OAK RIDGE National Laboratory

Efficient tensor contractions for Nuclear Physics with NTCL

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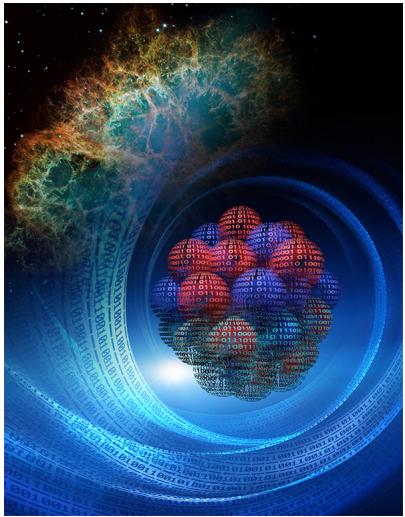
Tensor contractions in NuCCOR

- Hartree-Fock
- Coupled-Cluster
- Eigenvalue solver
- Expectation values



Conceptual art by LeJean Hardin and Andy Sproles

The Coupled-Cluster

- Schrödinger Equation

$$H|\Psi\rangle = E|\Psi\rangle$$

- Exponential anzats

$$|\Psi_{CCD}\rangle = e^{T}|\phi\rangle$$

- Energy equation

$$E_{CCD} = \langle\phi|e^{-T}He^{T}|\phi\rangle$$

- Cluster equations

$$\left\langle \phi_{i,j,\ldots}^{a,b,\ldots} \middle| e^{-T}He^{T} \middle| \phi \right\rangle = 0$$

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Coupled-Clusters Doubles

$$T = \sum_{a>b,i>j} t_{ij}^{ab} c_a^\dagger c_b^\dagger c_i c_j$$

$$\Delta E_{CCD} = \sum_{i>j,a>b} \langle ij|V|ab\rangle \, t_{ij}^{ab}$$

$$\varepsilon_{ij}^{ab} t_{ij}^{ab} = \langle ab|V|ij\rangle + \frac{1}{2} \sum_{cd} \langle ab|V|cd\rangle \, t_{ij}^{cd} + \cdots$$

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Transition between hardware

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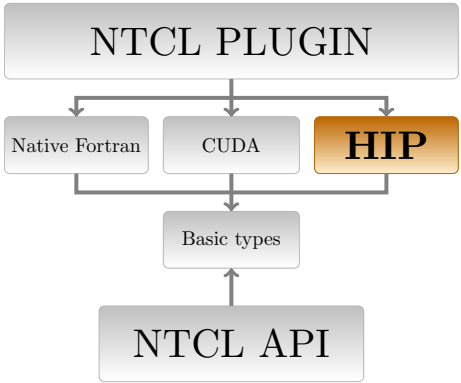
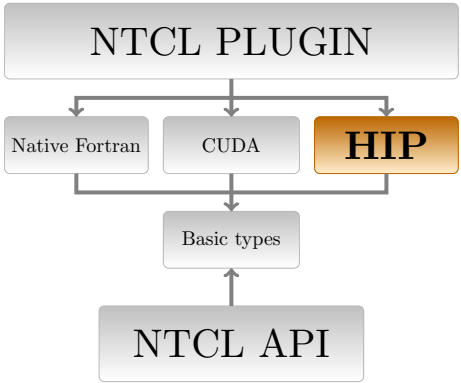
NTCL

- Written in modern object-oriented Fortran (Fortan 2018)
- Test-driven development to ensure correctness
- Hardware-independent frontend
- Hardware-dependent backend

