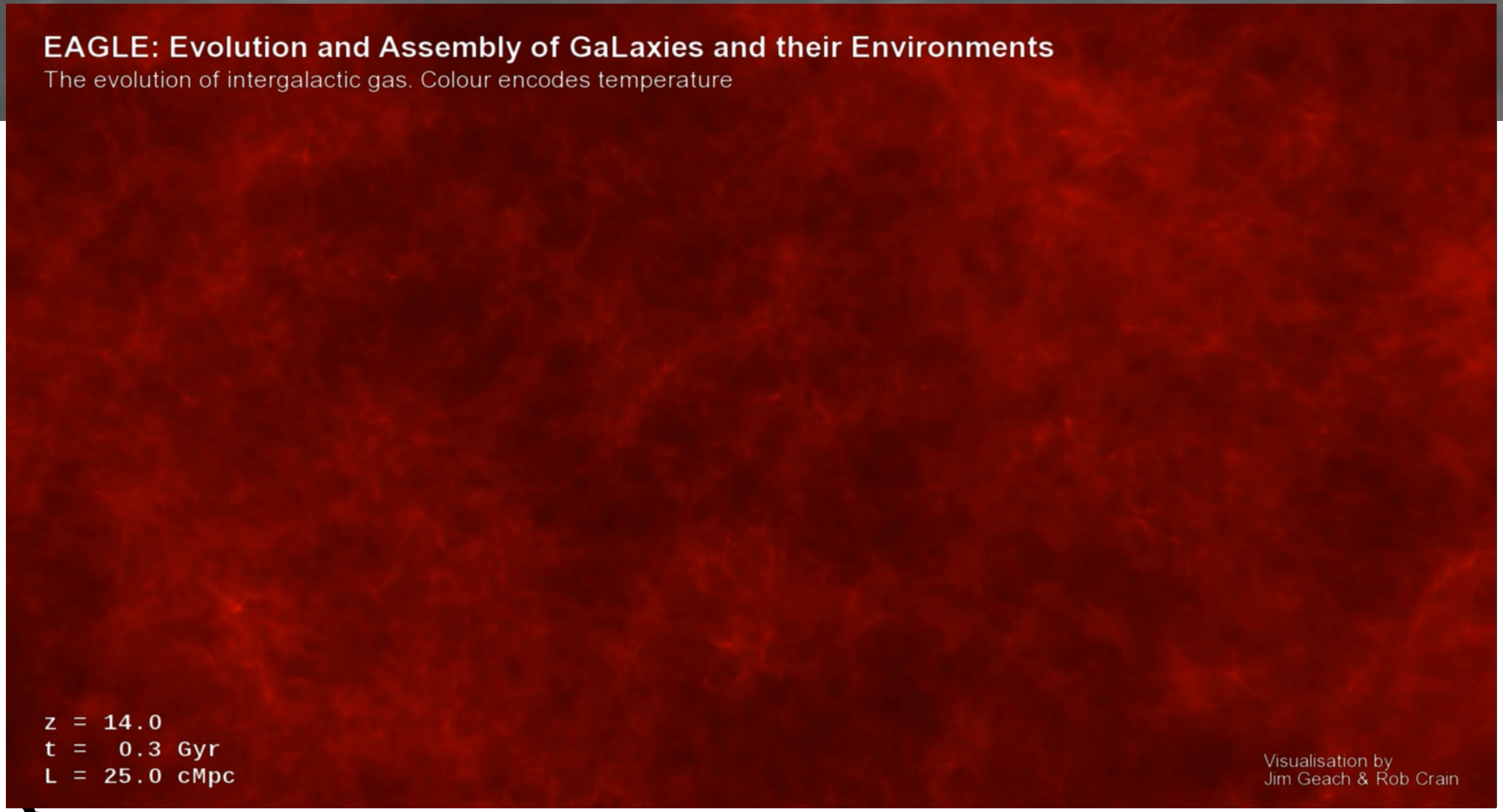
- Cosmological simulations of the formation of the Universe and galaxy formation.

- EAGLE project: 48 days of computing on 4096 cores. >500 TBytes of data products (post-processed data is public!). Most cited astronomy paper of 2015.



Trayford+2015, MNRAS

http://www.eaglesim.org/


EAGLE: Evolution and Assembly of GaLaxies and their Environments
The evolution of intergalactic gas. Colour encodes temperature
z = 14.0
t = 0.3 Gyr
L = 25.0 cMpc
Visualisation by
Jim Geach & Rob Crain

What we do and how we do it

- Solve coupled equations of gravity and hydrodynamics using particle-based methods (SPH, FVPM, …).
- Consider the interaction between gas and stars/black holes as part of a large and complex *subgrid* model with free parameters to be calibrated.
- Evolve multiple matter species at the same time.
- Dynamic range of >6 orders of magnitude in “particle size”.
- Typically have >2M time-steps.

Hydrodynamics scheme: The problem to solve

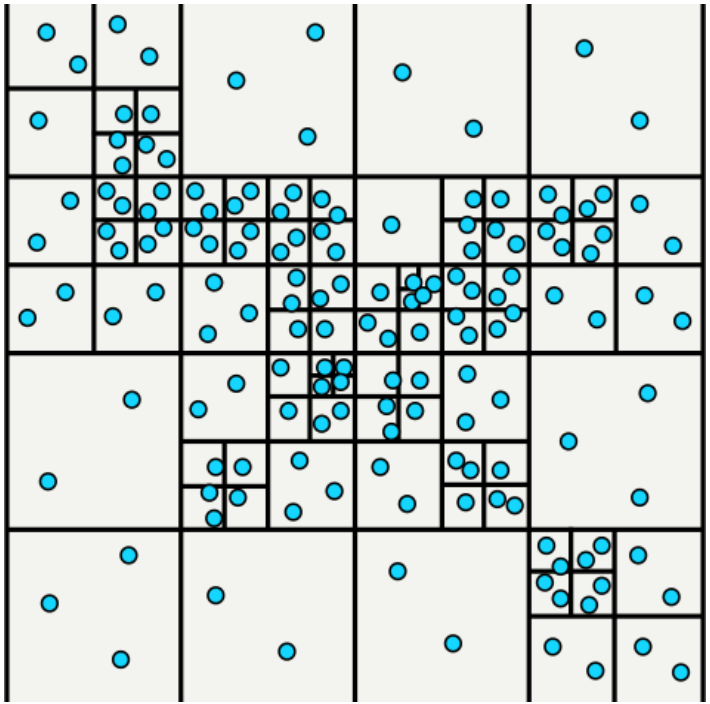
For a set of N (>10^{10}) particles, we want to exchange hydrodynamical forces between all neighbouring particles within a given (time and space variable) search radius. Large density imbalances develop over time.

Challenges:

- Particles are unstructured in space, large density variations.
- Particles will move and the neighbour list of each particle evolves over time.
- Interaction between two particles is computationally cheap (low FLOP/byte).
- Individual time-steps for each particle.

