This document details the input parameters needed to reproduce all results in our forthcoming publication (`https://arxiv.org/abs/2005.00654`). More methodological details for each of these methods are provided in the paper. The statistics reported for each calculation can be obtained using the `calc_stats.py` Python script provided in this directory.

FCI-FRI calculations

The following results were obtained using the systematic FCI-FRI method without the semi-stochastic extension, using the original heat-bath Power-Pitzer factorization.

Ne (aug-cc-pVDZ)

These results are for the Neon atom in the aug-cc-pVDZ basis. The Hartree-Fock data for this system, generated using pyscf, can be found in the directory `Input_Data/Neon_augccpvdz`. As an example, the results in the second line of this table were generated by running the following command:

```
mpirun -n 4 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/Neon_augccpvdz/ --target 100000 --distribution HB
--vec_nonz 100000 --mat_nonz 100000 --max_dets 50000 --initiator 0.5 --ini_vec Input_Data/Neon_augccpvdz/cisd_
```

Vec. nonz.	Matr. nonz.	Target[1]	n_a^2	Trial vec.[3]	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)[4]	Efficiency (E_h^{-2})	Figures[5]
100k	100k	100k	0.0	HF	CISD	40k	1M	4.4561 ± 16.5977	0.0151	1
100k	100k	100k	0.5	HF	CISD	40k	1M	2.3959 ± 4.4132	0.2139	1
100k	100k	100k	1.0	HF	CISD	40k	1M	0.0223 ± 0.0070	85802	1, 2, 4
100k	100k	100k	1.5	HF	CISD	40k	1M	0.0282 ± 0.0064	100190	1
100k	100k	100k	2.0	HF	CISD	40k	1M	0.0321 ± 0.0065	97480	1
50k	50k	50k	1	HF	CISD	40k	1M	0.0103 ± 0.0095	46368	2, 4
150k	150k	150k	1	HF	CISD	40k	1M	0.0102 ± 0.0055	135837	2, 3, 4
200k	200k	200k	1	HF	CISD	40k	1M	0.0052 ± 0.0095	206821	2, 3, 4
250k	250k	250k	1	HF	CISD	40k	1M	0.0038 ± 0.0040	259087	2, 3
24k	52k	50k	3	HF	CISD	40k	1M	0.0038 ± 0.0101	40798	5
42k	104k	100k	3	HF	CISD	40k	1M	0.0196 ± 0.0064	100854	5
58k	157k	150k	3	HF	CISD	40k	1M	0.0247 ± 0.0051	158244	5
73k	209k	200k	3	HF	CISD	40k	1M	0.0251 ± 0.0043	229864	5

[1] Indicates the target one-norm of the iterates.

[2] n_a indicates the initiator threshold.

[3] Because no trial vector was specified in the input options, Hartree-Fock was used.

[4] The exact FCI ground-state energy was subtracted from these estimates.
[5] Indicates the figures in our paper in which the data appears.

H_2O (cc-pVDZ)

These results are for H_2O in the cc-pVDZ basis. The Hartree-Fock data for this system, generated using pyscf, can be found in the directory `Input_Data/H2O_ccpvdz`. As an example, the results in the second line of this table were generated by running the following command:

```
mpirun -n 16 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/H2O_ccpvdz/ --target 1000000 --distribution HB
--vec_nonz 1000000 --mat_nonz 1000000 --max_dets 100000 --initiator 0.5 --ini_vec Input_Data/H2O_ccpvdz/cisd_
```

Vec. nonz.	Matr. nonz.	Target	n_a	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	1M	1M	0.0	HF	CISD	40k	1M	173.9337 ± 49.0249	0.00173	1
1M	1M	1M	0.5	HF	CISD	40k	1M	2.4213 ± 3.1589	0.4176	1
1M	1M	1M	1.0	HF	CISD	40k	1M	0.0171 ± 0.0067	92963	1,2
1M	1M	1M	1.5	HF	CISD	40k	1M	0.0273 ± 0.0064	102492	1
1M	1M	1M	2.0	HF	CISD	40k	1M	0.0298 ± 0.0069	86657	1
3M	3M	3M	1	HF	CISD	40k	524k	0.0172 ± 0.0048	358168	2, 3, 4
5M	5M	5M	1	HF	CISD	40k	319k	0.0124 ± 0.0044	732651	2, 3, 4
528k	1.1M	1M	3	HF	CISD	40k	1M	0.0444 ± 0.0059	119583	5
3.4M	11.0M	10M	3	HF	CISD	40k	424k	0.0174 ± 0.0019	2773910	5
9.9M	52.3M	50M	3	HF	CISD	40k	621k	0.0155 ± 0.0004	42184887	5

