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## Automating Data Layout Conversion in a Large Cosmological Simulation Code

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## Intro: The Gadget cosmological code

- Large-scale structure formation (galaxies and clusters)
- Publicly available [1], cosmological TreePM N-body + SPH code
- MPI/OpenMP-parallel; up to O(100k) Xeon cores (SuperMUC@LRZ)
- Several teams and several versions (>200 kLoC each)

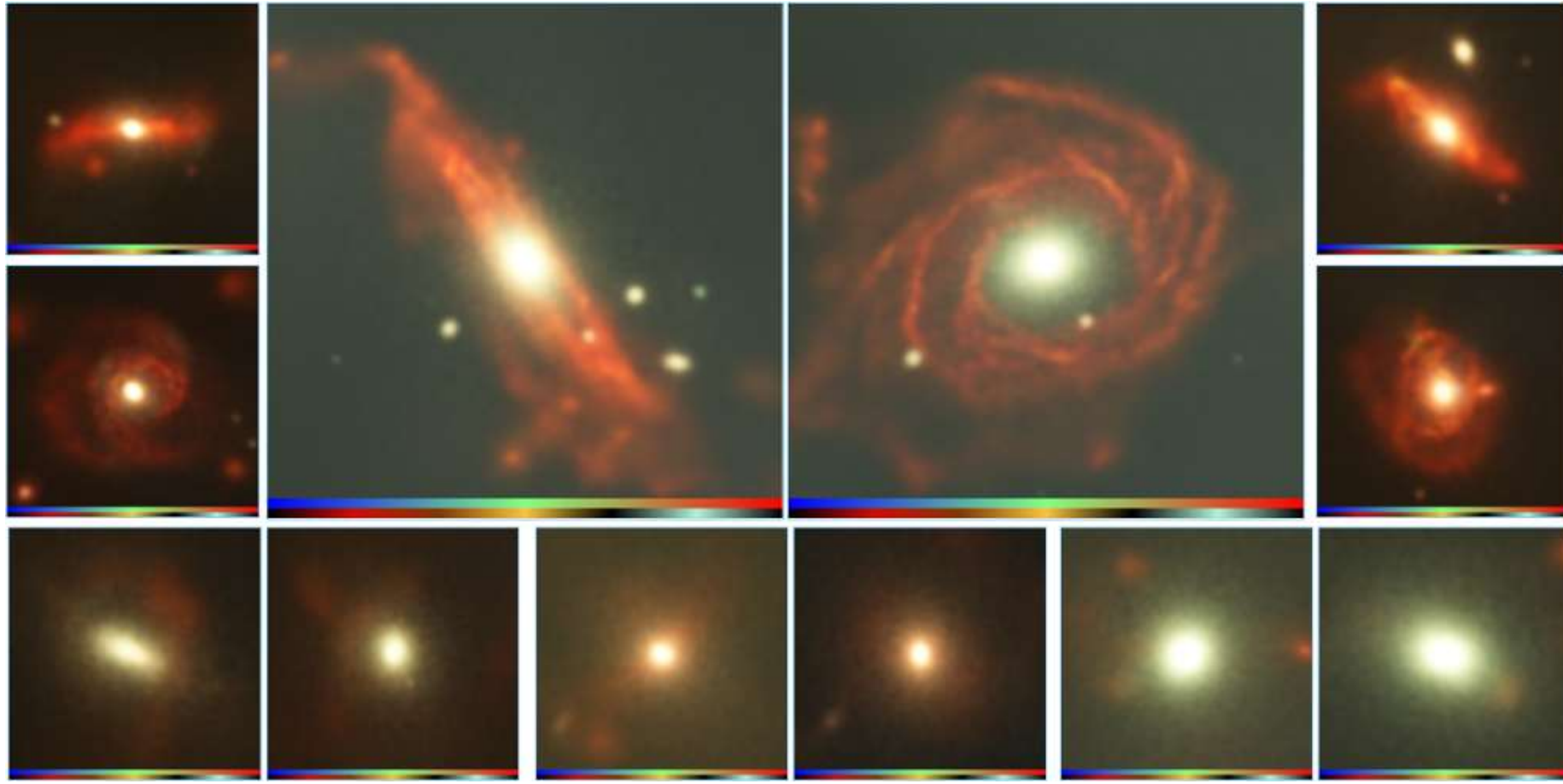


Figure 1: Galaxies simulated with Gadget – courtesy Magneticum Project [2] / <http://magneticum.org>

