Automating Many-Body QM

Ed Valeev
Department of Chemistry
Virginia Tech

ESNT Workshop “Automated Tools for Many-Body Theory”
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Saclay, France

Talk Synopsis

need to raise the level of abstraction to enable many-body QM

symbolic techniques are a component of the needed many-body QM technology stack

particularly needed for supporting tensor compressed/factorized methods (e.g., PNO)

ideas are old, let's learn from the pioneers and make this sustainable

Outline

- Motivation: Richness of Tensor Algebras in Quantum Mechanics
- Technology Roadmap for Many-Body QM
- SeQuant
  - Overview
  - Key innovations
- Ongoing/Future work

Tensors

Tensors in Quantum Mechanics

Tensor structures arise naturally, and with great(est) variety

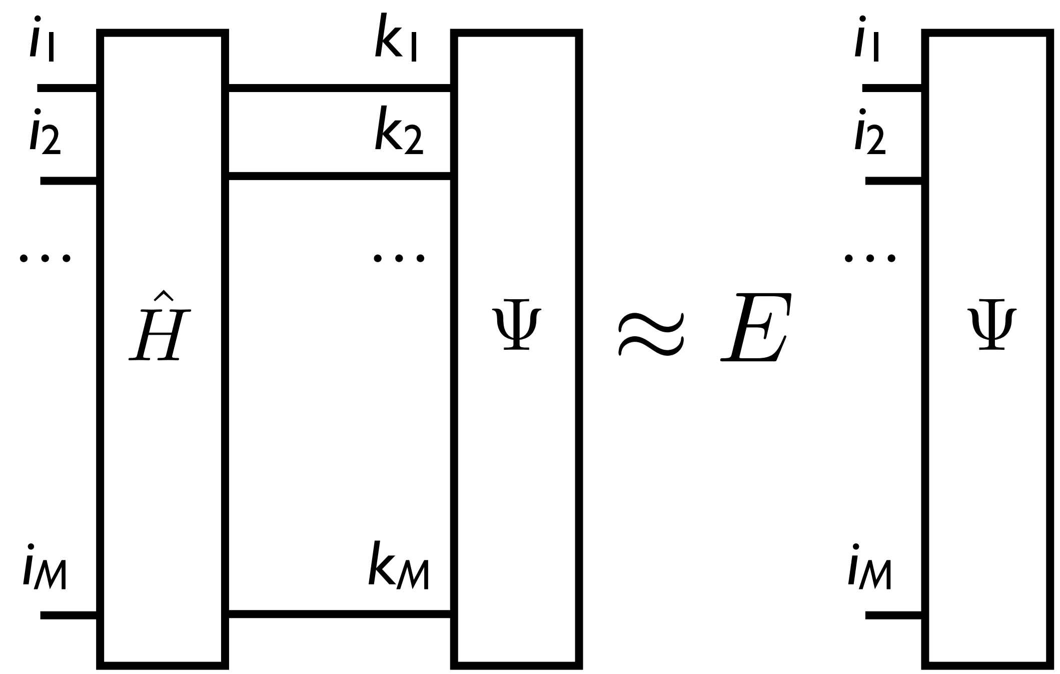
key objects are *fields* i.e. functions of space(time) coordinates	➧	tensor *meshes* and other PDE technologies
n-particle QM is *polylinear* state = tensor of order O(n)	➧	*high*-order tensors
states are *data-sparse* at least all(?) states we care about	➧	tensor *networks* of *many* kinds built out of *block/rank-sparse* tensors

To make sense of this and understand the relevant problem scales let's start with a few pictures

QM States and Their Properties/Changes Are Tensors

N-Body Schrödinger Equation = Tensor Eigenvalue Problem

$$\hat{H}\Psi = E\Psi \quad \Longrightarrow$$



Important simplifications

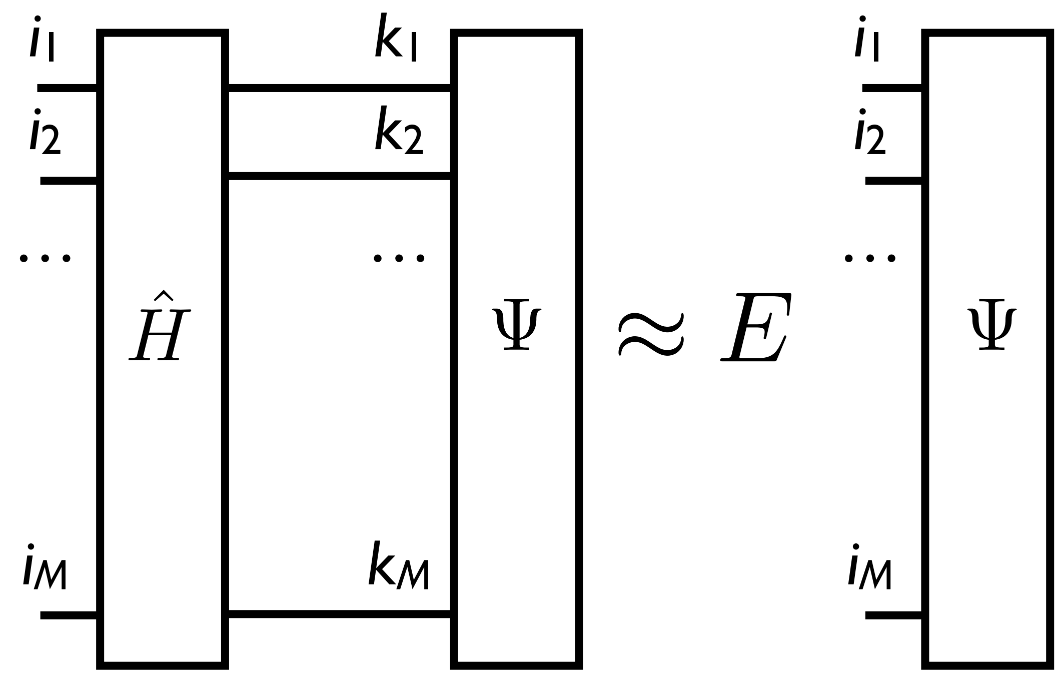
1. *H* is very sparse: up to 2 output indices can differ from the input indices for 2-body *H*

2. For most important states **Ψ** is also sparse in good basis

Properties of Quantum States Are Also Tensors

N-Body Schrödinger Equation = Tensor Eigenvalue Problem

$$\hat{H}\Psi = E\Psi \quad \Longrightarrow$$



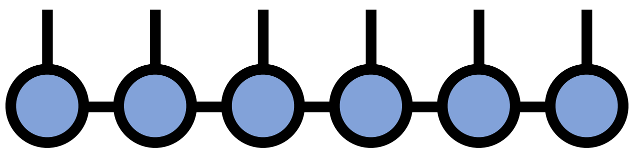
Example: N_2 molecule

N=14 M=60 (cc-pVTZ basis)

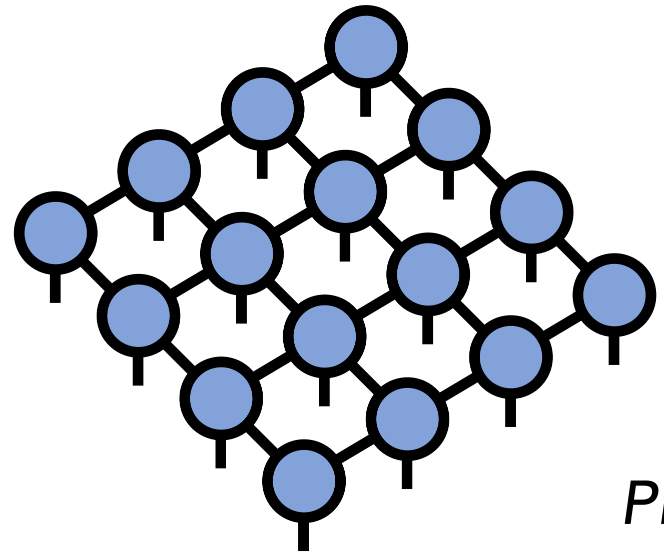
size(**Ψ**) = 1.5 x 10^{17} but only <10^9 elements are significant!

element sparsity can be useful, but essential to exploit general data sparsity in H and **Ψ**

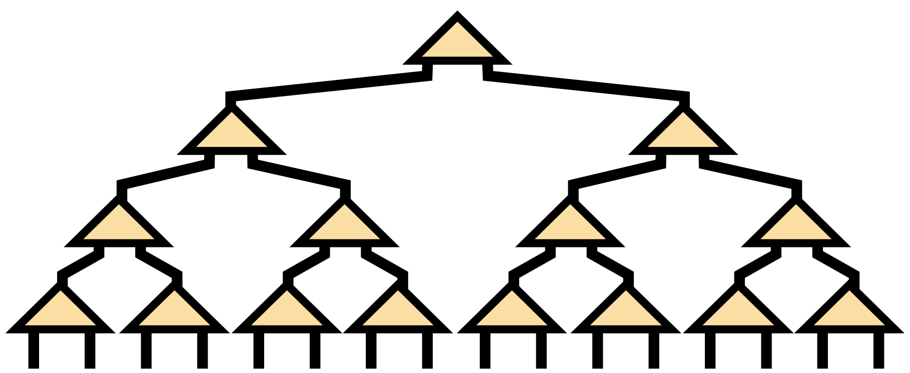
Reducing Complexity v1: Tensor Networks



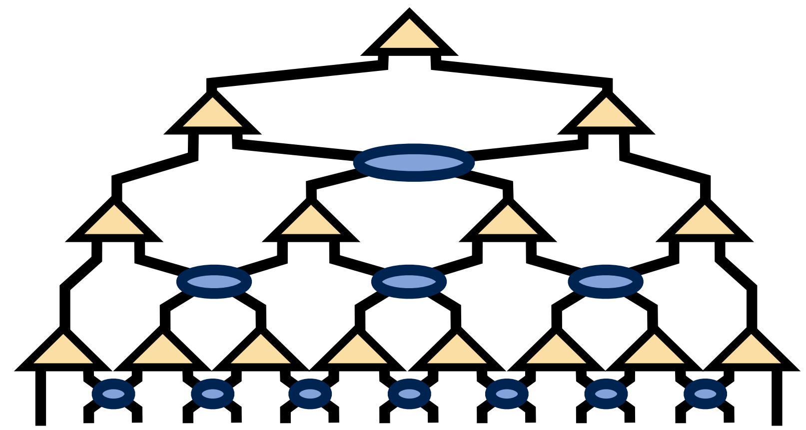
matrix product state (MPS), or tensor-train



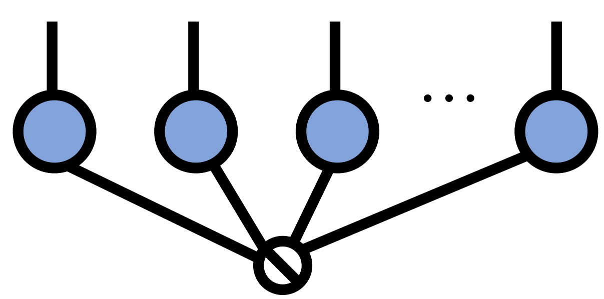
PEPS



tree tensor network (TTN)



MERA



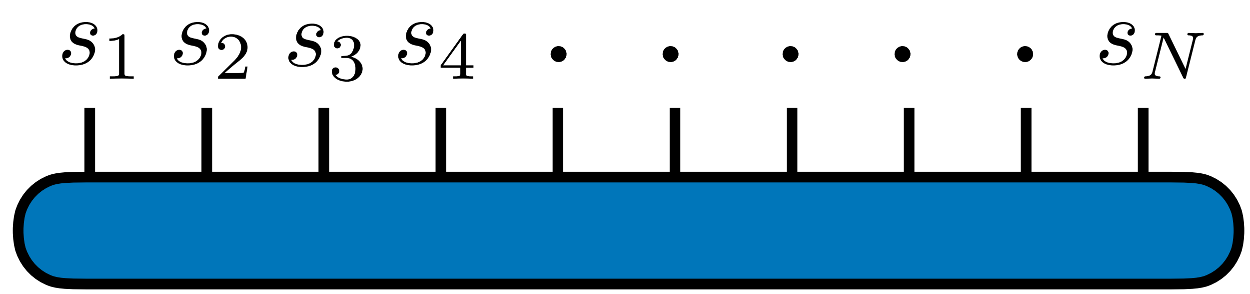
CP

physics, sometimes chemistry

Reducing Complexity v2: Cumulant/Perturbative Expansion

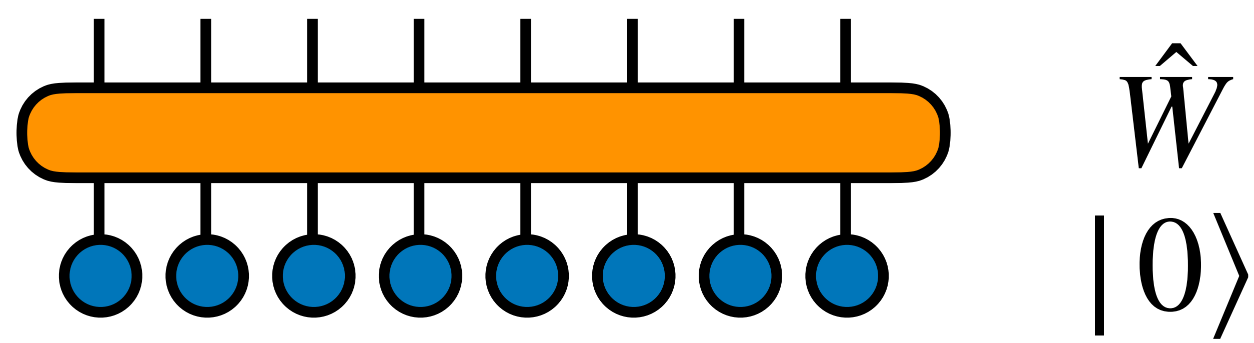
instead of encoding joint probability amplitudes

$$|\Psi\rangle \equiv$$



encode differences in probability amplitudes relative to simple (usually, uncorrelated) state

$$|\Psi\rangle \approx \hat{W}|0\rangle$$



efficient if *W* limited to a sum of few-body terms (e.g, 2-body in CCSD)

tensor ≈ sum of tensor networks

chemistry and physics

Cumulant/Perturbative Expansion: Coupled-Cluster

$$|\Psi\rangle = \exp(\hat{T}_2 + \hat{T}_3 + \ldots + \hat{T}_N) \;\times\; \widetilde{|0\rangle}$$

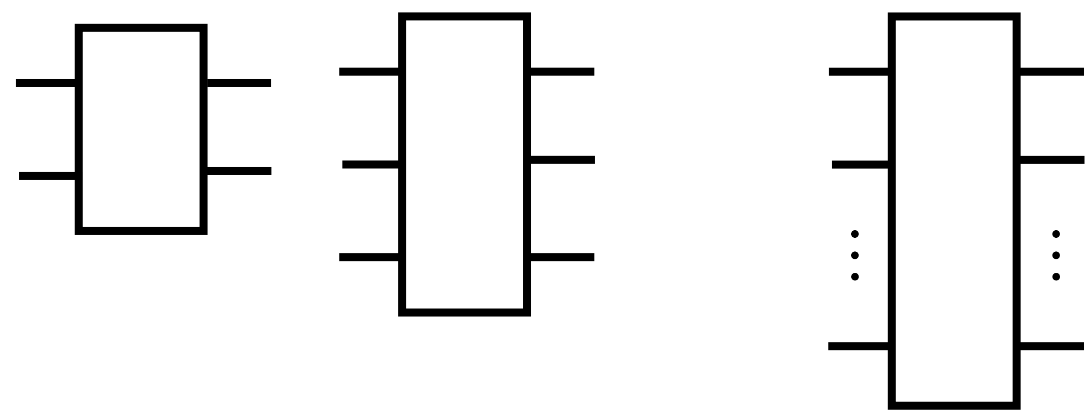
N correlated particles

2-body correlator

3-body correlator

N-body correlator

N independent particles



$\mathcal{O}(N^4)$ parameters

$\mathcal{O}(N^6)$ parameters

$\mathcal{O}(N^{2N})$ parameters

Roadmap for Automation

What Is Automation?

What Is Automation?

International Society of Automation

Standards Certification Training

About ISA / What is Automation?

What is Automation?

The dictionary defines *automation* as "the technique of making an apparatus, a process, or a system operate automatically."

We define automation as "the creation and application of technology to monitor and control the production and delivery of products and services."

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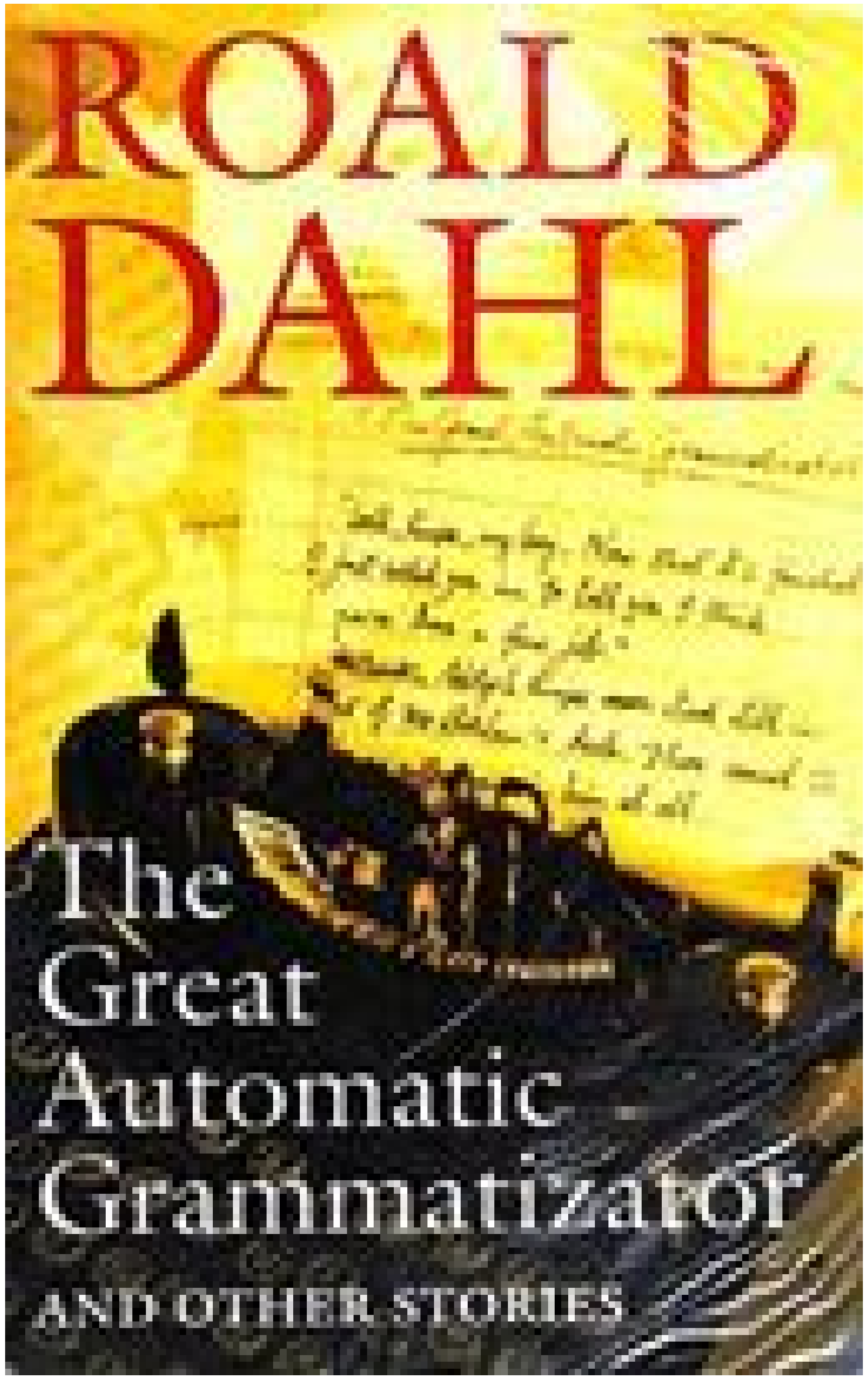
funding agency: product is manuscript

isa.org

Clearly, not a new idea …



wicked funny

oddly relevant

What Is Automation?

