**HACI User Guide**

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1. The first step in running a HACI calculation is to source the desired wavefunction you wish to approximate by running a CASCI wavefunction with the keyword “cassavevectors.”

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This will produce a “.dat” file in the scratch directory for each respective wavefunction the calculation has built. For example, if you want the ground state singlet, and lowest energy triplet wavefunction the input is the following.

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This will produce two binary files which are wavefunctions.



1. Now we need to compress the “.dat” files using the HACI algorithm by running the python script, “HACI\_4-14-23.” By changing the value of “thres=” in this python program we can tune the storage and accuracy of the method. The storage for a given calculation will be output as,

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Where “Dense” is the uncompressed storage cost of the input matrix, and “CMatrix” is the compressed storage cost. “Memory” is the number of double needed to store the matrix, while “RelError” approximates the error introduced to the matrix (larger is worse). The output of this program will be a file named recn\_init.bin. This will be the file we need for the next step.

1. The next step is to run a TDCI calculation. The version of Terachem you are running should be compiled from the TDCI testing branch to get the energy and spin calculations for an input “.dat” file. The version HACI was tested on was TeraChem v1.9-2022.10-dev. This can be done on Seawulf by using my compiled version of Terachem by exporting the following.

**export TeraChem=/gpfs/projects/LevineGroup/kberard/terachem\_current/build**

**export LD\_LIBRARY\_PATH=/gpfs/projects/LevineGroup/kberard/terachem\_current/build/lib:\$LD\_LIBRARY\_PATH**

**export PATH=/gpfs/projects/LevineGroup/kberard/terachem\_current/build/bin:\$PATH**

For the TDCI calculation to calculate the energy and spin (<S2>) of the input wavefunction (ren\_init.bin) you must include the keyword,



1. Once the calculation has completed you will see,

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And,



To the right of these prompts, you will see the output spin and energy of the input wavefunction. For example, an output would look like,





1. For comparison we often run an SVD approximation of the wavefunction using different ranks. This can also be accomplished using python by reading in the “.dat” files, running SVD, then multiplying the decomposition back to a single matrix. The final matrix should be output to a binary file named “recn\_init.bin. The storage can be calculated as the number of elements of the three matrices which make up the SVD.

**Examples of a HACI and SVD calculation will be included for reference!**

**There will also be other compression schemes that were tested in the alternative compression scheme folder.**

**Best, Ken.**