

Optimización de la estructura electrónica del átomo de Be

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Algunas variables importantes en la optimización de Be

- ▶ Configuraciones en CI
 - N parámetros
- ▶ Potencial modelo $V_{nl}^{\text{eff}}(r)$
 - Tipo de potencial: TFDA o STO
 - nl parámetros: λ_{nl}
- ▶ Potencial de polarización $V_l^{\text{pol}}(r)$
 - Tipo de potencial: Norcross o Bayliss
 - $2(l+1)$ parámetros: $\xi_l = \{\alpha_l, \rho_l\}$

Parámetros de la optimización

- ▶ Espacio de hiper-parámetros
- ▶ Diseño inicial
 - ▶ Tipo de mapeo (random, latin hypercube, etc.)
 - ▶ Número de datos iniciales
- ▶ Kernel (squared exponential, periodic, etc.)
- ▶ Función de adquisición (EI, MPI, etc.)
- ▶ Presupuesto (máximo número de evaluaciones)
- ▶ Función costo:
 - ▶ Suma de errores relativos de energías absolutas de n niveles
 - ▶ Suma de errores relativos de coeficientes de Einstein de t transiciones

¿Cómo saber si el mínimo hallado en una optimización es el mínimo global?

→ Evaluación del modelo usando 100 semillas diferentes ←

Potencial de polarización

- ▶ Número de configuraciones en CI: `mxconf=6`
- ▶ Potencial de Norcross (1976)

$$V_{\text{pol}}(r) = -\frac{\alpha_l}{r^4} \left[1 - e^{-\left(\frac{r}{\rho_l}\right)^6} \right]$$

- ▶ Espacio de hiper-parámetros: `npolvar=6`

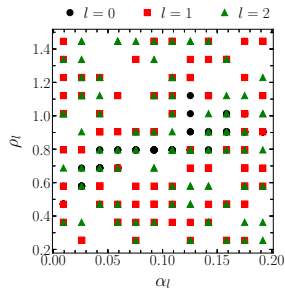
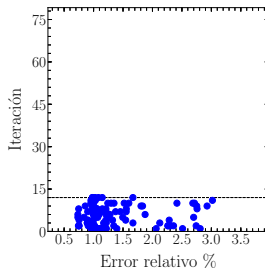
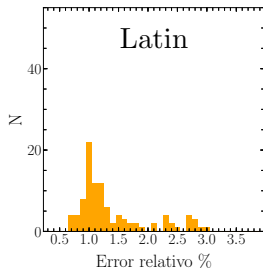
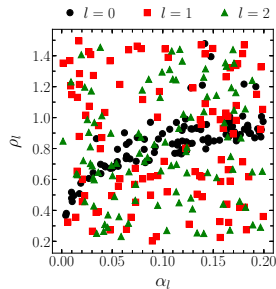
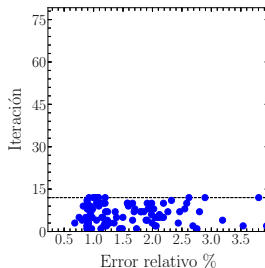
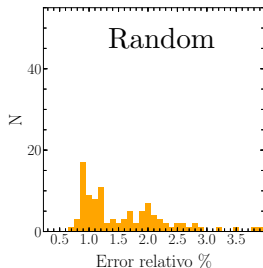
$$\alpha_l = [0.0010, 0.2000]$$

$$\rho_l = [0.2000, 1.5000] \quad : \quad l = 0, 1, 2$$

- ▶ Diseño inicial:
 - ▶ Tipo de mapeo (random, latin hypercube, etc.)
 - ▶ Número de datos iniciales: `initer`
- ▶ Kernel: RBF (squared exponential)
- ▶ Función de adquisición: EI
- ▶ Presupuesto: `maxeval`
- ▶ Función costo: $\sum_i (E_i^{\text{obs.}} - E_i^{\text{comp.}}) / E_i^{\text{obs.}}$