- Here: replacing tedious human work by machine work
  - Formal manipulation
  - Algorithm design/optimization
  - Code transformation
  - Code generation
  - Performance Analysis/Optimization
  - Graphics/table generation …
- Not everything can or should be automated
- Automation needs to be controlled, hence understandable
- Automation needs to be high-quality

Purposes of Automation

- Correctness for new (and old) methods
- Future-proofing
- Optimization: execution speed, resource use

automation = use of technology to *enable* many-body QM simulation

Wishlist for Automation

automation = use of technology to *enable* many-body QM simulation

- High level of abstraction: algebraic or graphical
- Ability to lower level of abstraction gradually (operator algebra/TN -> tensor algebra -> tensor data structures + algorithms -> generic IR
- Non-monolithic
- Deployable to large machines
- Open source

Again, This Has Been Known and Realized

Theor Chim Acta (1991) 79: 1–42

Theoretica
Chimica Acta

The automated solution of second quantization equations with applications to the coupled cluster approach*

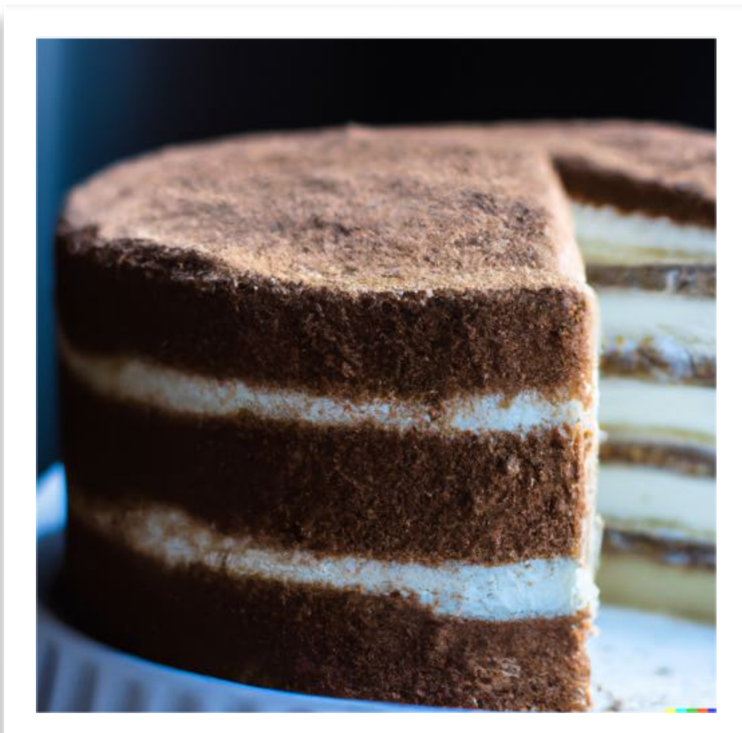
Curtis L. Janssen and Henry F. Schaefer III

Center for Computational Quantum Chemistry, University of Georgia, Athens, GA 30602, USA

Received August 14, 1990; received in revised form/Accepted September 26, 1990

Technology
~~Automation~~ Vision

many-body physics runtime stack



solvers

operator algebra / TN “compiler” as embedded DSL / library

tensor algebra engine

QM operator evaluation

Technology ~~Automation~~ Vision

many-body physics runtime stack

solvers

operator algebra / TN "compiler" as embedded DSL / library

ValeevGroup/SeQuant

tensor algebra engine

ValeevGroup/TiledArray

QM operator evaluation

ValeevGroup/Libint{,X} **m-a-d-n-e-s-s/madness**

Technology ~~Automation~~ Vision

many-body physics runtime stack

solvers — ValeevGroup/mpqc

operator algebra / TN "compiler" as embedded DSL / library

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ValeevGroup/Libint{,X} m-a-d-n-e-s-s/madness

Reusable Layers Highlight 1: Fast Hybrid All-Electron Kohn-Sham

arXiv > physics > arXiv:2303.14280

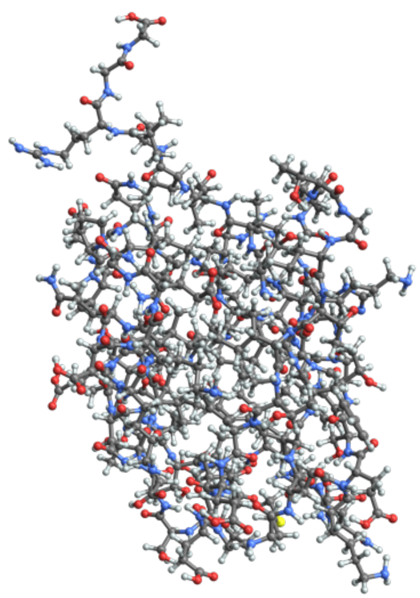
Help | Advanced

Physics > Computational Physics

[Submitted on 24 Mar 2023]

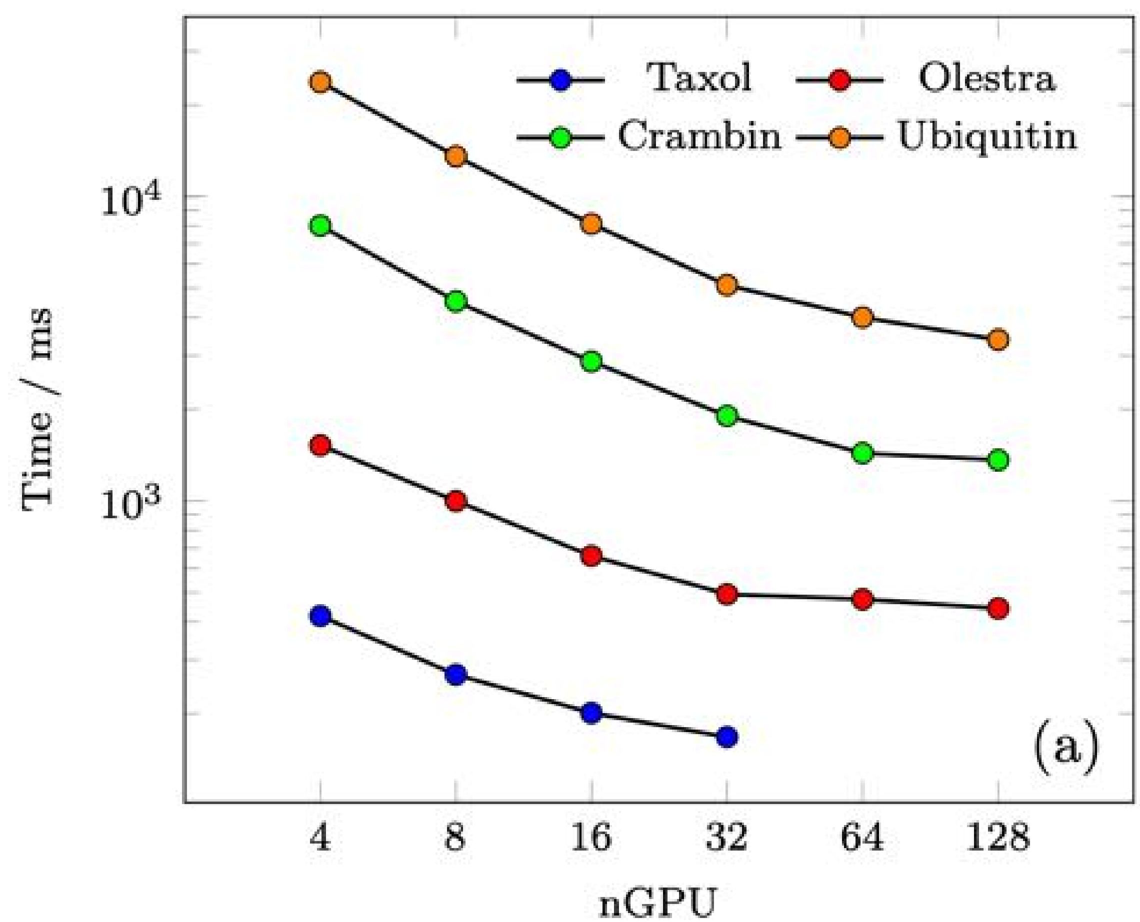
Distributed Memory, GPU Accelerated Fock Construction for Hybrid, Gaussian Basis Density Functional Theory

David B. Williams-Young, Andrey Asadchev, Doru Thom Popovici, David Clark, Johnathan Waldrop, Theresa Windus, Edward F. Valeev, Wibe A. de Jong



ubiquitin (1k+ atoms, 10k+ bf)

GPU-accelerated hybrid Fock build



Reusable Layers Highlight 1: Fast Hybrid All-Electron Kohn-Sham

arXiv > physics > arXiv:2303.14280

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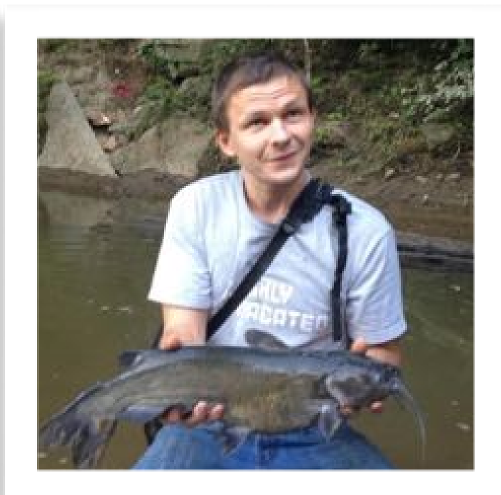
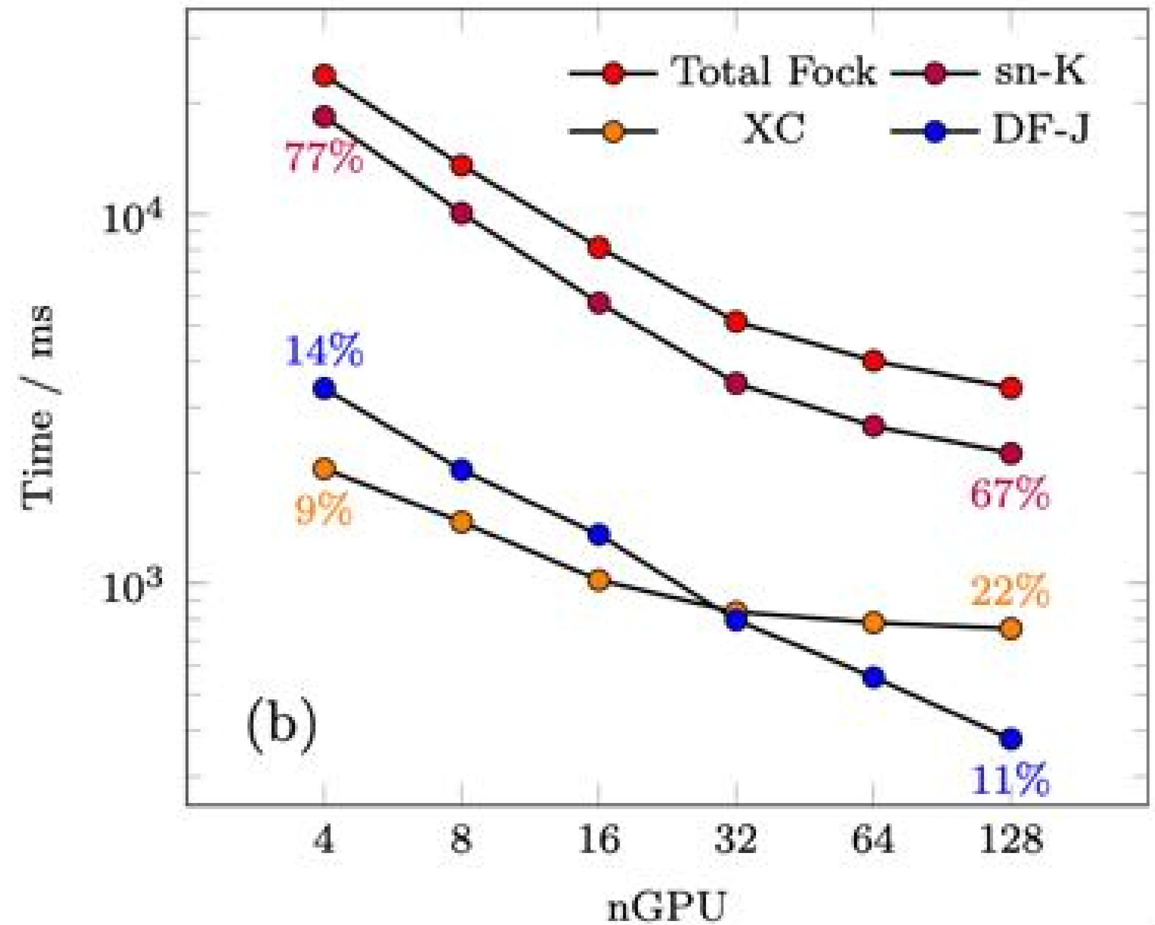


Dr. Andrey Asadchev

ValeevGroup/LibintX



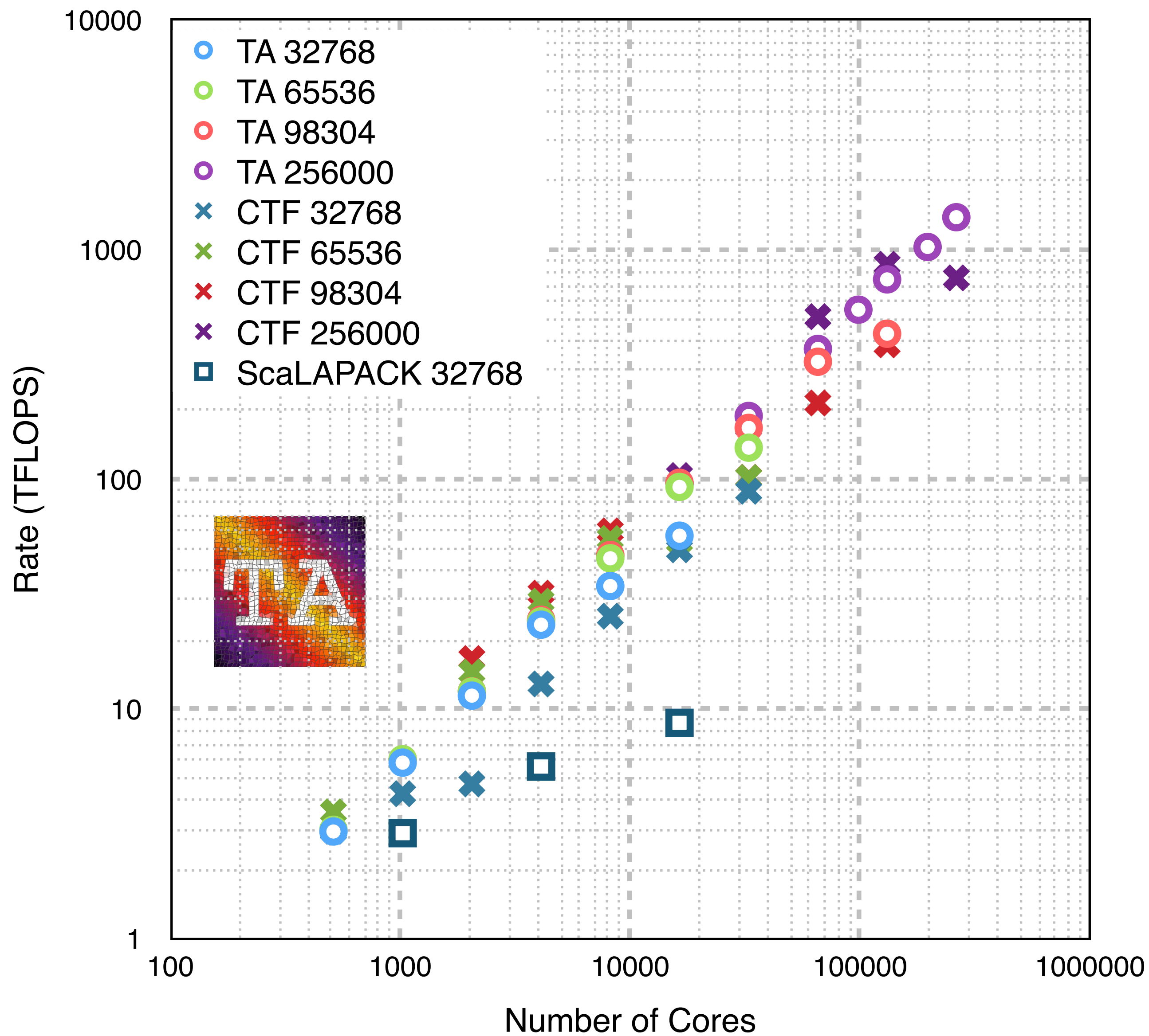
N.B. Open-source parallel GPU-accelerated J-engine … soon fast high-L 4-center AO integrals

Reusable Layers Highlight 2: TiledArray Framework

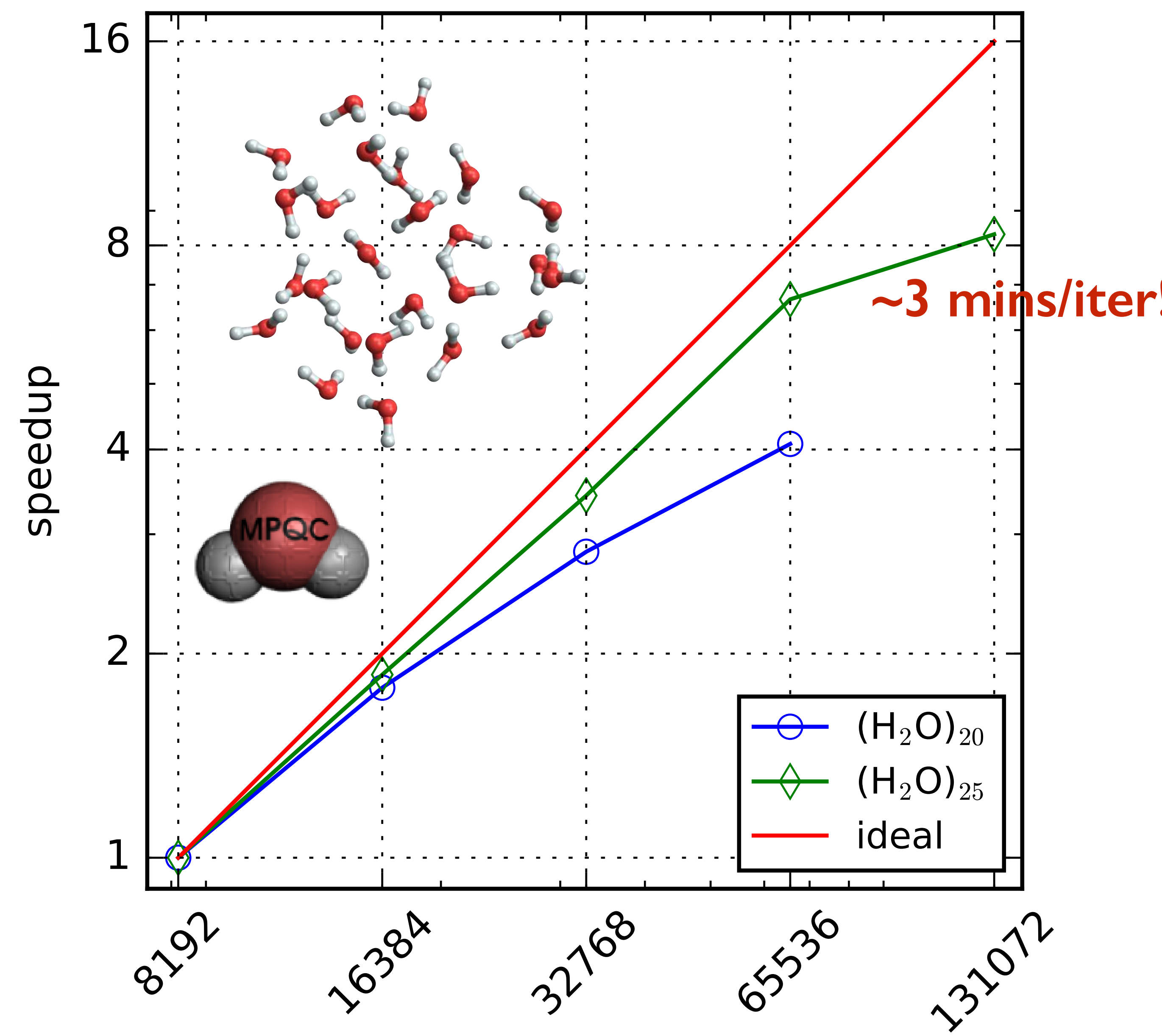
- **covers many domains**: dense and block-sparse arrays/tensors
- **general purpose**: no domain concepts, applicable to chemistry/physics/engineering
- **for users**: high-level post-einsum DSL
- **for developers**: powerful STL-like abstractions
- **scalable**: intra- and inter-node, >10^5 cores
- h**igh-performance**: CUDA, other backends in progress
- **free and open source**: GPL
- **open development**: central repo on Github

