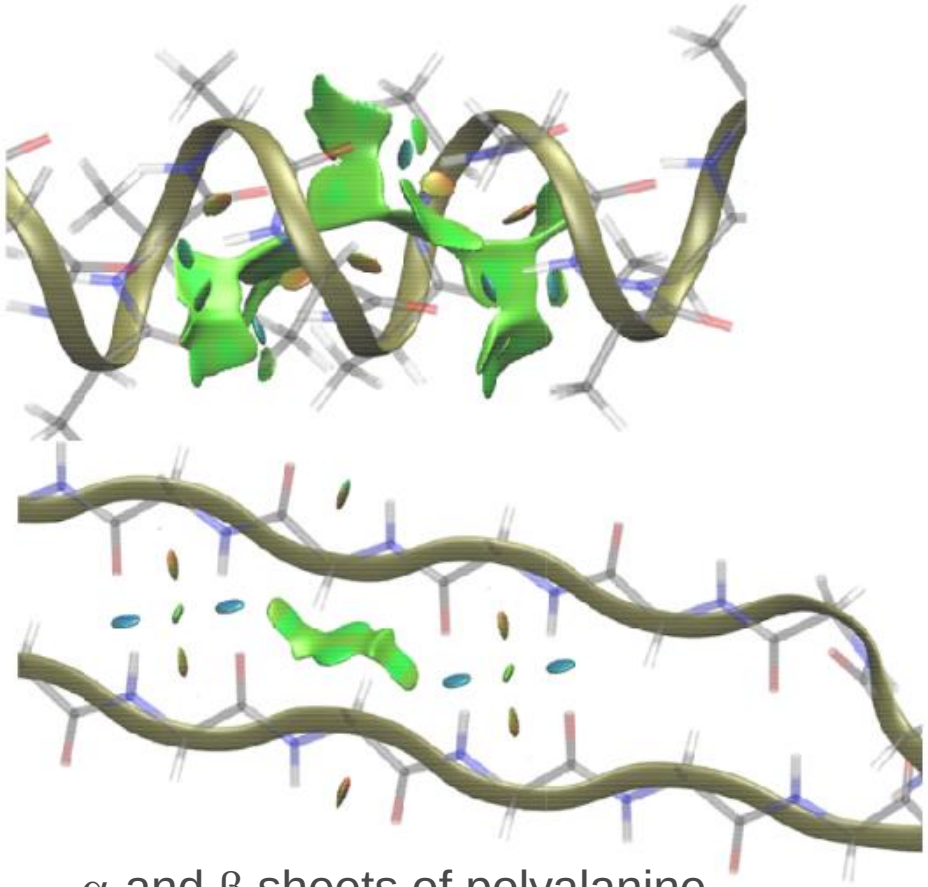
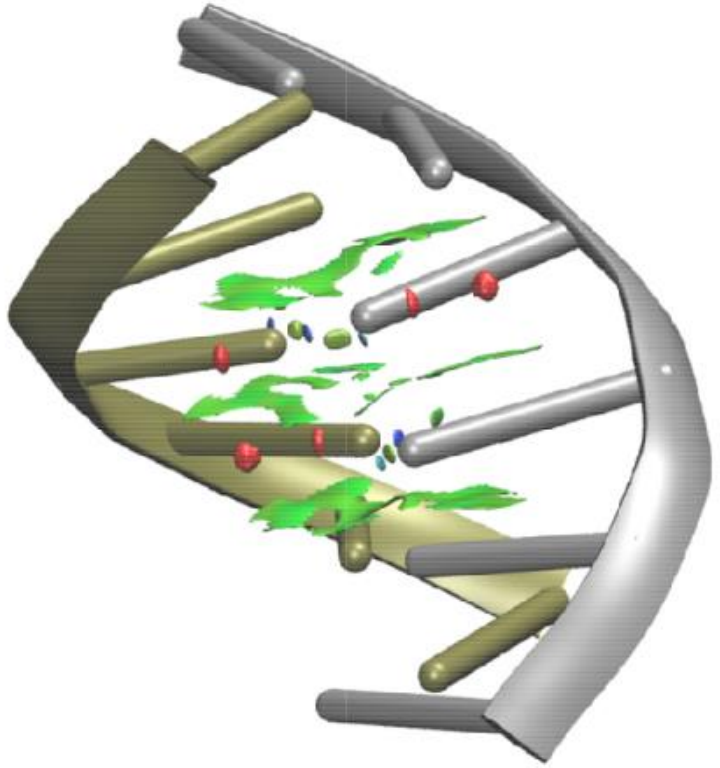
Application examples