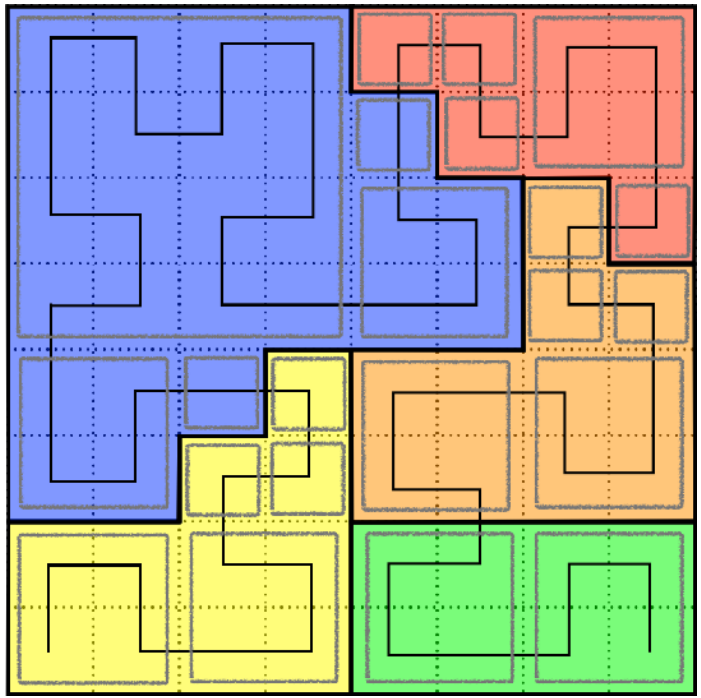
SPH scheme: The traditional method

- “Industry standard” code is *Gadget* (Springel+2005).
- MPI-only code.
- Neighbour search based on oct-tree.
- Domain decomposition based on a space-filling curve.



Domain Decomposition

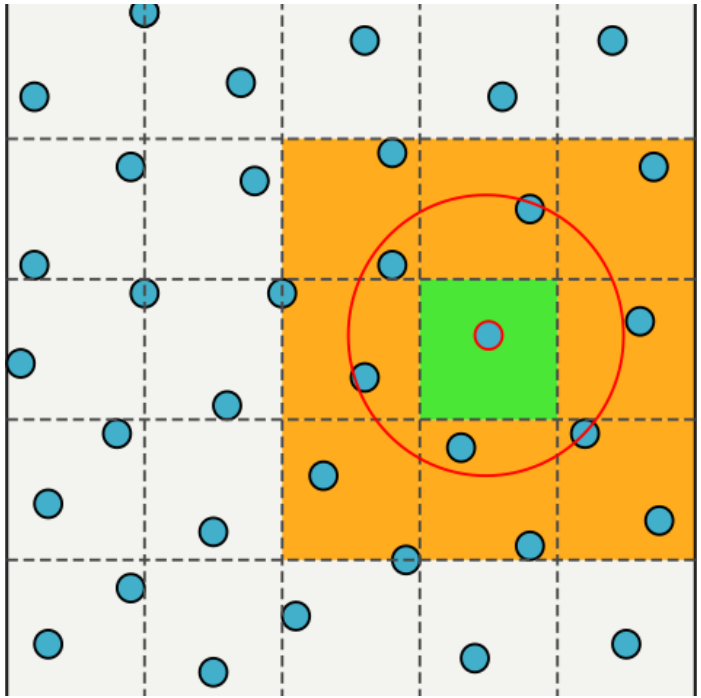
1. Sort the data along a space-filling curve.
2. Split the curve such that each node gets the same number of particles.
3. Do this at the top-level or close to the top.



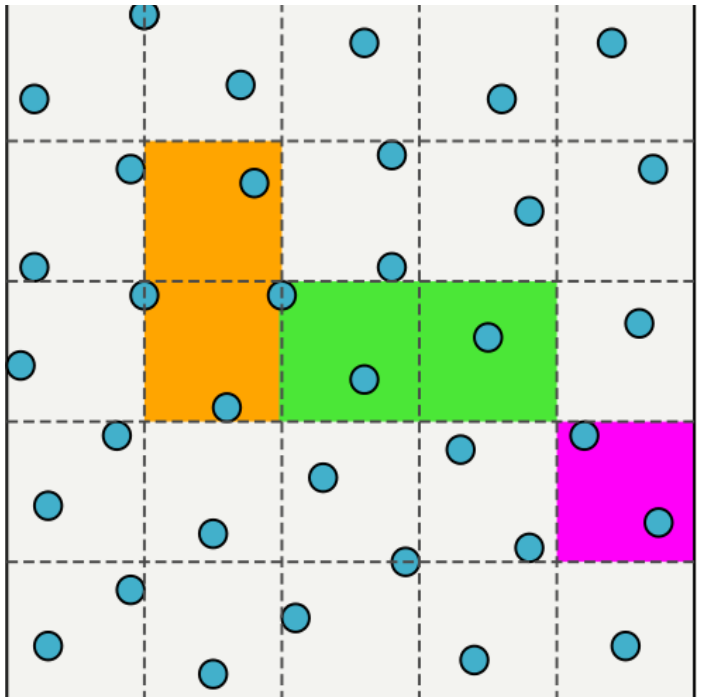
SWIFT basics

- Use an AMR-grid-based Verlet-list neighbour search.
- Use Task-based parallelism on the node.
- Use asynchronous MPI communications in the task framework.
- Use SIMD intrinsics for the core of the calculation.

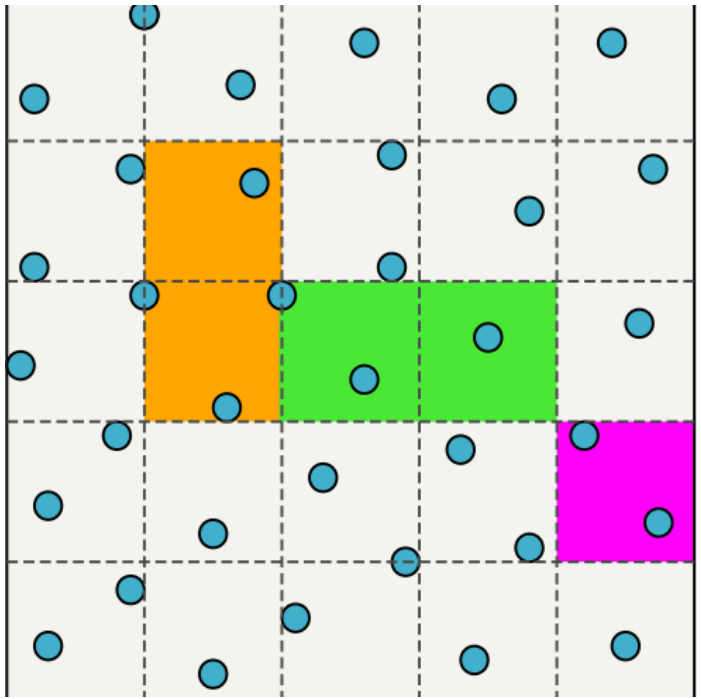
AMR Verlet-list neighbour search



- Target ~500 particles per cell via adaptive mesh refinement.
- Cell size naturally matches particle neighbour search radius.
- Particles only interact with particles in the same cell or any direct neighbouring cell.



- Cells pairs do not need to be processed in any pre-defined order.
- Only need to make sure two threads do not work on the same cell.
- Cell pairs can have vastly different work-loads.