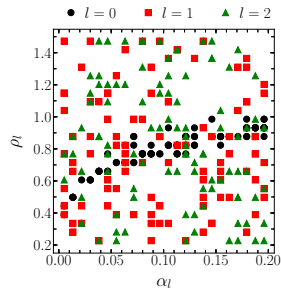
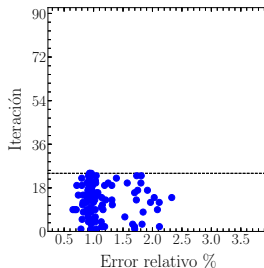
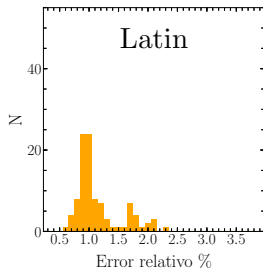
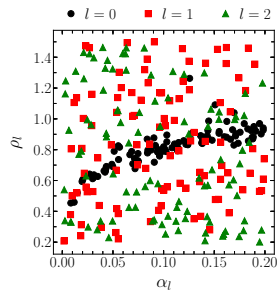
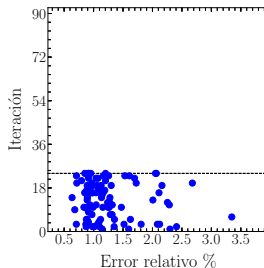
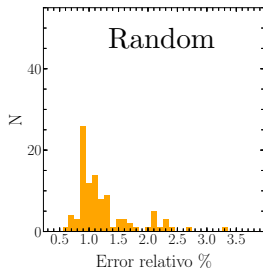
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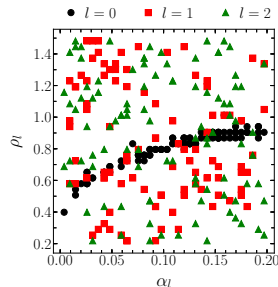
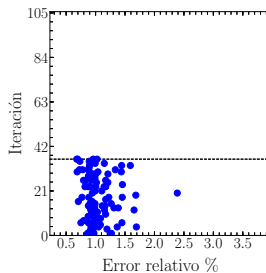
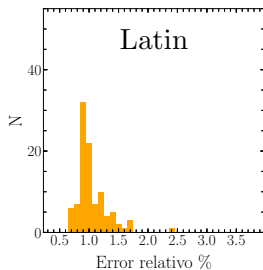
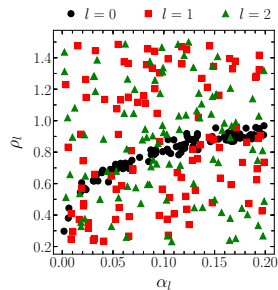
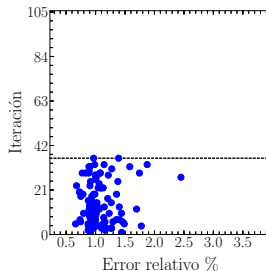
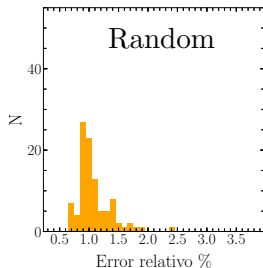
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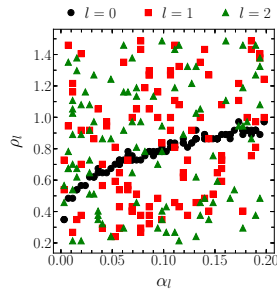
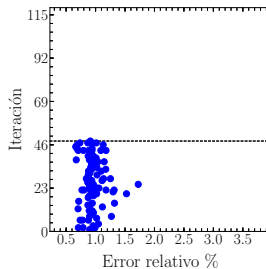
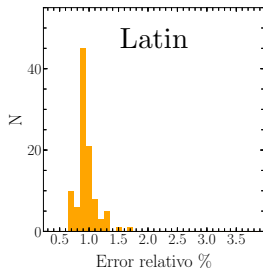
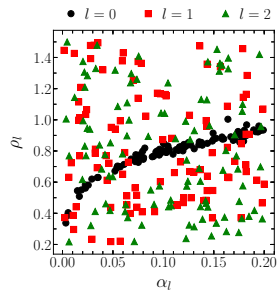
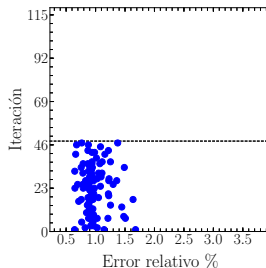
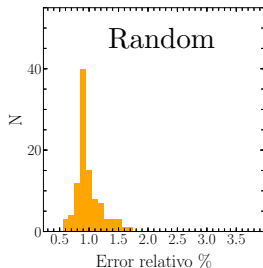
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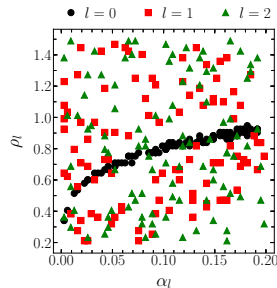
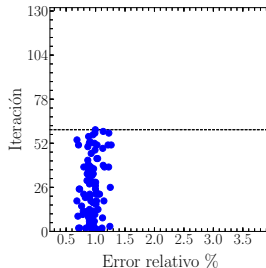
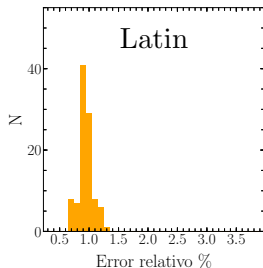
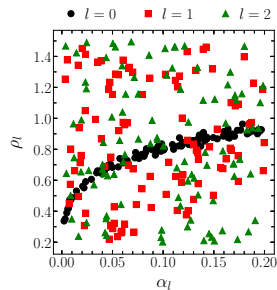
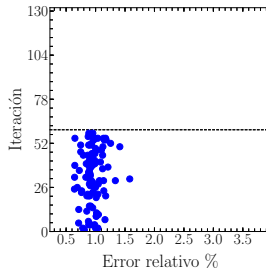
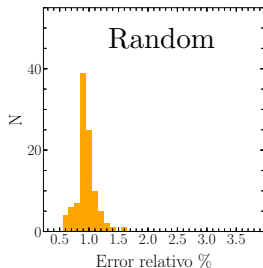
Estudio de mapeo inicial:

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Estudio de mapeo inicial:

initer=60

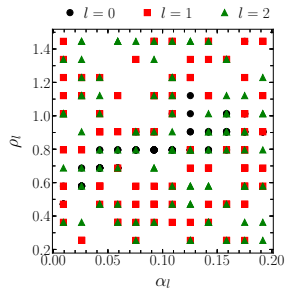
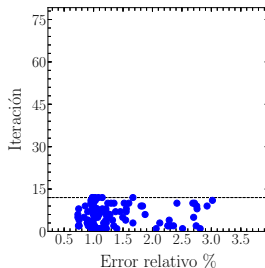
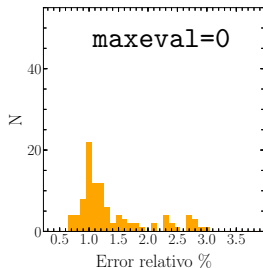
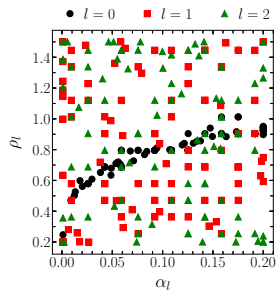
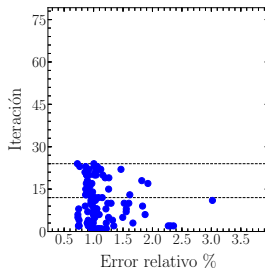
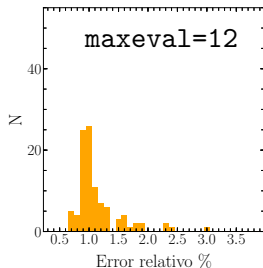


Conclusión:

- ▶ Latin hypercube es la mejor herramienta para hacer el muestreo inicial.
- ▶ El número de elementos en el muestreo inicial **initer** es crucial para reducir el valor máximo que puede tomar la función de costo.

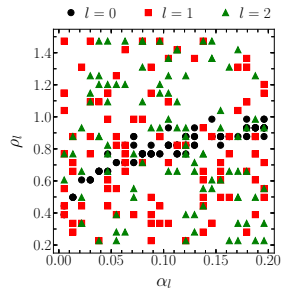
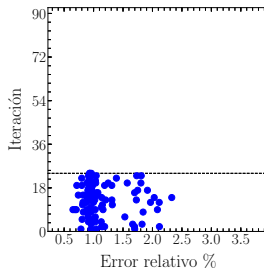
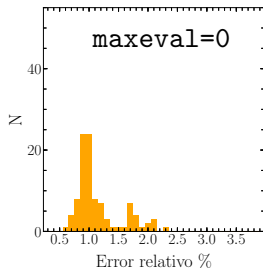
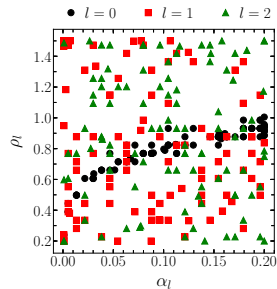
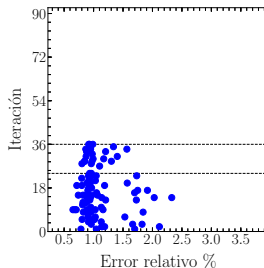
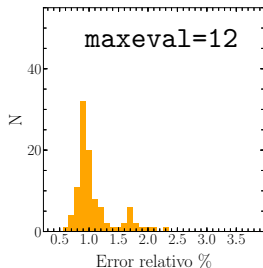
Estudio de presupuesto vs mapeo inicial:

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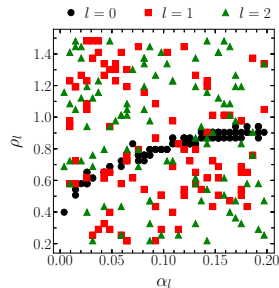
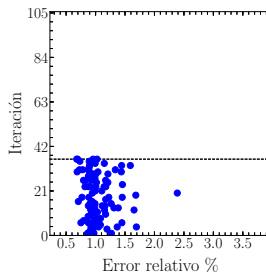
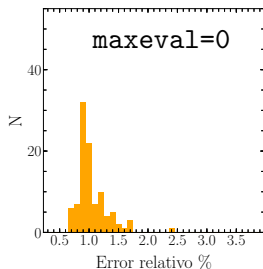
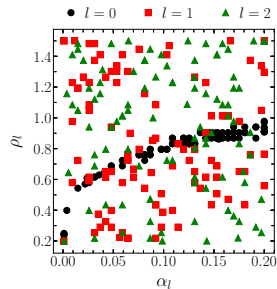
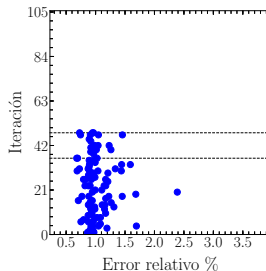
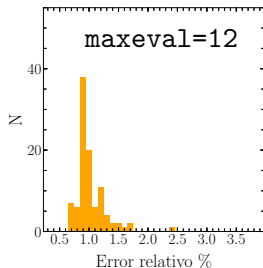
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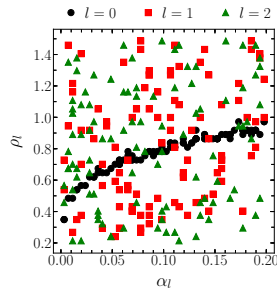
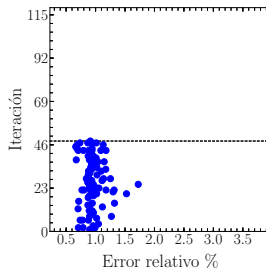
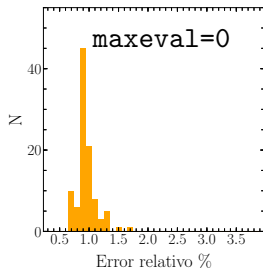
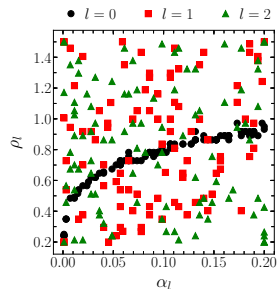
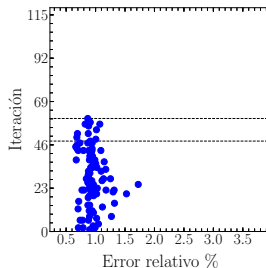
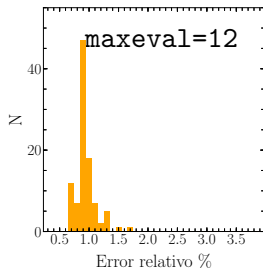
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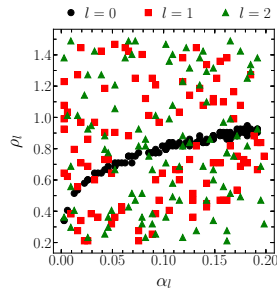
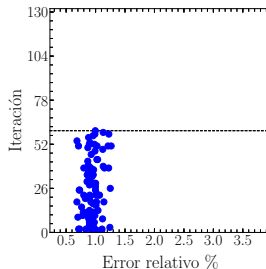
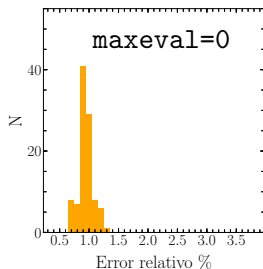
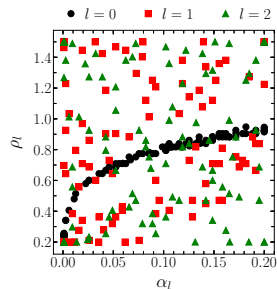
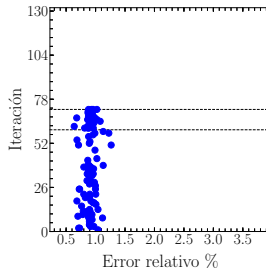
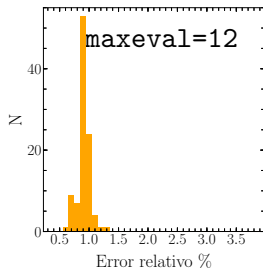
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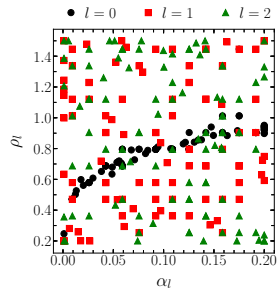
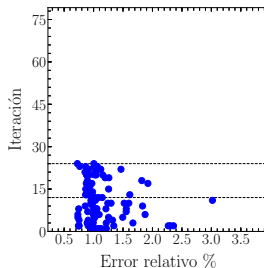
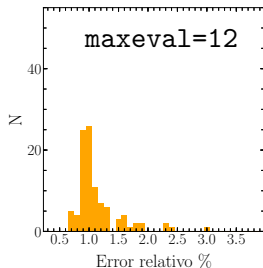
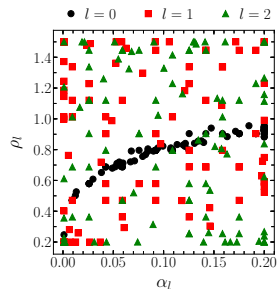
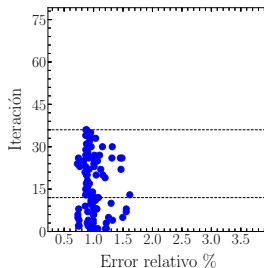
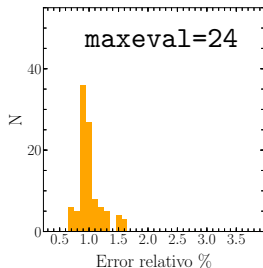
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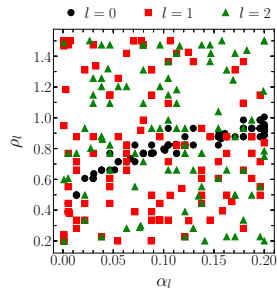
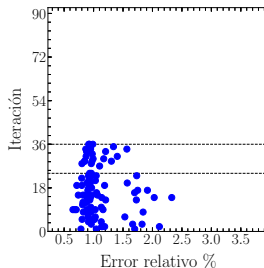
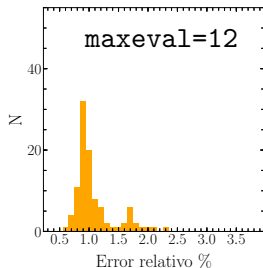
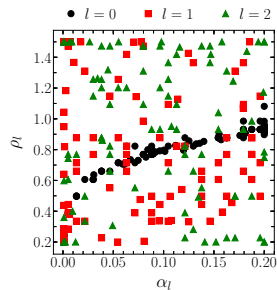
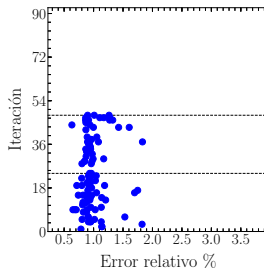
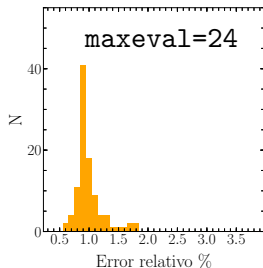
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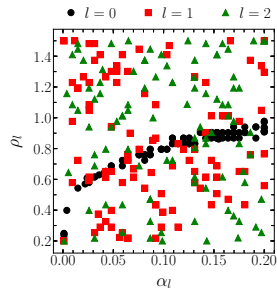
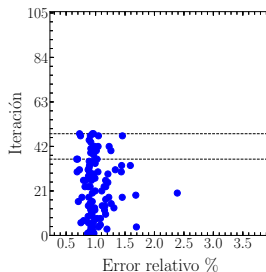
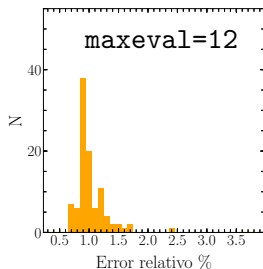
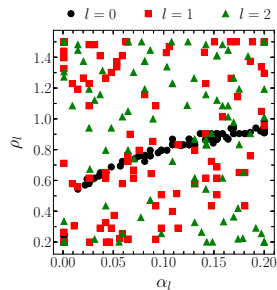
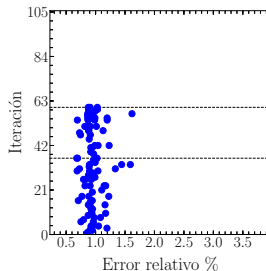
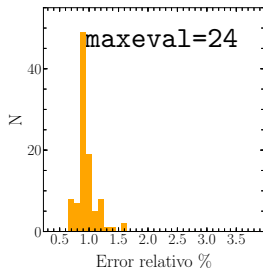
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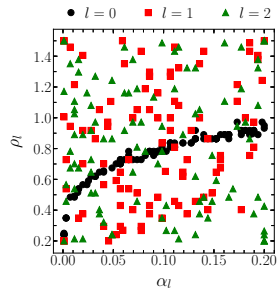
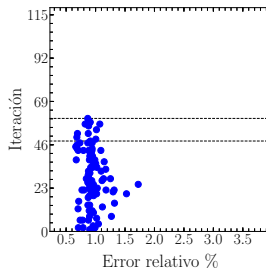
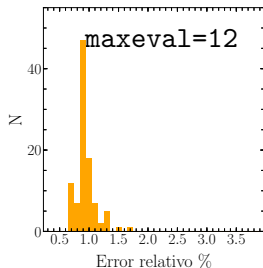
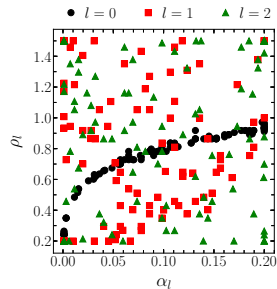
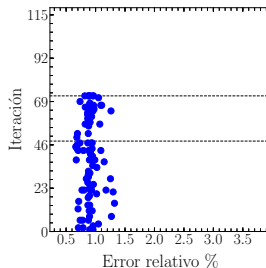
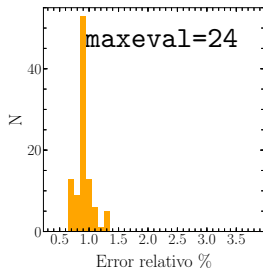
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initer=36