N_2 (equilibrium, cc-pVDZ)

These results are for N_2 at the equilibrium geometry ($r_{NN} = 2.068a_0$) in the cc-pVDZ basis. The Hartree-Fock data for this system, generated using pyscf, can be found in the directory `Input_Data/N2_ccpvdz`. As an example, the results in the second line of this table were generated by running the following command:

```
mpirun -n 20 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/N2_ccpvdz/ --target 1000000 --distribution HB --vec_nonz
1000000 --mat_nonz 1000000 --max_dets 100000 --initiator 0.5 --ini_vec Input_Data/N2_ccpvdz/cisd_
```

Vec. nonz.	Matr. nonz.	Target	n_a	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	1M	1M	0.0	HF	CISD	40k	1M	1593.6500 ± 8414.6232	5.88e-8	1
1M	1M	1M	0.5	HF	CISD	40k	1M	284.2253 ± 83.8154	0.000593	1
1M	1M	1M	1.0	HF	CISD	40k	1M	0.0275 ± 0.0208	9592	1,2
1M	1M	1M	1.5	HF	CISD	40k	1M	0.0645 ± 0.0161	16103	1
1M	1M	1M	2.0	HF	CISD	40k	1M	0.1103 ± 0.0154	17610	1
3M	3M	3M	1	HF	CISD	40k	1M	0.0080 ± 0.0101	40632	2, 3, 4
5M	5M	5M	1	HF	CISD	40k	760k	0.0087 ± 0.0082	83285	2, 3, 4
652k	1.2M	1M	3	HF	CISD	40k	1M	0.1431 ± 0.0127	25676	5
4.8M	11.0M	10M	3	HF	CISD	40k	579k	0.0167 ± 0.0046	348800	5
18.2M	53.4M	50M	3	HF	CISD	40k	272k	0.0074 ± 0.0022	3684000	5

Ne (cc-pVQZ)

These results are for Ne in the cc-pVQZ basis. The Hartree-Fock data for this system, generated using pyscf, can be found in the ZIP archive at `Input_Data/Neon_ccpvqz.zip`. After it is unzipped, the results in this table can be generated by running the following command:

```
mpirun -n 10 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/Neon_ccpvqz/ --target 500000 --distribution HB --vec_nonz
500000 --mat_nonz 500000 --max_dets 60000 --initiator 1
```

Vec. nonz.	Matr. nonz.	Target	n_a	Trial vec.	Ini vec.[1]	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
500k	500k	500k	1	HF	HF	40k	1M	-333.3856 ± 0.0264	5994	-

[1] Because no initial vector was specified in the input options, Hartree-Fock was used.

N_2 (stretched, cc-pVDZ)

These results are for stretched N_2 ($r_{NN} = 4.2a_0$) in the cc-pVDZ basis. The Hartree-Fock data for this system, generated using pyscf, can be found in the directory `Input_Data/N2_str_ccpvdz`. The results in this table were generated by running the following command:

```
mpirun -n 20 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/N2_str_ccpvdz/ --target 5000000 --distribution HB
--vec_nonz 5000000 --mat_nonz 5000000 --max_dets 400000 --initiator 3 --ini_vec Input_Data/N2_str_ccpvdz/cisd_
```

Vec. nonz.	Matr. nonz.	Target	n_a	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
500k	500k	500k	3	HF	CISD	80k	350k	0.0234 ± 0.1140	1140	-

Semi-stochastic FCI-FRI calculations

The following results were obtained using the systematic FCI-FRI method with the semi-stochastic extension, using the original heat-bath Power-Pitzer factorization.

Ne (aug-cc-pVDZ)

These results are for the Neon atom in the aug-cc-pVDZ basis, using the same Hartree-Fock data described above. As an example, the results in the first line of this table were generated by running the following command:

```
mpirun -n 4 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/Neon_augccpvdz/ --target 150000 --distribution HB
--vec_nonz 150000 --mat_nonz 150000 --max_dets 50000 --initiator 1.0 --ini_vec Input_Data/Neon_augccpvdz/cisd_ --det_space
Input_Data/Neon_augccpvdz/50_big_cisd_dets.txt
```

Nonz.[1]	n_a^2	Trial vec.	Ini vec.	Deterministic subspace[3]	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
150k	1	HF	CISD	50 largest CISD	40k	1M	0.0113 ± 0.0048	179568	3
200k	1	HF	CISD	50 largest CISD	40k	1M	0.0038 ± 0.0039	276718	3
250k	1	HF	CISD	50 largest CISD	40k	1M	0.0041 ± 0.0034	351606	3
150k	1	HF	CISD	50 smallest CISD	40k	1M	0.0146 ± 0.0069	86276	3
200k	1	HF	CISD	50 smallest CISD	40k	1M	0.0042 ± 0.0056	134809	3
250k	1	HF	CISD	50 smallest CISD	40k	1M	0.0015 ± 0.0046	351606	3

[1] Indicates the number of nonzero elements used in matrix and vector compressions. This number was also used as the target one-norm for all calculations in this section.

