Large-scale and user-friendly exact diagonalization in Chapel

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Radboud University

- Located in Nijmegen — the oldest city in the Netherlands;
- In 2010 Andre Geim and Konstantin Novoselov got a Nobel Prize in Physics for the discovery of graphene;
- Strong Programming Languages department: Clean, SAC (Single Assignment C);

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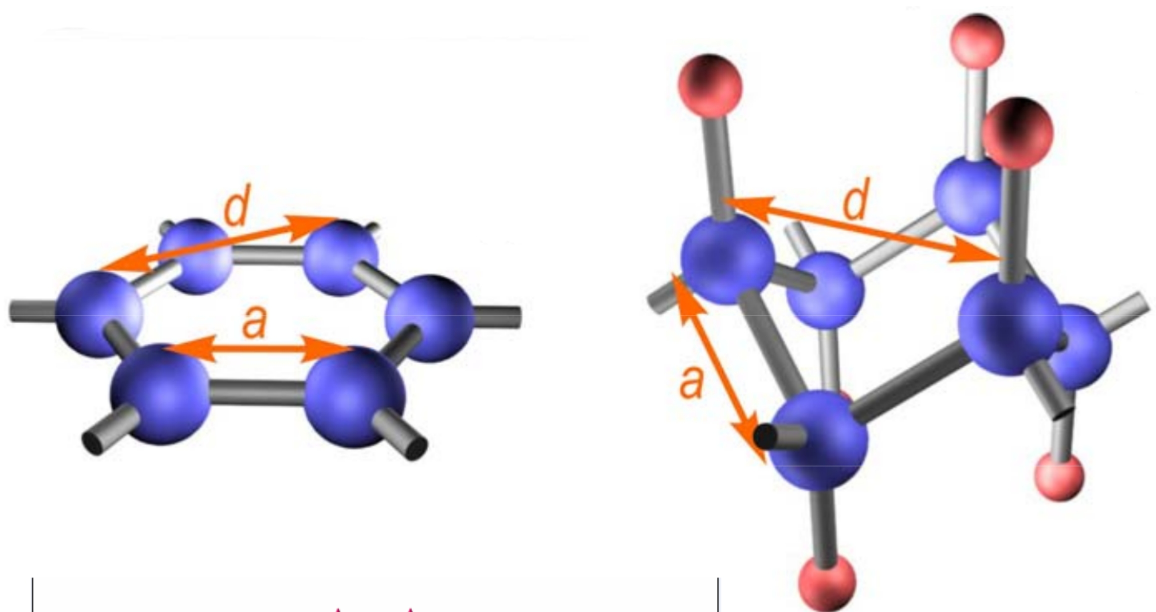
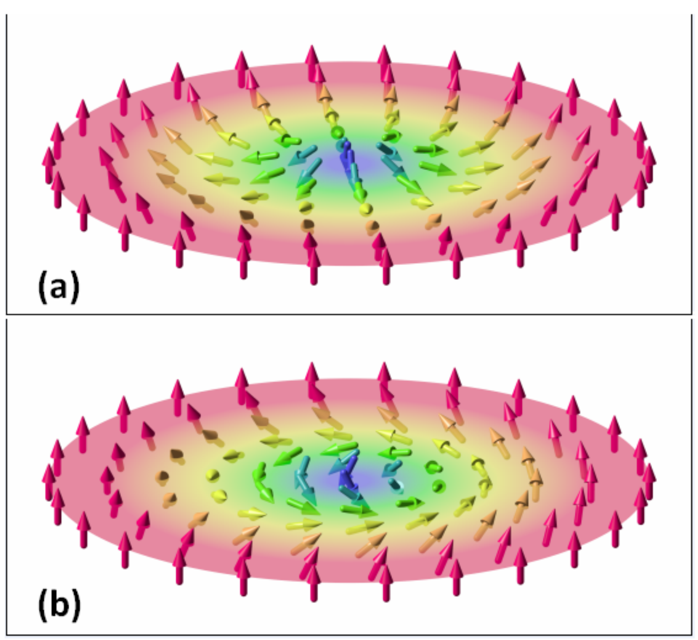
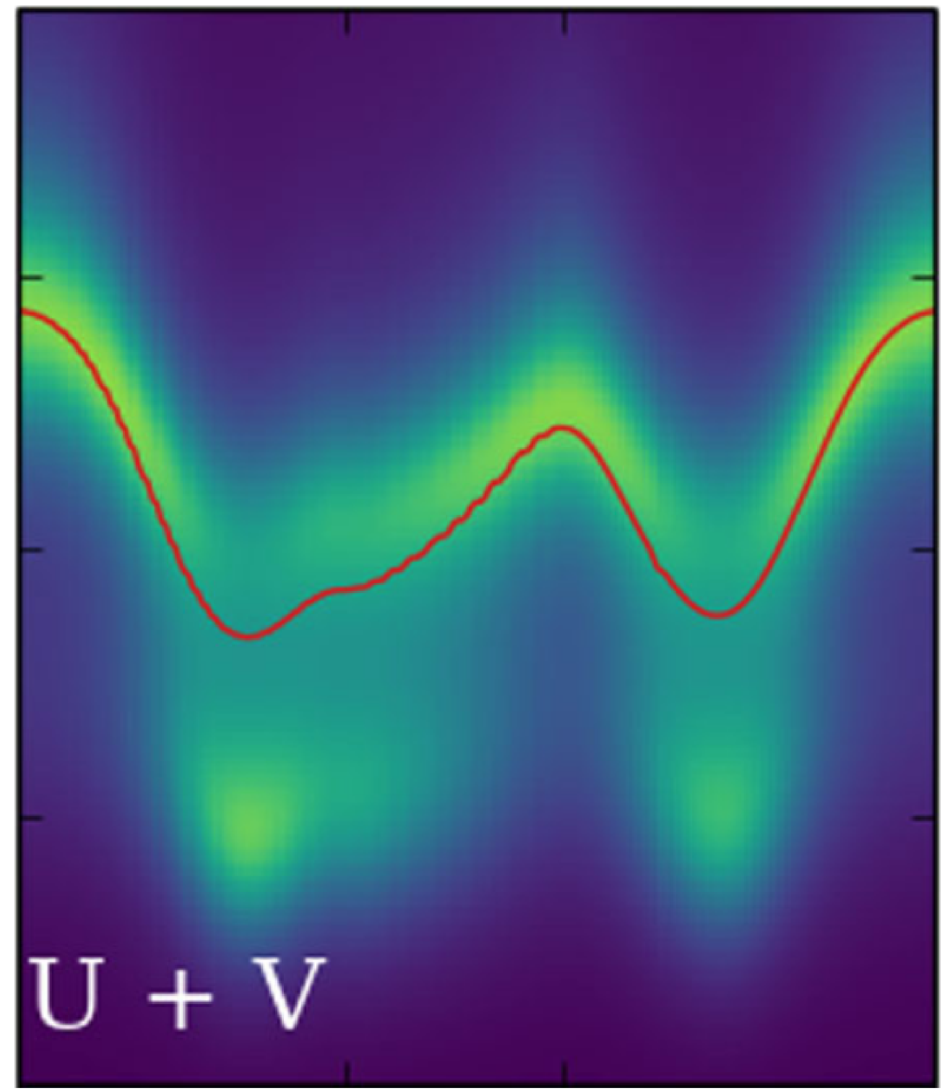
Theory of Condensed Matter department

