PyRETIS — RETIS analysis

RETIS analysis report generated by PyRETIS version 3.0.0.dev0+098fc56 on 13.02.2023 09:16:42.
The main results are:

- The crossing probability: $P_{\mathrm{cross}} = 5.828589643 \times 10^{-7} \pm 2.906370120\ \%$
- The initial flux (unit: 1/reduced): $f_A = 0.441497339 \pm 0.152807745\ \%$
- The rate constant (unit: 1/reduced): $k_{AB} = 2.573306817 \times 10^{-7} \pm 2.910384422\ \%$

Detailed results are given below for the different path ensembles and the overall results are summarized in the last section.

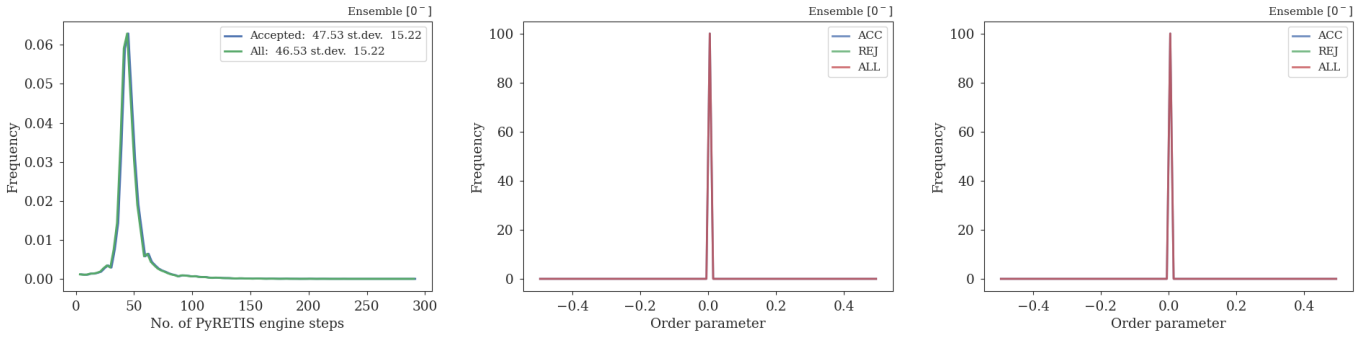
1 Results for $[0^-]$

Table 1: Interfaces

Ensemble	Left	Middle	Right
$[0^-]$	$-inf$	−0.9900	−0.9900

Table 2: Path lengths

Ensemble	Accepted	All	All/Accepted
$[0^-]$	47.528607	46.528607	0.978960



2 Results for path ensembles

The following interfaces were used in the simulation and in the analysis:

Table 3: Interfaces

Ensemble	Left	Middle	Right	Detect
$[0^+]$	−0.9900	−0.9900	1.0000	−0.8000
$[1^+]$	−0.9900	−0.8000	1.0000	−0.7000
$[2^+]$	−0.9900	−0.7000	1.0000	−0.6000
$[3^+]$	−0.9900	−0.6000	1.0000	−0.5000
$[4^+]$	−0.9900	−0.5000	1.0000	−0.4000
$[5^+]$	−0.9900	−0.4000	1.0000	−0.3000
$[6^+]$	−0.9900	−0.3000	1.0000	1.0000

