Software development strategy in the TREX Center of Excellence

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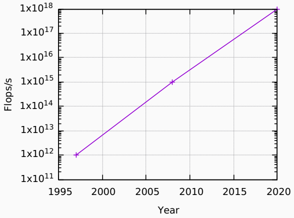
Disclaimer: Currently in the process of signing the Grant Agreement with the EU

Exascale

The supercomputing race

Worldwide technological competition

- 1997 : Teraflops/s[1]
- 2008 : Petaflops/s
- 2020? : Exaflops/s



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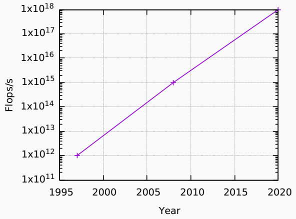

- Expected increase of computational power is *exponential*
- Moore's Law is ending
- Technological breakthrough needed (quantum computing?)

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Peak flops/s improved by $1000\times$. What about

- Memory capacity per core?
- Memory bandwidth? latency?
- I/O bandwidth? latency?
- Network bandwidth? latency?

Simple Math

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Computational power

- 24 cores
- 2.5 GHz $= 2.5\,10^9$ cycles/s
- Fused multiply-add (FMA) : 2 flops/FMA
- 512 bit vectors : $\times 8$ flops in double precision
- $24 \times 2.5\,10^9 \times 8 \times 2 =$ 960 Gflops/s

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Memory bandwidth

- 2666 MHz $= 2.666\,10^9$ cycles/second
- 8 bytes / cycle
- 6 memory channels
- $2.666\,10^9 \times 6 \times 8 =$ 128 GB/s

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- 2 flops
- 3 loads + 1 store : $4 \times 8 = 32$ bytes
- Arithmetic intensity : $2/32 =$ 0.0625 flops/byte

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0.8% of the peak is expected for this loop, if streamed from memory.

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A100 GPU

- 9.7 Tflops/s
- 1.555 TB/s
- Required arithmetic intensity on GPU: (9.7 Tflops/s) / (1.555 TB/s) = 6.2 flops/byte

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Streaming from memory is slower than on CPU

A few words on Quantum Monte Carlo

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- Scalable : YES

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  We can trivially run many trajetories in parallel
- Easily : NO!

For *exascale simulations*, we need to be massively parallel *and* efficient.

A few words on Quantum Monte Carlo

Efficiency

- Small systems $\equiv$ small matrices $\Longrightarrow$ *low arithmetic intensity*
- Very large systems $\Longrightarrow$ linear-scaling algorithms $\Longrightarrow$ very low arithmetic intensity by nature

Parallelism within a trajectory

- DMC trajectories need to be *ergodic*, and one trajectory is *sequential* by nature
- One trajectory performs $\sim$10M–100M steps $\Longrightarrow$ one step $\sim$ 1 millisecond

Exploiting parallelism improve the efficiency is difficult

Software development

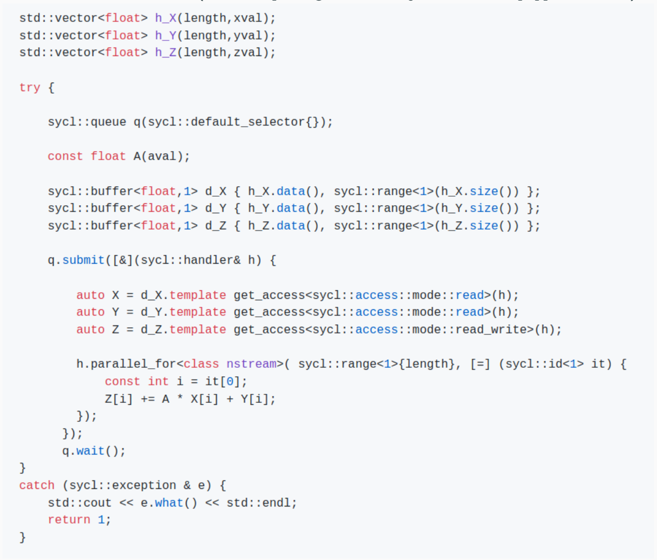
Programming for the exascale

- Progress in quantum chemistry may require codes with new ideas/algorithms
- New ideas/algorithms are implemented by physicists/chemists
- Exascale machines will be horribly complex

Is it reasonable to ask physicists/chemists to write codes for exascale machines?

No: Proof

Vector addition (from `https://github.com/jeffhammond/dpcpp-tutorial`)



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try {

    sycl::queue q(sycl::default_selector{});

    const float A(aval);

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        h.parallel_for<class nstream>( sycl::range<1>{length}, [=] (sycl::id<1> it) {
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        });
      });
      q.wait();
}
catch (sycl::exception & e) {
    std::cout << e.what() << std::endl;
    return 1;
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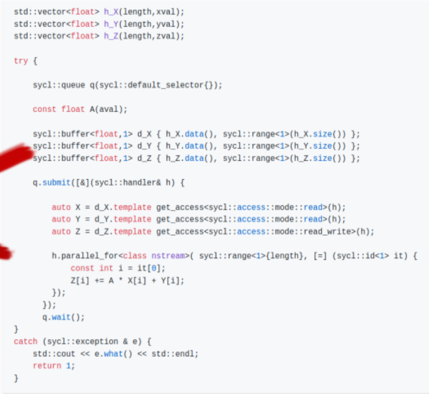