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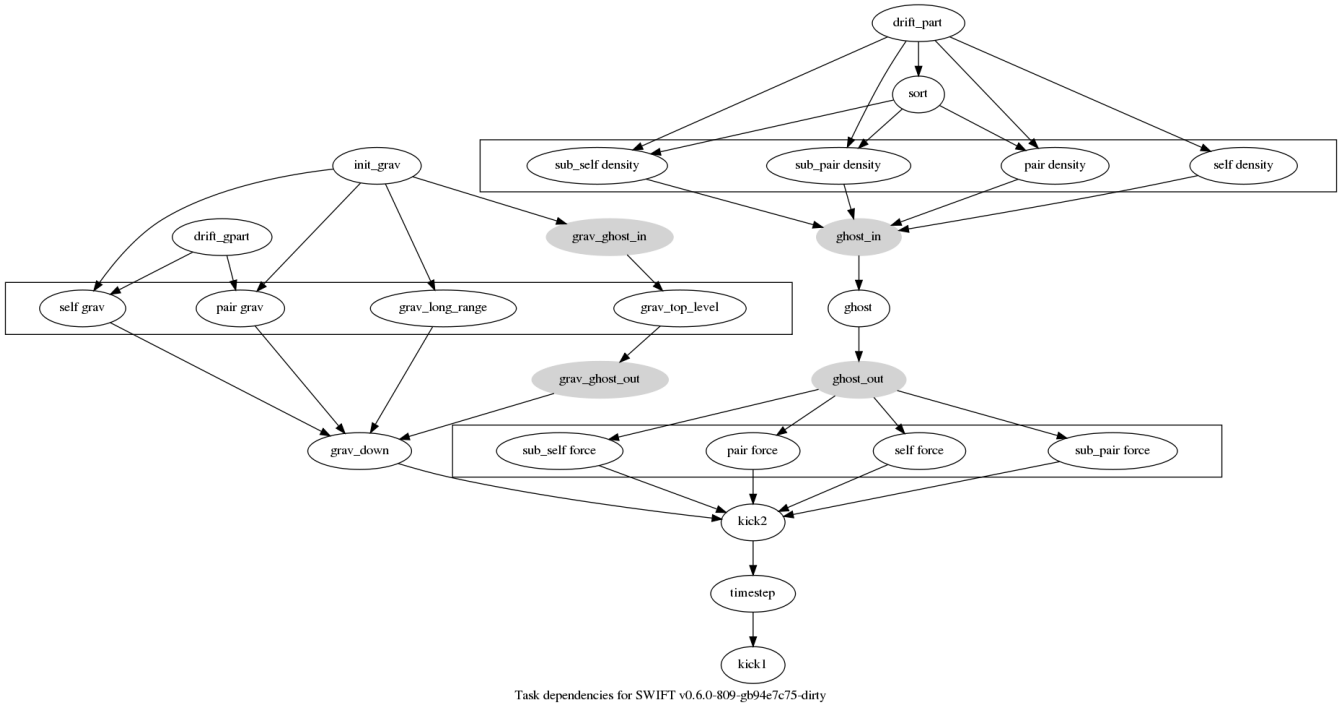
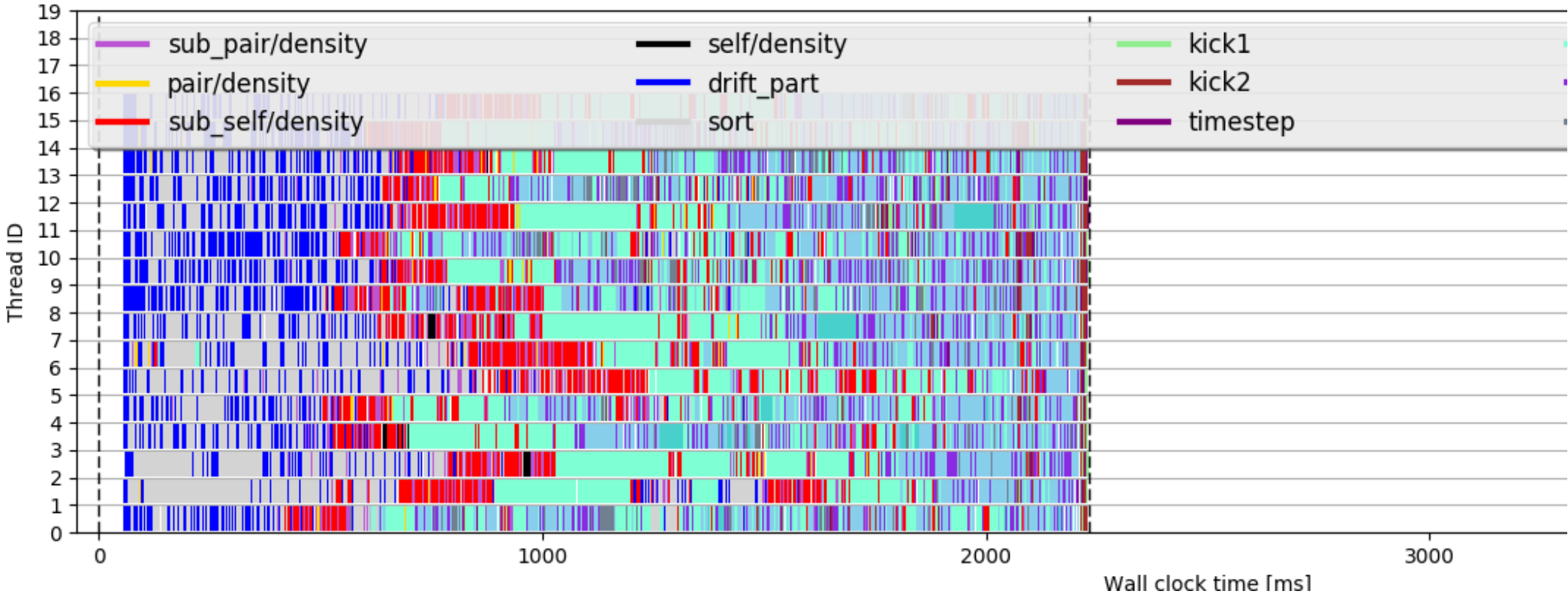
→ Need runtime dynamic scheduling