ValeevGroup/TiledArray

Our Tensor Framework TiledArray Allows Us To Simulate Electrons on Largest Machines



dense matrix multiplication benchmark



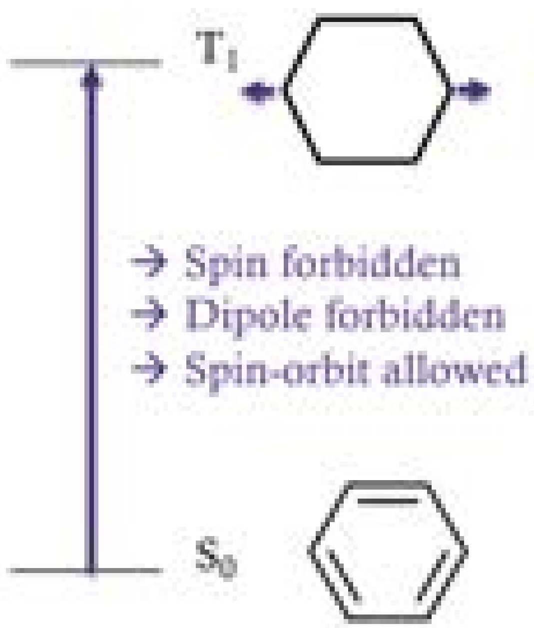
production CCSD-F12 solver
IBM BG/Q "Mira"

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

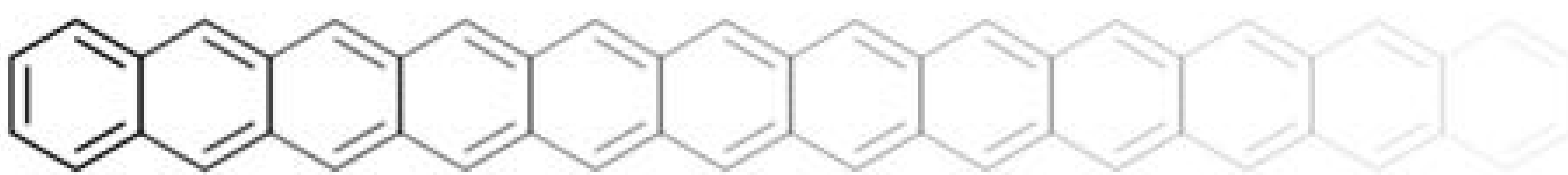
Reusable Layers Highlight 2: TiledArray Framework

others are starting to use it too, e.g.

Phosphorescent lifetimes of the $S_0 \rightarrow T_1$ transition



	Benzene	Naphthalene	Anthracene
Predicted Energy	3.25 eV	2.26 eV	1.53 eV
Exp. Energy	3.66 eV	2.63 eV	1.83 eV
Oscillator Strength	3.6e-10	2.89e-10	2.07e-10
Predicted Lifetime	6 s	15 s	48 s
Exp. Lifetime	10 s	18 s	60 s



relativistic ground and excited state massively-parallel CCSD in ChronusQ

SciDAC collaboration with Eugene DePrince (FSU), Xiaosong Li (UW) and Chao Yang (LBL)

TiledArray Arithmetic: DSL

Math

$$R_{iajb} = G_{iajb} + F_{ac}T_{icjb} + F_{bc}T_{iajc} - F_{ik}T_{kajb} - F_{jk}T_{iakb}$$
$$E = (G_{iajb} + R_{iajb})(2T_{iajb} - T_{ibja})$$

C++

```
TArrayD R(world, ovov);

R("i,a,j,b") = G("i,a,j,b") + Fv("a,c") * T("i,c,j,b") +
                Fv("b,c") * T("i,a,j,c") - Fo("i,k") * T("k,a,j,b") -
                Fo("j,k") * T("i,a,k,b");

double energy =
     (G("i,a,j,b") + R("i,a,j,b")).dot(2 * T("i,a,j,b") - T("i,b,j,a"));
```

TiledArray Arithmetic: DSL

Math

$$
\begin{aligned}
R_{iajb} =& G_{iajb} + F_{ac} T_{icjb} + F_{bc} T_{iajc} - F_{ik} T_{kajb} - F_{jk} T_{iakb} \\
E =& (G_{iajb} + R_{iajb})(2T_{iajb} - T_{ibja})
\end{aligned}
$$

C++

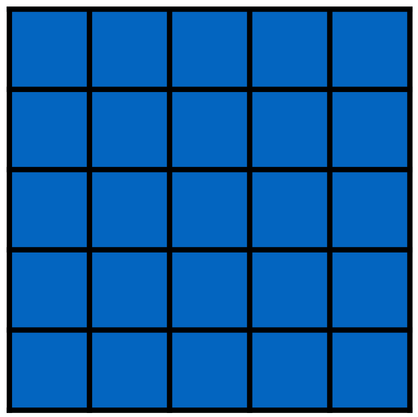
```
TArrayD R(world, ovov);

R("i,a,j,b") = G("i,a,j,b") + Fv("a,c") * T("i,c,j,b") +
                Fv("b,c") * T("i,a,j,c") - Fo("i,k") * T("k,a,j,b") -
                Fo("j,k") * T("i,a,k,b");

double energy =
     (G("i,a,j,b") + R("i,a,j,b")).dot(2 * T("i,a,j,b") - T("i,b,j,a"));
```

***deeply* customizable:**

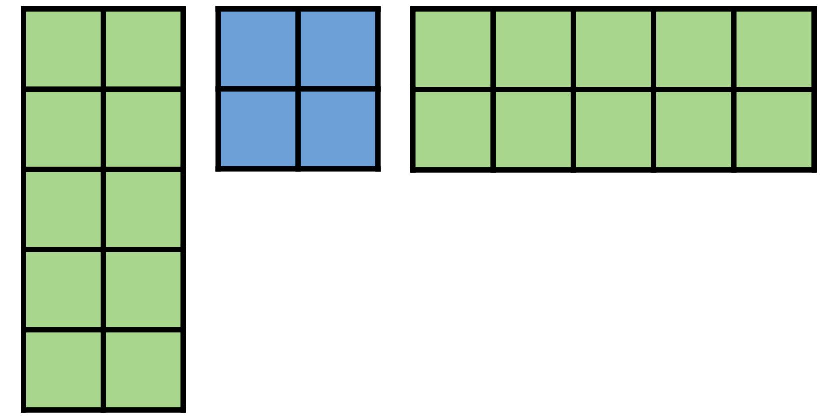
```
TArrayD = DistArray<Tensor<double>, DensePolicy>
```

can do lazily-evaluated tiles, tensors of tensors, sparse tensors, etc.

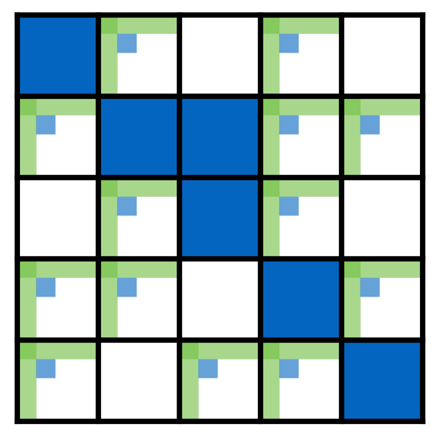
TiledArray Supports General Data Sparsity



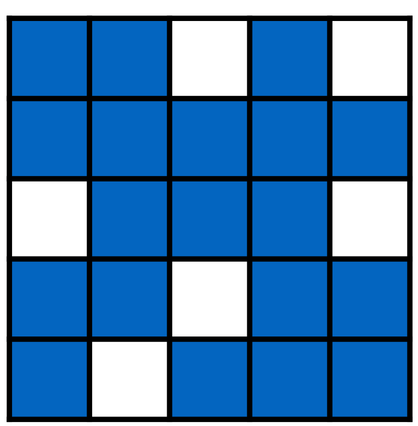
dense



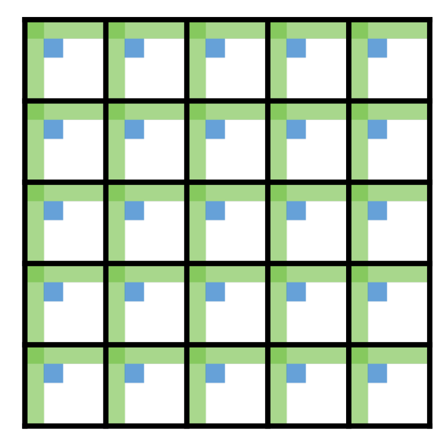
rank sparse



Clustered Low Rank



element/block sparse



block-rank sparse

Lewis, Calvin, Valeev, *J. Chem. Theor. Comp.* **12**, 5868 (2016).

SeQuant

SeQuant Synopsis

fast symbolic algebra of tensors

interpreter using parallel data-sparse tensor engine TiledArray

reusable open-source C++ library

old ideas in modern form, with some twists

SeQuant: **Se**cond **Quant**ization Algebra System

- SeQuant v1 (2002-now)
  - Implemented in Mathematica
  - Original objective to support R12 methods development (incl. CC-R12)
  - Extended by Martin Torheyden and Chong Peng (2007-2010) to support extended WT w.r.t. multi-determinant vacuum
  - Sufficient for CCSD, MR-F12, etc.
  - Slow, imperfect expression reduction, no factorization, etc.
  - Publicly available at github.com/ValeevGroup/SeQuant
- SeQuant2 (2018-now)
  - Implemented in C++17
  - Online symbolic manipulation now possible
  - Can interpret expressions using external tensor backend
  - github.com/ValeevGroup/SeQuant2

SeQuant2: Getting Started

- TL;DR

```
$ git clone https://github.com/ValeevGroup/SeQuant2
$ cmake -S SeQuant2 -B SeQuant2/build -DCMAKE_PREFIX_PATH="path-to-boost;path-to-eigen3"
$ cmake --build SeQuant2/build --target check
```

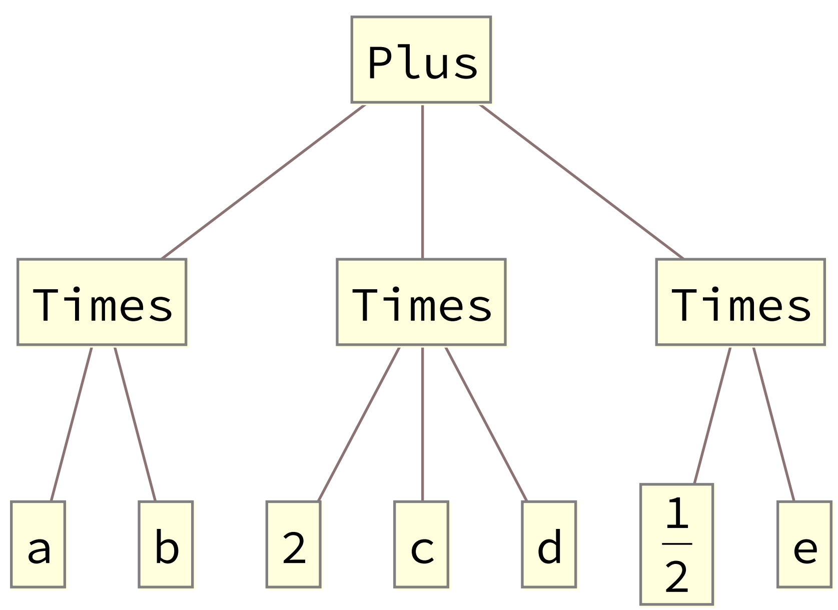
- Prereqs:
  - Boost 1.67+ (can't use 1.70, 1.77, 1.78)
  - Range-v3 (can autobuild)
  - (Unless BOOST_TESTING=OFF): Eigen3

SeQuant2: Core

- Core of SeQuant2 provides basic support for representing and manipulating *expressions*
  - SeQuant1 leveraged Mathematica for this job (hence its choice)
- Expressions are traditionally represented as trees/graphs

In[10]:= `TreeForm[a*b+c*2*d+(1/2)*e]`

Out[10]//TreeForm=



- But actual representation is some recursive data structure

In[14]:= `FullForm[a*b+c*2*d+(1/2)*e]`

Out[14]//FullForm=

```
Plus[Times[a, b], Times[2, c, d], Times[Rational[1, 2], e]]
```

SeQuant2: Core

- Expr = node on an expression tree
- Every type of expression (Constant, Product, Sum, etc.) must derive from Expr
  - Since expressions are polymorphic they should be stored on heap and held via a shared_ptr; use shortcuts ExprPtr ≡ shared_ptr<Expr> and ex<Type>(…) ≡ static_pointer_cast<Expr>(make_shared<Type>(…))
- Expr is a polymorphic *range* of pointers (ExprPtr) to subexpressions

```
auto prod = ex<Constant>(1) * ex<Constant>(2);
for(auto& factor: *(prod)) {
  std::wcout << "factor = " << to_wolfram(factor) << std::endl;
}
```

```
factor = 1.000000
factor = 2.000000
```

- Iteration over the tree trivially implemented by iterating over subexprs

SeQuant2: Core

- The `Expr` range is *mutable* for many expressions, this makes it possible to transform expressions

```
auto prod = ex<Constant>(1) * ex<Constant>(2);
std::wcout << "Old prod = " << to_wolfram(prod) << std::endl;
for(auto& factor: *(prod)) {
  factor = ex<Constant>(factor->as<Constant>().value() * 2.);
}
std::wcout << "New prod = " << to_wolfram(prod) << std::endl;
```

⇒

```
Old prod = Times[1.000000,2.000000]
New prod = Times[2.000000,4.000000]
```

- To make it easier dealing with polymorphic ranges, type ID of an `Expr` can be examined at runtime via `Expr::is<Type>` and it can be cast to `Type` via `Expr::as<Type>`(this does not use RTTI! See `Expr::get_type_id()`)

```
auto x = ex<Constant>(1) * (ex<Constant>(2) + ex<Constant>(3));
for(auto& factor: *(x)) {
  std::wcout << "factor is constant? “
             << (factor->is<Constant>() ? “true” : “false”) << std::endl;
}
```

⇒

```
factor is Constant? true
factor is Constant? false
```

SeQuant2: Core

- Most operations on expressions involve traversing the tree and invoking a function on (*visiting*) every node (optionally only invoking it on leaves only).

```
auto x = ex<Constant>(1) * (ex<Constant>(2) + ex<Constant>(3));
x->visit([](const ExprPtr& ex){
  std::wcout << to_wolfram(ex)
             << (ex->is<Constant>() ? " is" : " is not”)
             << " a Constant" << std::endl;
});
```

```
1.000000 is a Constant
2.000000 is a Constant
3.000000 is a Constant
Plus[2.000000,3.000000] is not a Constant
Times[1.000000,Plus[2.000000,3.000000]] is not a Constant
```

- e.g. `to_wolfram(ExprPtr)` ~~can be~~ is implemented by a visitor

SeQuant2: Core

- Most operations on expressions involve traversing the tree and invoking a function on (*visiting*) every node (optionally only invoking it on leaves only).
- Visitor can change its argument arbitrarily! This is another way expressions can be transformed.

```
auto x = ex<Constant>(1) * (ex<Constant>(2) + ex<Constant>(3));
std::wcout << “Old expr = " << to_wolfram(x) << std::endl;
x->visit([](ExprPtr& subx){
  if (subx->is<Constant>())
    subx = ex<Constant>(2);
});
std::wcout << “New expr = " << to_wolfram(x) << std::endl;
```

⇩

```
Old expr = Times[1.000000,Plus[2.000000,3.000000]]
New expr = Times[2.000000,Plus[2.000000,2.000000]]
```

SeQuant2: Core

- `Tensor` represents abstract tensorial quantities of finite order
  - Covariant and contravariant modes in Einstein notation are referred to as *bra* and *ket* modes (in the sense of Dirac notation for matrix elements of operators)
  - `Tensor` modes are represented by `Index` objects, composed of a label and an `IndexSpace`
  - `IndexSpace` represents a vector space; it has a type (`Type`) and quantum number attributes (`QuantumNumbers`).