## Optimization study of Gkernel

- Gkernel is:
  - isolated representative Gadget code kernel (“halo finder”)
  - stand-alone application, avoids simulation overhead
- Node-level optimization study [3] in the frame of the IPCC [4]
- Target computing systems:
  - Knights Corner (KNC), Ivy Bridge (IVB)
  - Haswell (HSW), Broadwell (BDW), Knights Landing (KNL)
- Main changes:
  - Data layout optimization
  - Better threading parallelism

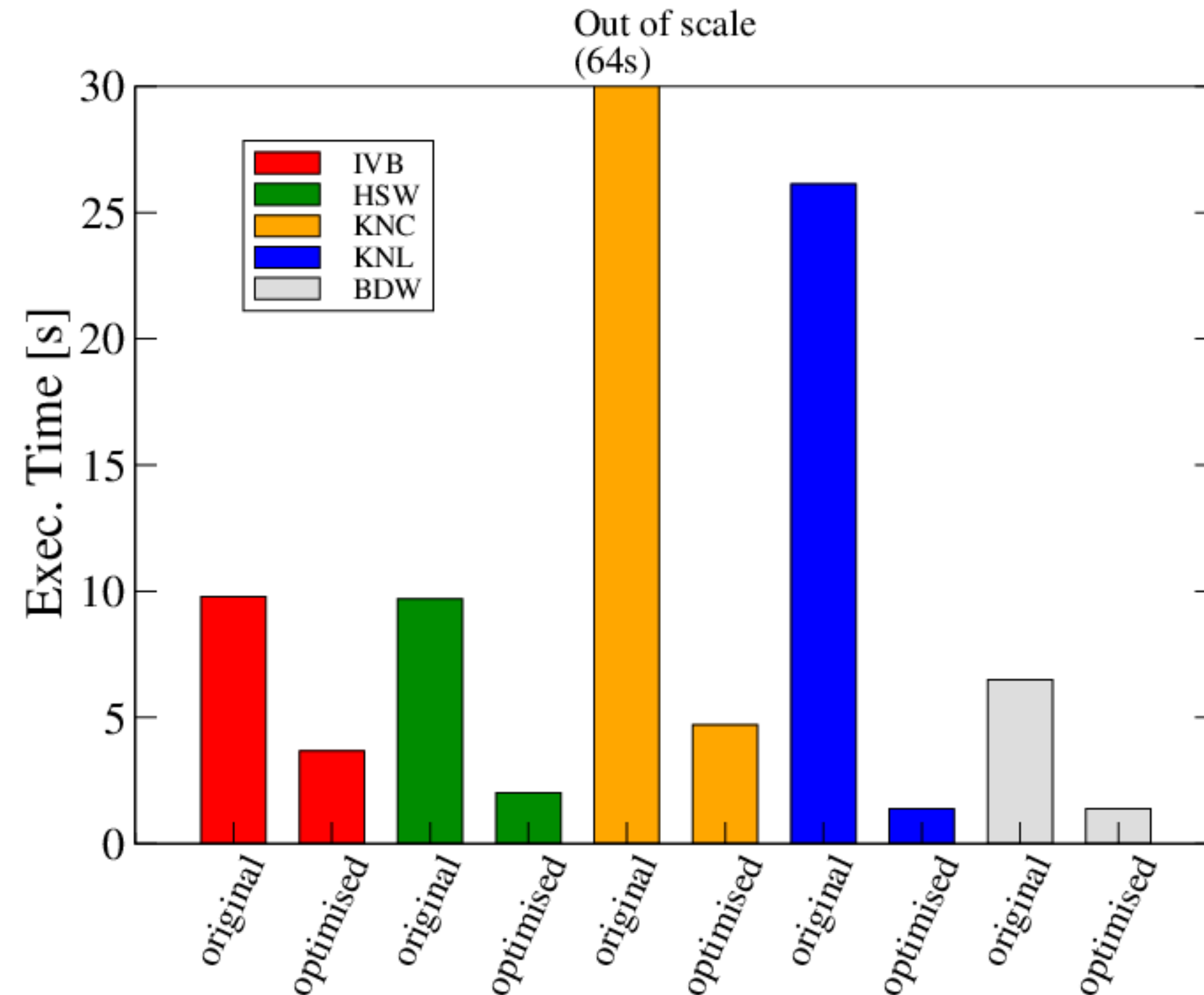


Figure 2: Tests on one-socket Xeon systems; 240 threads (4 thr./core) for KNC; 128 threads (2 thr./core) for KNL. Performance improvement: up to 19x faster on KNL; 13.6x on KNC, ca. for 2-5x on Xeon.

## Data layout optimization

From Array of Structures to Structure of Arrays (AoS ⇒ SoA)

- Sample code changes in Fig. 3 and Fig. 4
- Leads to better memory access
- Eases compiler auto-vectorization
- SoA-specific performance benefit (over OpenMP improvement):
  - +13% on IVB
  - +48% on KNC

```

1 // Before:
2 // one structure per particle
3 struct particle {
4     double Mass, Hsml, ...;
5     ...
6 };
7
8 ...
9 // Array of Structures
10 struct particle *P;

1 // After:
2 // One array for each quantity
3 struct particle_soa_t {
4     double *Mass, *Hsml, ...;
5     ...
6 };
7
8 ...
9 // Structure of Arrays
10 struct particle_soa_t P_SoA;
    
```

Figure 3: A “Structure of Arrays” struct definition introduction example. Only a dozen arrays have been introduced this way in Gkernel. Gadget would need over a hundred.

```

1 // may not vectorize
2 ...P[i].Mass + P[i]...

1 // vectorizes better
2 ...P_SoA.Mass[i] + P_SoA...
    
```

Figure 4: AoS to SoA transition sample. Impacts a few hundreds statements in Gkernel. Would impact many thousands in full Gadget. Notice that i could be any expression.

## Perspective for Gadget

- Obtained and validated performance guidelines for Gadget
- Limitations of [3] study:
  - single kernel only, no MPI
  - relying on AoS ⇒ SoA ⇒ AoS at each kernel call
- Left open questions:
  - what to do with members like Pos [3] or DV [3] [3] ?
  - ...and anonymous unions ?
  - ...and other kernels/quantities?
- How to backport >>200 kLoC to Gadget ?