- Our research aims to predict and explain the properties of condensed matter.
- We utilize and develop advanced mathematical frameworks and state-of-the-art numerical approaches.







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Exact diagonalization

A numerical technique to simulate small quantum systems.

Goal:

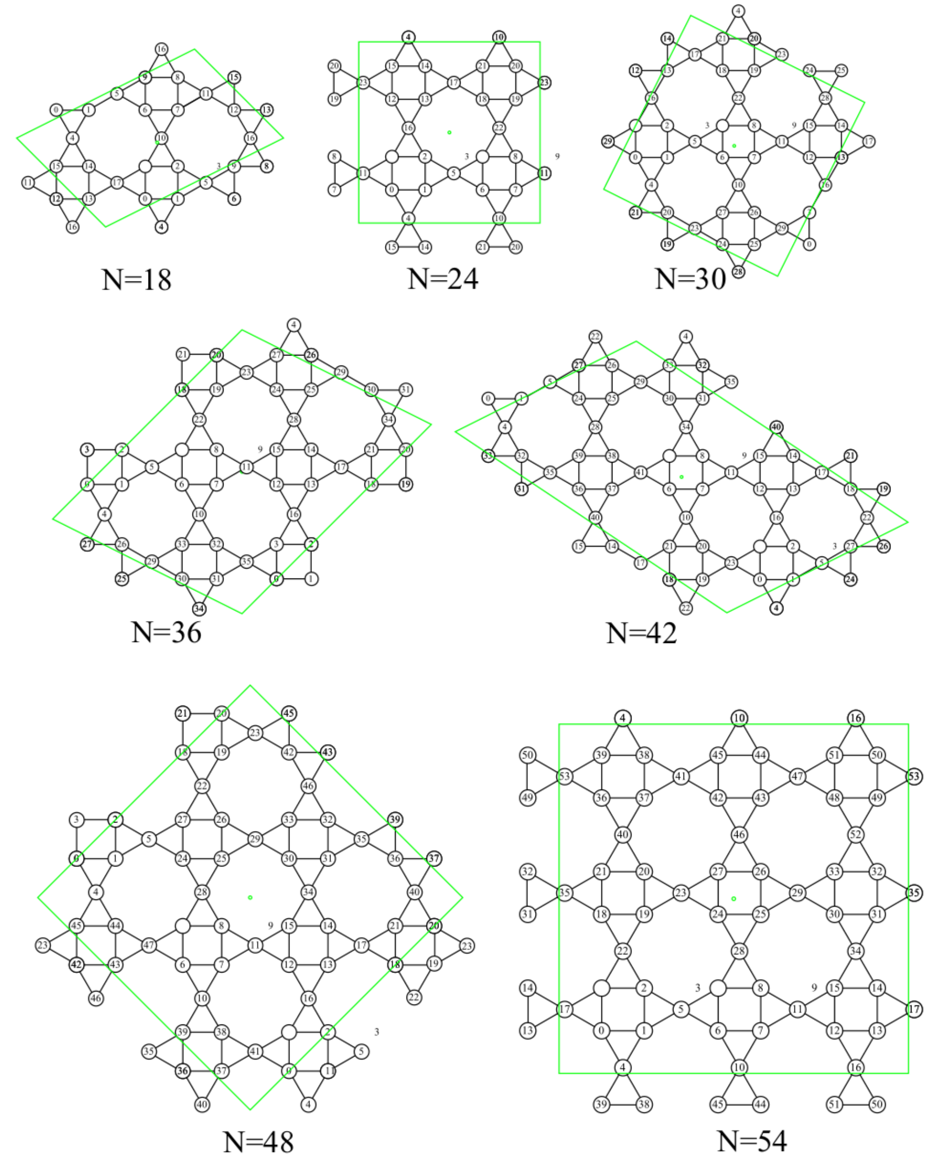
Competitive performance
while preserving user friendliness.

Constraint:

Limited developer time.

Approach:

A mix of languages among which Chapel.



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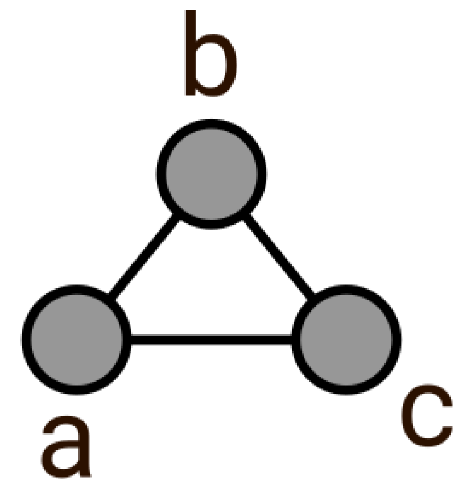
Exact diagonalization

- Physical system is described by a matrix H, the *Hamiltonian*.
- Eigenvalue problem (i.e. find a scalar E and a vector v such that $Hv = Ev$).

$$
\begin{aligned}
H &= \sigma_a \otimes \sigma_b + \sigma_b \otimes \sigma_c + \sigma_a \otimes \sigma_c \\
&= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \mathbb{I} \\
&+ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \mathbb{I} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&+ \ldots
\end{aligned}
$$

$|\uparrow\rangle$ $|\downarrow\rangle$



$$
\begin{gathered}
|\downarrow\downarrow\downarrow\rangle \\
|\downarrow\downarrow\uparrow\rangle \\
|\downarrow\uparrow\downarrow\rangle \\
|\downarrow\uparrow\uparrow\rangle \\
\ldots
\end{gathered}
$$

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Challenges

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Fix Hamming weight

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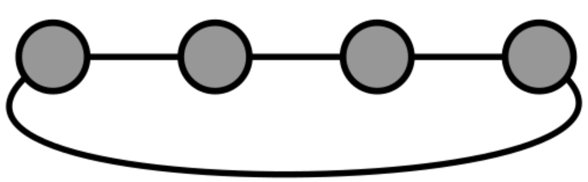