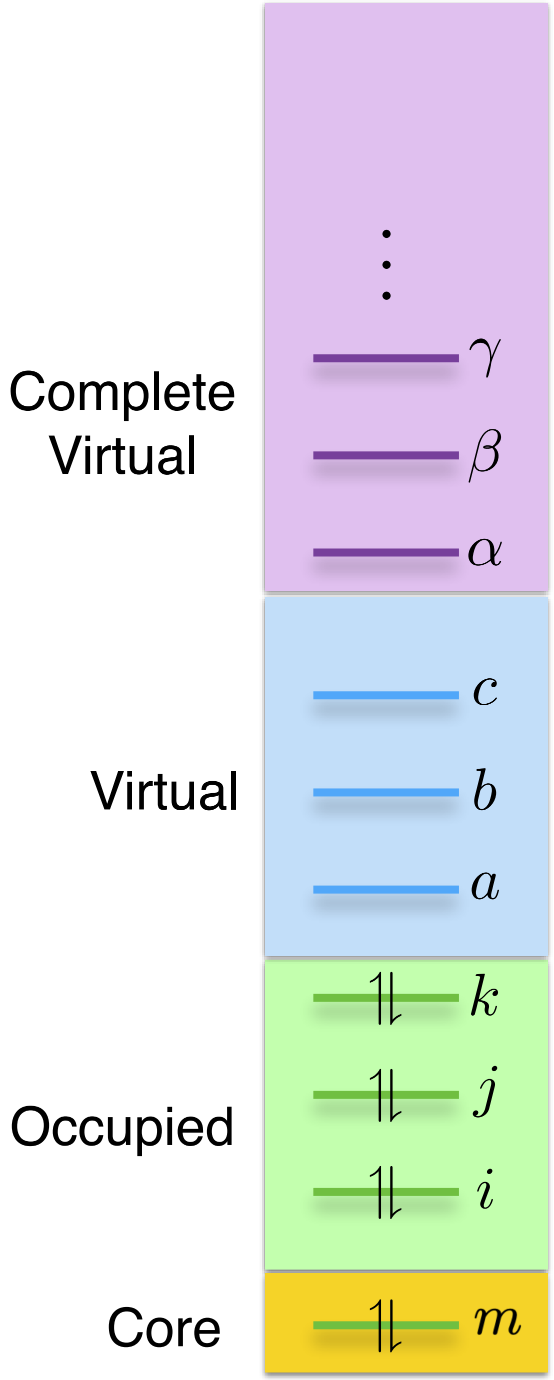
SeQuant DSL

- Index Type

i_1
```
Index i1(L"i_1");
```
a_1
```
Index a1(L"a_1");
```
p_1^α
```
auto p1A = Index(L”p⁺_1", IndexSpace::alpha);
```
p_1^β
```
auto p1B = Index(L"p⁻_1", IndexSpace::beta);
```
$a_3^{i_1 i_2}$
```
Index a3(L”a_3", IndexSpace::active_occupied,
         {i1, i2});
```

- Tensor Type

$F_{i_1}^{i_2}$
```
Tensor(L"F", {L"i_1"}, {L"i_2"});
```
$\bar{g}_{i_1 i_2}^{i_3 i_4}$
```
Tensor(L"g", {Index{L"i_1"}, Index{L"i_2"}},
       {Index{L”i_3"}, Index{L"i_4"}},
       Symmetry::antisymm);
```



SeQuant DSL

- Operators

$$\tilde{a}^{i_1 i_2}_{a_1 a_2}$$

```
auto nop1 = FNOperator({L"i_1", L"i_2"}, {L"a_1", L"a_2"},
                       Vacuum::SingleProduct);
```

$$\tilde{a}^{i_1 i_2}_{\quad a_2}$$

```
auto nop2 = FNOperator({L"i_1", L"i_2"}, {L"a_2"},
                       Vacuum::SingleProduct);
```

- Operator sequence

$$\tilde{a}^{i_1 i_2}_{a_1 a_2} \tilde{a}^{i_1 i_2}_{\quad a_2}$$

```
auto nopseq = FNOperatorSeq({nop1, nop2});
```

- Wick's theorem

$$\tilde{a}^{i_1 i_2}_{a_1 a_2} \tilde{a}^{a_3 a_4}_{i_3 i_4}$$

```
auto wick = FWickTheorem{opseq};
```

$$s^{i_4}_{i_1} s^{i_3}_{i_2} s^{a_3}_{a_2} s^{a_4}_{a_1} - s^{i_4}_{i_1} s^{i_3}_{i_2} s^{a_4}_{a_2} s^{a_3}_{a_1} - s^{i_3}_{i_1} s^{i_4}_{i_2} s^{a_3}_{a_2} s^{a_4}_{a_1} + s^{i_3}_{i_1} s^{i_4}_{i_2} s^{a_4}_{a_2} s^{a_3}_{a_1}$$

SeQuant DSL

- Expression transcription: operator algebra

$$F^{i_2}_{i_1} \tilde{a}^{i_1}_{i_2}$$

```
auto h1 = ex<Tensor>(L"F",{L"i_1"},{L"i_2"}) *
          ex<FNOperator>({L"i_1"},{L"i_2"});
```

- Expression transcription: tensor products

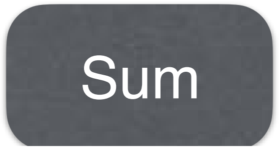
$$\frac{1}{8} \bar{g}^{a_4 a_5}_{i_4 i_5} \bar{t}^{i_1 i_2}_{a_1 a_4} \bar{t}^{i_3 i_4 i_5}_{a_2 a_3 a_5}$$

```
auto input = ex<Constant>(1./8) *
             ex<Tensor>(L"g",{L"i_4", L"i_5"},
                        {L"a_4", L"a_5"}, Symmetry::antisymm) *
             ex<Tensor>(L"t",{L"a_1", L"a_4"},
                        {L"i_1", L"i_2"}, Symmetry::antisymm) *
             ex<Tensor>(L"t",{L"a_2",L"a_3", L"a_5"},
                        {L"i_3", L"i_4",L"i_5"}, Symmetry::antisymm);
```

SeQuant DSL

Expressions are represented as trees

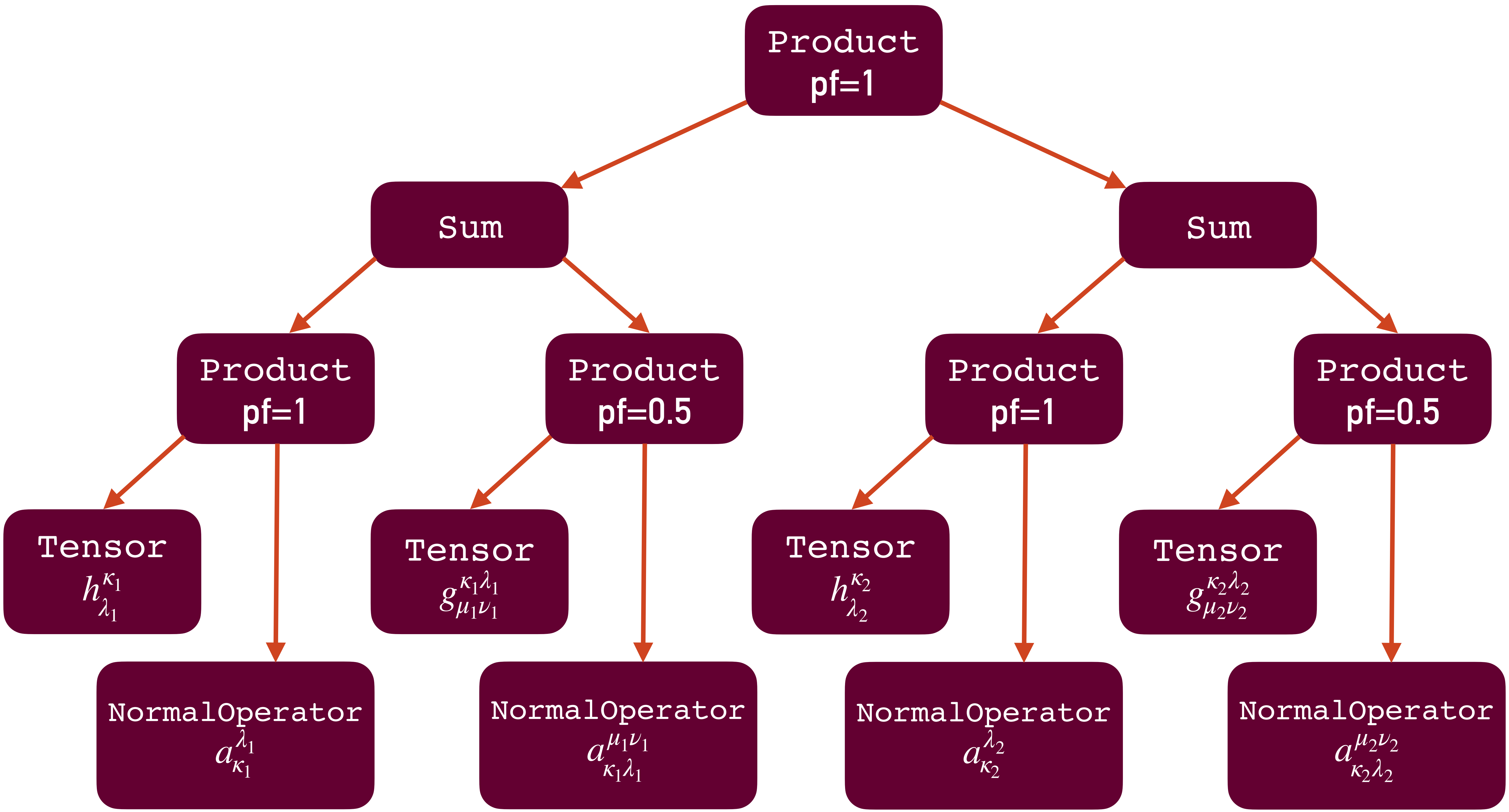
$$\frac{1}{4} A^{a_1 a_2}_{i_1 i_2} \bar{g}^{i_1 i_2}_{a_1 a_2} + \frac{1}{2} A^{a_1 a_2}_{i_1 i_2} f^{i_1}_{i_3} \bar{t}^{i_2 i_3}_{a_1 a_2} + \dots$$



math: $$\hat{H}^2 \equiv \left(h^{\kappa}_{\lambda} a^{\lambda}_{\kappa} + \frac{1}{2} g^{\kappa\lambda}_{\mu\nu} a^{\mu\nu}_{\kappa\lambda} \right)^2 = \left(h^{\kappa_1}_{\lambda_1} a^{\lambda_1}_{\kappa_1} + \frac{1}{2} g^{\kappa_1\lambda_1}_{\mu_1\nu_1} a^{\mu_1\nu_1}_{\kappa_1\lambda_1} \right) \left(h^{\kappa_2}_{\lambda_2} a^{\lambda_2}_{\kappa_2} + \frac{1}{2} g^{\kappa_2\lambda_2}_{\mu_2\nu_2} a^{\mu_2\nu_2}_{\kappa_2\lambda_2} \right)$$

SeQuant:

```
#include <SeQuant/domain/mbpt/sr/sr.hpp>
using namespace sequant::mbpt::sr::so;
auto H2 = H() * H();
```



SeQuant DSL

- Custom expression elements

```
namespace sequant::mbpt {
  template <typename QuantumNumbers, Statistics S>
  class Operator : public Expr {
      // ...
  };

  namespace sr {
    template <Statistics S>
    class Operator : public mbpt::Operator<QuantumNumberSet<2>> {
        // ...
    };
  }
}
```

SeQuant DSL

- compose CC equations at high level

```
using namespace SeQuant::mbpt;

// 1. construct hbar(op) in canonical form
auto hbar = op::H();
auto H_Tk = hbar;
for (int64_t k = 1; k <= 4; ++k) {
  H_Tk = simplify(ex<Constant>(rational{1, k}) * H_Tk * op::T(N));
  hbar += H_Tk;
}

for(auto p : range(0,P)) {
  // 2.a screen by ex level

  // 2.b multiply by A(P)
  auto A_hbar = simplify(op::A(p) * hbar_p);

  // 2.c compute vacuum average
  auto R_p = op::vac_av(A_hbar);
  simplify(R_p);
}
```

SeQuant2: Key Algorithms

- Tensor network automorphizer
- Fast(er) Wick engine
- Spin tracing
- Expression optimization
- Expression evaluation

SeQuant2: Tensor network automorphizer

- Maps tensor network onto (symmetry-preserving) colored graph and determines its automorphism group
- Used to manipulate tensor networks
  - e.g. find topologically-equivalent parts
- Used to manipulate expressions involving TNs
  - e.g. recognizing equivalent terms produced by the Wick engine

Example: CCSD

$$\langle 0 | \hat{L}_2 (\hat{W}\hat{T}_2^2)_c | 0 \rangle = (-\frac{1}{4} \times A^{a_1a_2}_{i_1i_2} g^{a_3a_4}_{i_3i_4} t^{i_1i_2}_{a_1a_3} t^{i_3i_4}_{a_2a_4} +$$

equivalent

$$A^{a_1a_2}_{i_1i_2} g^{a_3a_4}_{i_3i_4} t^{i_1i_3}_{a_1a_3} t^{i_2i_4}_{a_2a_4} +$$

$$-\frac{1}{4} \times A^{a_1a_2}_{i_1i_2} g^{a_3a_4}_{i_3i_4} t^{i_3i_4}_{a_1a_3} t^{i_1i_2}_{a_2a_4} +$$

$$\frac{1}{8} \times A^{a_1a_2}_{i_1i_2} g^{a_3a_4}_{i_3i_4} t^{i_3i_4}_{a_1a_2} t^{i_1i_2}_{a_3a_4} +$$

$$-\frac{1}{2} \times A^{a_1a_2}_{i_1i_2} g^{a_3a_4}_{i_3i_4} t^{i_1i_3}_{a_1a_2} t^{i_2i_4}_{a_3a_4})$$

Example: CCSDT

$$\langle 0 | \hat{L}_3(\hat{W}\hat{T}_2\hat{T}_3)_c | 0 \rangle = (\frac{1}{48} \times A^{a_1a_2a_3}_{i_1i_2i_3} g^{a_4a_5}_{i_4i_5} t^{i_1i_2}_{a_4a_5} t^{i_3i_4i_5}_{a_1a_2a_3} +$$

$$\frac{1}{24} \times A^{a_1a_2a_3}_{i_1i_2i_3} g^{a_4a_5}_{i_4i_5} t^{i_1i_4}_{a_4a_5} t^{i_2i_3i_5}_{a_1a_2a_3} +$$

$$\frac{1}{24} \times A^{a_1a_2a_3}_{i_1i_2i_3} g^{a_4a_5}_{i_4i_5} t^{i_4i_5}_{a_1a_4} t^{i_1i_2i_3}_{a_2a_3a_5} +$$

$$\frac{1}{4} \times A^{a_1a_2a_3}_{i_1i_2i_3} g^{a_4a_5}_{i_4i_5} t^{i_1i_4}_{a_1a_4} t^{i_2i_3i_5}_{a_2a_3a_5} +$$

$$\frac{1}{8} \times A^{a_1a_2a_3}_{i_1i_2i_3} g^{a_4a_5}_{i_4i_5} t^{i_1i_2}_{a_1a_4} t^{i_3i_4i_5}_{a_2a_3a_5} +$$

$$\frac{1}{8} \times A^{a_1a_2a_3}_{i_1i_2i_3} g^{a_4a_5}_{i_4i_5} t^{i_1i_4}_{a_1a_2} t^{i_2i_3i_5}_{a_3a_4a_5} +$$

$$\frac{1}{48} \times A^{a_1a_2a_3}_{i_1i_2i_3} g^{a_4a_5}_{i_4i_5} t^{i_4i_5}_{a_1a_2} t^{i_1i_2i_3}_{a_3a_4a_5})$$

Example: PNO CCSD

$$\langle 0|\hat{L}_2(\hat{W}\hat{T}_2^2)_c|0\rangle = (\frac{1}{8}\times A^{a_1^{i_1i_2}a_2^{i_1i_2}}_{i_1i_2} g^{a_3^{i_1i_2}a_4^{i_1i_2}}_{i_3i_4} t^{i_3i_4}_{a_5^{i_3i_4}a_6^{i_3i_4}} t^{i_1i_2}_{a_3^{i_1i_2}a_4^{i_1i_2}} S^{a_5^{i_3i_4}}_{a_1^{i_1i_2}} S^{a_6^{i_3i_4}}_{a_2^{i_1i_2}} +$$

$$-\frac{1}{2}\times A^{a_1^{i_1i_2}a_2^{i_1i_2}}_{i_1i_2} g^{a_3^{i_1i_3}a_4^{i_1i_3}}_{i_3i_4} t^{i_1i_3}_{a_3^{i_1i_3}a_4^{i_1i_3}} t^{i_2i_4}_{a_5^{i_2i_4}a_6^{i_2i_4}} S^{a_5^{i_2i_4}}_{a_1^{i_1i_2}} S^{a_6^{i_2i_4}}_{a_2^{i_1i_2}} +$$

equivalent

$$\frac{1}{2}\times A^{a_1^{i_1i_2}a_2^{i_1i_2}}_{i_1i_2} g^{a_3^{i_1i_3}a_4^{i_2i_4}}_{i_3i_4} t^{i_1i_3}_{a_3^{i_1i_3}a_5^{i_1i_3}} t^{i_2i_4}_{a_4^{i_2i_4}a_6^{i_2i_4}} S^{a_5^{i_1i_3}}_{a_1^{i_1i_2}} S^{a_6^{i_2i_4}}_{a_2^{i_1i_2}} +$$

$$-\frac{1}{2}\times A^{a_1^{i_1i_2}a_2^{i_1i_2}}_{i_1i_2} g^{a_3^{i_1i_3}a_4^{i_2i_4}}_{i_3i_4} t^{i_1i_3}_{a_3^{i_1i_3}a_5^{i_1i_3}} t^{i_2i_4}_{a_4^{i_2i_4}a_6^{i_2i_4}} S^{a_6^{i_2i_4}}_{a_1^{i_1i_2}} S^{a_5^{i_1i_3}}_{a_2^{i_1i_2}} +$$

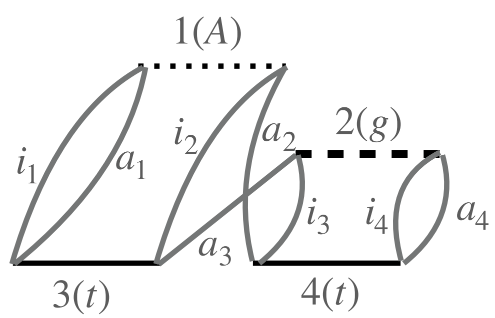
$$-\frac{1}{2}\times A^{a_1^{i_1i_2}a_2^{i_1i_2}}_{i_1i_2} g^{a_3^{i_3i_4}a_4^{i_1i_2}}_{i_3i_4} t^{i_3i_4}_{a_3^{i_3i_4}a_5^{i_3i_4}} t^{i_1i_2}_{a_1^{i_1i_2}a_4^{i_1i_2}} S^{a_5^{i_3i_4}}_{a_2^{i_1i_2}})$$

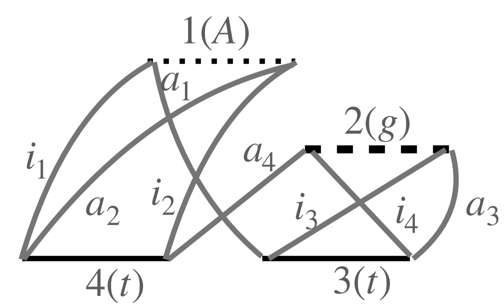
need *complete* canonization

Example: tensor network canonization

$$-\frac{1}{4} \times A_{i_1 i_2}^{a_1 a_2} g_{i_3 i_4}^{a_3 a_4} t_{a_1 a_3}^{i_1 i_2} t_{a_2 a_4}^{i_3 i_4}$$

$$-\frac{1}{4} \times A_{i_1 i_2}^{a_1 a_2} g_{i_3 i_4}^{a_3 a_4} t_{a_1 a_3}^{i_3 i_4} t_{a_2 a_4}^{i_1 i_2}$$





how to determine if 2 diagrams are equivalent?

