N-body memory layout exploration

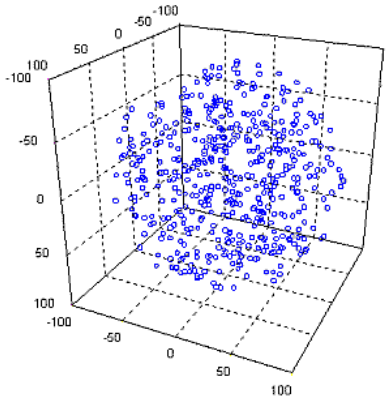
Oliver Geisel & Lisa Hentschke

January 30, 2021

Structure

The n-body simulation

- simulate the interaction of n particles
- each particle has
  - position x
  - position y
  - position z
  - velocity x
  - velocity y
  - velocity z
  - mass



http://astro.dur.ac.uk/~nm/pubhtml/nbody/nbody.html

Recap: AoS vs SoA

Array of Structures (AoS)

```
struct Pixel {
  float r;
  float g;
  float b;
  float a;
} pixels[N];
```

Structure of Arrays (SoA)

```
struct Pixel {
  float r[N];
  float g[N];
  float b[N];
  float a[N];
} pixels;
```

from the slides 04-GPU-Memory

Solution Strategies

- rewrite CPP-code in CUDA: implement AoS, SoA and AoSoA memory layouts
- implemented shared memory variants
- for SoA: implemented two sub-variants: B and T
  - B: compute one particle per block
  - T: compute one particle per thread
- We tested on several devices

Example on K80

16 k particles (448.000 kiB)

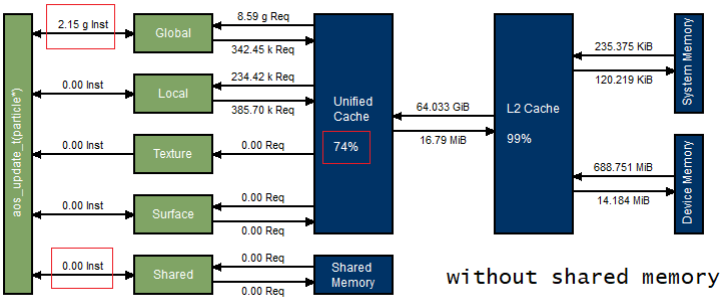
Benchmarks:			Thread,	Thread_shared,	Move
AoS			56.5121ms	17.3868ms	0.036544ms
AoS			56.4797ms	17.4133ms	0.033280ms
AoS			54.9357ms	15.6404ms	0.033632ms
AoS			50.7257ms	15.6060ms	0.032544ms
AoS			50.7504ms	15.5858ms	0.032768ms
AVG:			53.8807ms	16.3264ms	0.033754ms

Benchmarks:	Block,	Block_shared,	Thread,	Thread_shared,	Move
SoA	55.0906ms	21.4492ms	22.8277ms	14.2324ms	0.0110ms
SoA	54.3634ms	21.4436ms	22.8197ms	13.0962ms	0.0083ms
SoA	49.3135ms	19.3027ms	20.4029ms	12.7189ms	0.0083ms
SoA	48.4277ms	18.4641ms	18.8272ms	11.7521ms	0.0092ms
SoA	44.3154ms	17.7516ms	18.8140ms	11.7349ms	0.0092ms
AVG:	50.3021ms	19.6823ms	20.7383ms	12.7069ms	0.009184ms

Benchmarks:			Thread,	Thread_shared,	Move
AoSoA			28.2286ms	43.9762ms	0.222112ms
AoSoA			28.2296ms	43.6562ms	0.220672ms
AoSoA			28.2461ms	43.9120ms	0.221504ms
AoSoA			28.2501ms	43.8764ms	0.222688ms
AoSoA			28.2302ms	44.0284ms	0.218080ms
AVG:			28.2369ms	43.8898ms	0.221011ms