Translation invariance

$|\downarrow\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\uparrow\downarrow\rangle, |\uparrow\uparrow\downarrow\downarrow\rangle, |\uparrow\downarrow\downarrow\uparrow\rangle$
$|\downarrow\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow\uparrow\downarrow\rangle$

Target: 50 spins

- $10^{15} \times 10^{15}$ matrix (8PB for one vector);
- with symmetries — $10^{11} \times 10^{11}$ (15.5TB for the simulation);

- Exponential scaling of resources (both memory and compute);
- Trading memory for computations;

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lattice_symmetries
(old architecture)

high-level functions;
algorithm prototyping

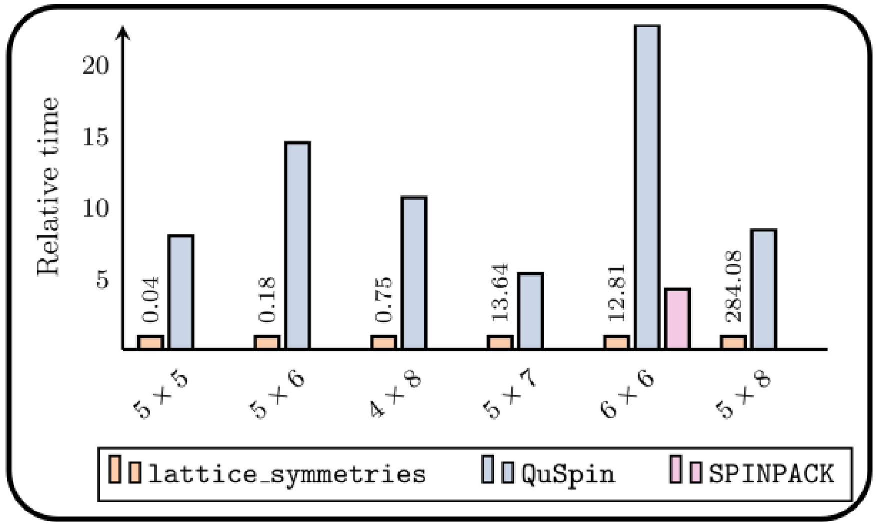
Python wrapper module

simple interface;
portable static executable

Haskell application

C++ library
SIMD for kernels

kernels for a few processors;
runtime dispatch to the right one;
x86-64 only



Tom Westerhout. Journal of Open Source Software 6, 64 (2021), 3537.

C++ library
SIMD for kernels

high-level Haskell code

low-level C code

Halide kernels

How about embedding Halide into Chapel?

Faster than my hand-written intrinsics kernels;
can now compile to x86, ARM, and GPUs!

"Halide is a programming language designed to make it easier to write high-performance image and array processing code on modern machines."

```
Func blur_3x3(Func input) {
  Func blur_x, blur_y;
  Var x, y, xi, yi;
  // The algorithm - no storage or order
  blur_x(x, y) = (input(x-1, y) + input(x, y)
                 + input(x+1, y))/3;
  blur_y(x, y) = (blur_x(x, y-1) + blur_x(x, y)
                 + blur_x(x, y+1))/3;
  // The schedule - defines order, locality;
  // implies storage
  blur_y.tile(x, y, xi, yi, 256, 32)
        .vectorize(xi, 8).parallel(y);
  blur_x.compute_at(blur_y, x).vectorize(x, 8);
  return blur_y;
}
```