this is a *graph isomorphism* problem

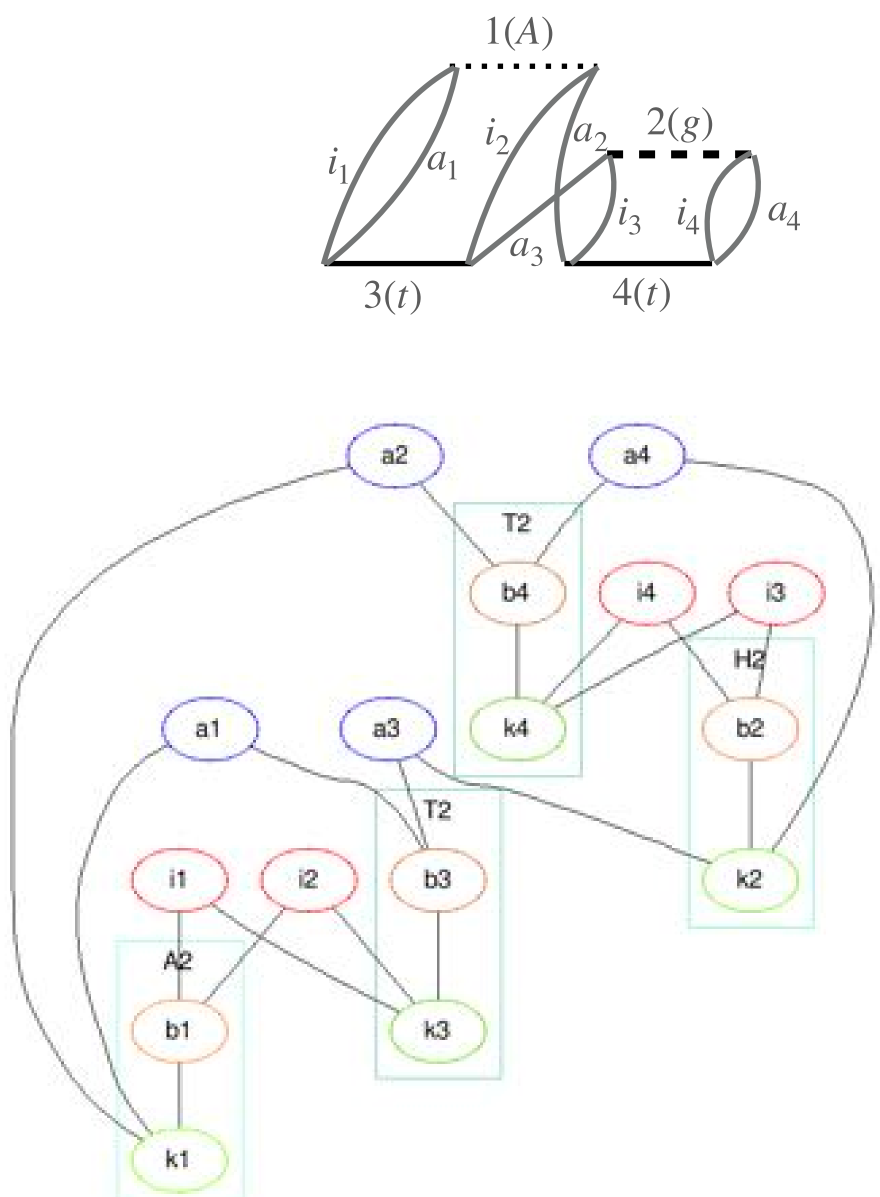
Tensor network canonization

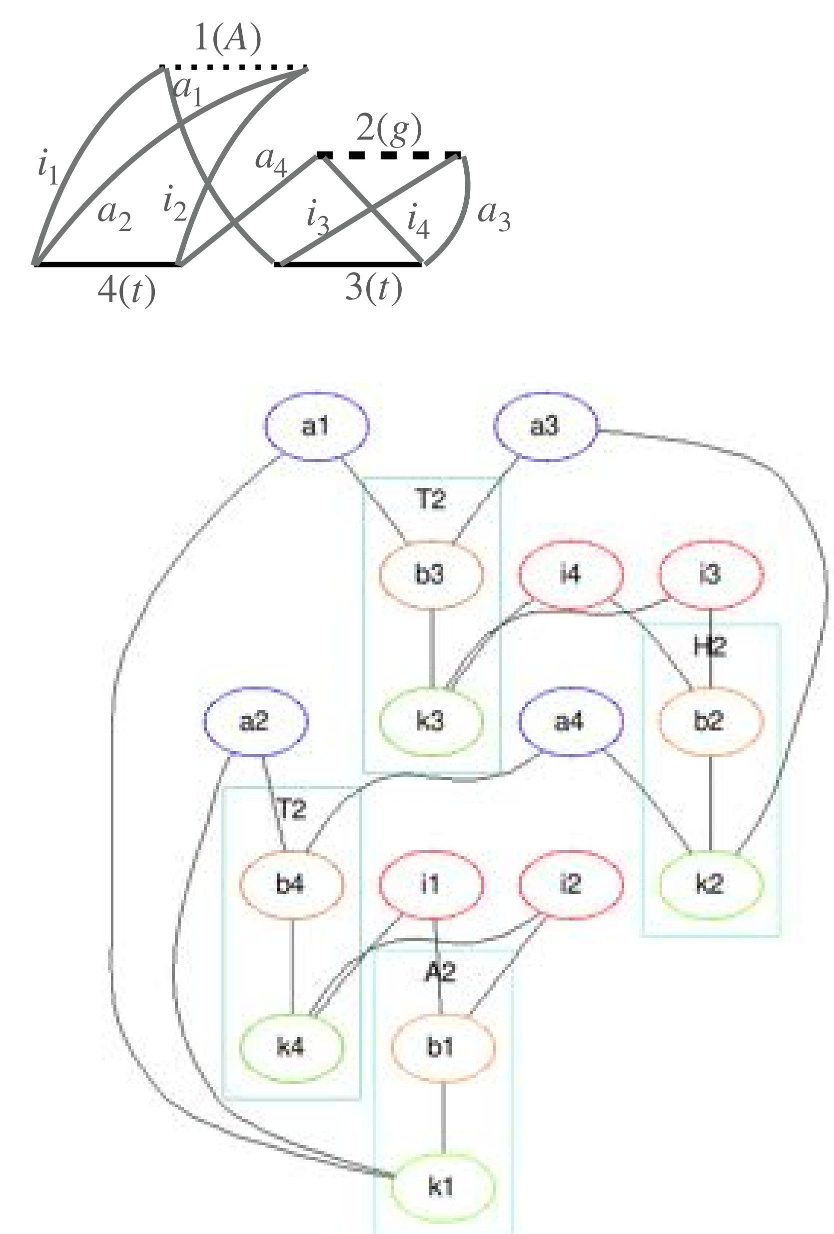
represent diagram as a colored graph whose structure and vertex colors reflect the symmetries of the diagram …

diagram	graph
line	vertex (color = line type)
operator	linked bra and ket vertices (color = operator type)

Tensor network canonization

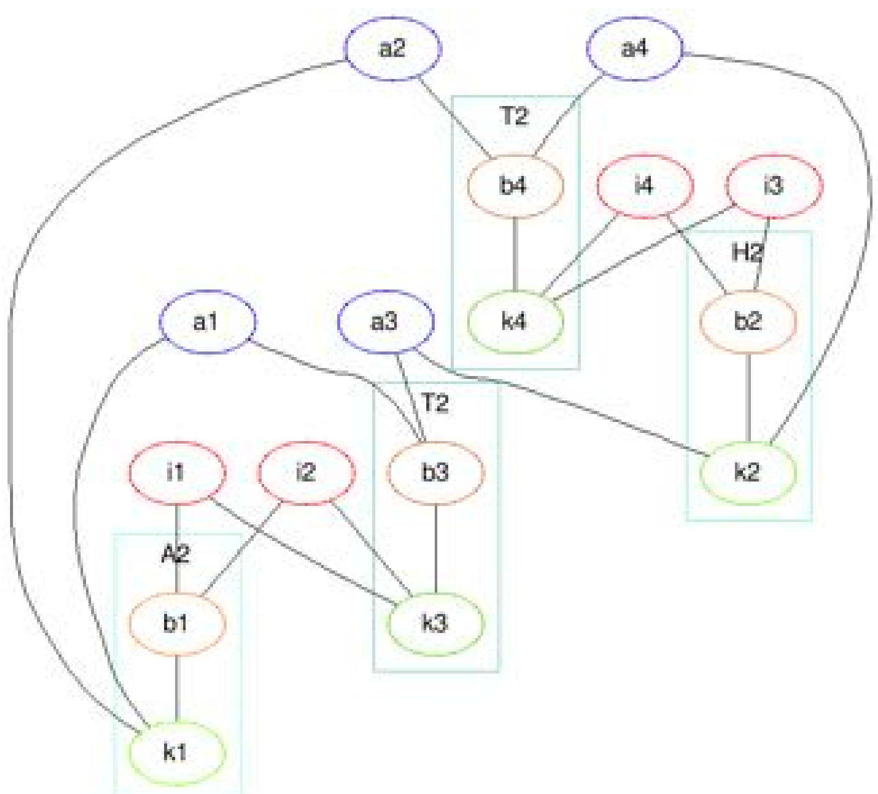
represent diagram as a colored graph whose structure and vertex colors reflect the symmetries of the diagram …

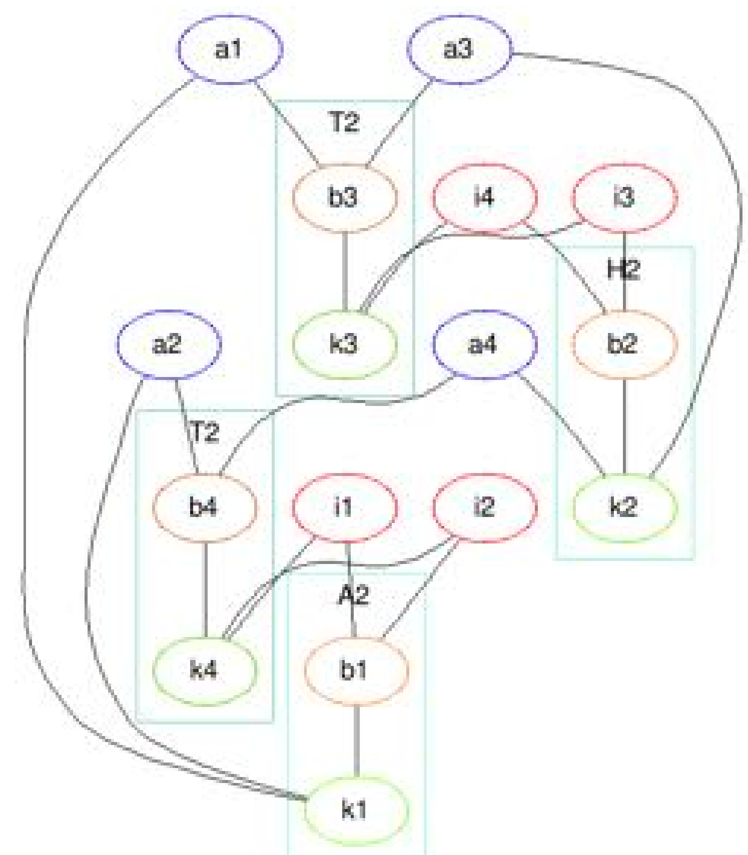




Tensor network canonization

… determine **canonical** order of its vertices …



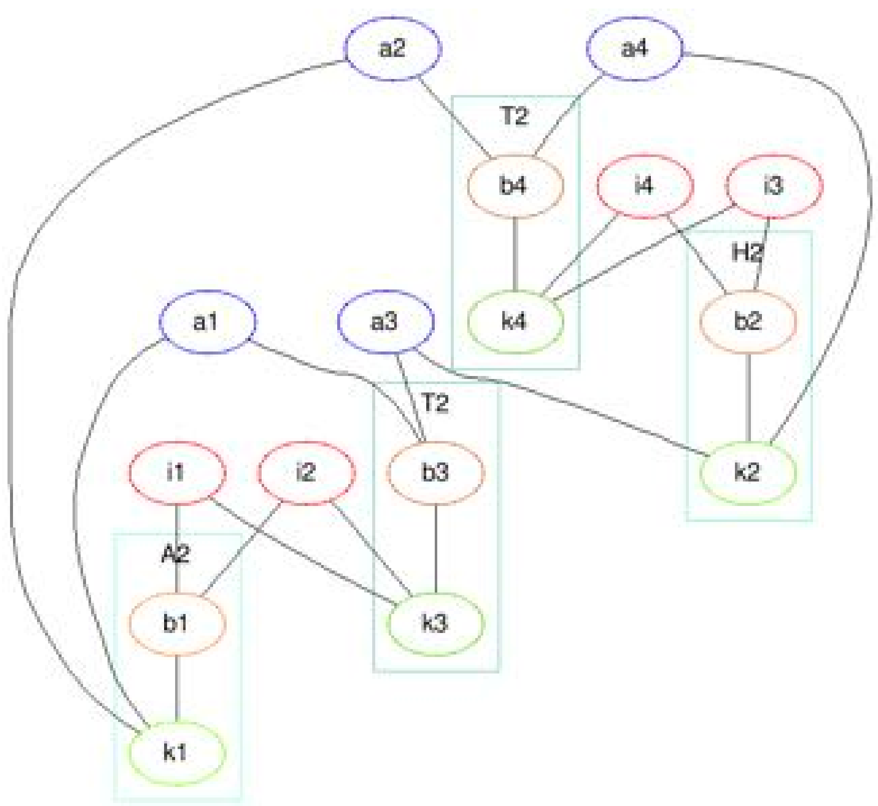


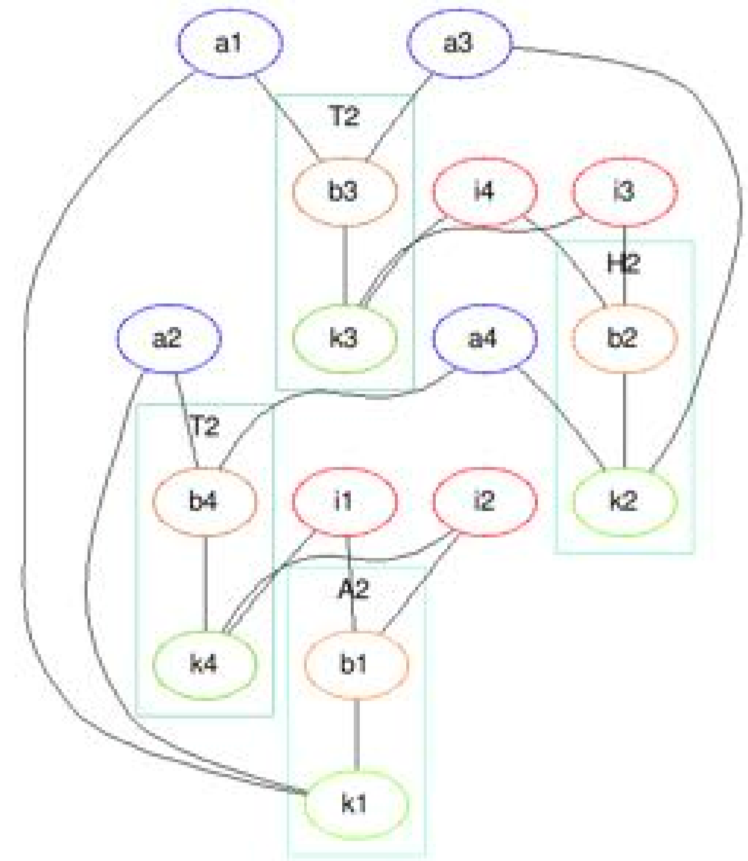

```
b1=>0 k1=>1 b2=>2 k2=>3 b3=>4 k3=>6 b4=>5 k4=>7
i1=>8 i2=>9 i3=>10 i4=>11 a1=>13 a2=>12 a3=>15 a4=>14
```

```
b1=>0 k1=>1 b2=>2 k2=>3 b3=>6 k3=>4 b4=>7 k4=>5
i1=>8 i2=>9 i3=>10 i4=>11 a1=>12 a2=>13 a3=>14 a4=>15
```

Tensor network canonization

… compare the vertices in canonical order …





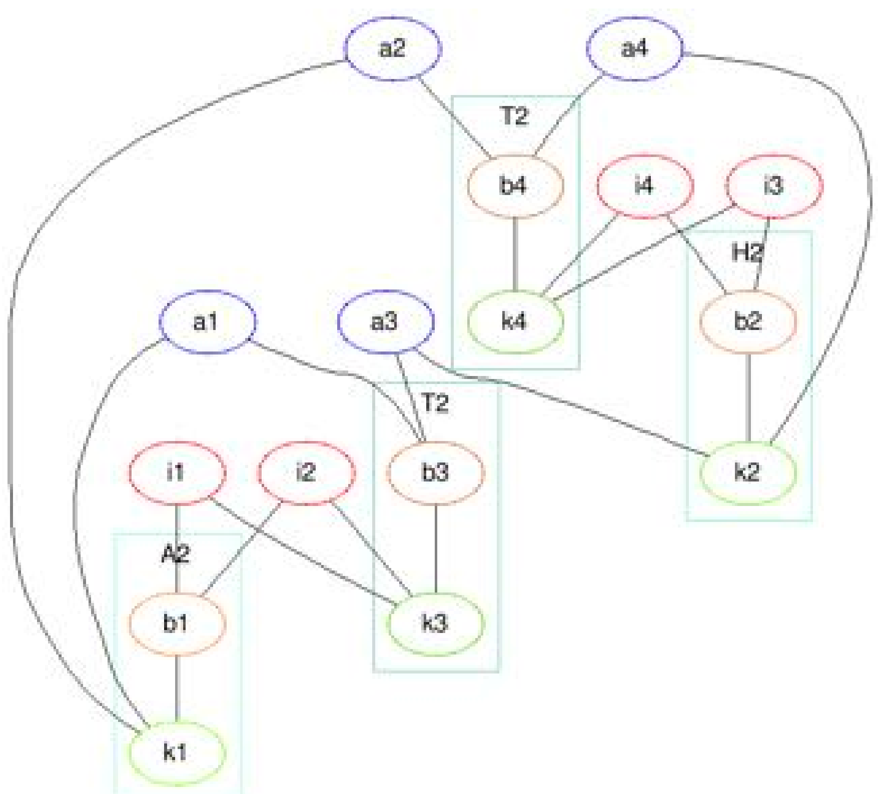

```
 b1=>0 k1=>1 b2=>2 k2=>3 b3=>4 k3=>6 b4=>5 k4=>7
i1=>8 i2=>9 i3=>10 i4=>11 a1=>13 a2=>12 a3=>15 a4=>14
```

```
 b1=>0 k1=>1 b2=>2 k2=>3 b3=>6 k3=>4 b4=>7 k4=>5
i1=>8 i2=>9 i3=>10 i4=>11 a1=>12 a2=>13 a3=>14 a4=>15
```

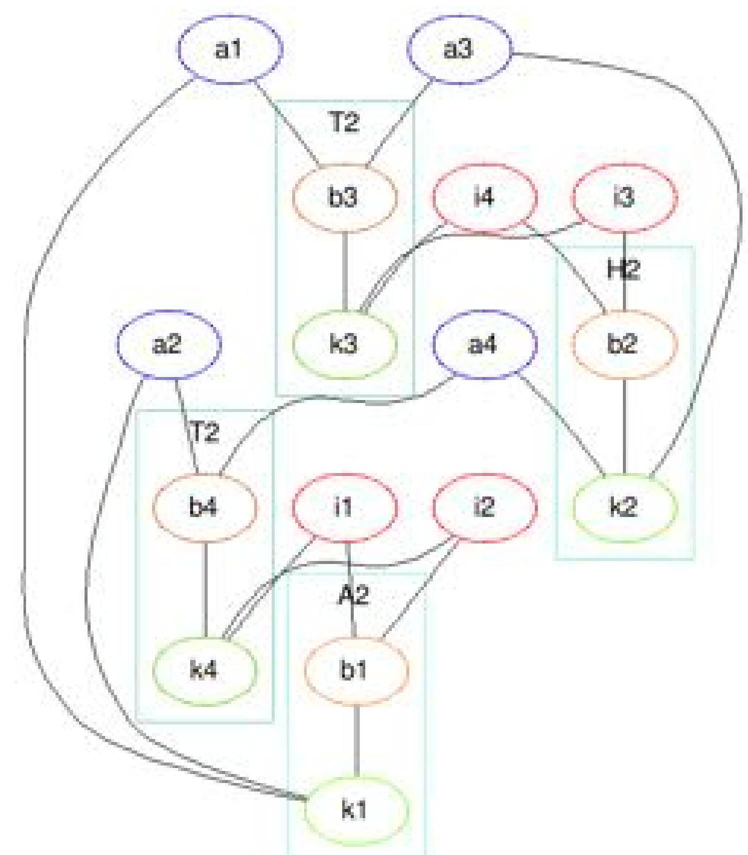
```
b1=>b1 k1=>k1 b2=>b2 k2=>k2 b3=>b4 k3=>k4 b4=>b3 k4=>k3
i1=>i1 i2=>i2 i3=>i3 i4=>i4 a1=>a2 a2=>a1 a3=>a4 a4=>a3
```