Used Profilers

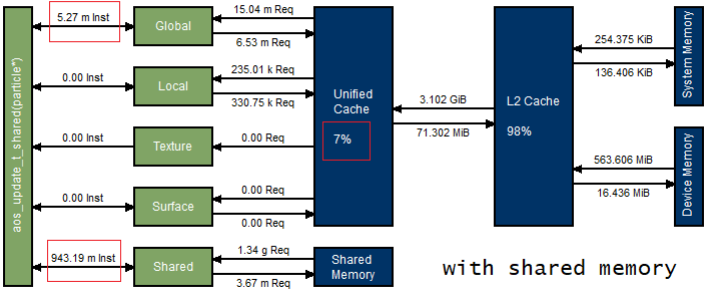
- nvprof on Taurus
- Nvidia Visual Profiler version 11.2



tested on 1070; version 128k paricles on mem layout AoS; subversion T

Used Profilers

- nvprof on Taurus
- Nvidia Visual Profiler version 11.2



tested on 1070; version 128k paricles on mem layout AoS; subversion T

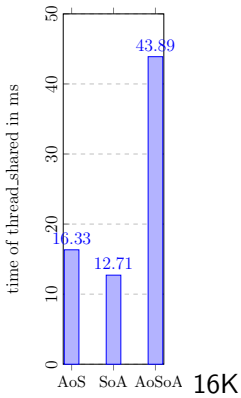
Compare the memory structures

We tested on K80 (Taurus), v100 (Taurus), 1070 (private, driver version 461.09), and RTX 2080 (private, driver version 461.40) respectively

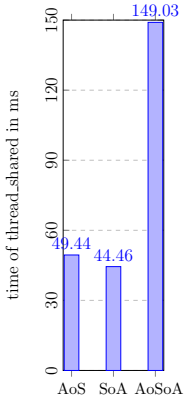
Memory Layout:

- K80 - GDDR 5 with SDRAM
- v100 - HBM 2
- 1070 - GDDR 5
- RTX 2080 - GDDR 6

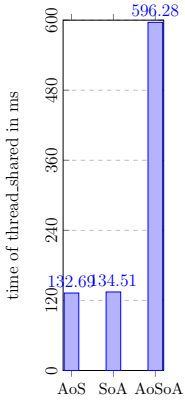
Compare the memory structures - on K80



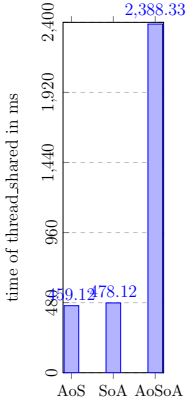
16K



32K

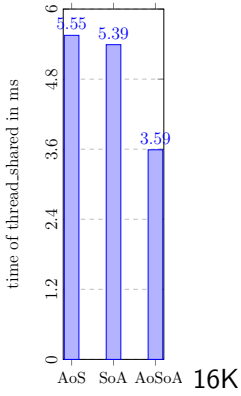


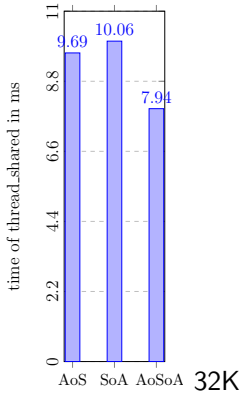
64K

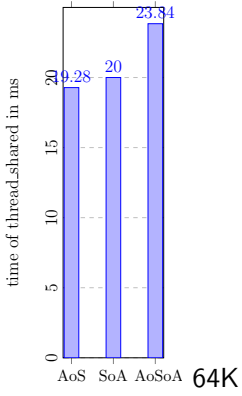


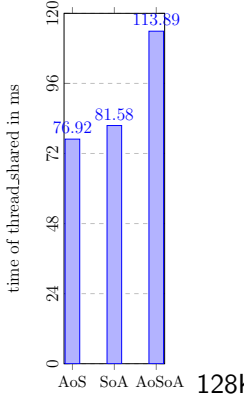
128K

Compare the memory structures - on v100

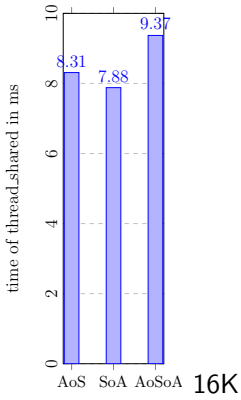


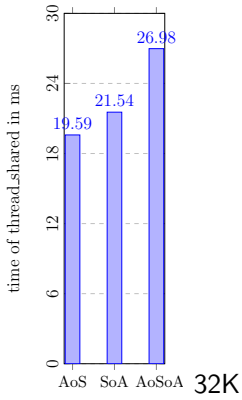


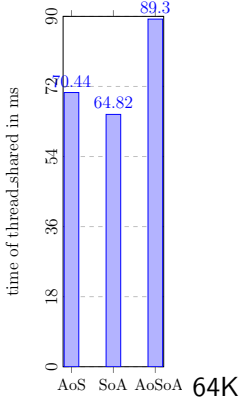


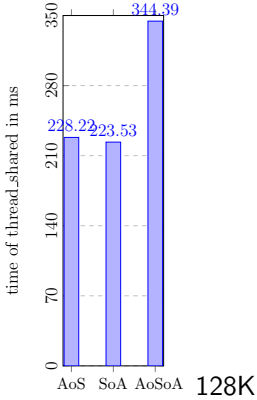


Compare the memory structures - on 1070

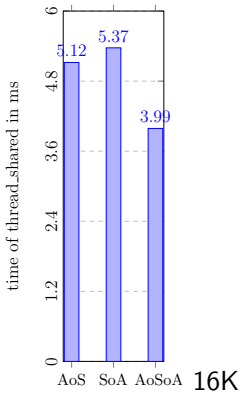


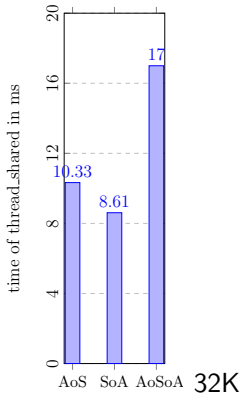


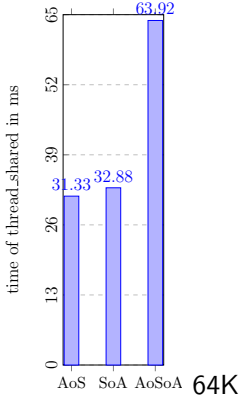


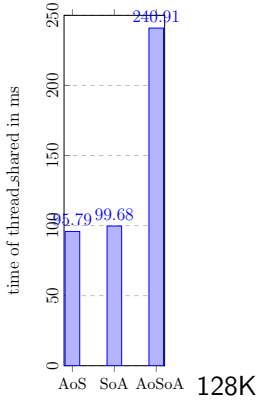


Compare the memory structures - on RTX 2080









Conclusion

- AoSoA can be optimized, but ...
- AoS or SoA heavily depends on architecture $\rightarrow$ just take the easier implementation

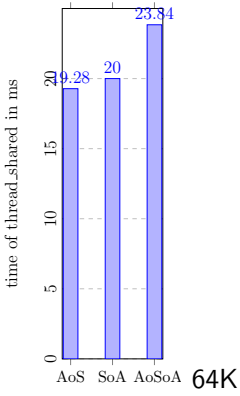
Performance of AoSoA on 16K

- has nothing to do with the mem layout
- SMs aren't fully occupied
- we configured 32 threads per block

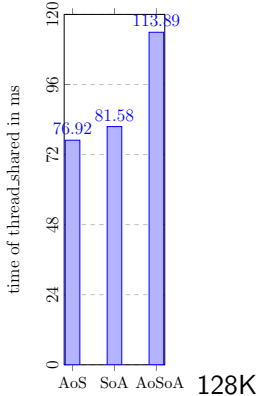
AoS vs SoA

- performance AoS vs SoA are somewhat equally
- contrary to facts from the lecture $\rightarrow$ WHY?
- K80, v100, and RTX 2080 have configurable L1 chaches (we chose 32KiB)
- also read-only data cache for K80 (48KiB), for 1070 (no RODC) $\rightarrow$ AoS behaves differently
- that could be the reason why AoS can be better than SoA (bigger chache)
- guess: at bigger n AoS can't catch up? but ...

On v100 with 2 million particles

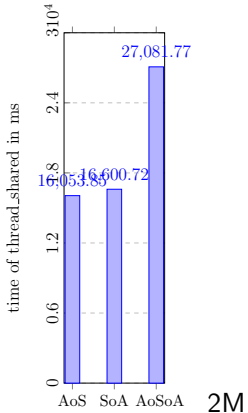


64K



128K

...



2M

The Explanation?

- we don't really know
- cache hierarchy is dynamic and complex, e.g.

K80	48 RODC	dyn. 16-48 L1	(it's 32 in our case)
V100	128 UDC	rest L1	(it's 96 in our case)
RTX 2080	96 UDC	rest L1	(it's 64 in our case)
1070	– RODC	48 L1	

*values are given in KiB

RODC ... read-only data cache
UDC ... unified memory cache

What else could we try?

- use texture memory (indirectly we already do that)
  - $\rightarrow$ mass never changes
- use surface memory? tensor cores?
- change computation (not part of the task)
- optimize AoSoA (not sure if it will be better compared to SoA)

Validation

Two ways:

- **visualize** a 3-body problem with our code, see if it's right
- **compare** with reference computation (use reference values)