[2] Indicates the initiator threshold.

[3] The deterministic subspace was constructed from the Slater determinants corresponding to the largest- or smallest-magnitude elements in the CISD ground-state eigenvector.

H_2O (cc-pVDZ)

These results are for H_2O in the cc-pVDZ basis, using the same Hartree-Fock data described above. As an example, the results in the first line of this table were generated by running the following command:

```
mpirun -n 16 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/H2O_ccpvdz/ --target 1000000 --distribution HB
--vec_nonz 1000000 --mat_nonz 1000000 --max_dets 100000 --initiator 1.0 --ini_vec Input_Data/H2O_ccpvdz/cisd_ --det_space
Input_Data/H2O_ccpvdz/150_big_cisd_dets.txt
```

Nonz.	n_a	Trial vec.	Ini vec.	Deterministic subspace	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	1.0	HF	CISD	150 largest CISD	40k	1M	0.0440 ± 0.0203	10107	3
3M	1.0	HF	CISD	150 largest CISD	40k	1M	0.0135 ± 0.0035	344228	3
5M	1.0	HF	CISD	150 largest CISD	40k	661k	0.0178 ± 0.0029	777820	3
1M	1.0	HF	CISD	150 smallest CISD	40k	1M	0.0247 ± 0.0102	40239	3
3M	1.0	HF	CISD	150 smallest CISD	40k	590k	0.0178 ± 0.0054	249487	3
5M	1.0	HF	CISD	150 smallest CISD	40k	642k	0.0153 ± 0.0042	385820	3

N_2 (equilibrium, cc-pVDZ)

These results are for equilibrium N_2 in the cc-pVDZ basis, using the same Hartree-Fock data described above. As an example, the results in the first line of this table were generated by running the following command:

```
mpirun -n 20 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/N2_ccpvdz/ --target 1000000 --distribution HB
--vec_nonz 1000000 --mat_nonz 1000000 --max_dets 100000 --initiator 1.0 --ini_vec Input_Data/N2_ccpvdz/cisd_ --det_space
Input_Data/N2_ccpvdz/150_big_cisd_dets.txt
```

Nonz.	n_a	Trial vec.	Ini vec.	Deterministic subspace	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	1.0	HF	CISD	150 largest CISD	40k	1M	0.0408 ± 0.0172	14145	3
3M	1.0	HF	CISD	150 largest CISD	40k	1M	0.0085 ± 0.0072	80267	3
5M	1.0	HF	CISD	150 largest CISD	40k	756k	0.0159 ± 0.0063	141279	3
1M	1.0	HF	CISD	150 smallest CISD	40k	1M	277.6687 ± 52.1335	0.0015	3
3M	1.0	HF	CISD	150 smallest CISD	40k	1M	0.0306 ± 0.0146	19612	3
5M	1.0	HF	CISD	150 smallest CISD	40k	769k	0.0141 ± 0.0098	57082	3

FCI-FRI Calculations with the Alternative HB-PP Factorization

The following results were obtained using the systematic FCI-FRI method with the alternative, "un-normalized" HB-PP factorization, without the semi-stochastic extension.

Ne (aug-cc-pVDZ)

These results are for the Neon atom in the aug-cc-pVDZ basis, using the same Hartree-Fock data described above. As an example, the results in the first line of this table were generated by running the following command:

```
mpirun -n 4 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/Neon_augccpvdz/ --target 50000 --distribution HB_unnorm
--vec_nonz 50000 --mat_nonz 50000 --max_dets 50000 --initiator 1.0 --ini_vec Input_Data/Neon_augccpvdz/cisd_
```

Nonz.	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
50k	1.0	HF	CISD	40k	1M	0.0073 ± 0.0079	67108	4
100k	1.0	HF	CISD	40k	1M	0.0114 ± 0.0056	132196	4
150k	1.0	HF	CISD	40k	1M	0.0098 ± 0.0042	239832	4
200k	1.0	HF	CISD	40k	1M	0.0048 ± 0.0035	333066	4

