Towards a Unified Numerical Framework for Quantum Mechanical Simulations

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Abstract

- State-of-the-art simulations often need to utilize high-performance computing (HPC) to be feasible...
- ..., but HPC architectures are getting more complex and diverse.
- No optimization → 4 - 5 orders of magnitude slowdown
- Manual optimization might not be viable for everybody.
- We have developed the Qubus tensor framework to mitigate this problem.

Key features

- Syntax inspired by mathematical notation.
- Architecture-independent interface + auto-parallelizing optimizer and runtime
- →no need to ...
  - know about architecture specifics (SIMD, Caches, ...).
  - manually parallelize and synchronize execution.
  - worry about data distribution and communication via MPI.
- Out-of-the-box support for a diverse set of architectures (x86, CUDA, Xeon Phi, ...).

Efficiency via high-level optimizations

Math

$$\Sigma_{ij}^{<,\mathrm{2B}}(t_a,t_b) = \sum_{klmnrs} w_{ikms}\left(w_{ljrm} - w_{njrl}\right) G_{kl}^{<}(t_a,t_b) G_{mn}^{<}(t_a,t_b) G_{rs}^{>}(t_b,t_a)$$

User code

```
tensor_expr<double, 4> w = get_interaction(params); // Polymorphic function

tensor_expr<complex<double>, 4> Sigma =
   def_tensor (i, j, ta, tb) [ sum(w(i, k, m, s) * (w(l, j, r, n) - w(n, j, r, l)) *
                                   Gl(k, l, ta, tb) * Gl(m, n, ta, tb) * Gg(r, s, tb, ta), {k, l, m, n, r, s}) ];
```

Interaction tensor

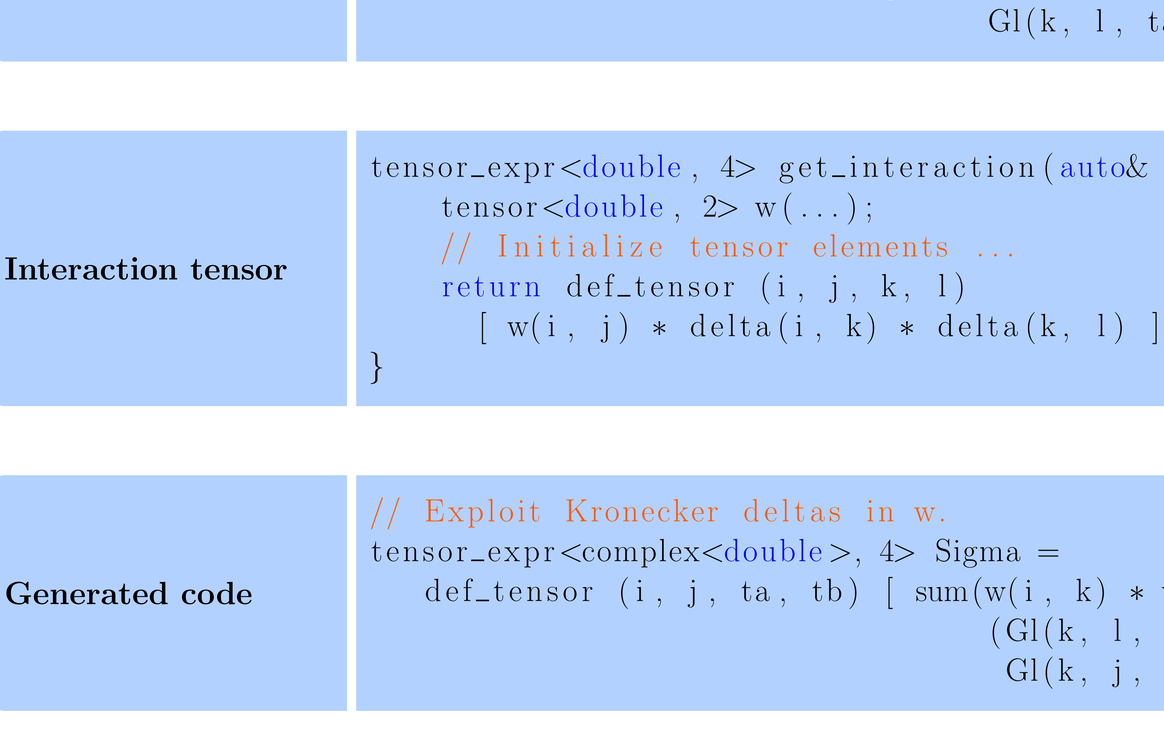
```
tensor_expr<double, 4> get_interaction(auto& params) {
    tensor<double, 2> w(...);
    // Initialize tensor elements ...
    return def_tensor (i, j, k, l)
      [ w(i, j) * delta(i, k) * delta(k, l) ];
}
```

Just one possible implementation.

Generated code

```
// Exploit Kronecker deltas in w.
tensor_expr<complex<double>, 4> Sigma =
   def_tensor (i, j, ta, tb) [ sum(w(i, k) * w(l, j) * Gg(l, k, tb, ta) *
                                   (Gl(k, l, ta, tb) * Gl(i, j, ta, tb) -
                                    Gl(k, j, ta, tb) * Gl(i, l, ta, tb)) , {k, l}) ];
```

Matrix multiplication benchmark



Matrix multiplication using Qubus

Math $C_{ij} = \sum_k A_{ik} B_{kj}$

Code

```
index i, j, k; // Declare abstract indices.

// Declare double-precision tensor variables of order 2.
tensor<double, 2> A(N, N);
tensor<double, 2> B(N, N);
tensor<double, 2> C(N, N);

C = def_tensor(i, j) [ sum(A(i, k) * B(k, j), k) ];
```

Example is fully parallelized.

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LaTeX TikZposter