Leibniz-Rechenzentrum
der Bayerischen Akademie der Wissenschaften

# Performance optimization of the Smoothed Particle Hydrodynamics code Gadget3 on 2nd generation Intel Xeon Phi

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# Work main contributors

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- Member of the Intel Parallel Computing Center (IPCC) @ LRZ/TUM

- Expert in computational astrophysics and simulations

- Some of the results shown here are based on work performed with Dr. Fabio Baruffa (now at Intel)



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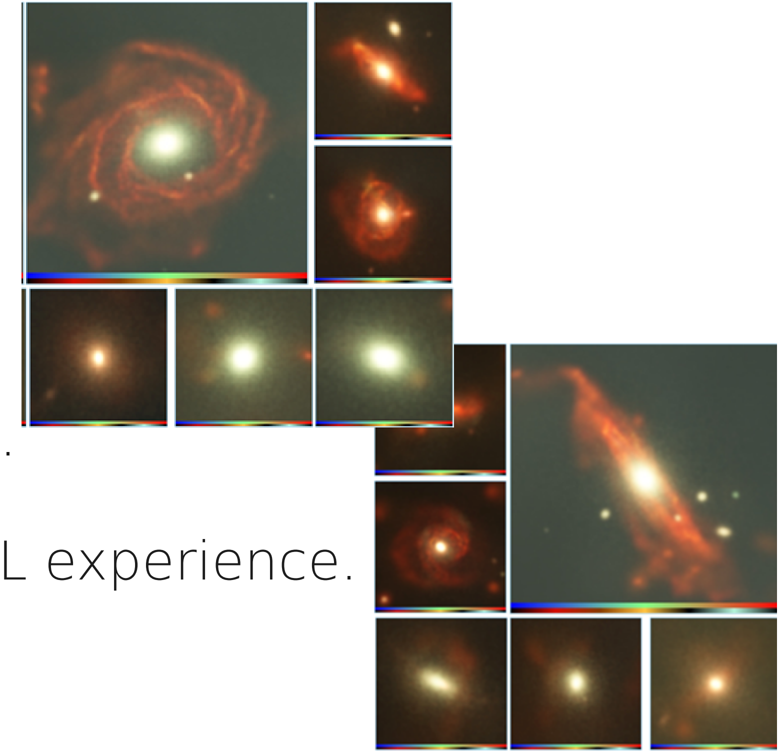
# Outline of the talk

- Overview of the code: P-Gadget3.
- Modernization of a code kernel.
- Back-porting to the full code.
- Optimization steps on Knights Landing (KNL).
- Performance results, takeaways from our KNL experience.

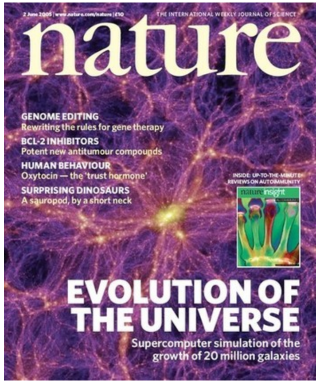




Simulation details:
www.magneticum.org

# Gadget intro

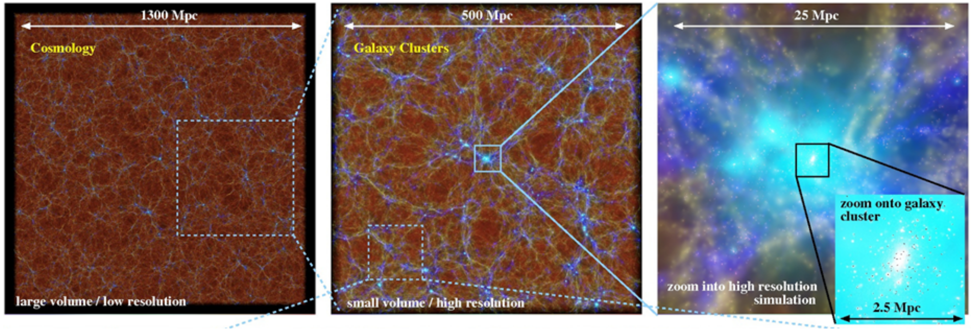
- Leading application for simulating the formation of the cosmological large-scale structure (galaxies and clusters) and of processes at sub-resolution scale (e.g. star formation, metal enrichment).