H_2O (cc-pVDZ)

These results are for H_2O in the cc-pVDZ basis, using the same Hartree-Fock data described above. As an example, the results in the first line of this table were generated by running the following command:

```
mpirun -n 16 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/H2O_ccpvdz/ --target 1000000 --distribution HB_unnorm
--vec_nonz 1000000 --mat_nonz 1000000 --max_dets 100000 --initiator 1.0 --ini_vec Input_Data/H2O_ccpvdz/cisd_
```

Nonz.	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	1	HF	CISD	40k	1M	0.0283 ± 0.0058	122875	4
3M	1	HF	CISD	40k	1M	0.0184 ± 0.0027	583227	4
5M	1	HF	CISD	40k	1M	0.0167 ± 0.0023	1148398	4

N_2 (equilibrium, cc-pVDZ)

These results are for equilibrium N_2 in the cc-pVDZ basis, using the same Hartree-Fock data described above. As an example, the results in the first line of this table were generated by running the following command:

```
mpirun -n 20 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/N2_ccpvdz/ --target 1000000 --distribution HB_unnorm
--vec_nonz 1000000 --mat_nonz 1000000 --max_dets 100000 --initiator 1.0 --ini_vec Input_Data/N2_ccpvdz/cisd_
```

Nonz.	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	1	HF	CISD	40k	1M	0.0697 ± 0.0179	13025	4
3M	1	HF	CISD	40k	1M	0.0262 ± 0.0080	65667	4
5M	1	HF	CISD	40k	1M	0.0154 ± 0.0058	146051	4

Ne (aug-pVQZ)

These results are for Ne in the cc-pVQZ basis. The Hartree-Fock data for this system, generated using pyscf, can be found in the ZIP archive at `Input_Data/Neon_ccpvqz.zip`. After it is unzipped, the results in this table can be generated by running the following command:

`mpirun -n 10 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/Neon_ccpvqz/ --target 500000 --distribution HB_unnorm --vec_nonz 500000 --mat_nonz 500000 --max_dets 60000 --initiator 1`

Nonz.	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
500k	1	HF	HF	40k	1M	-333.4149 ± 0.0167	14967	-

N_2 (stretched, cc-pVDZ)

These results are for stretched N_2 ($r_{NN} = 4.2a_0$) in the cc-pVDZ basis. The Hartree-Fock data for this system, generated using pyscf, can be found in the directory `Input_Data/N2_str_ccpvdz`. The results in this table were generated by running the following command:

`mpirun -n 20 ./build/FRIES_bin/frisys_mol --hf_path Input_Data/N2_str_ccpvdz/ --target 5000000 --distribution HB_unnorm --vec_nonz 5000000 --mat_nonz 5000000 --max_dets 500000 --initiator 3 --ini_vec Input_Data/N2_str_ccpvdz/cisd_`

Vec. nonz.	Matr. nonz.	Target	n_a	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
500k	500k	500k	3	HF	CISD	80k	350k	0.1025 ± 0.1019	1205	-

FCIQMC (integer) Calculations

These results were obtained using our implementation of the FCIQMC method in which vector elements are constrained to be integers. The heat-bath Power-Pitzer matrix factorization was used in these calculations, along with the initiator approximation. The semi-stochastic extension was not used.

Ne (aug-cc-pVDZ)

These results are for the Neon atom in the aug-cc-pVDZ basis, using the same Hartree-Fock data described above. All calculations were initialized from a population of 5000 walkers distributed among determinants in proportion to the values of elements in the CISD unit vector. As an example, the results in the first line of this table were generated by running the following command:

`mpirun -n 4 ./build/FRIES_bin/fciqmc_mol --hf_path Input_Data/Ne_augccpvdz/ --target 50000 --initiator 3 --max_dets 20000 --distribution HB --ini_vec Input_Data/Neon_augccpvdz/cisd_int_`

Target walkers	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
50k	3	HF	CISD	40k	1M	0.0099 ± 0.0734	773	5
100k	3	HF	CISD	40k	1M	-0.0136 ± 0.0546	1400	5
150k	3	HF	CISD	40k	1M	-0.0062 ± 0.0457	1998	5
200k	3	HF	CISD	40k	1M	0.0178 ± 0.0382	2851	5

H_2O (cc-pVDZ)