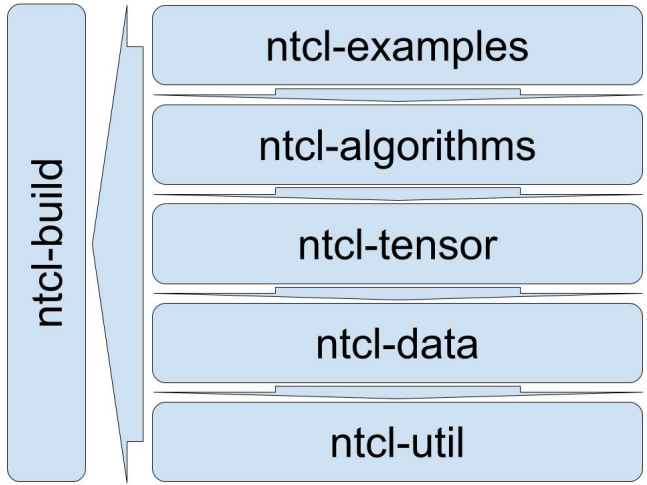
NTCL



NTCL



NTCL



NTCL

- ntcl-comm: Manages MPI distribution
- ntcl-manybody: Implements sparse tensors for many-body physics both for J-scheme and M-scheme
- ntcl-diagrams: Implements sparse tensor contractions relevant for CC

User friendly API

```
1  class(tensor), allocatable :: my_tensor1, my_tensor2, my_tensor3
2  class(tensor_contraction), allocatable :: my_contraction
3  real(real64), dimension(:,:,:,:), ... :: fortran_tensor1, ...
4  real(real64), dimension(:,:,:,:), pointer :: result_pointer
5  ...
6  call allocate_and_copy_tensor(my_tensor1, fortran_tensor1)
7  ...
8  call tensor_contraction_factory%create(my_contraction, &
9                                         'C(a,b,c,d)=A(a,e,c,f)*B(e,b,f,d)')
10 ...
11 call my_contraction%contract(my_tensor3, my_tensor1, my_tensor2)
12 ...
13 call secure_fortran_pointer_from_tensor(result_pointer, my_tensor3)
14 fortran_tensor3 = result_pointer
15 call release_pointer_from_remote_tensor(result_pointer, my_tensor3)
```

User friendly API

```
1  real(real64), dimension(:,:,:,:), ... :: my_tensor1, &
2                                           my_tensor2, &
3                                           my_tensor3
4  call contract('C(a,b,c,d)=A(a,e,c,f)*B(e,b,f,d)', &
5                my_tensor1, my_tensor2, my_tensor3)
```

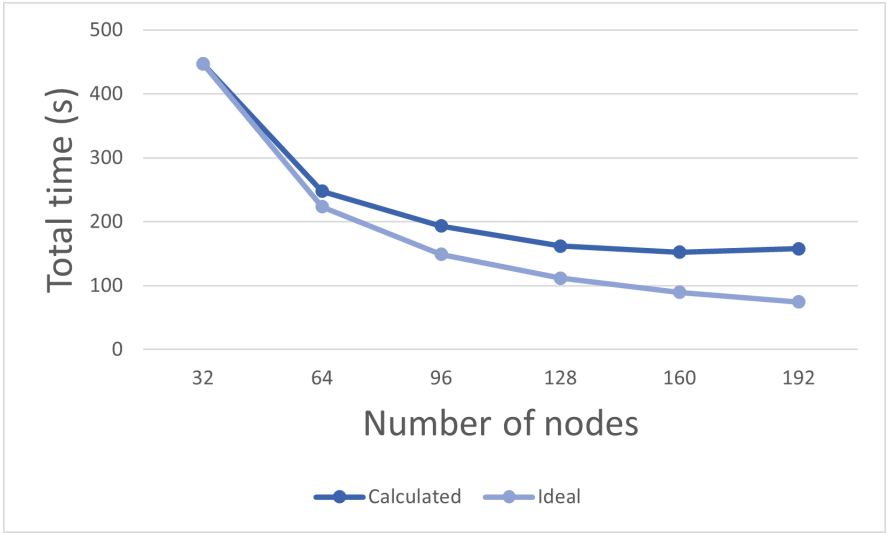
User friendly API

```
1  real(real64), dimension(m,k), ... :: A
2  real(real64), dimension(k,n), ... :: B
3  real(real64), dimension(m,n), ... :: C
4  ...
5  call ntcl_gemm('N', 'N', m, n, k, 1.0D0, A, m, B, k, 0.0D0, C, m)
```