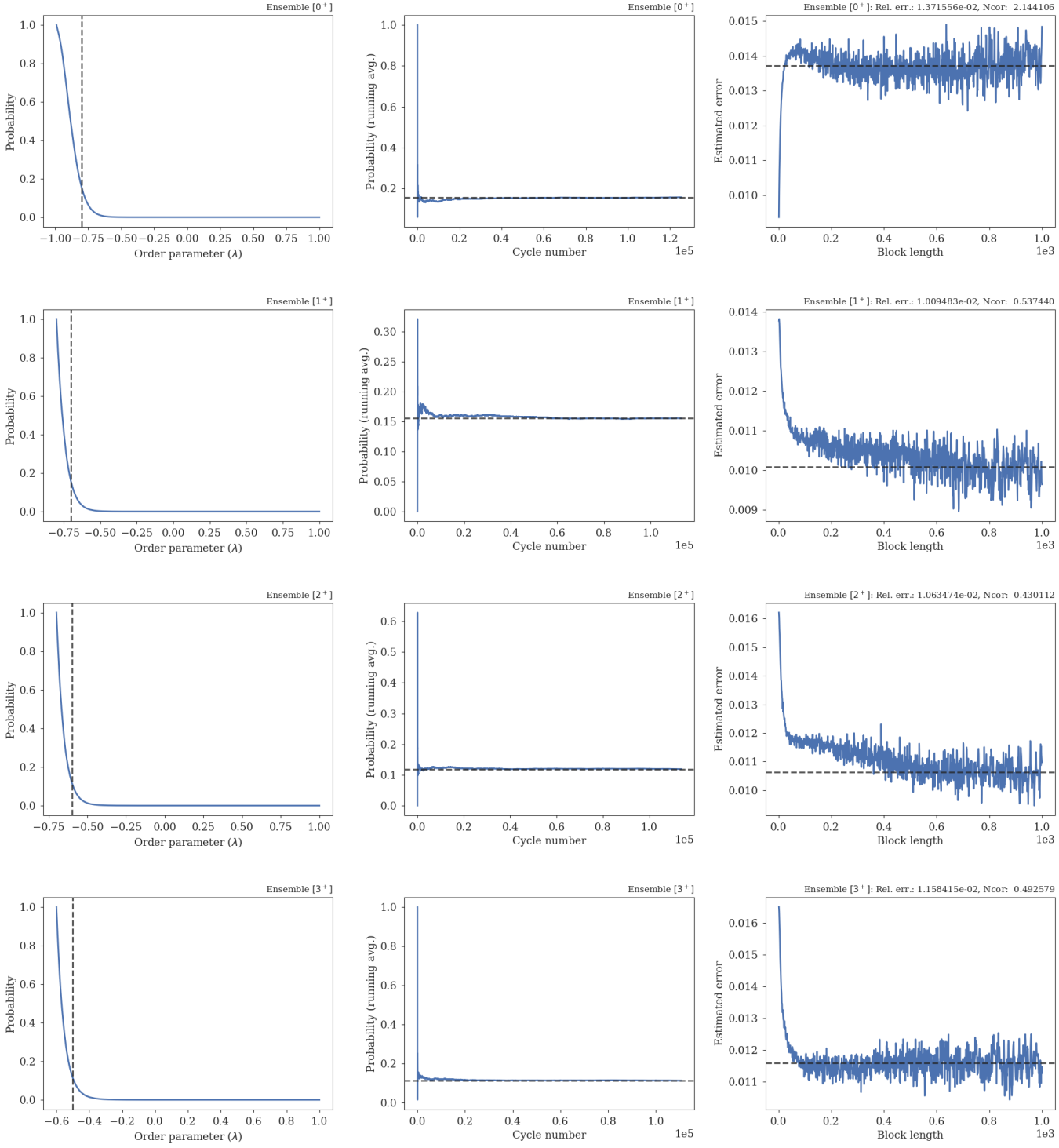
The calculated crossing probabilities are:

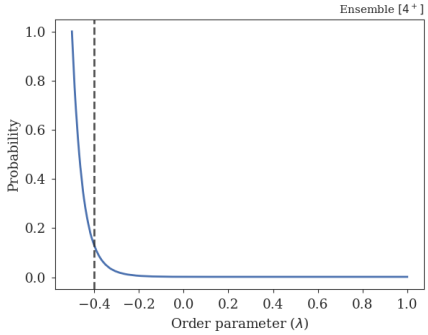
Table 4: Probabilities

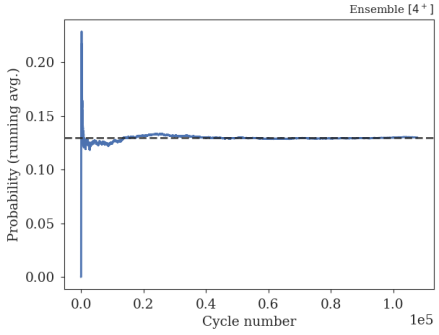
Ensemble	P_{cross}	Error	Rel. error (%)
$[0^+]$	0.158091	0.002168	1.371556
$[1^+]$	0.155359	0.001568	1.009483
$[2^+]$	0.118868	0.001264	1.063474
$[3^+]$	0.112638	0.001305	1.158415
$[4^+]$	0.129853	0.001319	1.015812
$[5^+]$	0.170829	0.001668	0.976631
$[6^+]$	0.079902	0.000834	1.043159