Tensor network canonization

… and combine the diagrams



$$a1 \leftrightarrow a2$$
$$a3 \leftrightarrow a4$$
$$b3 \leftrightarrow b4$$
$$k3 \leftrightarrow k4$$



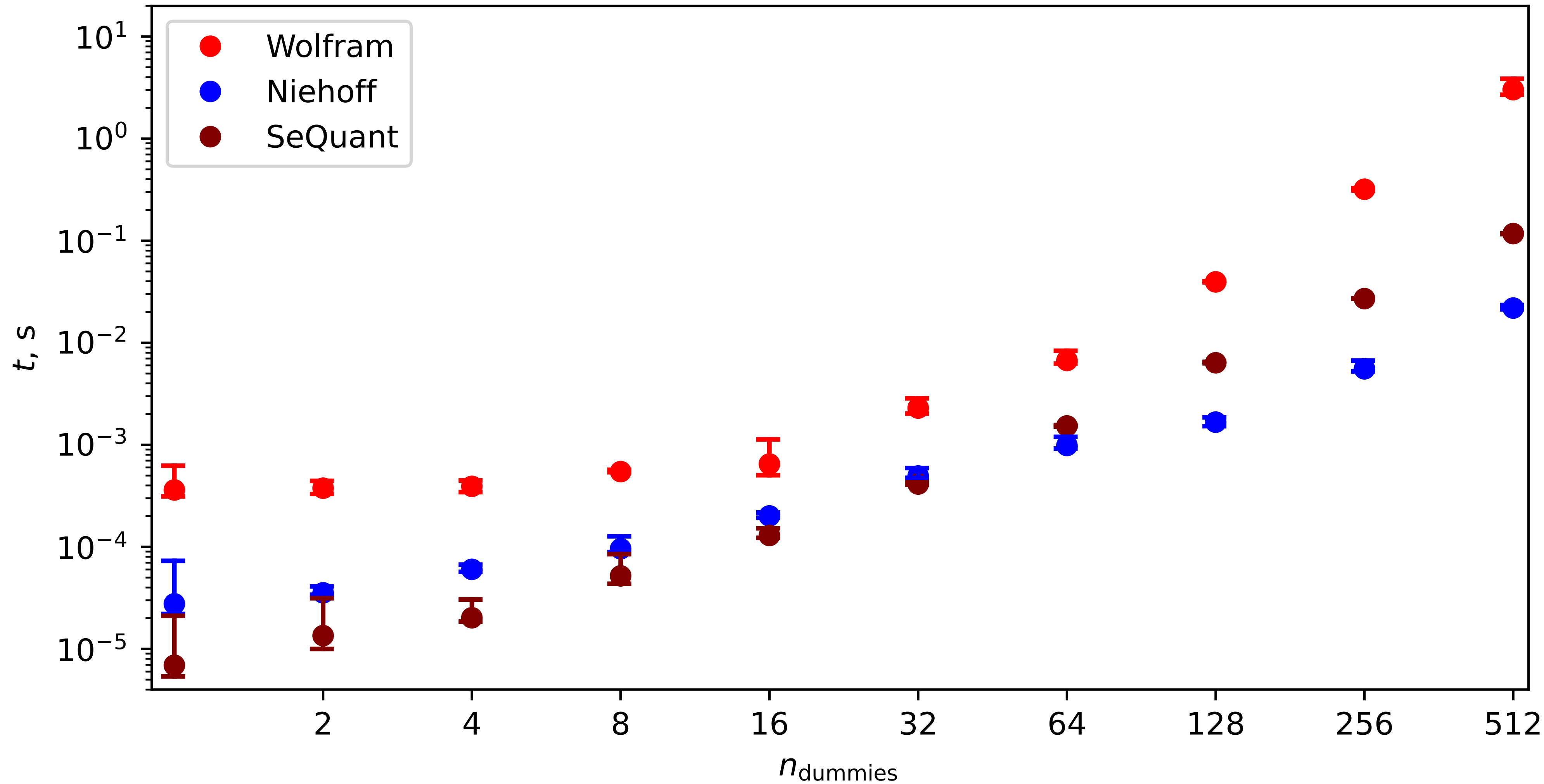
$$-\frac{1}{4} \times A^{a_1 a_2}_{i_1 i_2} g^{a_3 a_4}_{i_3 i_4} t^{i_1 i_2}_{a_1 a_3} t^{i_3 i_4}_{a_2 a_4} - \frac{1}{4} \times A^{a_1 a_2}_{i_1 i_2} g^{a_3 a_4}_{i_3 i_4} t^{i_3 i_4}_{a_1 a_3} t^{i_1 i_2}_{a_2 a_4} = -\frac{1}{2} \times A^{a_1 a_2}_{i_1 i_2} g^{a_3 a_4}_{i_3 i_4} t^{i_1 i_2}_{a_1 a_3} t^{i_3 i_4}_{a_2 a_4}$$

still need extra structure to support protoindices and non-symmetric tensors …

Tensor network canonization: colored graph vs others

canonicalizing $D_{i_1 \ldots i_N} U^{\pi[i_1 \ldots i_N]}$

asymmetric D and U

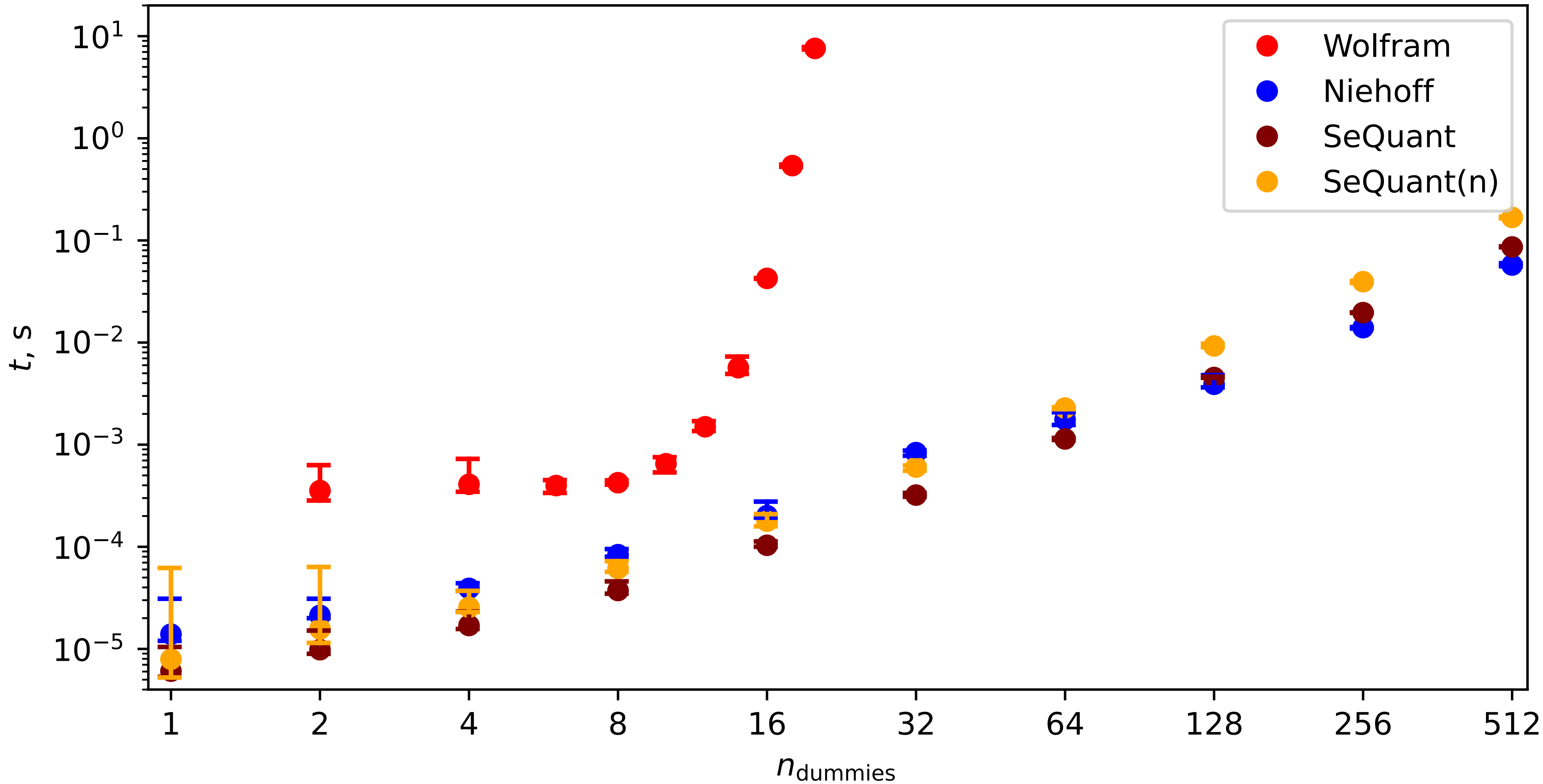


group-theoretic Butler-Portugal algorithm ("Wolfram") is near optimal for asymmetric tensors

Tensor network canonization: colored graph vs others

canonicalizing $D_{i_1 \ldots i_N} U^{\pi[i_1 \ldots i_N]}$

totally-symmetric D, asymmetric U



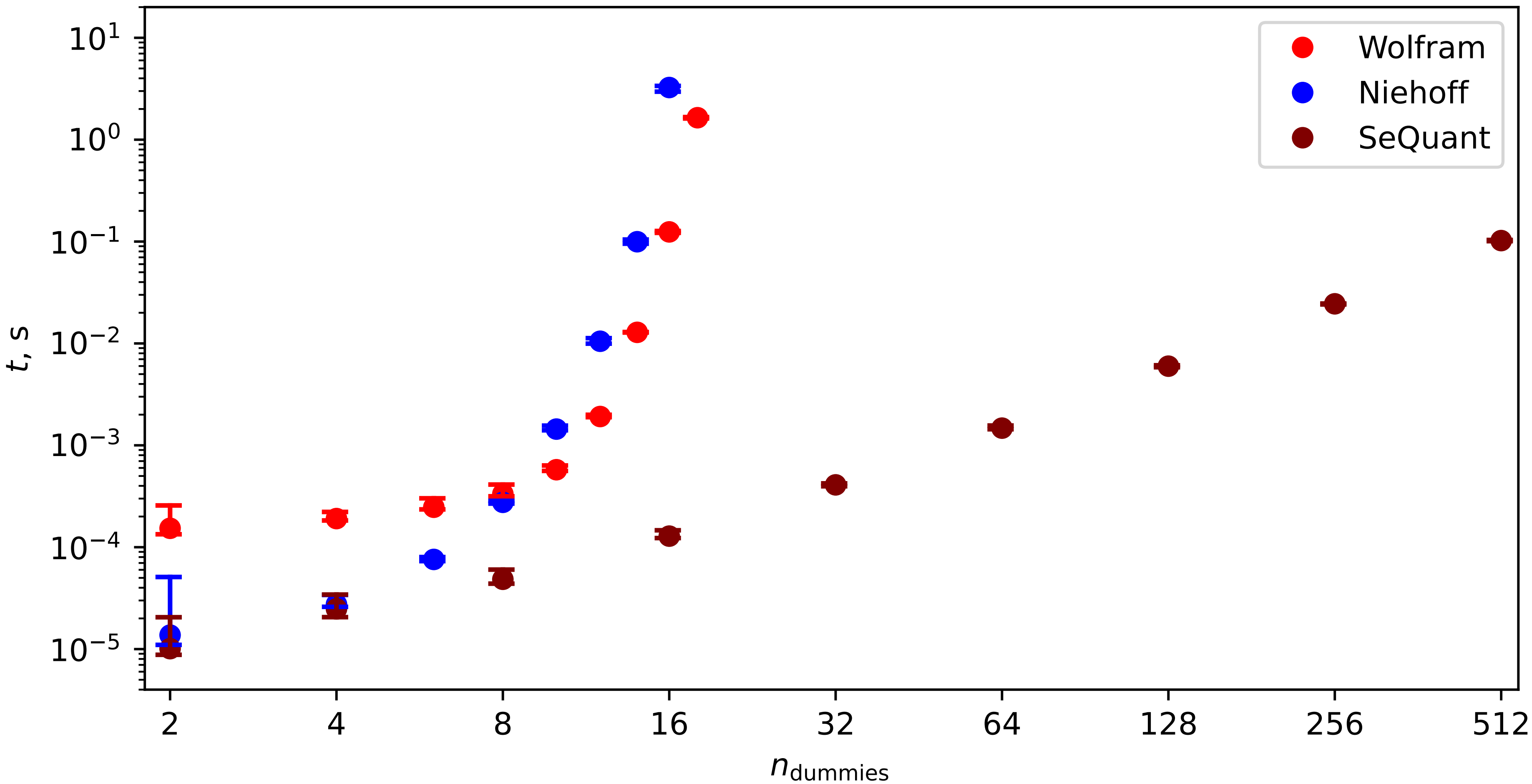
graph-theoretic extension of Butler-Portugal ("Niehoff") can handle some symmetric cases

Niehoff, Comp. Phys. Comm. 228, 123-145 (2018).

Tensor network canonization: colored graph vs others

canonicalizing $D_{i_1 i_2} D_{i_3 i_4} \ldots D_{i_{N-1} i_N} U^{\pi[i_1 \ldots i_N]}$

asymmetric D **and** U



our group-theoretic algorithm is fast for general tensor networks

SeQuant2: Fast(er) Wick Engine

- Thread-level concurrency (C++ threads or std::execution::par)
- Avoid equivalent contractions by topological info generated by tensor network automorphizer

Wick Theorem Optimization

- Further optimizations are possible if vacuum expectation values are wanted:
  - By tracking quasiparticle numbers (esp. easy if normal operators are pure (quasi)particle creators/annihilators e.g. in single-reference coupled-cluster)
  - By using topological symmetry of the expression* (this is similar to diagram-based approaches)
    - Topologically-equivalent ops in normal operators, e.g. $\langle 0 | \hat{T}_3^\dagger \hat{T}_3 | 0 \rangle$

$$\tilde{a}^{i_1 i_2 i_3}_{a_1 a_2 a_3} \tilde{a}^{a_4 a_5 a_6}_{i_4 i_5 i_6} \rightarrow \times 3 \quad \tilde{a}^{i_1 i_2 i_3}_{a_1 a_2 a_3} \tilde{a}^{a_4 a_5 a_6}_{i_4 i_5 i_6} \rightarrow \times 0 \quad \tilde{a}^{i_1 i_2 i_3}_{a_1 a_2 a_3} \tilde{a}^{a_4 a_5 a_6}_{i_4 i_5 i_6} \rightarrow \times 2$$

    - Topologically-equivalent normal operators in product, e.g. $\langle 0 | \hat{W} \hat{T}_1^2 | 0 \rangle$

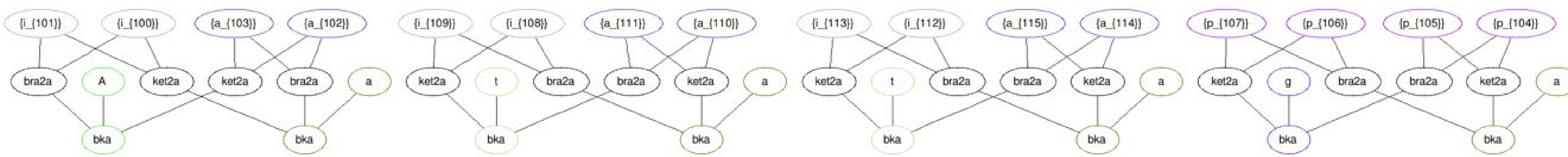
$$\tilde{a}^{p_1 p_2}_{p_3 p_4} \tilde{a}^{a_4}_{i_4} \tilde{a}^{a_5}_{i_5} \rightarrow \times 2 \quad \tilde{a}^{p_1 p_2}_{p_3 p_4} \tilde{a}^{a_4}_{i_4} \tilde{a}^{a_5}_{i_5} \rightarrow \times 0 \quad \tilde{a}^{p_1 p_2}_{p_3 p_4} \tilde{a}^{a_4}_{i_4} \tilde{a}^{a_5}_{i_5} \rightarrow \times 1 \quad \tilde{a}^{p_1 p_2}_{p_3 p_4} \tilde{a}^{a_4}_{i_4} \tilde{a}^{a_5}_{i_5} \rightarrow \times 1$$

e.g. see Xiao, Wang, Zhu, Comp. Phys. Comm. 184, 1966 (2013)

Wick Theorem Optimization: Details

- Topological symmetry of the input expression is determined by colored graph mapping and analysis similar to that used previously for canonization
  - Step 1: input expression is mapped to colored graph

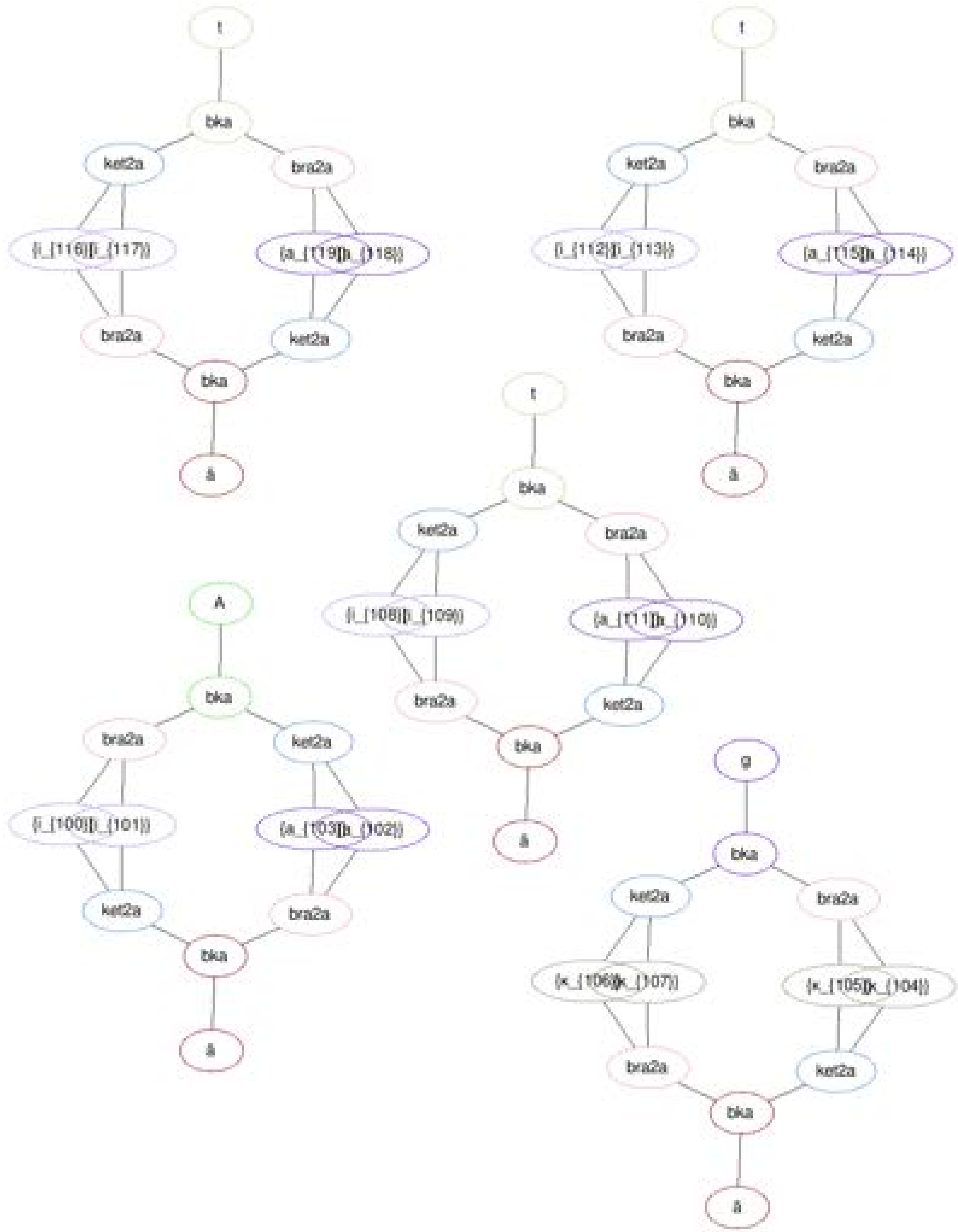
$$\langle 0|\hat{A}_2\hat{W}\hat{T}_2\hat{T}_2|0\rangle \equiv \frac{1}{256} \times A^{a_{102}a_{103}}_{i_{100}i_{101}}\tilde{a}^{i_{100}i_{101}}_{a_{102}a_{103}} \times g^{p_{106}p_{107}}_{p_{104}p_{105}}\tilde{a}^{p_{104}p_{105}}_{p_{106}p_{107}} \times t^{i_{108}i_{109}}_{a_{110}a_{111}}\tilde{a}^{a_{110}a_{111}}_{i_{108}i_{109}} \times t^{i_{112}i_{113}}_{a_{114}a_{115}}\tilde{a}^{a_{114}a_{115}}_{i_{112}i_{113}}$$