Supported datatypes

- real32
- real64
- complex64
- complex128

Nuccor on Frontier for $^{48}\mathrm{Ti}$ $N_{\max} = 8$ Strong scaling



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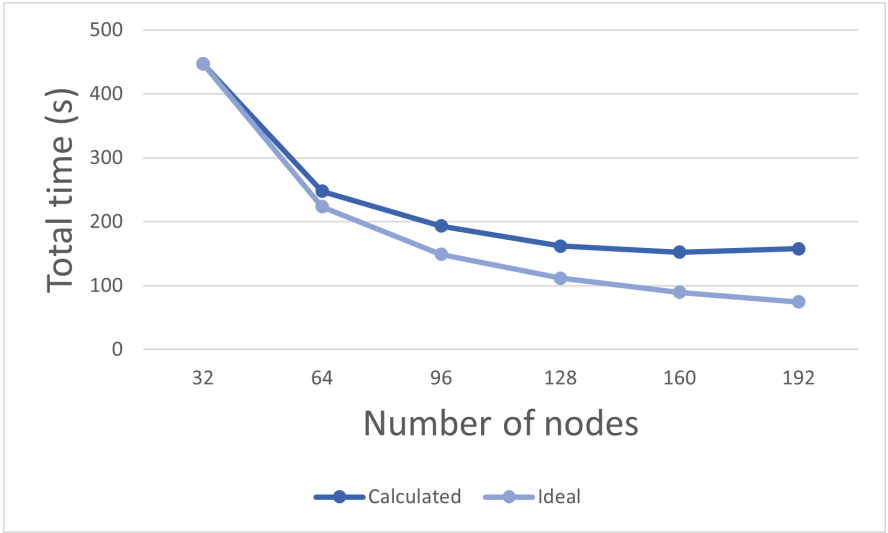

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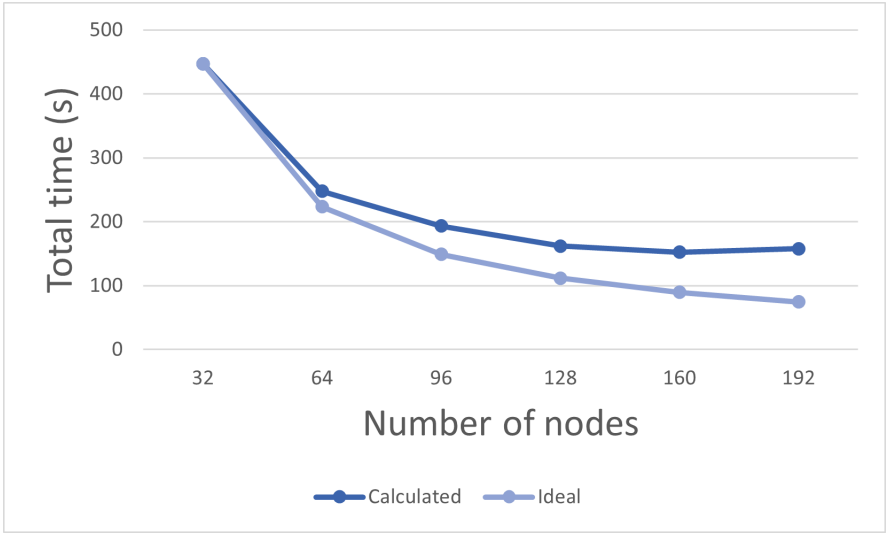

Conclusion

- Coupled-Cluster needs efficient tensor-contractions
- NTCL provides a hardware-independent interface to do tensor-contractions on different hardware
- Simple user interface

Conclusion

To get access to NTCL email us

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- Tor Djärv: djarvtr@ornl.gov