- Publicly available, cosmological TreePM N-body + SPH code.

- First developed in the late 90s as serial code, later evolved as an MPI and a hybrid code.

- Good scaling performance up to O(100k) Xeon cores (SuperMUC@LRZ).





Simulation details:
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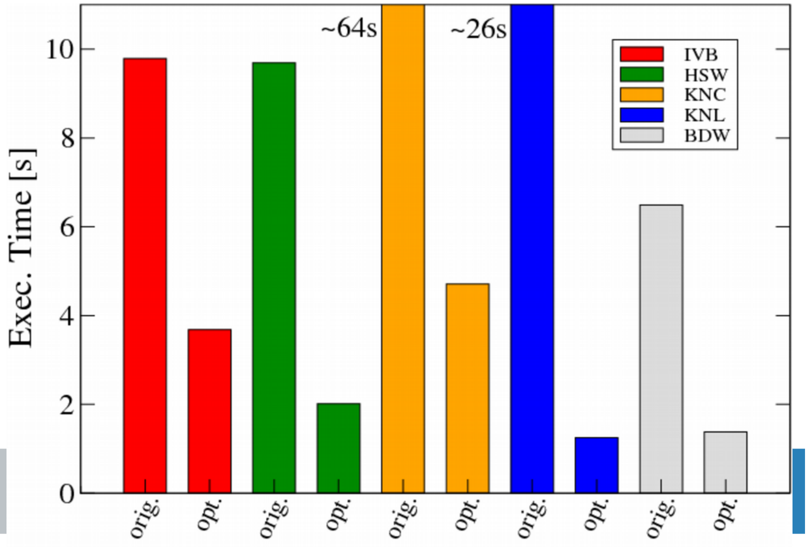
# Previous optimization work
## (Baruffa, Iapichino, Hammer & Karakasis, proceedings of HPCS 2017)