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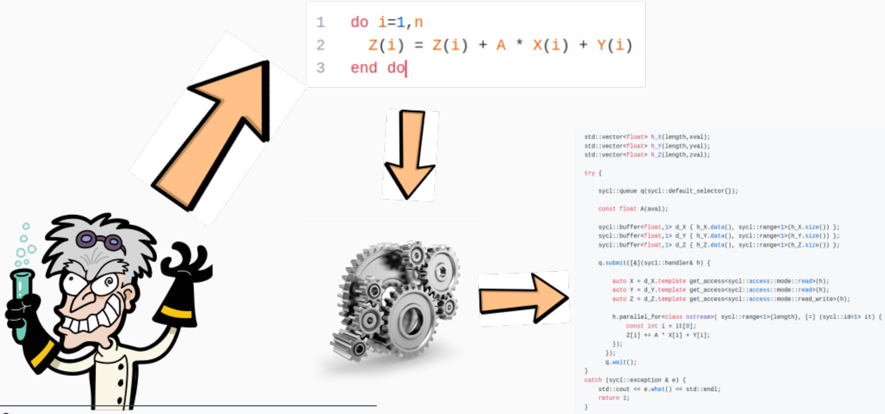
The dream

A compiler[2] that can read an average researcher's code and transform it into highly efficient code on an exascale machine.



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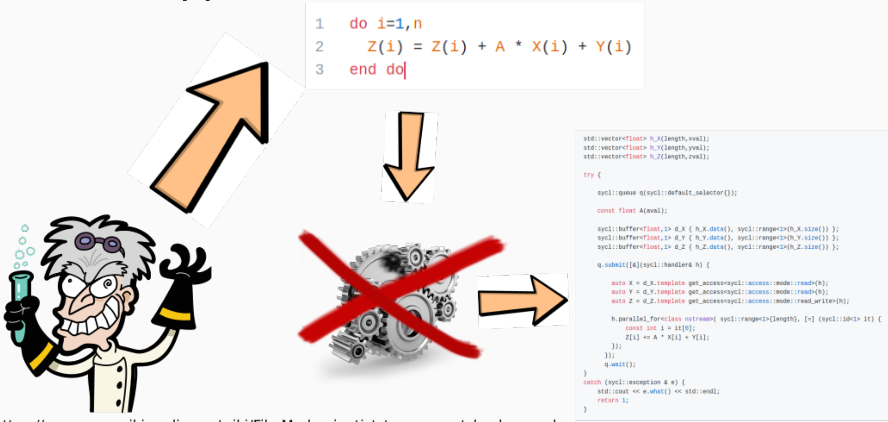
[2]Wikipedia: A compiler is a computer program that translates computer code written in one programming language (the source language) into another language (the target language)

Reality

“AI” is not ready yet . . .



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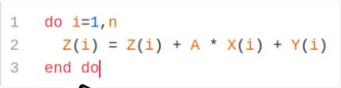
Reality

. . . so let's use "NI" and add a human layer between the machine and the researchers : a *bio-compiler*



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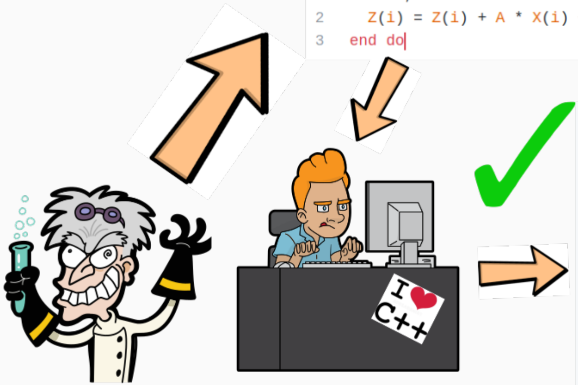

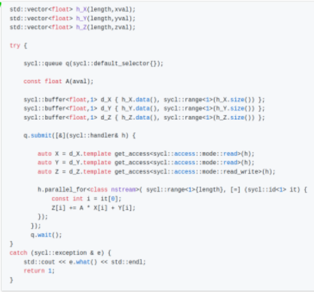

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5. HPC experts *bio-compile* it in high-performance implementations
6. Integrate the library in TREX codes

A very old and successful practice

- BLAS/Lapack (Linear Algebra)
- MPI (Communication)
- FFTW (Fourier transforms)
- OpenMP (shared-memory parallelism)
- OpenGL (3D graphics)
- MPEG (Audio/Video encoding/decoding)
- Video game rendering engines

$\vdots$

Benefits of this model

For scientists

- We don't impose a programming language
- Codes will not die with a change of architecture

Separation of concerns

- Scientists will never have to manipulate low-level HPC code
- HPC experts will not be required to be experts in theoretical physics

Conclusion

"*QMC can scale easily*" assumes that one can efficiently compute one trajectory.
Using efficiently the hardware to accelerate the realization of one trajectory is the challenge that will be taken by QMCkl to enable easy scalability.