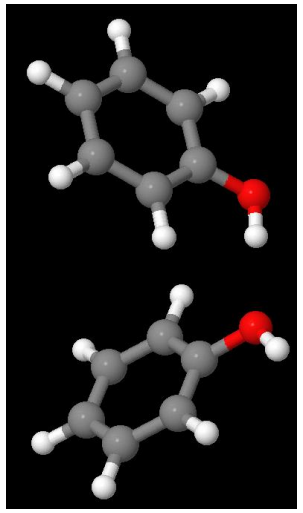
α and β sheets of polyalanine



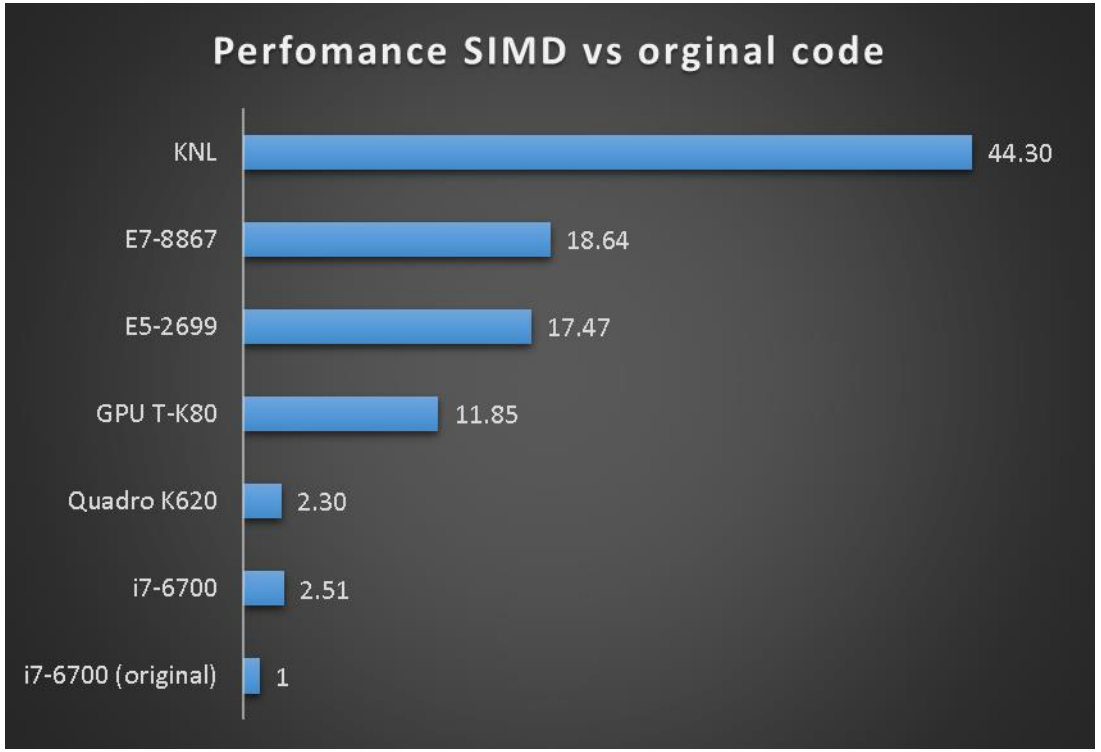
Double helix DNA strands

*Author: nciplot team