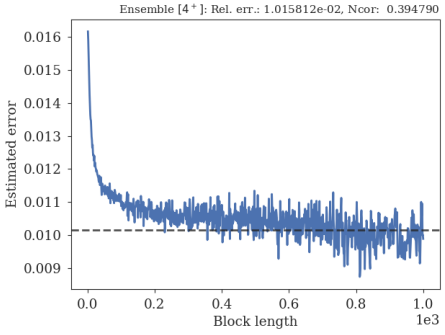
The crossing probabilities are also displayed in the figures below

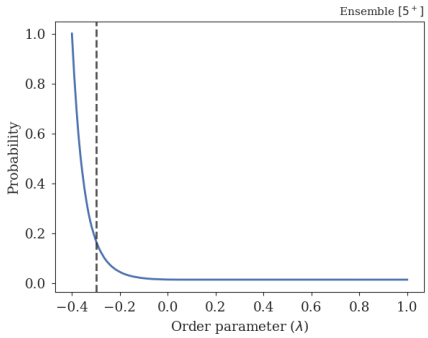
2.1 Crossing probabilities

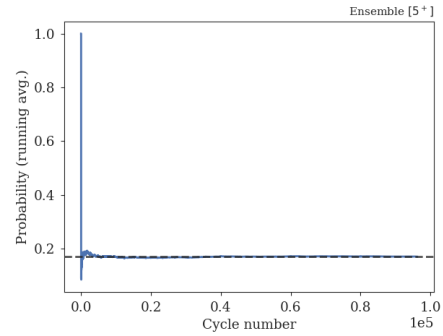


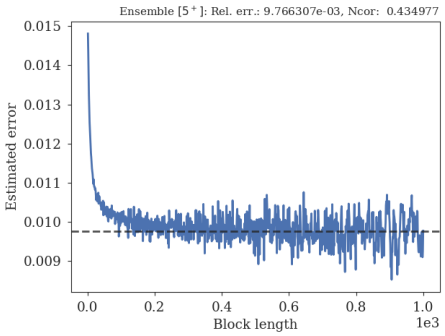

Ensemble [4⁺]
Probability
Order parameter (λ)

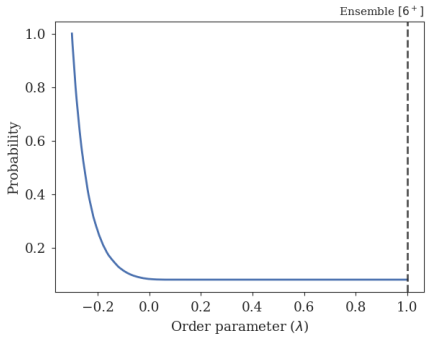

Ensemble [4⁺]
Probability (running avg.)
Cycle number
1e5

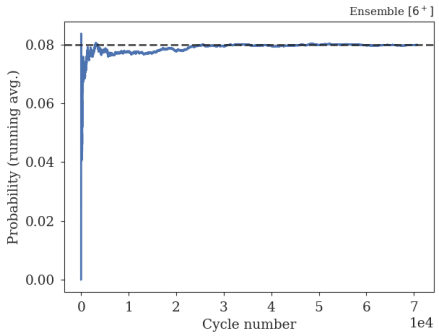

Ensemble [4⁺]: Rel. err.: 1.015812e-02, Ncor: 0.394790
Estimated error
Block length
1e3