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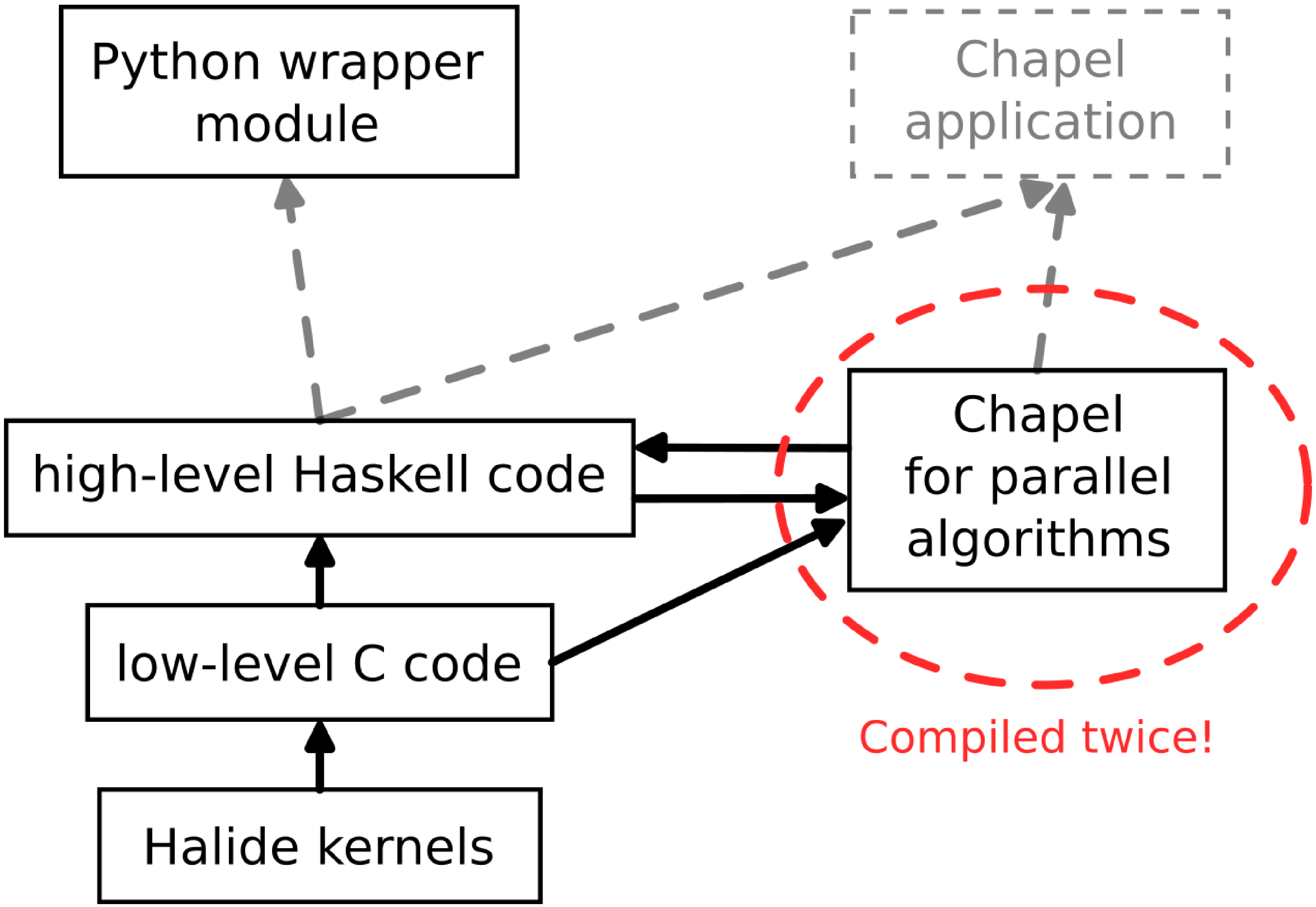
OpenMP → Chapel

- Potential for multi-node parallelism;
- In single-locale setting, we can still generate a standalone shared library;
- Simpler and shorter code;

New architecture



Singularity

1. Debian with custom OpenMPI;
2. Chapel with `CHPL_LAUNCHER=none`:
    - `CHPL_COMM=none`
    - `CHPL_COMM=gasnet` & `CHPL_COMM_SUBSTRATE=mpi`
    - `CHPL_COMM=gasnet` & `CHPL_COMM_SUBSTRATE=ibv`
3. Our project;
4. Minimal release container based on Busybox;

```
# On your laptop
singularity exec hello-world.sif /project/bin/none/hello6-taskpar-dist
# On our local cluster (ethernet)
mpirun -np 3 singularity exec hello-world.sif /project/bin/mpi/hello6-taskpar-dist -nl 3
# On the Dutch National supercomputer
salloc -N 20 --ntasks-per-node=1 --exclusive \
  srun -n 20 singularity exec hello-world.sif /project/bin/ibv/hello6-taskpar-dist -nl 20
```

Current limitations

- Performance of distributed implementation should be improved;
  Thanks to Engin Kayraklioglu and Ben Harshbarger we now have a plan 😃
- Non x86-64 architectures should work, but ...

Chapel feature requests

- Compile times;
- Tools for profiling;
- `ref` record & class attributes
  (currently using `c_ptr` as a hack);

Conclusion

- Exact diagonalization — a method to simulate small quantum systems;
- Exponential scaling of compute resources — need distributed parallelism;
- We mix Halide, C, Haskell, Python, and Chapel to reduce the amount of code (800 lines of C, 3500 lines of Haskell, 2000 lines of Chapel) vs. other projects with >25000 lines;
- Singularity as the packaging mechanism;

Next step: performance tuning

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