Task-based parallelism for SPH



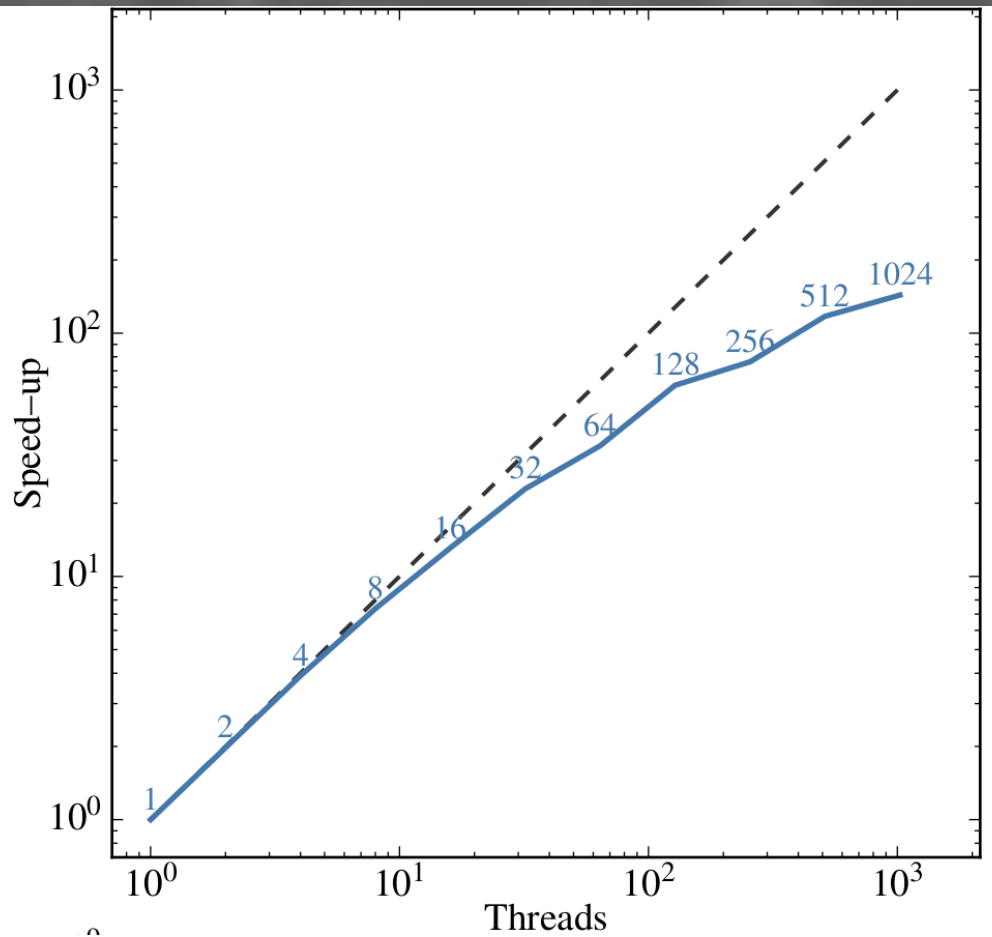
- Task-graph describing the science.
- Arrows depict dependencies.

Task-based parallelism in action

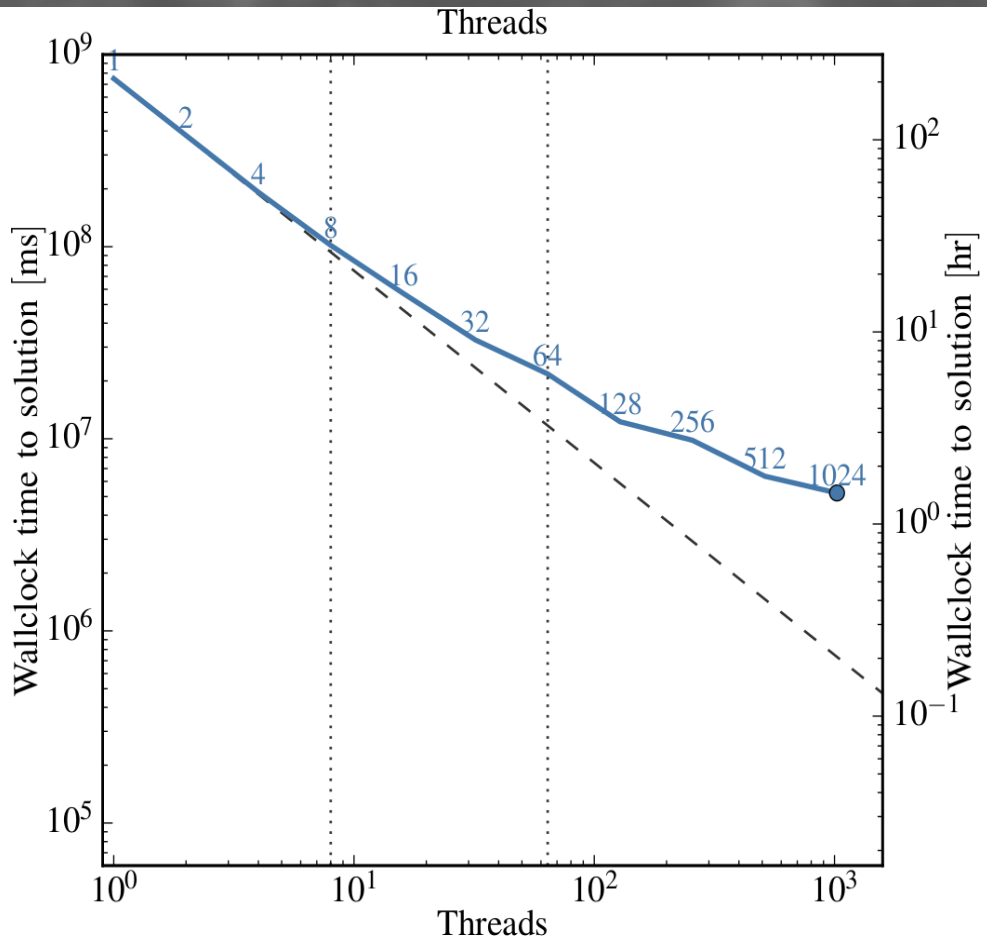


Task-graph for one time-step. Colours correspond to different task types.
Almost perfect load-balance achieved on 16 cores.