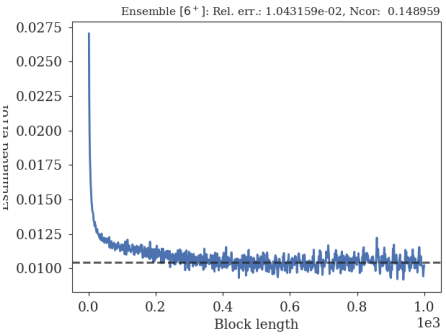

Ensemble [5⁺]
Probability
Order parameter (λ)


Ensemble [5⁺]
Probability (running avg.)
Cycle number
1e5


Ensemble [5⁺]: Rel. err.: 9.766307e-03, Ncor: 0.434977
Estimated error
Block length
1e3


Ensemble [6⁺]
Probability
Order parameter (λ)


Ensemble [6⁺]
Probability (running avg.)
Cycle number
1e4

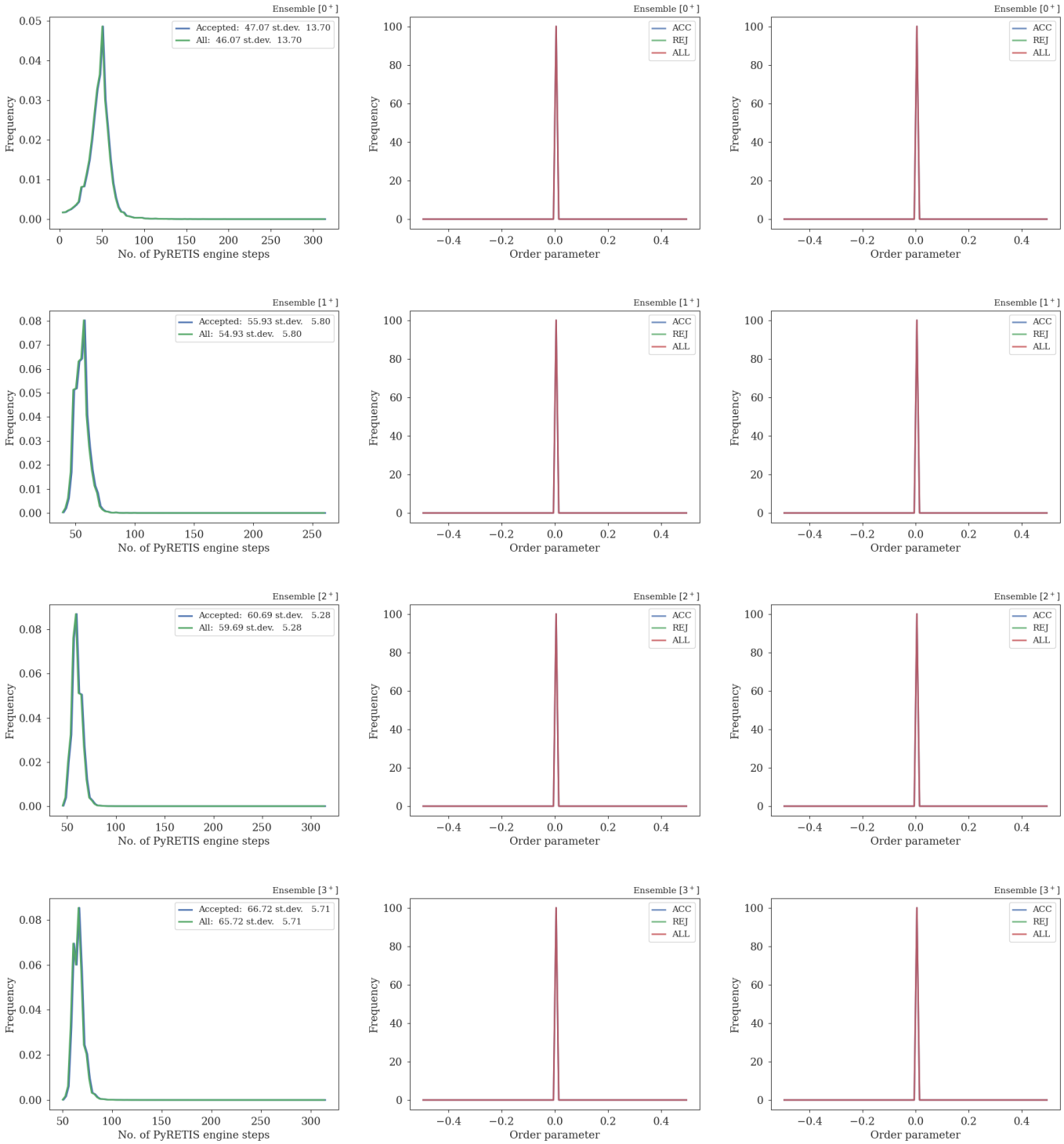

Ensemble [6⁺]: Rel. err.: 1.043159e-02, Ncor: 0.148959
Block length
1e3

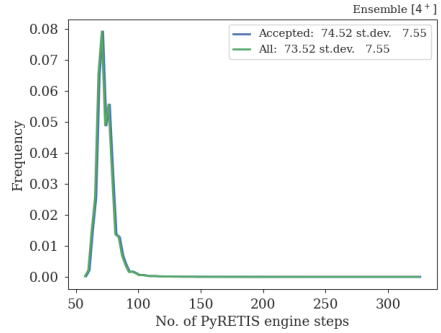
2.2 Distributions for path lengths and shooting moves

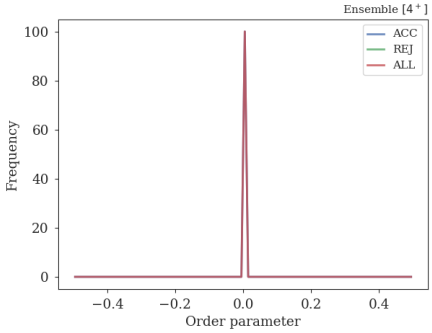
