Leibniz-Rechenzentrum
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Improving node-level performance in Gadget: data structure and data locality

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Optimisation strategy

- Gadget3: publicly available, cosmological TreePM N-body + SPH code. Good scaling performance up to 130,000 Sandy Bridge cores (SuperMUC, Extreme Scaling workshop 2013 @ LRZ).
- However: performance optimization at node level and the use of accelerators had gone largely unexplored before our work.
- Initial analysis: most of the code components consist of two sub-phases of nearly equal execution time (40 to 45% for each of them).
- The most suitable for the optimization and execution on Intel® Xeon Phi™ (higher floating-point rate, sustainable cache and memory b/w requirements, but data cache misses) will be the target of our work.
- Isolation of a typical kernel (subfind_density):
  - Run as a stand-alone separate kernel (same input as original: sandbox model!).
  - Avoid the overhead of the whole simulation → Quick prototyping, allows native mode on the Xeon Phi™.
  - Later: port optimizations back to the original code.

Code status before our work

- Current data organisation: Array of Structures (AoS), 224 bytes per particle.
- Motivation: highly optimized for performance at large MPI task numbers.
- Outcome: data cache misses, code is memory latency bound. Data structure hinders vectorisation.
- In the kernel: ~ 17 iterations, 1.5M particles to be processed.

Proposed solution: SoA

- New particle data structure: defined as Structure of Arrays (SoA).
- From the original set, only variables used in the kernel are included in the SoA: ~ 60 bytes per particle.
- Software gather / scatter routines.
- Gather from old to new data structure, compute with it, scatter back to old. Example of change in the data structure approach:

```
struct new_particle_data
{
MyDoublePos *Pos[3];
MyFloat *Vel[3];
short int *Type;
MyIDType *ID;
MyFloat *Mass;
int *DM_NumNgb;
MyFloat *DM_Hsml;
MyFloat *DM_Density;
MyFloat *DM_VelDisp;
};
```

```
v2 += P[j].Vel[0]*P[j].Vel[0] +
P[j].Vel[1]*P[j].Vel[1] + P[j].Vel[2]*P[j].Vel[2];
```

↓

```
v2 += NewPart.Vel[0][j]*NewPart.Vel[0][j]
+ NewPart.Vel[1][j]*NewPart.Vel[1][j] +
NewPart.Vel[2][j]*NewPart.Vel[2][j];
```

```
void gather_particle_data(struct new_particle_data
*dst, const struct particle_data *src, size_t N)
{
int i;

#pragma omp parallel for
for (i = 0; i < N; i++) {
:
dst->Vel[1][i] = src[i].Vel[1];
dst->Vel[2][i] = src[i].Vel[2];
dst->Type[i] = src[i].Type;
dst->ID[i] = src[i].ID;
:
```

Outcome

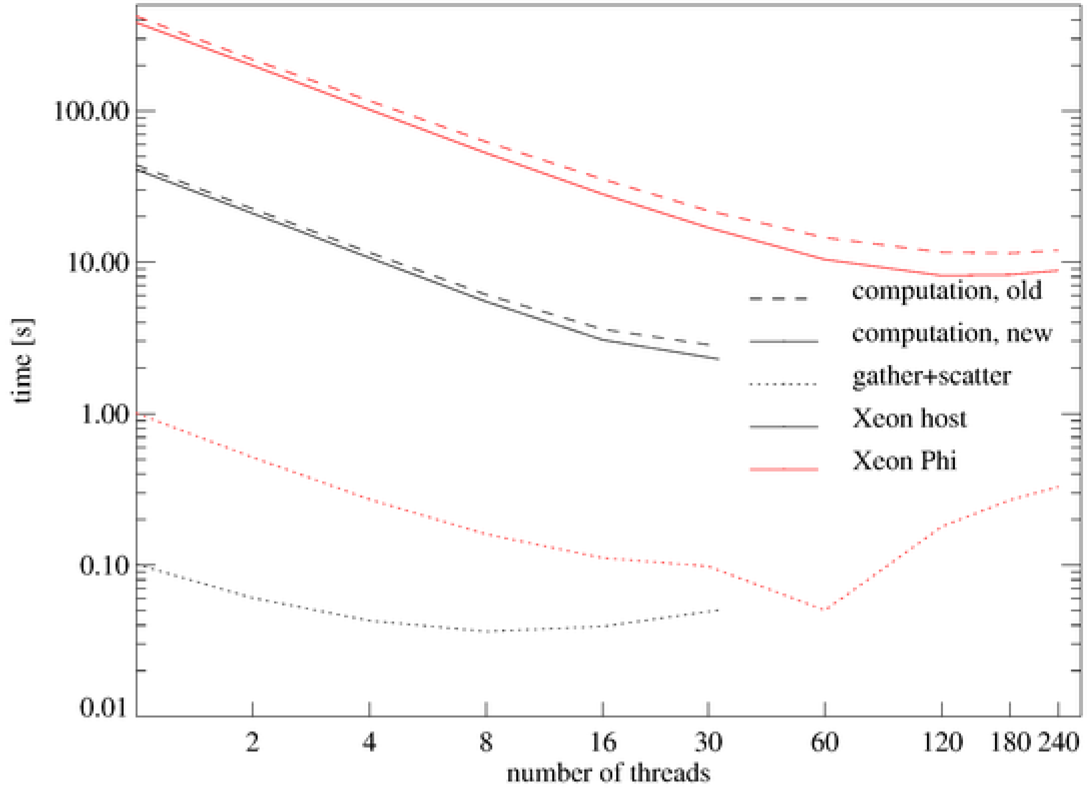
- Gather+scatter overhead small when compared both to execution time and to performance gain.
- Node-level performance improvement: +22% on the Xeon, +41% on the Xeon Phi™. Xeon/Xeon Phi™: 0.28
- Bottleneck on memory latency is solved: *Memory latency* metric (VTune) from 0.208 to 0.098.
- Data structure is now vectorisation-ready, although vectorisation has been completely disabled at this stage.
- Cache behaviour: improved performance by ~40%.

AoS

Stall type	**% cycles**
L1D miss	8.49 %
L2 miss	7.99 %
LLC miss	16.27 %
TOTAL	**32.75 %**

SoA

Stall type	**% cycles**
L1D miss	3.75 %
L2 miss	3.16 %
LLC miss	12.32 %
TOTAL	**19.23 %**



Insights and next steps

- Work on a representative Gadget3 kernel.
- Data structure and data locality: a first step towards vectorisation.
- Also part of our work:
  - Shared-memory parallelisation improvements
  - Other algorithmic improvements: selecting nearest particles.
- In general: optimisation is a win-win game, but the Xeon Phi™ wins more.
- Coming soon:
  - Lockless parallelisation scheme.
  - Port node-level code improvements back to Gadget3.