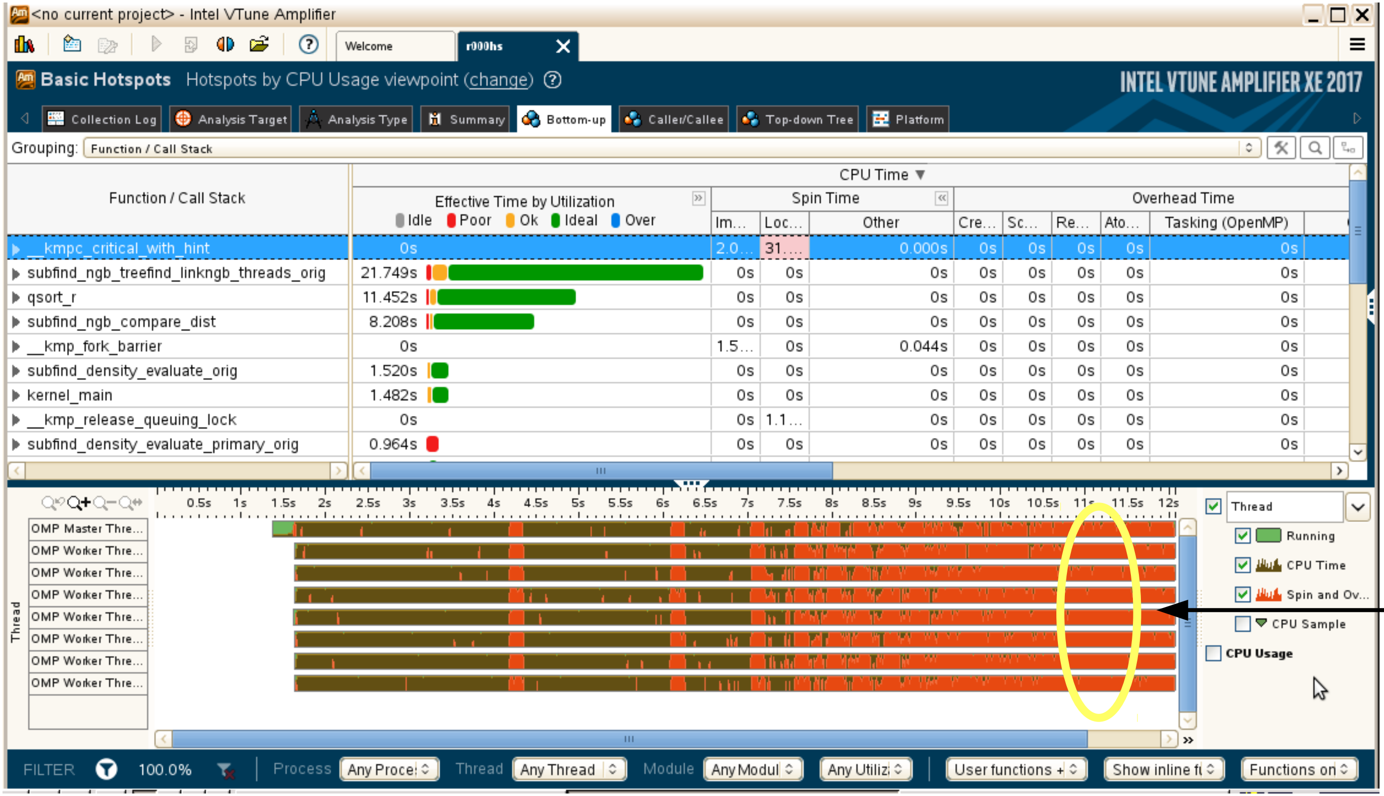
- The representative code kernel subfind_density was isolated and run as a stand-alone application, avoiding the overhead from the whole simulation.
- Focus on node-level performance, through minimally invasive changes.
- We use tools from the Intel® Parallel Studio XE (VTune Amplifier and Advisor).
- Code optimizazion through:
  - Better threading parallelism;
  - Data optimization (AoS → SoA);
  - Promoting more efficient vectorization.
- Up to 19x faster execution on KNL.