The average path lengths in the different ensembles are given in the table below and some distributions for the path lengths and shooting moves can also be found here:

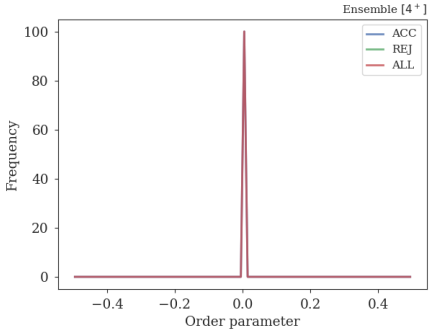
Table 5: Path lengths

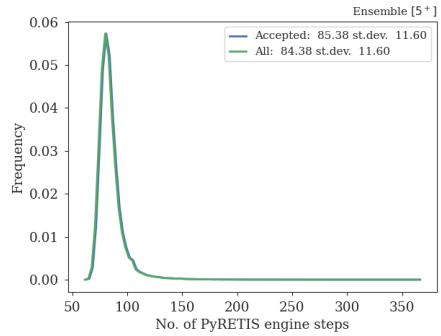
Ensemble	Accepted	All	All/Accepted
$[0^+]$	47.072165	46.072165	0.978756
$[1^+]$	55.932448	54.932448	0.982121
$[2^+]$	60.689634	59.689634	0.983523
$[3^+]$	66.717445	65.717445	0.985011
$[4^+]$	74.523973	73.523973	0.986581
$[5^+]$	85.379767	84.379767	0.988288
$[6^+]$	101.588626	100.588626	0.990156

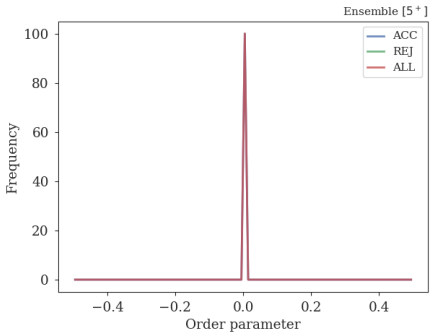


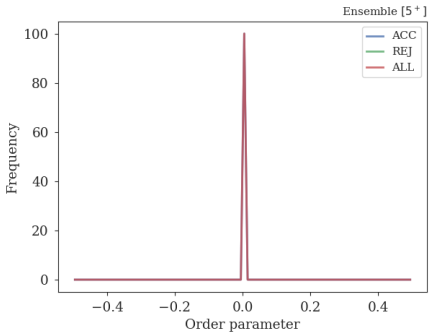

Ensemble [4+]
Accepted: 74.52 st.dev. 7.55
All: 73.52 st.dev. 7.55
Frequency
No. of PyRETIS engine steps