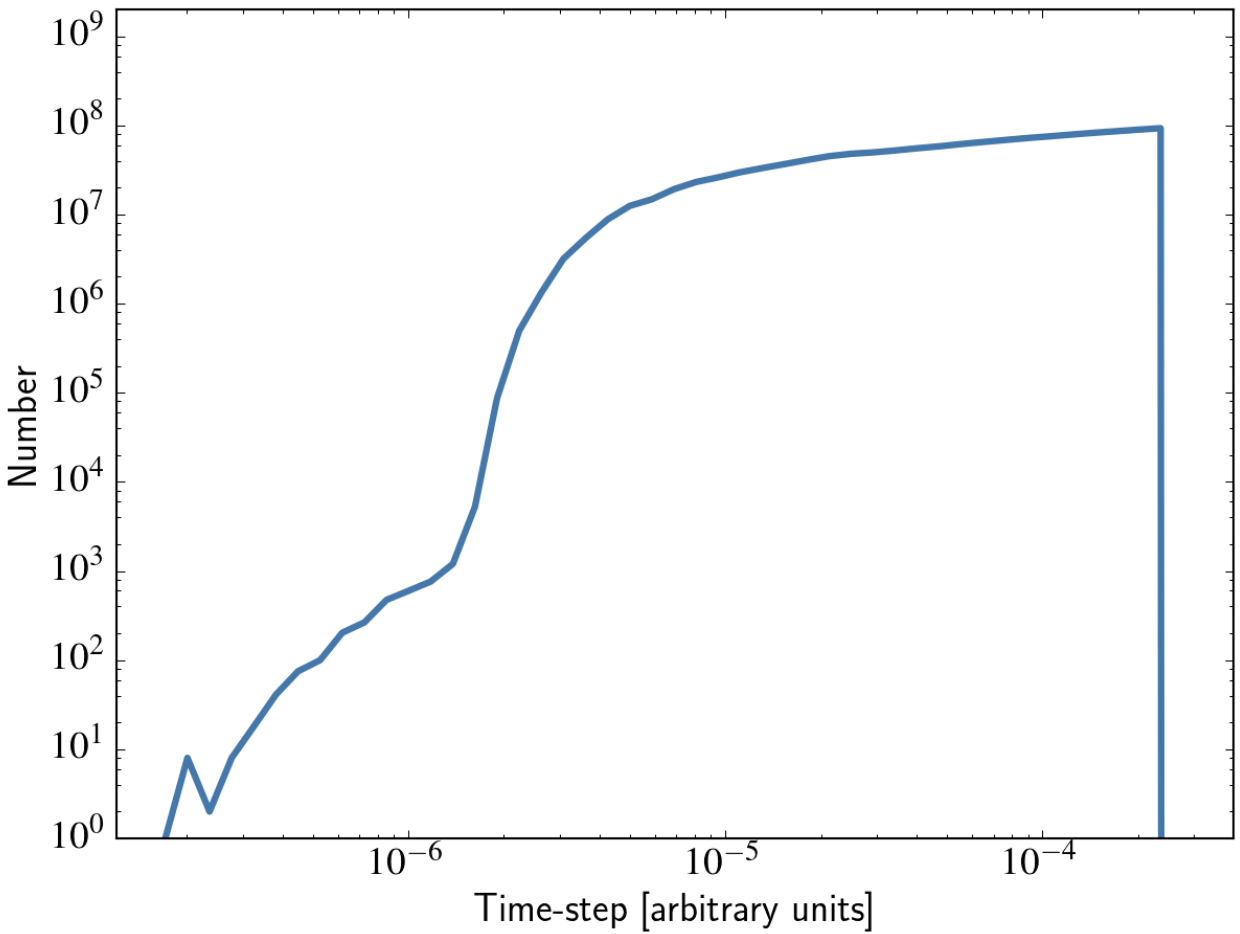
Scaling with a global time-step



Time-to-solution with a global time-step



Time-step hierarchy



Local time-stepping

Our particle methods for hydro-dynamics have a linear cost.

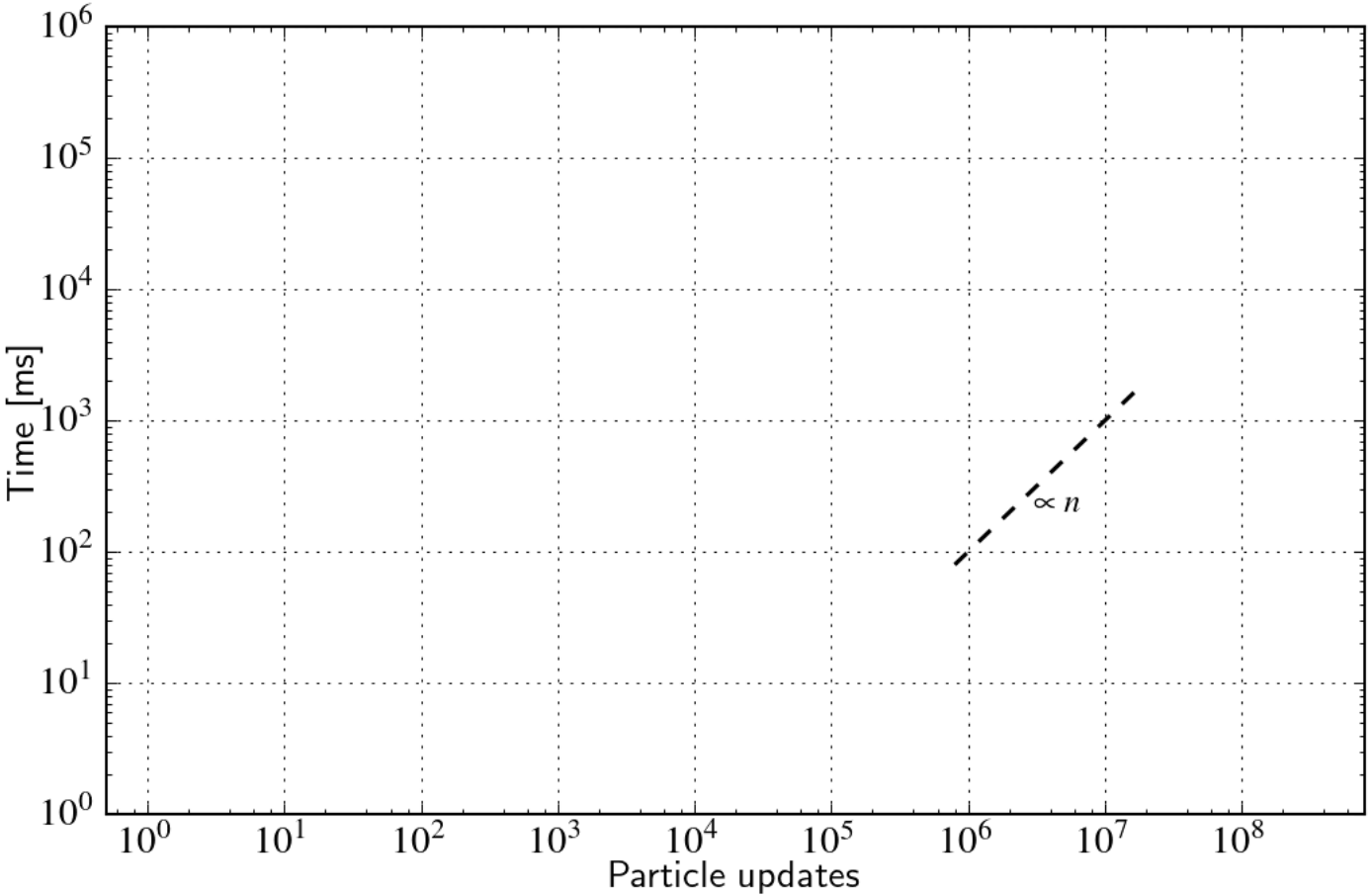
→ By only updating the particles on a short time-step we can gain orders of magnitude in run time.

(not a new idea. Been done since the 80s in astrophysics)

→ You also kill your scaling.

The question is then how to load-balance and parallelize this.
How do you update ~10 particles efficiently on 1000 nodes?