Also available as: https://arxiv.org/abs/1612.06090

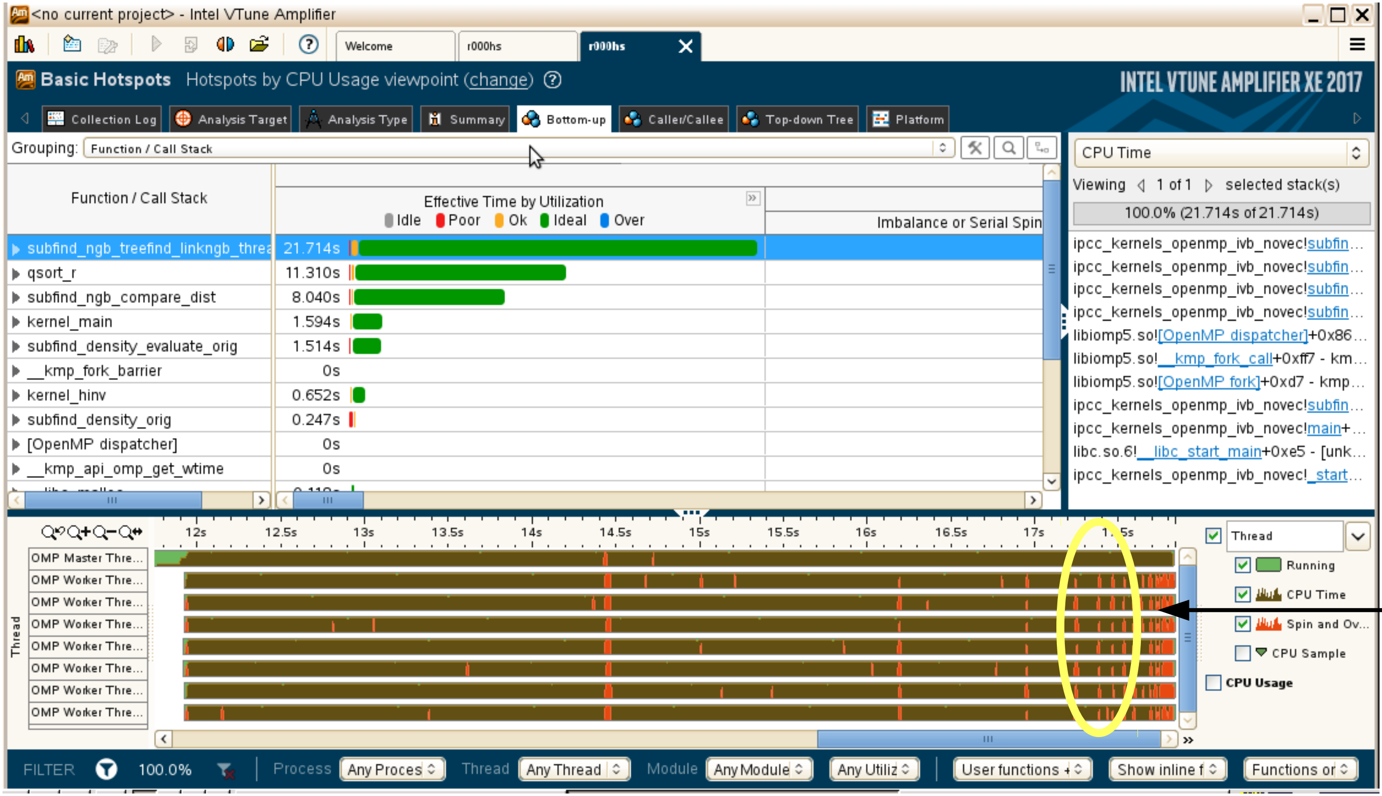
# Modernizing the threading parallelism of the isolated kernel




- Severe shared-memory parallelization overhead
- At later iterations, the particle list is locked and unlocked constantly due to the recomputation
- Spinning time 41%

***thread spinning***

# Improved performance




- Lockless scheme: lock contention removed through “todo” particle list and OpenMP dynamic scheduling.
- Time spent in spinning only 3%

***no spinning***

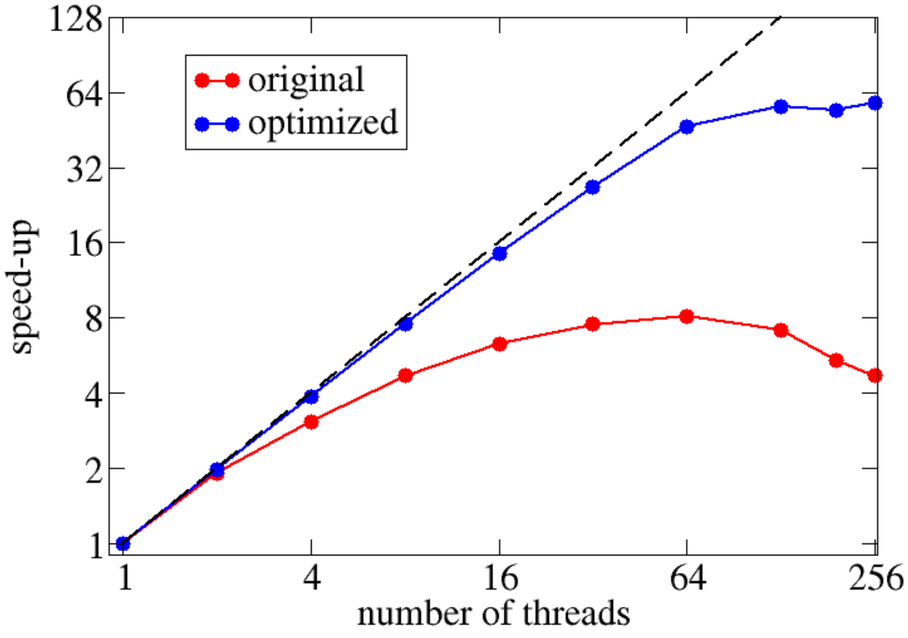
# Improved speed-up of the isolated kernel on KNL