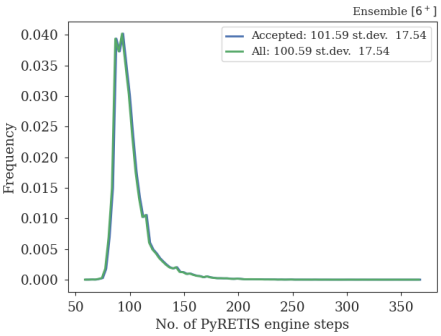

Ensemble [4+]
ACC
REJ
ALL
Frequency
Order parameter

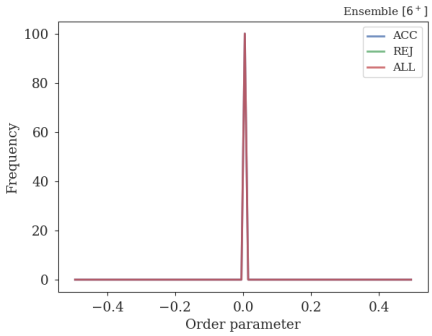

Ensemble [4+]
ACC
REJ
ALL
Frequency
Order parameter

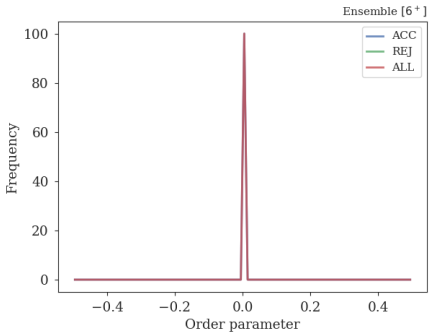

Ensemble [5+]
Accepted: 85.38 st.dev. 11.60
All: 84.38 st.dev. 11.60
Frequency
No. of PyRETIS engine steps


Ensemble [5+]
ACC
REJ
ALL
Frequency
Order parameter


Ensemble [5+]
ACC
REJ
ALL
Frequency
Order parameter


Ensemble [6+]
Accepted: 101.59 st.dev. 17.54
All: 100.59 st.dev. 17.54
Frequency
No. of PyRETIS engine steps


Ensemble [6+]
ACC
REJ
ALL
Frequency
Order parameter


Ensemble [6+]
ACC
REJ
ALL
Frequency
Order parameter

2.3 Efficiency analysis

Table 6: Efficiency

Ensemble	TIS cycles	Tot sim.	Acceptance ratio	Correlation	Efficiency
$[0^+]$	125274	5.7716×10^6	1.000000	2.144106	1.0857×10^3
$[1^+]$	113008	6.2078×10^6	1.000000	0.537440	632.609836
$[2^+]$	113646	6.7835×10^6	1.000000	0.430112	767.197278
$[3^+]$	110577	7.2668×10^6	1.000000	0.492579	975.155246
$[4^+]$	107599	7.9111×10^6	1.000000	0.394790	816.327028
$[5^+]$	96172	8.1150×10^6	1.000000	0.434977	774.012028
$[6^+]$	70671	7.1087×10^6	1.000000	0.148959	773.555261

3 Combined results

The overall matched probability distributions are shown in the left figure while the matched probability distribution is shown in the right figure below. The overall crossing rate as a function of cycles and its relative error block analysis are reported in the two following plots, respectively.