The challenge visually



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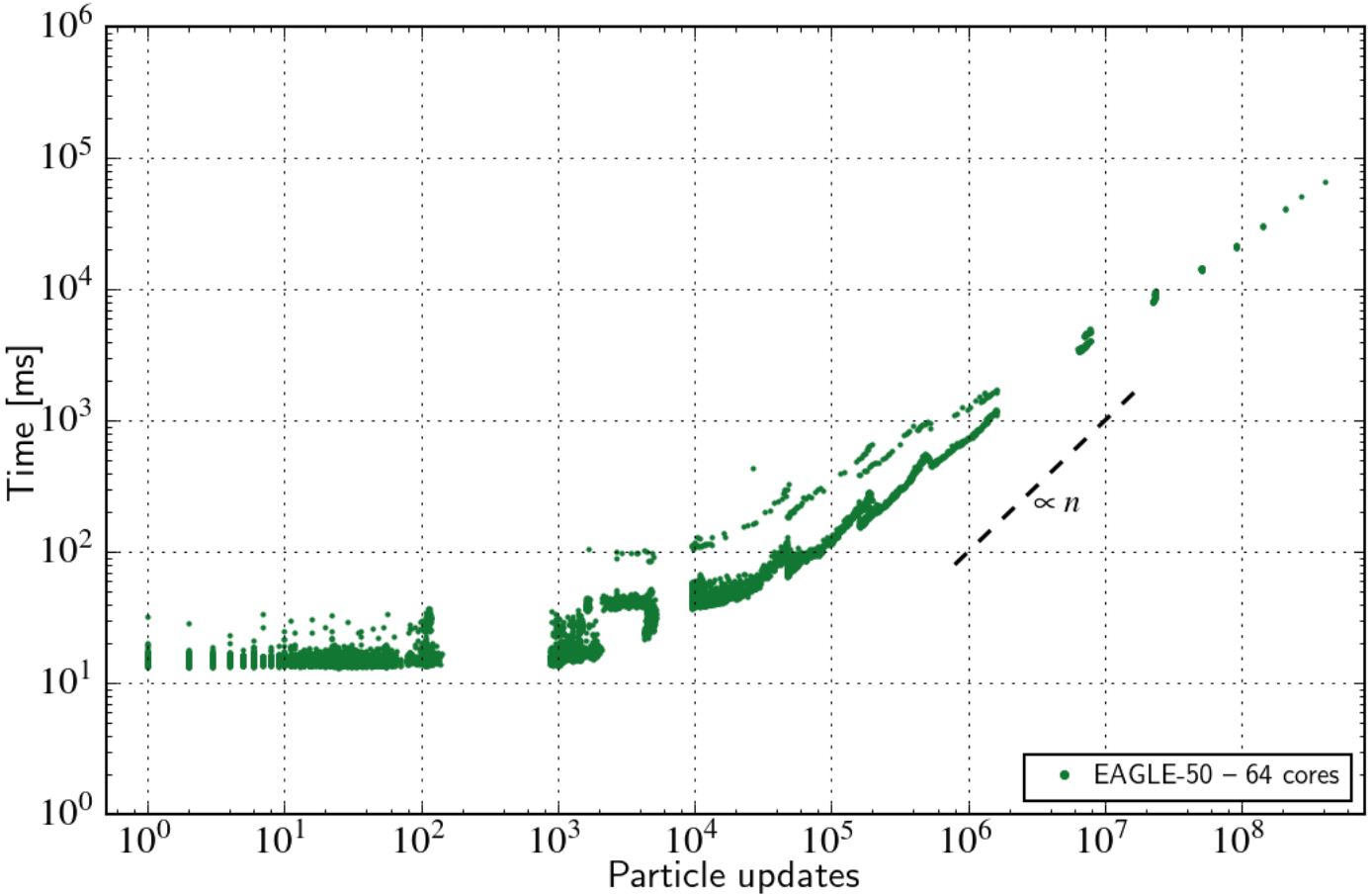

A hand-written solution

- Avoid MPI for small updates.
- The particles with the smallest time-steps should be at the centre of their domains and not require any “halo” particles.
- Small time-steps are at the centre of galaxies.

- Identify galaxies → Grow domains organically around them
  → Get efficient code.

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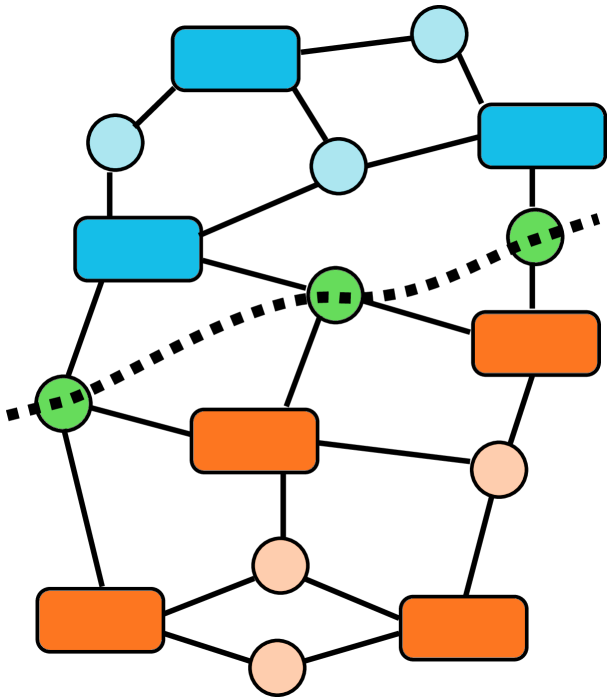
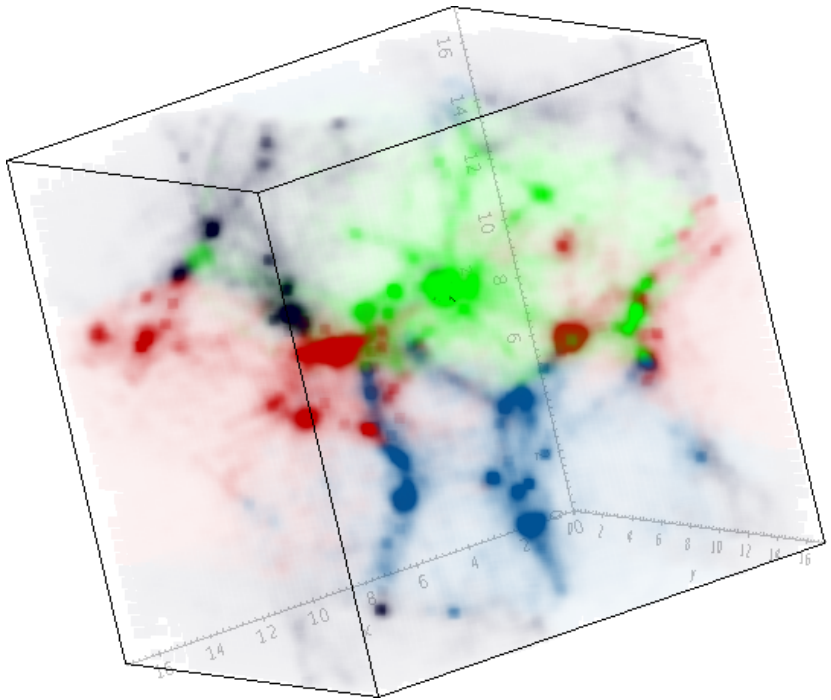
Drawbacks: Not generic. Identifying galaxies is not trivial.