- Knights Landing  Processor 7210 @ 1.3 GHz, 64 cores. KMP Affinity: scatter; Configuration Quadrant/Flat.

- On KNL @ 64 threads:
  - speed-up wrt original version: 5.7x
  - parallel efficiency: 73%

- Crucial for target performance: OpenMP threads per MPI task on the full code? On 16 threads on KNL, speed-up improvement 2.3x.

- Remark: the back-porting is based on a different physical workload, where the performance gain is lower (let's discuss this later...)



# Guideline for the optimization on KNL

Optimization for KNL seen as a three-step process:

| Step | Effort | Expected performance |
|---|---|---|
| Compilation “out of the box” | 1 hour | Lower than Haswell (~ 1.5x) |
| Optimization without coding (use of AVX512, explore configuration, MCDRAM, MPI/OpenMP) | 1 week | Up to 2x over previous step |
| Optimization with coding | 1-3 months (IPCC: 2 years) | Up to the level of Broadwell |



Freely adapted from Leijun Hu, Inspur @ ISC 2017

# Back-porting: development steps on KNL

| Code version | Description | Notes |
|---|---|---|
| Original | “Out-of-the-box” default environment, v. 2016 Intel compiler and libraries, no KNL-specific flags. | |
| Step 0 | v. 2018 Intel compiler and libraries, -xMIC-AVX512. | The code does not benefit from specific cluster or memory modes. |
| Optimized | Threading parallelism improved in subfind_density. Other minor improvements. | MPI/OpenMP configuration set by target, not by optimal performance. |



Freely adapted from Leijun Hu, Inspur @ ISC 2017

# Performance results

One-node tests, performed on an Intel Xeon Phi (KNL) 7210 @ 1.30GHz with 64 cores.
Configuration: Quad/flat with allocation on DDR. 4 MPI tasks, 16 OpenMP threads each.