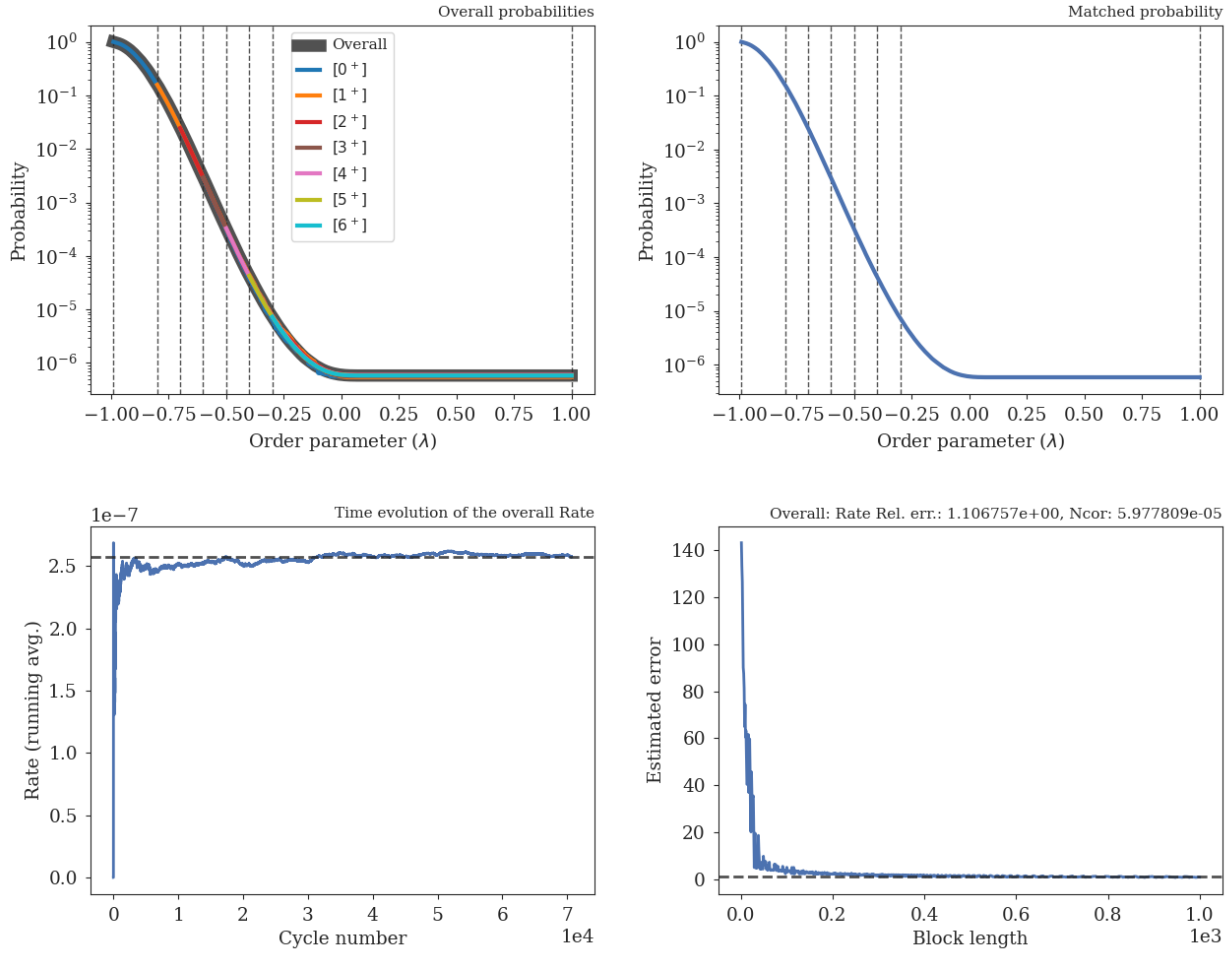


Table 7: Summary of main results

Property	Value	Relative error (%)
Crossing probability	$5.828589643 \times 10^{-7}$	2.906370120
Flux (1/reduced)	0.441497339	0.152807745
Rate constant (1/reduced)	$2.573306817 \times 10^{-7}$	2.910384422

Other statistics:

- sim.time: 4.916455237×10^7
- $\tau_{\text{eff}} = 4.152923483 \times 10^4$

- $\tau_{\text{eff}}^{\text{opt}} = 4.049492460 \times 10^4$