Application examples

\[ \alpha \text{ and } \beta \text{ sheets of polyalanine} \]

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

Weak Scaling

Cyclodextrine

Phenol

\[ p = \text{primitive functions} \]

*More is better
**Also more points

Computational Sciences Division & Argonne Leadership Computing Facility
GPUAM INSTRUMENTATION

3D density grid

GPUAM library

data adaptor

analysis adaptor

bridge

Analyst can be remote

Analysis performed on all timesteps → NO SCIENCE LOST

Image, File, Data Extracts, Analysis results

NWChem, GAMESS, etc

Analysis/Visualization

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