1 Past work

- Rys Quadrature CPU/GPU
- Fock Algorithm CPU/GPU
- MP2 Algorithm
  - Small memory footprint: $(M * N * O^2)/2$, eg 3.2 GB for 2000 virt, 200 occ , F shells
  - Arbitrary storage backend - distributed memory, disk, etc
  - Further enhancments possible
- Papers
  - Performance of Electronic Structure Calculations on Blue Gene and Cray XT4 Computers
  - Accelerating Quantum Chemistry Research Using GPUs - Two Electron Replusion Integrals

2 Current work

- Case for disk - cheap, scalable, SSD in future. E.g., 1TB SSD appr. $3000 CAD. 1TB RAM $100,000 CAD
- CCSD(T), ON^2 memory - very scalable - versus O^2N^2
  - (T) done
  - Integral transforms done $C(pa)C(qb)C(rc)C(sd) * g(pqrs) -> g'(abcd)$
  - S done
  - D almost done (this week)
- Papers
  - MP2
  - CCSD(T)

3 Future

Listing 1: Tensor operator expression

```
1
2    tensor::Tensor<3> A(10,20,10);
3    size_t size[] = { 10, 10, 20, 10 };
4    tensor::Tensor<4> B(size), C(size);
```

```
 5
 6    tensor::index<'a'> a;
 7    tensor::index<'b'> b;
 8    tensor::index<'c'> c;
 9    tensor::index<'d'> d;
10    tensor::index<'e'> e;
11    tensor::index<'i'> i;
12    tensor::index<'j'> j;
13
14    BOOST_AUTO(I, tensor::Operator::I);
15    BOOST_AUTO(P, tensor::Operator::P);
16
17    (I - P(j,i))(I - P(i,j))(A(i,j,0));
18
19    A(a,i,j) = 0.5*C(j,i,a,0) + (B(a,c,d,0)*C(i,j,c,d); // ok
20    A(a,i,j) = (B(a,c,d,0)*C(i,j,c,0); // error
21
22    C(a,b,c,d) = -B(b,a,d,c)
23
24    swap(A(b,0,0), A(0,b,0));
25    tensor::permute<1,0>(A(b,0,c));
26
27    contract(1, A(b,0,a), B(a,c,d,0), 0, C(b,c,d,0));
28    A(b,c,d) = contract(B(b,0,0,a), C(a,c,d,0));
29    A(b,c,d) = 5.0*contract(B(b,a,0,0), C(a,c,d,0));
```