  - Step 2: compute the automorphism group of the graph
  - Step 3: test topological equivalence of operators and indices

Wick Theorem Optimization: Details

$$\langle 0|\hat{A}_2\hat{W}\hat{T}_2^3|0\rangle \equiv \frac{1}{1024}\times A^{a_{102}a_{103}}_{i_{100}i_{101}}\tilde{a}^{i_{100}i_{101}}_{a_{102}a_{103}}\times g^{\kappa_{106}\kappa_{107}}_{\kappa_{104}\kappa_{105}}\tilde{a}^{\kappa_{104}\kappa_{105}}_{\kappa_{106}\kappa_{107}}\times t^{i_{108}i_{109}}_{a_{110}a_{111}}\tilde{a}^{a_{110}a_{111}}_{i_{108}i_{109}}\times t^{i_{112}i_{113}}_{a_{114}a_{115}}\tilde{a}^{a_{114}a_{115}}_{i_{112}i_{113}}\times t^{i_{116}i_{117}}_{a_{118}a_{119}}\tilde{a}^{a_{118}a_{119}}_{i_{116}i_{117}}$$



Automorphism Group Generators:

- ({κ_{106}},{κ_{107}})
- ({κ_{104}},{κ_{105}})
- ({a_{102}},{a_{103}})
- ({i_{100}},{i_{101}})
- ({a_{110}},{a_{111}})
- ({i_{108}},{i_{109}})
- ({a_{114}},{a_{115}})
- ({a_{118}},{a_{119}})
- ({i_{112}},{i_{113}})
- ({i_{116}},{i_{117}})
- ({a_{114}},{a_{118}})({a_{115}},{a_{119}})({i_{112}},{i_{116}})({i_{113}},{i_{117}})(t,t)(bra2a,bra2a)(ket2a,ket2a)(bka,bka)(ã,ã)(bra2a,bra2a)(ket2a,ket2a)(bka,bka)
- ({a_{110}},{a_{114}})({a_{111}},{a_{115}})({i_{108}},{i_{112}})({i_{109}},{i_{113}})(t,t)(bra2a,bra2a)(ket2a,ket2a)(bka,bka)(ã,ã)(bra2a,bra2a)(ket2a,ket2a)(bka,bka)

Example: SR CC timings (seconds)

	Screen*/Topology				Simple H**
	F/F	T/F	F/T	T/T	
SD	2.4	0.14	0.04	0.02	**0.02**
+T	6540	6.0	1.8	0.14	**0.07**
+Q	-	1210	115	1.35	**0.43**
+P	-	-	-	16.0	**3.5**
+H	-	-	-	-	**43**

Intel Core i7 7820HQ/ Apple Clang 10 / Hoard 3.13 malloc
* Screen operator products by possible excitation level
** Nonredundant BSH expansion of CC Hbar, i.e. combine H T1 T2 and H T2 T1

further screening improvements are straightforward …

SeQuant2: Optimization

- Evaluation of individual tensor networks uses exhaustive or heuristic search to determine optimized evaluation order

$$X = (AB)C = A(BC)$$

- Evaluation of sets (e.g., sums) of tensor networks uses CSE

$$X = AB + (AB)C = Y + YC; \quad Y = AB$$

- Fusion is also possible, not yet deployed in production

$$X = AB + AC = A(B + C)$$

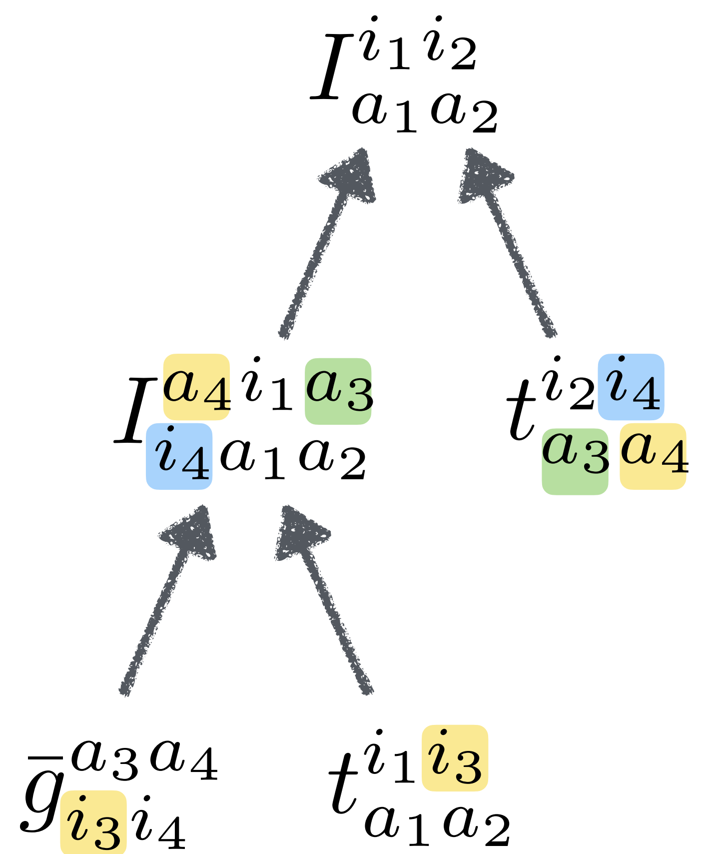
SeQuant2: Single Term Optimization / TN Binarization

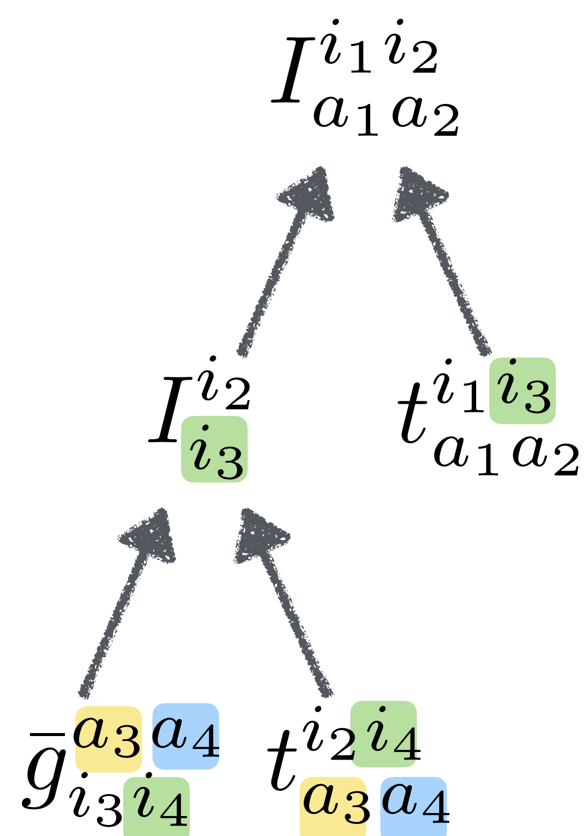
$$\left(\bar{g}^{a_3 a_4}_{i_3 i_4} t^{i_1 i_3}_{a_1 a_2}\right) t^{i_2 i_4}_{a_3 a_4}$$

$$\left(\bar{g}^{a_3 a_4}_{i_3 i_4} t^{i_2 i_4}_{a_3 a_4}\right) t^{i_1 i_3}_{a_1 a_2}$$

O^3V^4

O^3V^4

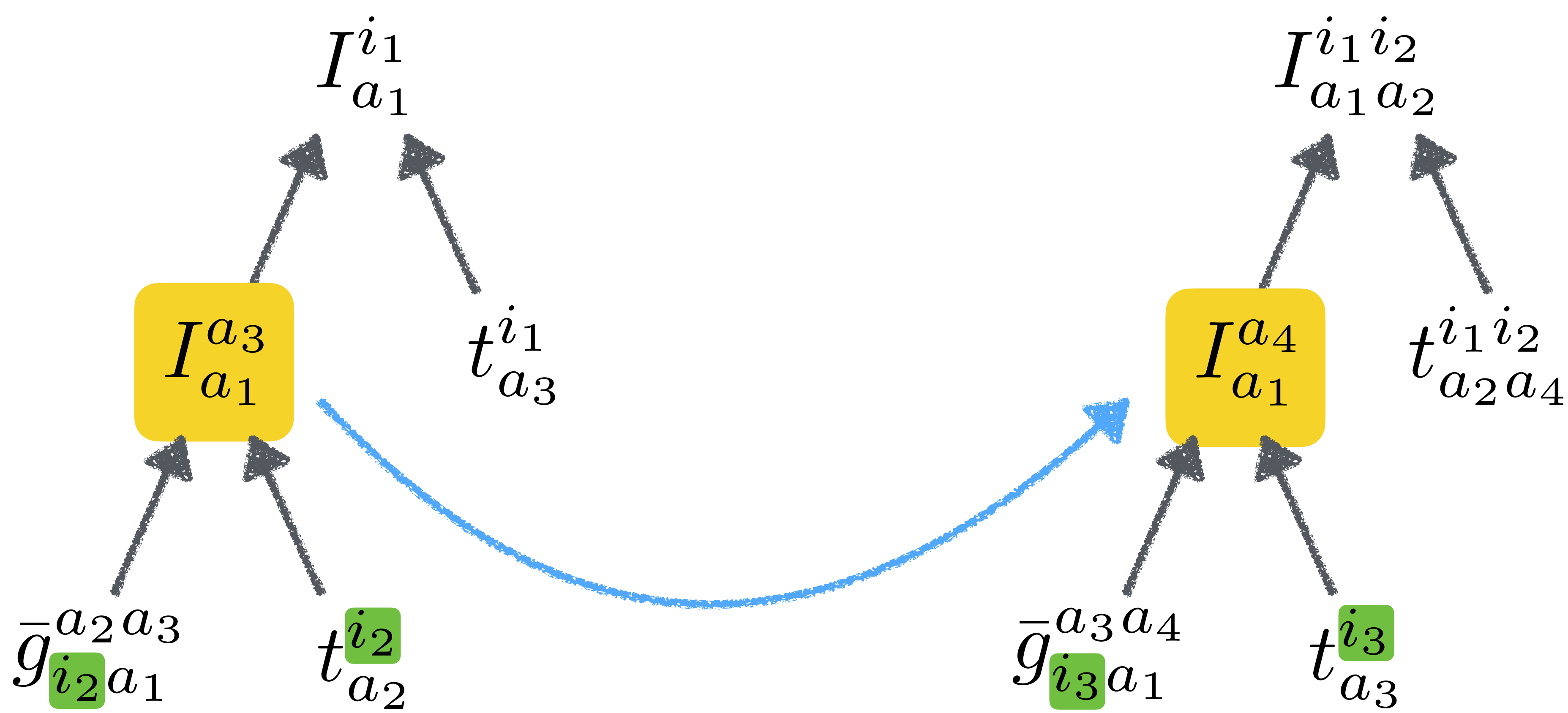




O^3V^2

O^3V^2

SeQuant2: TN Set CSE



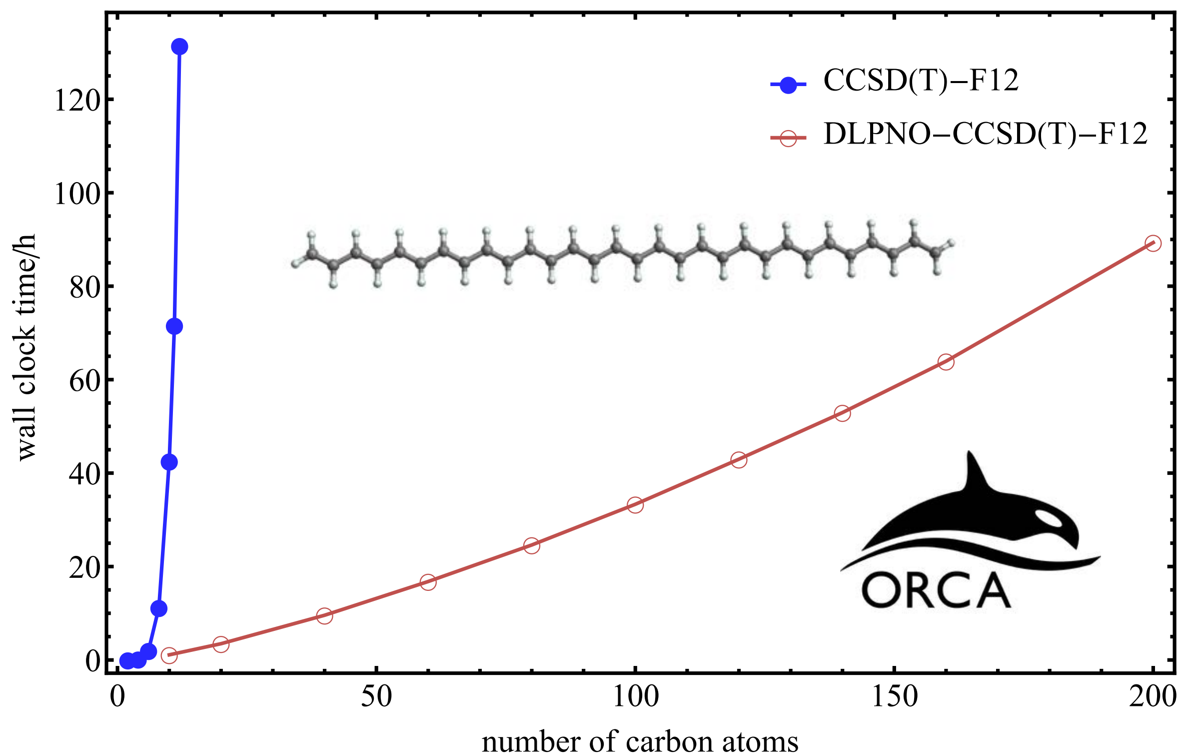
SeQuant2: Evaluation

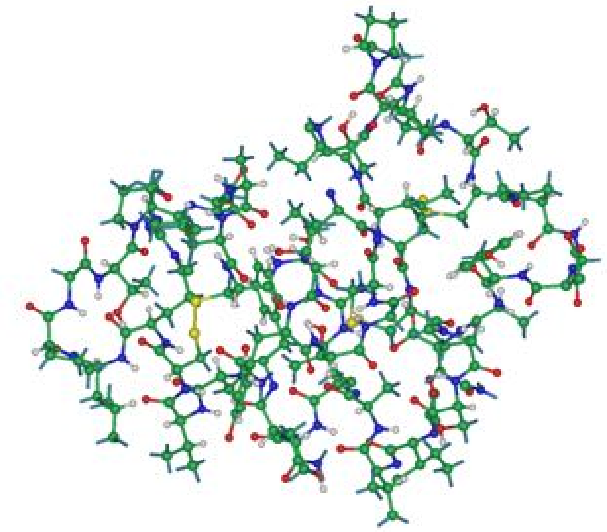
- Uses TiledArray (BTAS for reference testing; can add others)
- Rudimentary resource management
- Limited to conventional expressions (protoindex-free)
  - Work underway to extend to protoindex-containing expressions
    - Requires more functionality in TA

DATA-SPARSE TENSOR ALGEBRA

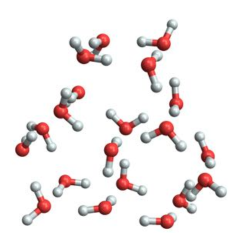
Better: Tensors in CC Networks are Data-Sparse!

conventional/dense CCSD(T) = O(N^7)   data-sparse CCSD(T) = O(N)





DLPNO-CC-F12 can be done on entire proteins now!