SIMD code comparison



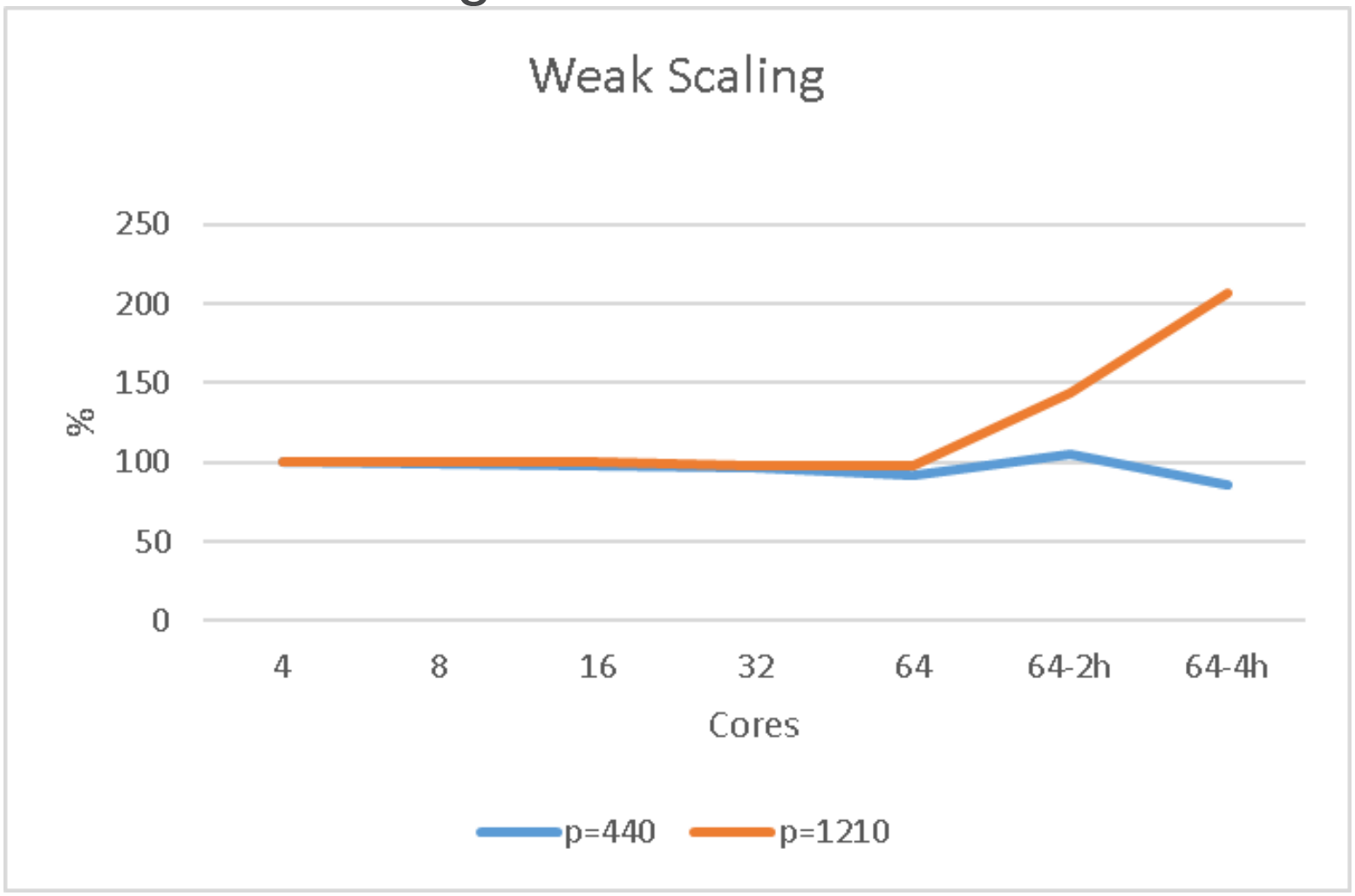
Phenol dimer - 2(C6OH6)
Method : B3LYP/6-31G*
Primitives : 440
Total points : 872040



