EMSL

Pacific Northwest NATIONAL LABORATORY

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U.S. DEPARTMENT OF ENERGY

Gaussian molecular electronic structure

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Acknowledgement

- Most material presented here: stolen from submitted whitepapers
- Re-digested and re-filtered through my own perspective

Computational Chemistry in 2020

- I don't know what the programming language of the future is going to look like, but it is going to be called **Fortran**
- I don't know what the parallel programming framework of the future is going to look like, but it is going to be based on **MPI**
- ….

HW changes requiring SW changes

- HW Changes: Multi-Core, Accelerators, etc …
- Intra-node parallelism to go beyond Message-Passing paradigm (or – in my case Global Arrays)

- Innovative Approaches:
  - Task-based approaches
  - Work stealing
  - Directed Acyclic Graph (DAG)
- ….

Hybrid computing a.k.a. Intra-node //sm

Complements the of MPI inter-node //sm

- Directives/Pragmas: OpenMP, OpenACC, LEO
- Cilk
- Intel TBB
- pThreads
- Multi-threaded BLAS

Advantages:

- Better memory utilization
- finer grain parallelism

Let's raise our voice!

Chemistry community input in emerging standards

- Is OpenMP emerging as a standard?
- Let's try to influence the inclusion of new features in OpenMP (e.g. acceletors)
- Become early adopters of new MPI features
- Play with PGAS

Community Effort & Open-Source

Why?

- Avoid wasting energies replicating the same effort too many times, e. g.
  - Evaluation of Gaussian Integrals
  - Tensor libraries
  - XC functional libraries
- Strengthen inter-operability among codes (so that users use code X when it's right to use code X)
- Adoption of open-source license the facilitate all of the above
- …

A Possible Community Effort?

Data Abstraction layer for

Distributed Multi-D Dense Matrices

- Global Arrays, DDI-, SIAL, DLSs, etc … why?
- Can't we agree to a common standard?
- Compile a small set of specifications, i.e. a common subset
- diversity still possible when building on top of this common kernel of specs

Educational Aspects

- Motivate young scientist towards the area of software development
- Stop the blind use of canned software packages
- Create SW development environments that are user-friendly?

thank you