A Graph-based strategy



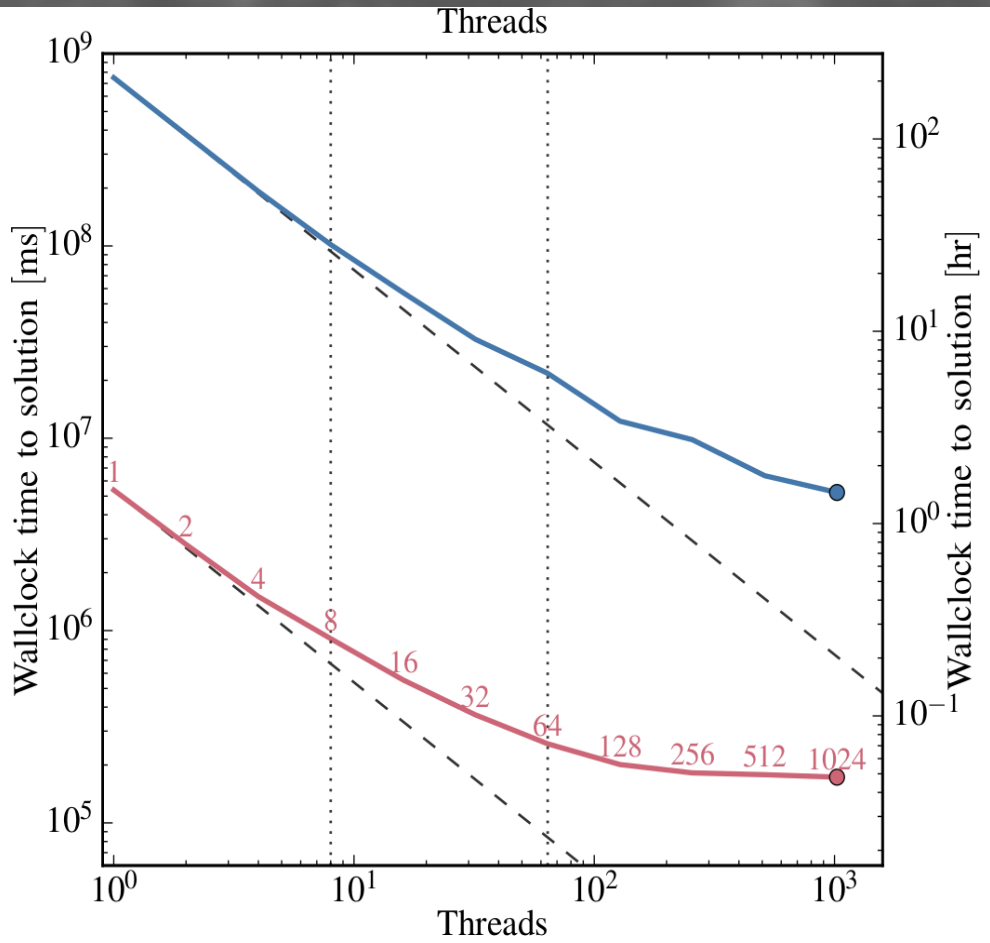
- For each task, we compute the amount of work (=runtime) required.
- We build a graph where the data are nodes and tasks are hyper-edges.
- METIS is used to split the graph such that the work (not the data!) is balanced.
- Extra cost added for communication tasks to minimise them.

What does it look like?



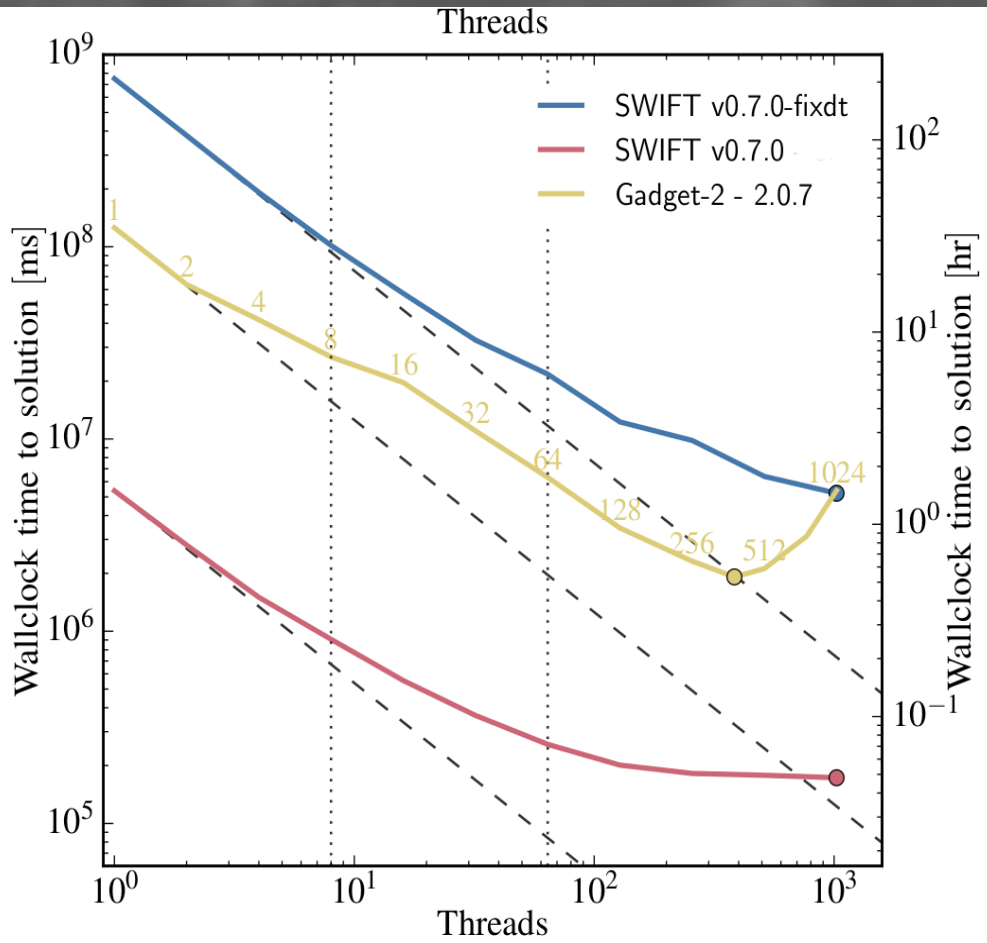
- No regular grid pattern.
- No space-filling curve pattern.
- Good (work) load-balancing by construction.
- The most dense regions are at the centre of their respective domains.

Time-to-solution with a local time-step



Time-to-solution with a local time-step

- Realistic problem
- Same accuracy.
- Same hardware.
- Same compiler.
- Same solution.