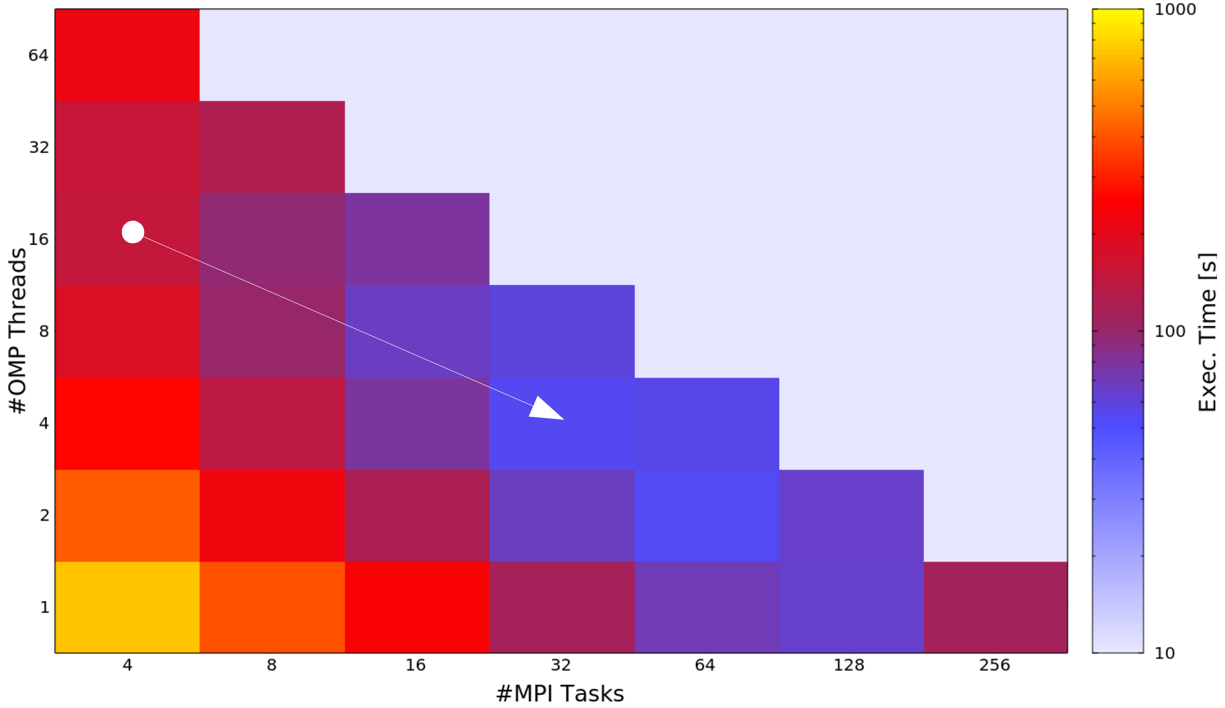
| Code version | Time (total) [s] | Time (subfind_density) [s], % of total |
|---|---|---|
| Original | 167.4 | 22.6 (13.5%) |
| Step 0 | 142.1 | 17.1 (12.1%) |
| Optimized | 137.1<br>1.2x | 12.7 (9.3%)<br>1.8x (isolated kernel: it was 1.4x) |



Freely adapted from Leijun Hu, Inspur @ ISC 2017

# Understanding results and performance targets

- Based on our experience 4-8 MPI tasks per KNL should be optimal.
- A complete back-porting should improve the OpenMP layer and move the best performance to the left.
- For comparison: currently the best performance on a Haswell node is for the pure-MPI case!
- Best performance KNL: 53.2s (total), 10.8s (subfind_density, 20.3%).
- Best performance HSW: 42.6s (total), 11.4s (subfind_density, 26.7%).




Parameter study of the MPI / OpenMP ratio on a KNL node.

# Summary and outlook

- Along the described development steps, performance improvement on KNL is 1.2x for the whole code, 1.8x for the optimized kernel subfind_density.
- Improvements are portable also on Xeon (ongoing tests on newer versions).
- The improvement of subfind_density is in line with predictions based on the isolated kernel (1.4x), thus verifying our approach.
- Performance gap with Haswell: the original code was 1.7x slower on KNL, the optimized is 1.3x slower. For subfind_density: the original version was 1.50x slower on KNL, the optimized one only 1.16x slower → closing the gap!
- Room for further improvement?
  - Complete back-porting of further steps (data layout, vectorisation);
  - Back-port to other two major routines (~70% total time);
  - Explore and modernize also the MPI layer of the code.

# Acknowledgements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- P-Gadget3 developers: Klaus Dolag, Margarita Petkova, Antonio Ragagnin.
- Research collaborator at Technical University of Munich (TUM): Nikola Tchipev.
- TCEs at Intel: Heinrich Bockhorst, Klaus-Dieter Oertel.
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- Special thanks to Colfax Research for granting access to their computing facilities.


More details: Baruffa, F., Iapichino, L., Karakasis, V., Hammer, N.J.: *Performance optimisation of Smoothed Particle Hydrodynamics algorithms for multi/many-core architectures.* 2017, proceedings of the 2017 International Conference on High Performance Computing & Simulation (HPCS 2017), 381. Awarded as Outstanding Paper (runner-up). DOI: 10.1109/HPCS.2017.64. arXiv: 1612.06090.