These results are for H_2O in the cc-pVDZ basis, using the same Hartree-Fock data described above. These calculations were initialized from a population of 500,000 walkers distributed among determinants in proportion to the values of elements in the CISD unit vector. As an example, the results in the first line of this table were generated by running the following command:

```
mpirun -n 16 ./build/FRIES_bin/fciqmc_mol --hf_path Input_Data/H2O_ccpvdz/ --target 1000000 --initiator 3 --max_dets 100000 --distribution HB --ini_vec Input_Data/H2O_ccpvdz/cisd_int_
```

Target walkers	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	3	HF	CISD	40k	1M	0.0491 ± 0.0332	3770	5
10M	3	HF	CISD	40k	574k	0.0120 ± 0.0147	34817	5
50M	3	HF	CISD	40k	339k	0.0147 ± 0.0022	2403490	5

N_2 (equilibrium, cc-pVDZ)

These results are for equilibrium N_2 in the cc-pVDZ basis, using the same Hartree-Fock data described above. These calculations were initialized from a population of 500,000 walkers distributed among determinants in proportion to the values of elements in the CISD unit vector. As an example, the results in the first line of this table were generated by running the following command:

```
mpirun -n 8 ./build/FRIES_bin/fciqmc_mol --hf_path Input_Data/N2_ccpvdz/ --target 1000000 --initiator 3 --max_dets 200000 --distribution HB --ini_vec Input_Data/N2_ccpvdz/cisd_int_
```

Target walkers	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	3	HF	CISD	40k	1M	0.1638 ± 0.0781	684	5
10M	3	HF	CISD	40k	543k	0.0061 ± 0.0398	5010	5
50M	3	HF	CISD	40k	462k	0.0089 ± 0.0189	24518	5

FCIQMC (non-integer) Calculations

These results were obtained using our implementation of the FCIQMC method in which only some vector elements are integerized, and the rest are allowed to be non-integers. The heat-bath Power-Pitzer matrix factorization was used in these calculations, along with the initiator approximation. The semi-stochastic extension was not used.

Ne (aug-cc-pVDZ)

These results are for the Neon atom in the aug-cc-pVDZ basis, using the same Hartree-Fock data and initial vector as described in the previous FCIQMC section. As an example, the results in the first line of this table were generated by running the following command:

`mpirun -n 4 ./build/FRIES_bin/fciqmc_fp_mol --hf_path Input_Data/Ne_augccpvdz/ --target 50000 --initiator 3 --max_dets 20000 --distribution HB --ini_vec Input_Data/Neon_augccpvdz/cisd_int_`

Target walkers	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
50k	3	HF	CISD	40k	1M	0.0307 ± 0.0176	13390	5
100k	3	HF	CISD	40k	1M	0.0313 ± 0.0126	26240	5
150k	3	HF	CISD	40k	1M	0.0336 ± 0.0103	39821	5
200k	3	HF	CISD	40k	1M	0.0290 ± 0.0090	51644	5

H_2O (cc-pVDZ)

These results are for H_2O in the cc-pVDZ basis, using the same Hartree-Fock data and initial vector as described in the previous FCIQMC section. As an example, the results in the first line of this table were generated by running the following command:

`mpirun -n 16 ./build/FRIES_bin/fciqmc_fp_mol --hf_path Input_Data/H2O_ccpvdz/ --target 1000000 --initiator 3 --max_dets 100000 --distribution HB --ini_vec Input_Data/H2O_ccpvdz/cisd_int_`

Target walkers	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	3	HF	CISD	40k	1M	0.0404 ± 0.0097	44495	5
10M	3	HF	CISD	40k	478k	0.0165 ± 0.0045	442339	5
50M	3	HF	CISD	5k	334k	0.0157 ± 0.0021	2818118	5

N_2 (equilibrium, cc-pVDZ)

These results are for equilibrium N_2 in the cc-pVDZ basis, using the same Hartree-Fock data and initial vector as described in the previous FCIQMC section. As an example, the results in the first line of this table were generated by running the following command:

`mpirun -n 8 ./build/FRIES_bin/fciqmc_fp_mol --hf_path Input_Data/N2_ccpvdz/ --target 1000000 --initiator 3 --max_dets 200000 --distribution HB --ini_vec Input_Data/N2_ccpvdz/cisd_int_`

Target walkers	Ini. thresh. (n_a)	Trial vec.	Ini vec.	Burn-in	Iterations	Mean $\pm 2\sigma$ (mE_h)	Efficiency (E_h^{-2})	Figures
1M	3	HF	CISD	40k	1M	0.1316 ± 0.0190	10574	5
10M	3	HF	CISD	40k	438k	0.0095 ± 0.0099	103387	5
50M	3	HF	CISD	40k	307k	0.0097 ± 0.0060	422516	5