$(H_2O)_{20}$
60 atoms
960 basis functions

Formulation	# of cores (nodes)	t(min)	Dissociation Energy (kcal/mol)
dense	32768 (2048)	94.1[a]	185.61
sparse	16 (1)	77.7[b]	184.75

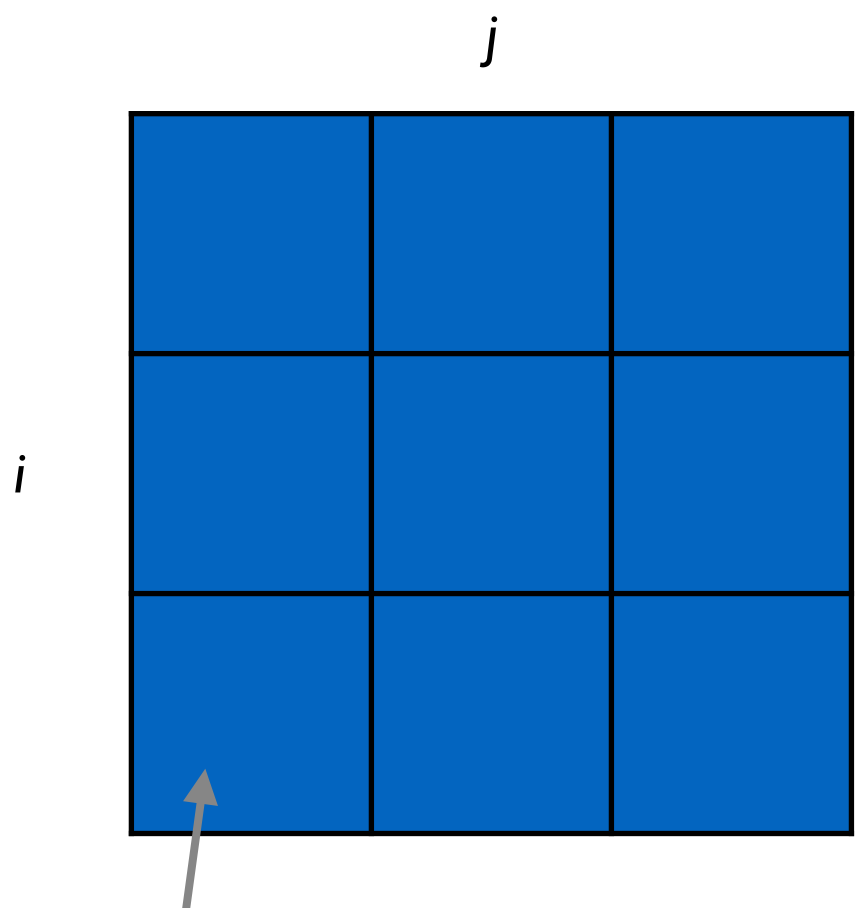
MPQC
ORCA

Pavosevic, Peng, Pinski, Riplinger, Neese, Valeev, J. Chem. Phys. (2017)

Data Sparsity Patterns Suggest New Tensor Formats

dense T2 tensor

order-4 tensor of scalars

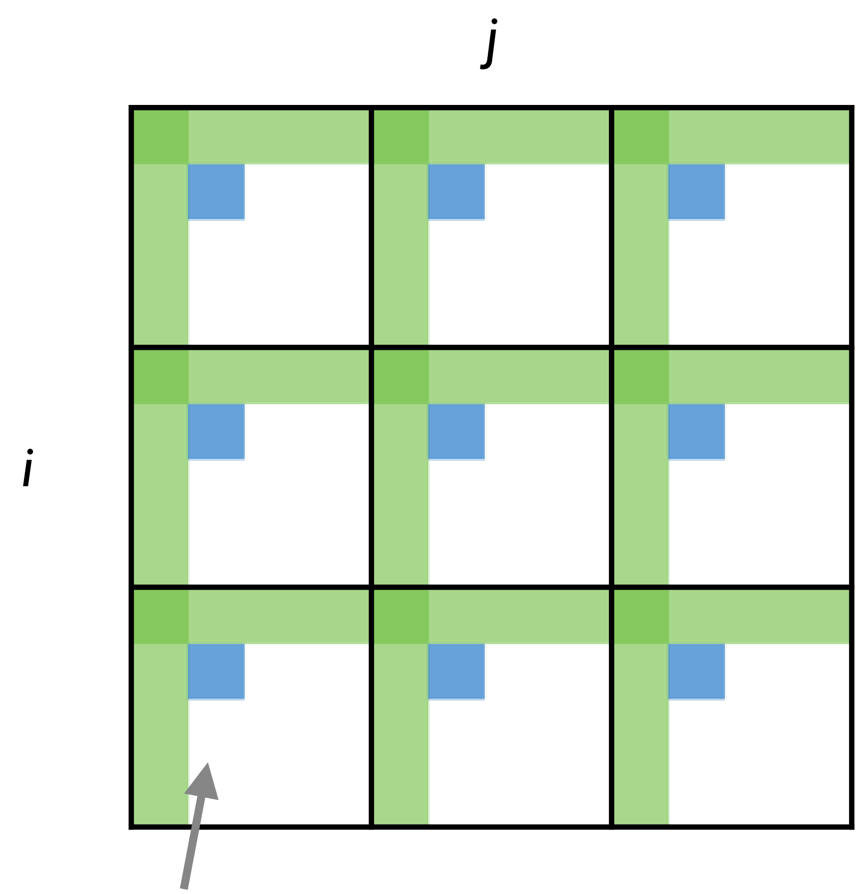


$$\mathbf{T}^{3,1} \equiv \{t_{ab}^{31}\}$$

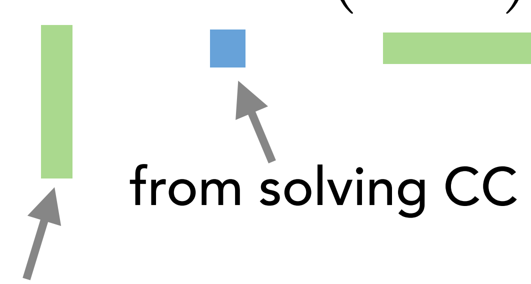
block-rank compressed (PNO) T2 tensor

Edmiston (1960s), Meyer (1970s), Neese (2000s)

order-2 tensor of order-2 tensors



$$\mathbf{T}^{3,1} \approx \mathbf{U}^{3,1}\ \mathbf{t}^{3,1}\ \left(\mathbf{V}^{3,1}\right)^{\dagger}$$



from solving CC eqn in subspace

fixed subspace from crude guess

Conventional vs PNO CC Methods

MP2 $R^{ij}_{ab} = G^{ij}_{ab} + F^c_a T^{ij}_{cb} + F^c_b T^{ij}_{ac} - F^i_k T^{kj}_{ab} - F^j_k T^{ik}_{ab}$

- familiar algebra of dense/block-sparse tensors with independent dimensions
- covariant algebra = affine loop nests, familiar optimization problems
- reduces to dense linear algebra kernels with high FLOP/MOP ratio

PNO MP2

$$R^{ij}_{a_{ij}b_{ij}} = G^{ij}_{a_{ij}b_{ij}} + F^{c_{ij}}_{a_{ij}} T^{ij}_{c_{ij}b_{ij}} + F^{c_{ij}}_{b_{ij}} T^{ij}_{a_{ij}c_{ij}}$$
$$- F^i_k T^{kj}_{a_{kj}b_{kj}} S^{a_{kj}}_{a_{ij}} S^{b_{kj}}_{b_{ij}} - F^j_k T^{ik}_{a_{ik}b_{ik}} S^{a_{ik}}_{a_{ij}} S^{b_{ik}}_{b_{ij}}$$

- algebra of block-sparse/element-sparse tensors with dependent dimensions
- noncovariant algebra = nonaffine loop nests
- sparsity patterns are *bootstrapped* iteratively, controlled by user-controlled thresholding
- reduces to dense linear algebra kernels with low FLOP/MOP ratio
- implementation complexity is largely driven by the sparsity computation/metadata manipulation

Complex Noncovariant Tensor Networks in PNO CC Methods

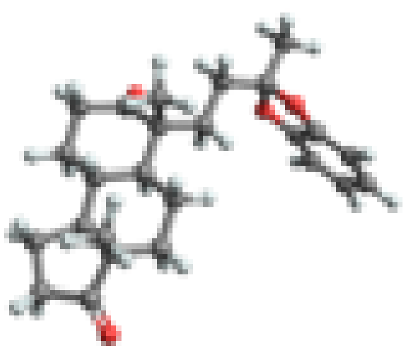
PNO MP2 $$G^{ij}_{a_{ij}b_{ij}} = C^{\tilde{\mu}_{ij}}_{a_{ij}} V^{iX_{ij}}_{\tilde{\mu}_{ij}} (\mathbf{V}^{-1})_{X_{ij}Y_{ij}} V^{jY_{ij}}_{\tilde{\nu}_{ij}} C^{\tilde{\nu}_{ij}}_{b_{ij}}$$

- high-level tensor notation doesn't capture complete details without undue complexity, hence need a mix of high-level DSL-like composition and imperative programming
- richer variety of data structures and algorithms, e.g. the above is implemented as a single 5-way contraction rather than a sequence of binary contractions

```
for i in [0,#occ):
  for all j in pair list of i:
    if i!=j:
      obtain unique parts of V(i,mu_i,X_i), V(i,mu_j,X_i), V(i,mu_i,X_j), V(i,mu_j,X_j) and
        merge into V(i,mu_ij,X_ij)
      obtain unique parts of V(j,mu_i,X_i), V(j,mu_j,X_i), V(j,mu_i,X_j), V(j,mu_j,X_j) and
        merge into V(j,mu_ij,X_ij)
      obtain unique parts of V(X_i,Y_i), V(X_i,Y_j), V(X_j,Y_i), V(X_j,Y_j), and
        merge into V(X_ij,Y_ij)
      concatenate OSVs C(a_i,mu_i) and C(a_j,mu_j) into C(a_ij,mu_ij)
      W(i,a_ij,X_ij) = C(a_ij,mu_ij) * V(i,mu_ij,X_ij)
      W(j,a_ij,X_ij) = C(a_ij,mu_ij) * V(i,mu_ij,X_ij)
      Vinv(X_ij,Y_ij) = inverse(V(X_ij,Y_ij))
      f(j,a_ij,X_ij) = W(j,a_ij,X_ij) * Vinv(X_ij,Y_ij)
      g(i,j,a_ij,b_ij) = W(i,a_ij,X_ij) * f(j,a_ij,X_ij)
    else: // i==j
      ..
```

composed as tasks generated by imperative code over local and distributed data

Manually-Written PNO MP2 Implementation in MPQC



- 31% of electron pairs screened out
- average pair domain = 729 bf
- average # of PNOs = 91
- recovered 99.7 % of DF-MP2 correlation energy

Performance (sec) vs. state-of-the-art PNO-MP2 in Molpro*

*Werner, et al, DOI 10.1021/ct500725e

Step	Molpro	MPQC
orbital domains (OSV)	43	54
integral transform	161	139
PNO generation	37	91
LMP2 solver	54	21
Total	265	341

20 cores x 2.8 GHz AVX

competitive performance with leading code already, but more optimizations possible

Progress: Automating PNO-CCSD implementation

$$\langle 0|\hat{A}_2\bar{H}|0\rangle = \frac{1}{8}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}}_{i_3i_4} t^{i_3}_{\alpha_5^{i_3}} t^{i_4}_{\alpha_6^{i_4}} t^{i_1i_2}_{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}} S^{\alpha_5^{i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_4}}_{\alpha_2^{i_1i_2}} + -1\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1\alpha_3^{i_2i_4}}_{i_3i_4} t^{i_3}_{\alpha_4^{i_3}} t^{i_2i_4}_{\alpha_3^{i_2i_4}\alpha_5^{i_2i_4}} S^{\alpha_5^{i_2i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_4^{i_3}}_{\alpha_2^{i_1i_2}} + \frac{1}{16}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}}_{i_3i_4} t^{i_3i_4}_{\alpha_5^{i_3i_4}\alpha_6^{i_3i_4}} t^{i_1i_2}_{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}} S^{\alpha_5^{i_3i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_3i_4}}_{\alpha_2^{i_1i_2}} +$$

$$\frac{1}{8}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}}_{i_3i_4} t^{i_3}_{\alpha_5^{i_3}} t^{i_4}_{\alpha_6^{i_4}} t^{i_1i_2}_{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}} S^{\alpha_5^{i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_4}}_{\alpha_2^{i_1i_2}} + -1\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1\alpha_3^{i_2i_4}}_{i_3i_4} t^{i_3}_{\alpha_4^{i_3}} t^{i_2i_4}_{\alpha_3^{i_2i_4}\alpha_5^{i_2i_4}} S^{\alpha_5^{i_2i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_4^{i_3}}_{\alpha_2^{i_1i_2}} + \frac{1}{16}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}}_{i_3i_4} t^{i_3i_4}_{\alpha_5^{i_3i_4}\alpha_6^{i_3i_4}} t^{i_1i_2}_{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}} S^{\alpha_5^{i_3i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_3i_4}}_{\alpha_2^{i_1i_2}} +$$

$$\frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_4}\alpha_4^{i_1i_2}}_{i_3i_4} t^{i_3}_{\alpha_5^{i_3}} t^{i_4}_{\alpha_3^{i_4}} t^{i_1i_2}_{\alpha_1^{i_1i_2}\alpha_4^{i_1i_2}} S^{\alpha_5^{i_3}}_{\alpha_2^{i_1i_2}} + -\frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} f^{\alpha_3^{i_1i_2}}_{i_3} t^{i_3}_{\alpha_4^{i_3}} t^{i_1i_2}_{\alpha_1^{i_1i_2}\alpha_3^{i_1i_2}} S^{\alpha_4^{i_3}}_{\alpha_2^{i_1i_2}} + -\frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_3}\alpha_4^{i_1i_2}}_{i_3\alpha_1^{i_1i_2}} t^{i_3}_{\alpha_3^{i_3}} t^{i_1i_2}_{\alpha_2^{i_1i_2}\alpha_4^{i_1i_2}} +$$

$$\frac{1}{8}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1}\alpha_4^{i_2}}_{i_3i_4} t^{i_1}_{\alpha_3^{i_1}} t^{i_2}_{\alpha_4^{i_2}} t^{i_3i_4}_{\alpha_5^{i_3i_4}\alpha_6^{i_3i_4}} S^{\alpha_5^{i_3i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_3i_4}}_{\alpha_2^{i_1i_2}} + \frac{1}{4}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1}\alpha_4^{i_2}}_{i_3i_4} t^{i_3}_{\alpha_5^{i_3}} t^{i_4}_{\alpha_6^{i_4}} t^{i_1}_{\alpha_3^{i_1}} t^{i_2}_{\alpha_4^{i_2}} S^{\alpha_5^{i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_4}}_{\alpha_2^{i_1i_2}} + A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1\alpha_3^{i_2i_3}}_{i_3\alpha_1^{i_1i_2}} t^{i_2i_3}_{\alpha_3^{i_2i_3}\alpha_4^{i_2i_3}} S^{\alpha_4^{i_2i_3}}_{\alpha_2^{i_1i_2}} +$$

$$-\frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} f^{\alpha_3^{i_1i_2}}_{\alpha_1^{i_1i_2}} t^{i_1i_2}_{\alpha_2^{i_1i_2}\alpha_3^{i_1i_2}} + \frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} f^{i_1}_{i_3} t^{i_2i_3}_{\alpha_3^{i_2i_3}\alpha_4^{i_2i_3}} S^{\alpha_3^{i_2i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_4^{i_2i_3}}_{\alpha_2^{i_1i_2}} + A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1\alpha_3^{i_2}}_{i_3\alpha_1^{i_1i_2}} t^{i_3}_{\alpha_4^{i_3}} t^{i_2}_{\alpha_3^{i_2}} S^{\alpha_4^{i_3}}_{\alpha_2^{i_1i_2}} +$$

$$\frac{1}{4}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1i_2}_{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}} + \frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1\alpha_3^{i_2}}_{i_3i_4} t^{i_3}_{\alpha_4^{i_3}} t^{i_4}_{\alpha_5^{i_4}} t^{i_2}_{\alpha_3^{i_2}} S^{\alpha_4^{i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_5^{i_4}}_{\alpha_2^{i_1i_2}} + \frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} f^{\alpha_3^{i_1}}_{i_3} t^{i_1}_{\alpha_3^{i_1}} t^{i_2i_3}_{\alpha_4^{i_2i_3}\alpha_5^{i_2i_3}} S^{\alpha_4^{i_2i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_5^{i_2i_3}}_{\alpha_2^{i_1i_2}} +$$

$$\frac{1}{4}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1i_2}_{i_3i_4} t^{i_3}_{\alpha_3^{i_3}} t^{i_4}_{\alpha_4^{i_4}} S^{\alpha_3^{i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_4^{i_4}}_{\alpha_2^{i_1i_2}} + -\frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1}\alpha_4^{i_3}}_{i_3i_4} t^{i_1}_{\alpha_3^{i_1}} t^{i_3}_{\alpha_4^{i_3}} t^{i_2i_4}_{\alpha_5^{i_2i_4}\alpha_6^{i_2i_4}} S^{\alpha_5^{i_2i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_2i_4}}_{\alpha_2^{i_1i_2}} + \frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1i_3}\alpha_4^{i_2i_4}}_{i_3i_4} t^{i_1i_3}_{\alpha_3^{i_1i_3}\alpha_5^{i_1i_3}} t^{i_2i_4}_{\alpha_4^{i_2i_4}\alpha_6^{i_2i_4}} S^{\alpha_5^{i_1i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_2i_4}}_{\alpha_2^{i_1i_2}} +$$

$$\frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1\alpha_3^{i_2}}_{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}} t^{i_2}_{\alpha_3^{i_2}} + -\frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1\alpha_3^{i_3}}_{i_3i_4} t^{i_3}_{\alpha_3^{i_3}} t^{i_2i_4}_{\alpha_4^{i_2i_4}\alpha_5^{i_2i_4}} S^{\alpha_4^{i_2i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_5^{i_2i_4}}_{\alpha_2^{i_1i_2}} + -\frac{1}{4}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_3i_4}\alpha_4^{i_1i_2}}_{i_3i_4} t^{i_3i_4}_{\alpha_3^{i_3i_4}\alpha_5^{i_3i_4}} t^{i_1i_2}_{\alpha_1^{i_1i_2}\alpha_4^{i_1i_2}} S^{\alpha_5^{i_3i_4}}_{\alpha_2^{i_1i_2}} +$$

$$\frac{1}{4}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}}_{i_3\alpha_1^{i_1i_2}} t^{i_3}_{\alpha_5^{i_3}} t^{i_1i_2}_{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}} S^{\alpha_5^{i_3}}_{\alpha_2^{i_1i_2}} + -1\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1}\alpha_4^{i_2i_4}}_{i_3i_4} t^{i_3}_{\alpha_5^{i_3}} t^{i_1}_{\alpha_3^{i_1}} t^{i_2i_4}_{\alpha_4^{i_2i_4}\alpha_6^{i_2i_4}} S^{\alpha_6^{i_2i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_5^{i_3}}_{\alpha_2^{i_1i_2}} + \frac{1}{4}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1}\alpha_4^{i_2}}_{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}} t^{i_1}_{\alpha_3^{i_1}} t^{i_2}_{\alpha_4^{i_2}} +$$

$$\frac{1}{4}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1\alpha_3^{i_2}}_{i_3i_4} t^{i_2}_{\alpha_3^{i_2}} t^{i_3i_4}_{\alpha_4^{i_3i_4}\alpha_5^{i_3i_4}} S^{\alpha_4^{i_3i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_5^{i_3i_4}}_{\alpha_2^{i_1i_2}} + A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1}\alpha_4^{i_2i_3}}_{i_3\alpha_1^{i_1i_2}} t^{i_1}_{\alpha_3^{i_1}} t^{i_2i_3}_{\alpha_4^{i_2i_3}\alpha_5^{i_2i_3}} S^{\alpha_5^{i_2i_3}}_{\alpha_2^{i_1i_2}} + \frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1i_2}_{i_3\alpha_1^{i_1i_2}} t^{i_3}_{\alpha_3^{i_3}} S^{\alpha_3^{i_3}}_{\alpha_2^{i_1i_2}} +$$

$$\frac{1}{2}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1}\alpha_4^{i_2}}_{i_3\alpha_1^{i_1i_2}} t^{i_3}_{\alpha_5^{i_3}} t^{i_1}_{\alpha_3^{i_1}} t^{i_2}_{\alpha_4^{i_2}} S^{\alpha_5^{i_3}}_{\alpha_2^{i_1i_2}} + \frac{1}{8}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{i_1i_2}_{i_3i_4} t^{i_3i_4}_{\alpha_3^{i_3i_4}\alpha_4^{i_3i_4}} S^{\alpha_3^{i_3i_4}}_{\alpha_1^{i_1i_2}} S^{\alpha_4^{i_3i_4}}_{\alpha_2^{i_1i_2}} + -\frac{1}{4}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_2i_4}\alpha_4^{i_2i_4}}_{i_3i_4} t^{i_1i_3}_{\alpha_5^{i_1i_3}\alpha_6^{i_1i_3}} t^{i_2i_4}_{\alpha_3^{i_2i_4}\alpha_4^{i_2i_4}} S^{\alpha_5^{i_1i_3}}_{\alpha_1^{i_1i_2}} S^{\alpha_6^{i_1i_3}}_{\alpha_2^{i_1i_2}} +$$

$$\frac{1}{8}\times A^{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}}_{i_1i_2} g^{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}}_{\alpha_1^{i_1i_2}\alpha_2^{i_1i_2}} t^{i_1i_2}_{\alpha_3^{i_1i_2}\alpha_4^{i_1i_2}}$$

Talk Synopsis

need to raise the level of abstraction to enable many-body QM

symbolic techniques are a component of the needed many-body QM technology stack

particularly needed for supporting tensor compressed/factorized methods (e.g., PNO)

ideas are old, let's learn from the pioneers and make this sustainable

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- Samuel Powell
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- Ashawini Thakur
- Kshitij Surjuse
- Ajay Melecamburath

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DE-SC0019374

postdoctoral positions available in methods and software development for electronic structure