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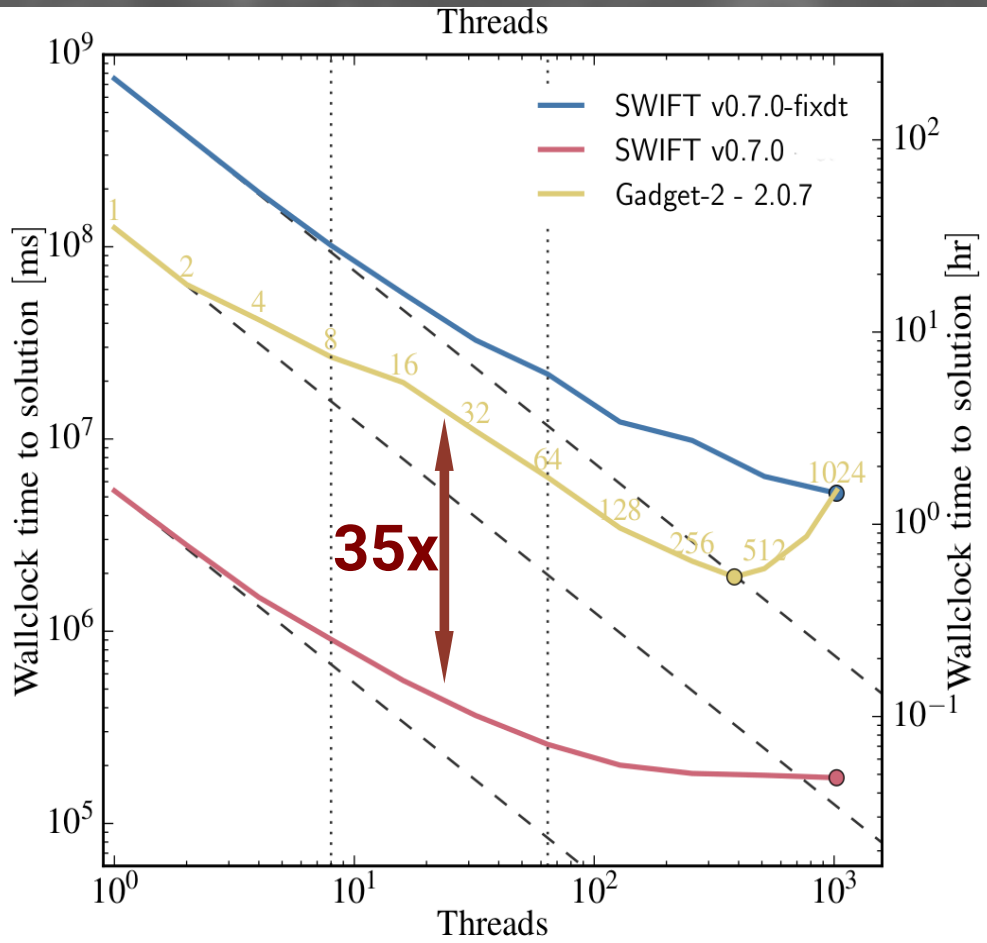
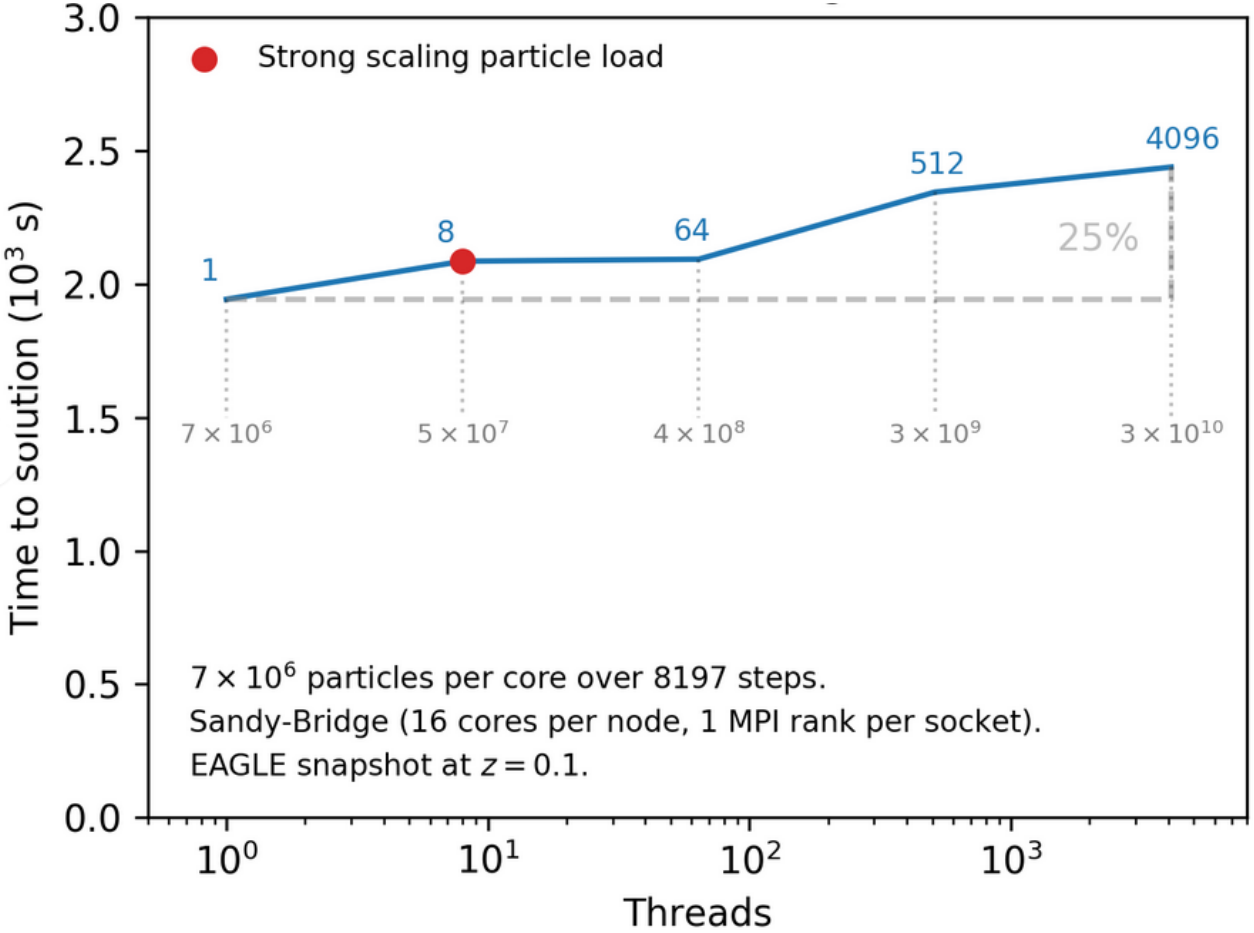


Half way to exa-scale!

Sustained performance in weak-scaling



Conclusions

- New algorithms can lead to significant speed-ups over conventional methods. Implicit methods vs. explicit local time-step based solvers.

  >30x over Gadget → “half way from peta-scale to exa-scale via algorithms”

- Task-based parallelism as a viable model for actual scientific applications.

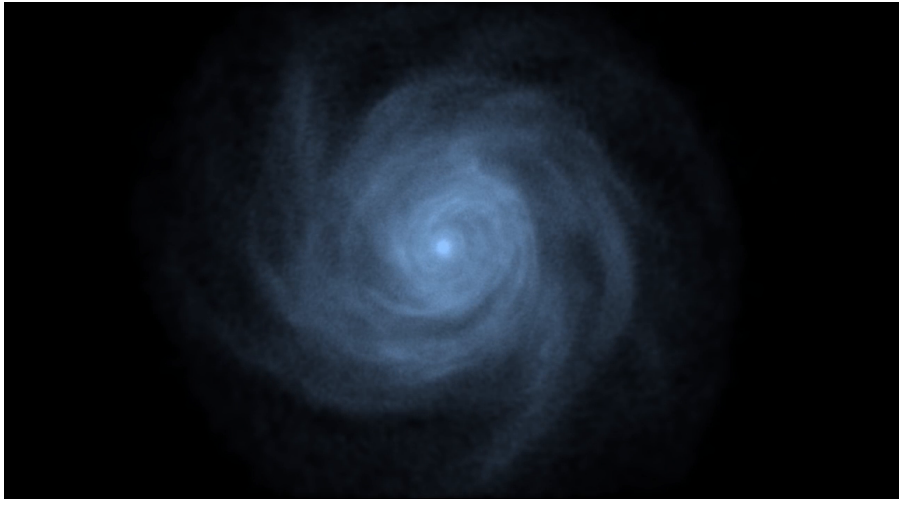
  → Not just a research concept.

- Pure scaling is not necessarily the best metric to judge an application or hardware.

  → “time-to-solution” or “time-to-science” should be considered.

@SwiftSimulation

www.swiftsim.com



Hausammann, Revaz, Schaller