## Discussion: Possible AoS ⇒ SoA breakdown

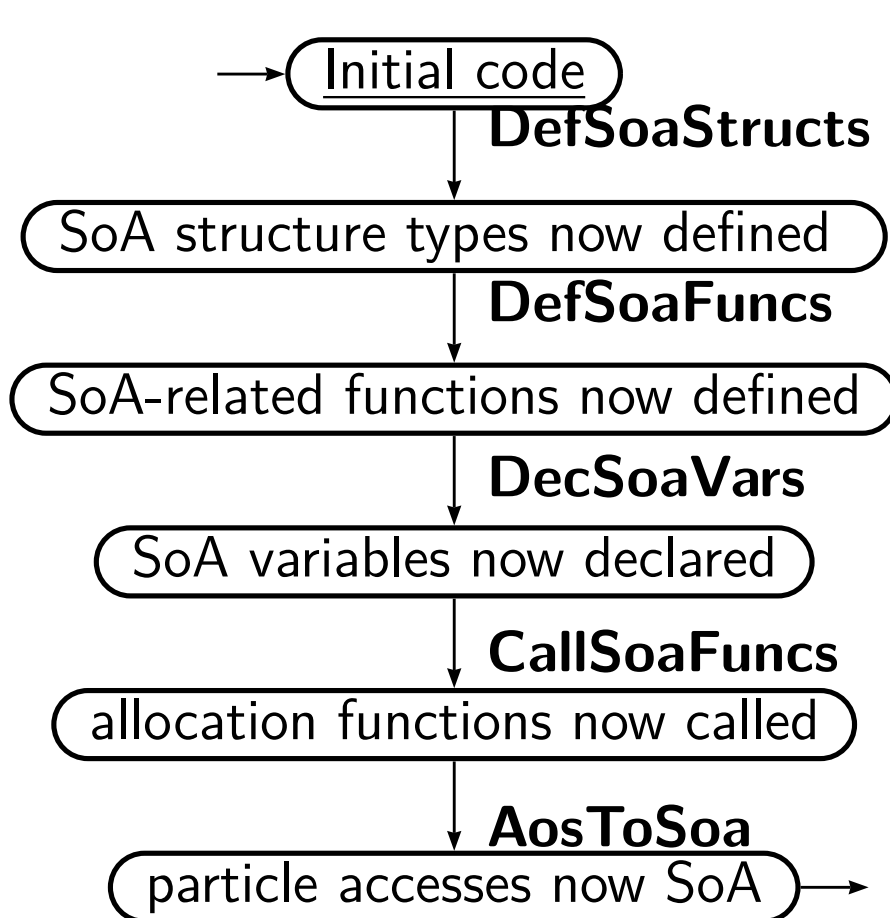


Figure 5: Transformation steps, ordered so that their introduction does not break code. The Gkernel study has performed this on a subset of Gadget ([3]).

- DefSoaStructs: define struct type with arrays instead of scalars
  - each member might depend on #ifdef...
- DefSoaFuncs: glue functions for SoA
  - like -allocate, -free, -convert, etc.
  - repetitive, time consuming

```

1 void aos_alloc(void)
2 {
3     P = (struct particle*) calloc(
4         All.MaxPart, struct particle);
5 }

1 void soa_alloc(void)
2 {
3     P_SoA.Hsml = (double*) calloc(
4         All.MaxPart, double);
5     P_SoA.Mass = (double*) calloc(
6         All.MaxPart, double);
7     ...
8 }
    
```

Figure 6: DefSoaFuncs. Transition to SoA in Gadget would require one allocation per quantity. Manual introduction of this and further glue functions (e.g. AoS ⇒ SoA copy functions) is error-prone and repetitive. Manual SoA accesses introduction (Fig. 4) can be worse.

- DecSoaVars: declare SoA structure variables
- CallSoaFuncs: call glue functions
- AosToSoa: replace relevant AoS accesses with SoA accesses
  - thousands of lines impacted (error prone and repetitive)
  - regular expressions help, but still error-prone and sloppy

## A more desirable approach

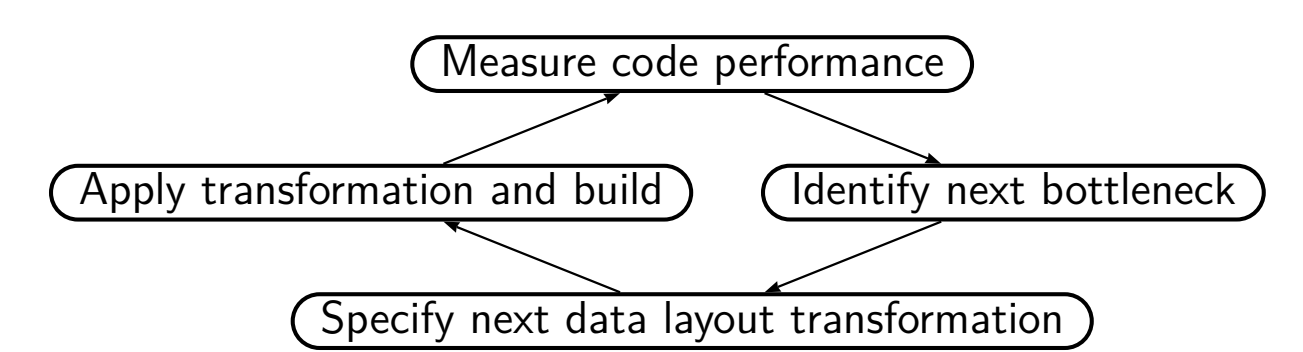


Figure 7: Tool-assisted automatic data layout transformation would greatly accelerate cycles of development and empirical performance optimization.