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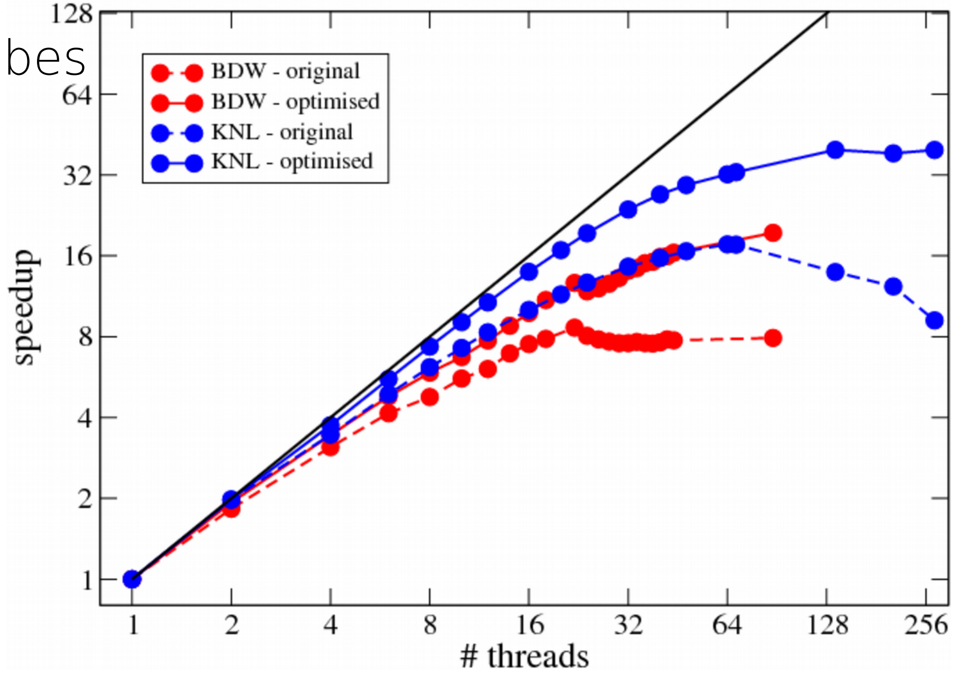
# Back-up:
# Back-porting the kernel optimizations to the full code

- To ease the back-porting, we defined a new Gadget test problem with a simplified but representative workload ($2 * 64^3$ particles).
- From a physical viewpoint, this workload probes advanced phases of the galaxy evolution (inter-galactic medium is strongly clumped).
- Computationally, a reduced effort for finding particle neighbors!
- Improvement in execution time: 2.3x on Broadwell (Xeon E5-2699v4, 22 cores/socket), 5.3x on KNL. It was 4.7x and 19.1x for the old workload.



# Back-up: removing lock contention

```
todo_partlist = partlist;

while(partlist.length){
  error=0;
  #pragma omp parallel for schedule(dynamic)
  for(auto p:todo_partlist){
    if(something_is_wrog) error=1;
    ngblist = find_neighbours(p);
    sort(ngblist);
    for(auto n:select(ngblist,K))
       compute_interaction(p,n);
  }

//...check for any error
  todo_particles = mark_for_recomputation(partlist);
}
```

creating a ***todo*** particle list

iterations over the ***todo*** list (*private ngblist*)

actual computation

***No-checks*** for computation

# Back-up: some more KNL wisdom

- Quad-cache is a good starting point, quad-flat with allocation on MCDRAM is worth being tested, SNC modes are for very advanced developers.
- It is unlikely to gain performance with more than 2 threads/core.
- Vectorize whenever possible, use compiler reports and tools to exploit low-hanging fruits.
- Know where your data are located and how they move.
- If optimizations are portable, the effort pays off!