i7-6700:	8 threads
Xeon E5-2699:	72 threads
Xeon E7-8867:	64 threads

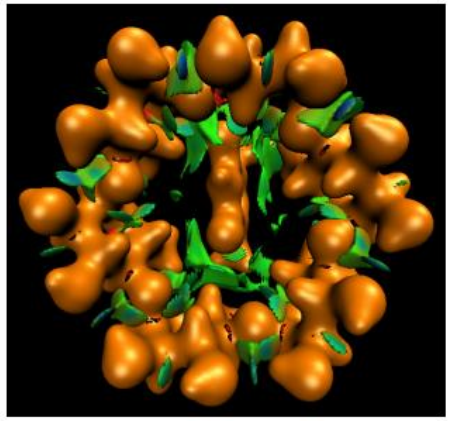
* More is better

Weak Scaling in KNL

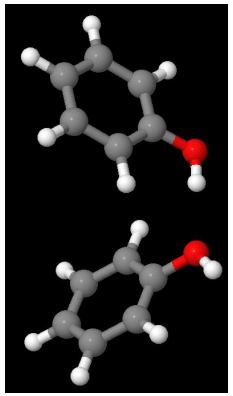


p = primitive functions

Ciclodextrine

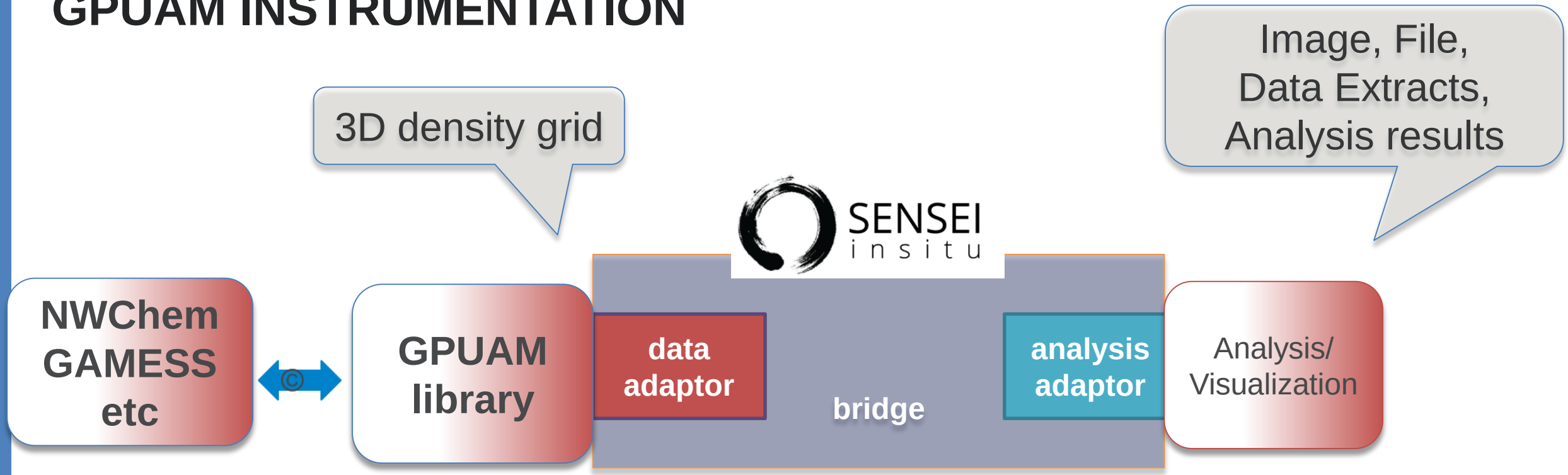


Phenol



*More is better
**Also more points

GPUAM INSTRUMENTATION



Analyst can be remote

Analysis performed on all timesteps
➔ NO SCIENCE LOST

Conclusions and Insights

- Reusing allocated memory space was key to beat accelerators
- Intensive workload per thread and vectorization matters in KNL more than in other many-core processors
- SIMD instructions used Xeon not always give faster code. But in KNL, SIMD could make a big difference.
- OpenMP affinity should be properly chosen to use cores and hyper threading more efficiently

- KNL could be used as visualization processor for chemical properties

- Future work
  - When is possible replace loops for vector operations and use of tiles to optimally saturate registers. More loop fission.
  - Offer a library for quantum chemistry and visualization codes for on-the-fly evaluations
  - MPI version, need partitioning of space to distribute over ranks
  - Bridge to Sensei is in progress