## Fine-grained AoS ⇒ SoA transition mechanism needed!

- transitory patch: generating AoS ⇔ SoA converter functions
- exclusion/inclusion of structure members based on
  - usage / occurrence in files
  - specific type
  - identifier whitelist

## Solution: Semantic patching

Coccinelle [5]: “...a program matching and transformation engine ... for specifying desired matches and transformations in C code”

- specification language inspired from UNIX patch (SmPL)
- SmPL can express steps in Fig. 5, enables Fig. 7 work style
- originally for collateral evolutions in the Linux kernel
- arbitrary C language transformations possible, model checking

```

1 @@
2 identifier id,I;
3 type T;
4 @@
5 struct id { ...
6     T I;
7     T *I;
8     ...
9 };

1 @@
2 expression E;
3 identifier AoS;
4 identifier J;
5 fresh identifier SoA=AoS##"_SoA";
6 @@
7 - AoS[E].J
8 + SoA.J[E]
9
    
```

Figure 8: Sample semantic patch for step DefSoaStructs, cf. Fig. 3. Lines 2-3 specify semantic elements of the C language. Lines 5 and 9 specify matching context, line 6 what to add, line 7 what to remove.

Figure 9: Semantic patch example for AOsToSoa, cf. Fig. 4. This patch requires no context apart from the elements to be replaced. Notice also introduction of a new identifier at line 5, used at line 8.

```

1 @str_flds@
2 identifier id,I;
3 type T;
4 @@
5 struct id { ...
6     T *I;
7     ...
8 };
9
10 @def_alloc_sig@
11 identifier str_flds.id;
12 @@
13 struct id { ... };
14 +void alloc(struct id*p,int n)
15 +{
16     @def_alloc_body@
17     type str_flds.T;
18     identifier str_flds.I, str_flds.id;
19     id;
20 void alloc(struct id*p, int n){
21     +p->I = calloc(n, sizeof(T));
22 }
23
24 @call_alloc@
25 identifier V, str_flds.id;
26 @@
27 struct id V;
28 + alloc(&V, 5);
29 +}
    
```

Figure 10: Semantic patch composed by four rules. This is similar to how DefSoaFuncs and CallSoaFuncs rules might look like. The first rule (line 1) matches a structure, the second (line 10) introduces an empty function, the third (line 16) populates it, the fourth (line 24) calls it. Notice inheritance of elements across rules, e.g. on line 11.

## Coccinelle advantages

- over other transformation engines (e.g. DMS, Rose Compiler):
  - straight-forward transformation language SmPL
  - fully free software-licensed (it serves the Linux kernel)
- over certain syntax-preserving C++ techniques (e.g. Intel SDLT)
  - code clarity (no operators and temporary objects involved)
  - preserves usability of -O0

## Results summary

- all scalar particle variables now SoA
- enables low effort extension to:
  - replay on several communities’ Gadget forks
  - arbitrary mixes of AoS/SoA
- patch: ≈ 10K +/- diff lines (with context: ≈ 20K)
- exploring Coccinelle usage for HPC

## Possible future work

- new performance studies possible
- rules for OpenMP optimizations backport [3]
- MPI-specific glue code

## References

[1] V. Springel, “The cosmological simulation code GADGET-2”, *MNRAS*, vol. 364, pp. 1105–1134, 2005.  
 [2] “Magneticum Home page (large-scale project based on Gadget)” <http://www.magneticum.org>.  
 [3] F. Baruffa, L. Iapichino, N. J. Hammer, and V. Karakasis, “Performance optimisation of smoothed particle hydrodynamics algorithms for multi-/many-core architectures”, in *2017 International Conference on High Performance Computing Simulation (HPCS)*, pp. 381–388, 2017.  
 [4] “Intel Parallel Computing Center: LRZ webpage”, <https://www.lrz.de/services/compute/labs/astro1ab/ipcc>.  
 [5] J. Lawall and G. Muller, “Coccinelle: 10 years of automated evolution in the Linux kernel”, in *2018 USENIX Annual Technical Conference, USENIX ATC*, pp. 601–614, 2018.