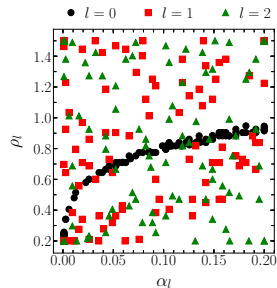
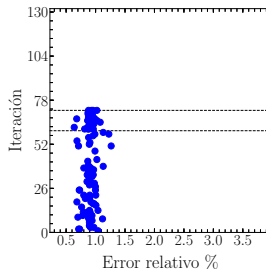
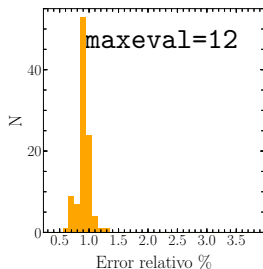
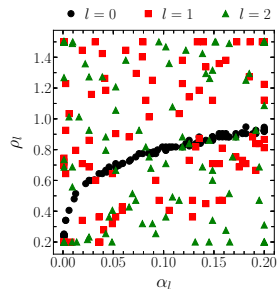
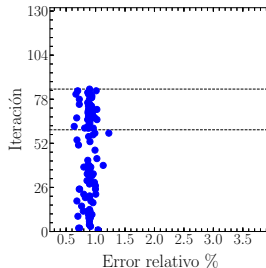
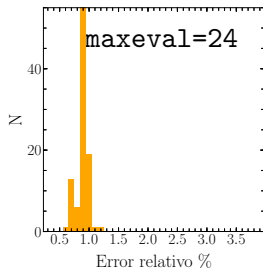
Estudio de presupuesto vs mapeo inicial:

initer=48



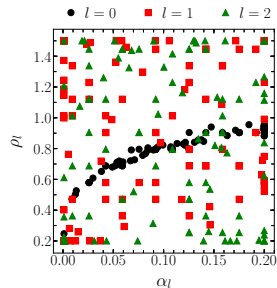
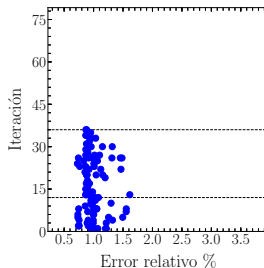
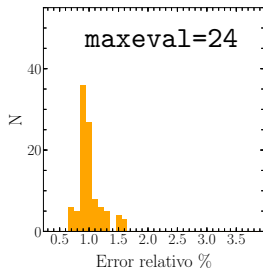
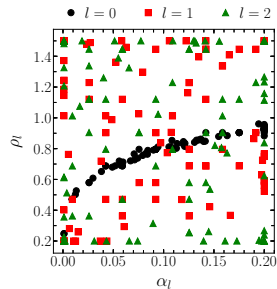
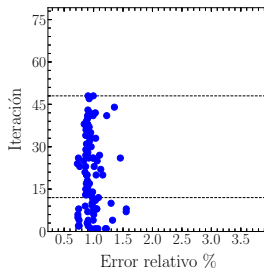
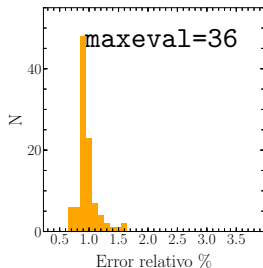
Estudio de presupuesto vs mapeo inicial:

initer=60



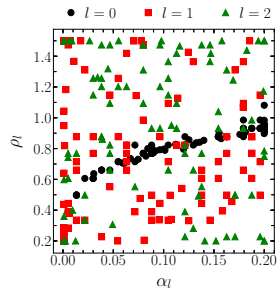
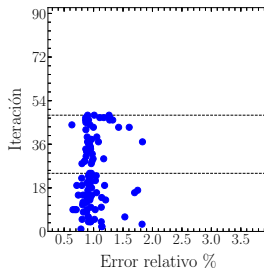
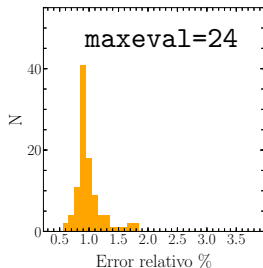
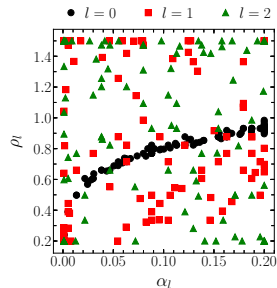
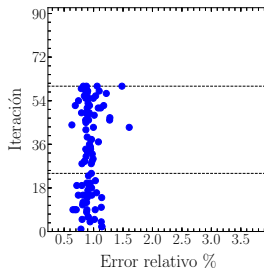
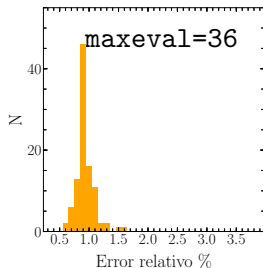
Estudio de presupuesto vs mapeo inicial:

initer=12



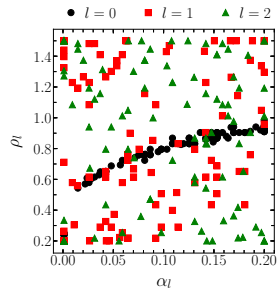
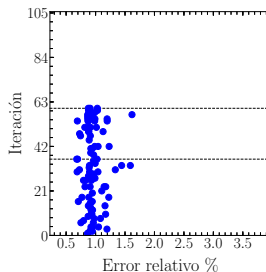
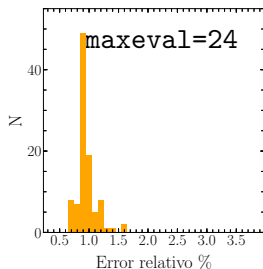
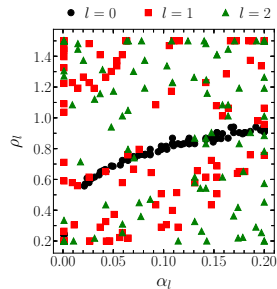
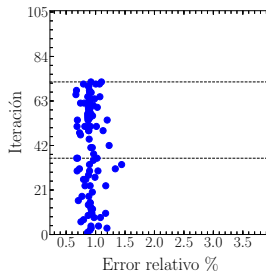
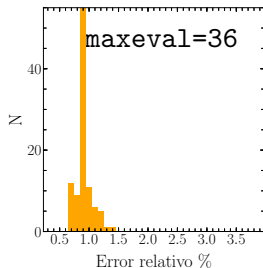
Estudio de presupuesto vs mapeo inicial:

initer=24



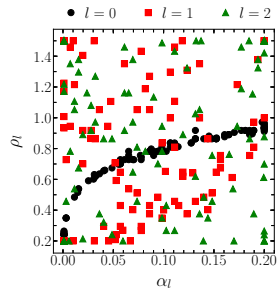
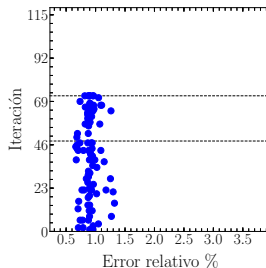
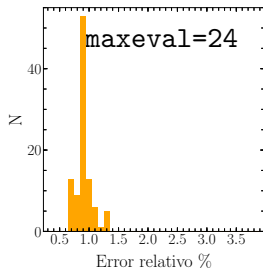
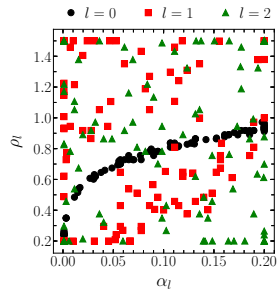
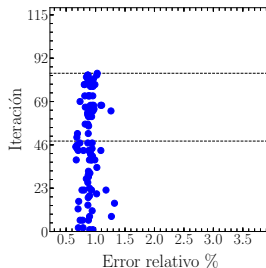
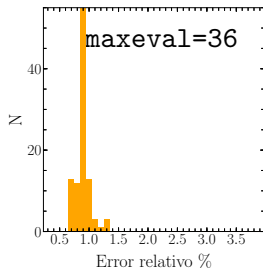
Estudio de presupuesto vs mapeo inicial:

initer=36



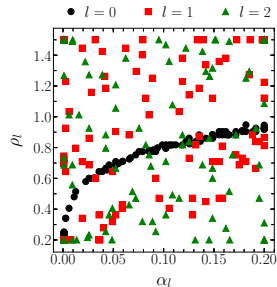
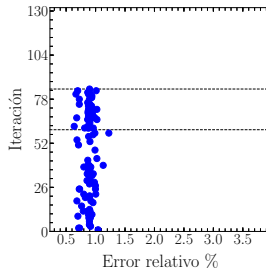
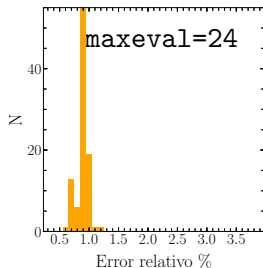
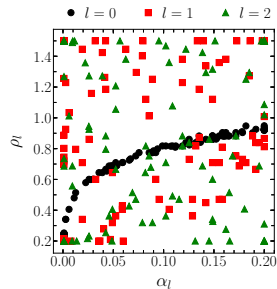
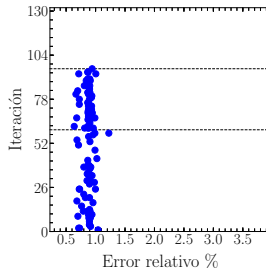
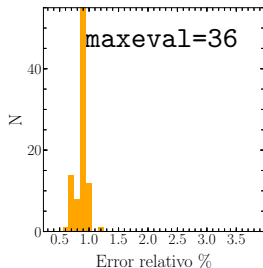
Estudio de presupuesto vs mapeo inicial:

initer=48



Estudio de presupuesto vs mapeo inicial:

initer=60



Potencial modelo

- ▶ Número de configuraciones en CI: `mxconf`
- ▶ Potencial Slater-Type-Orbital de Burgess
- ▶ Espacio de hiper-parámetros: `nlamvar`

$$\lambda_{nl} = [0.5, 1.5]$$

- ▶ Diseño inicial:
 - ▶ Latin hypercube
 - ▶ Número de datos iniciales: `initer`
- ▶ Kernel: RBF (squared exponential)
- ▶ Función de adquisición: EI
- ▶ Presupuesto: `maxeval`
- ▶ Función costo:
 - ▶ $\sum_i (E_i^{\text{obs.}} - E_i^{\text{comp.}}) / E_i^{\text{obs.}}$
 - ▶ $\sum_k (A_{ki}^{\text{obs.}} - A_{ki}^{\text{comp.}}) / A_{ki}^{\text{obs.}}$

Estudio de A_{ki}

- ▶ Número de configuraciones en CI: `mxconf=32`
- ▶ Espacio de hiper-parámetros: `nlamvar=6`

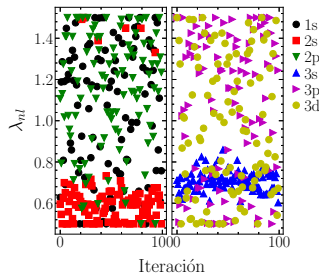
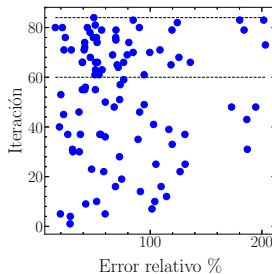
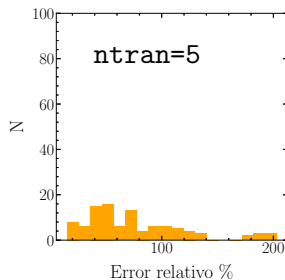
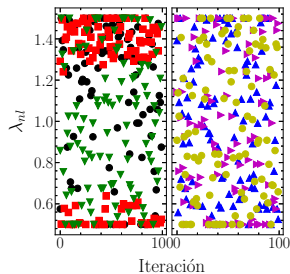
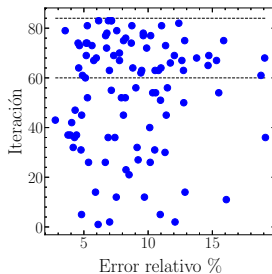
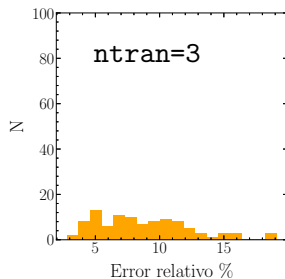
$$\lambda_{nl} = [0.5, 1.5] \quad : \quad n \leq 3, l \leq 2$$

- ▶ Diseño inicial:
 - ▶ Latin hypercube
 - ▶ Número de datos iniciales: `initer=60`
- ▶ Presupuesto: `maxeval=24`
- ▶ Función costo: `ntran= t`

$$J = \sum_k^t \frac{1}{e_t} \left| \frac{A_{ki}^{\text{obs.}} - A_{ki}^{\text{comp.}}}{A_{ki}^{\text{obs.}}} \right|$$

Minimización de t transiciones normalizadas:

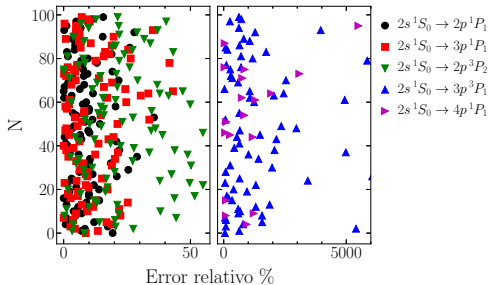
initer=60, maxevals=24



Minimización de t transiciones normalizadas:

initer=60, maxevals=24

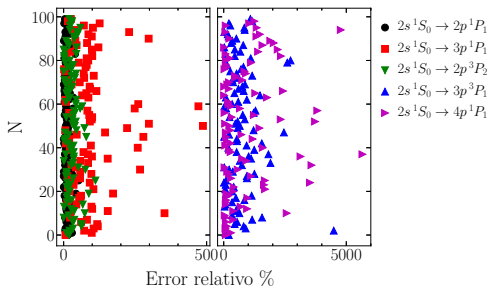
ntran=3



i	er%	observed	computed	acc
1	0.751896	-29.336884	-29.116301	0
2	0.659587	-29.136586	-28.944405	0
3	0.849625	-28.949000	-28.703042	0
4	0.775793	-28.862288	-28.638376	0
5	0.978053	-28.838628	-28.556571	0
6	0.758266	-28.818533	-28.600012	0
7	0.888515	-28.800078	-28.544185	0
8	0.556963	-28.792894	-28.632528	0
9	0.854502	-28.788417	-28.542419	0
10	0.908144	-28.771409	-28.510123	0

1	1.569E+00	5.520E+08	5.433E+08	3.0000
2	2.503E-02	7.230E+06	7.232E+06	3.0000
3	2.245E+01	1.650E-04	1.280E-04	10.0000
4	7.027E+03	4.400E-01	3.136E+01	50.0000
5	3.579E+04	1.200E+05	4.306E+07	50.0000
6	2.904E+02	4.200E-01	1.640E+00	100.0000

ntran=5

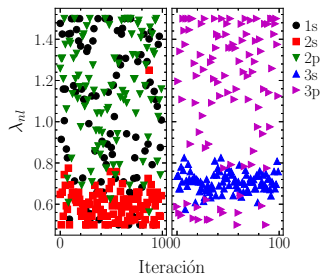
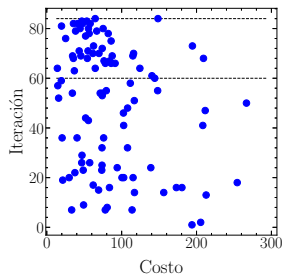
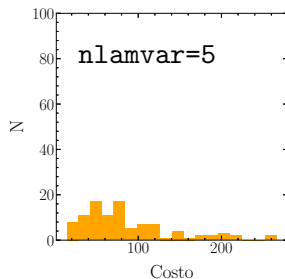
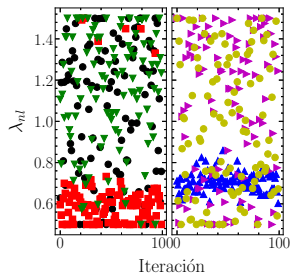
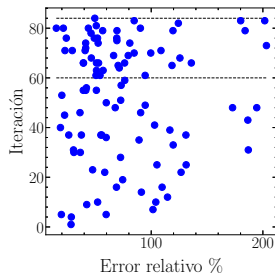
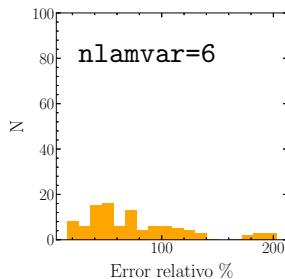


i	er%	observed	computed	acc
1	0.680740	-29.336884	-29.137176	X
2	0.641407	-29.136586	-28.949702	X
3	0.786642	-28.949000	-28.721275	X
4	0.558485	-28.862288	-28.701096	X
5	0.604849	-28.838628	-28.664198	X
6	1.043801	-28.818533	-28.517725	X
7	0.591408	-28.800078	-28.629752	X
8	0.659596	-28.792894	-28.602977	X
9	0.617514	-28.788417	-28.610644	X
10	0.556563	-28.771409	-28.611278	X

1	15.274638	5.520E+08	6.363E+08	3.0000
2	6.365698	7.230E+06	7.690E+06	3.0000
3	19.162424	1.650E-04	1.966E-04	10.0000
4	207.786364	4.400E-01	1.354E+00	50.0000
5	86.667500	1.200E+05	2.240E+05	50.0000
6	72.293810	4.200E-01	7.236E-01	100.0000

Minimización de t transiciones normalizadas:

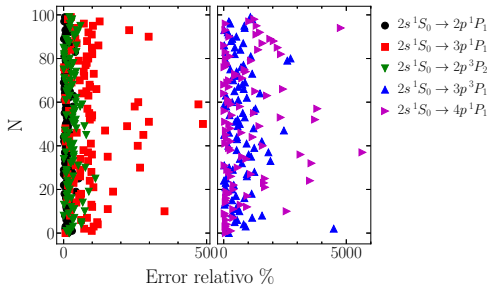
initer=60, maxevals=24



Minimización de t transiciones normalizadas:

initer=60, maxevals=24

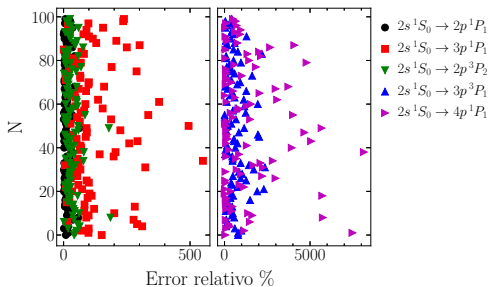
nlamvar=6



i	er%	observed	computed	acc
1	0.680740	-29.336884	-29.137176	X
2	0.641407	-29.136586	-28.949702	X
3	0.786642	-28.949000	-28.721275	X
4	0.558485	-28.862288	-28.701096	X
5	0.604849	-28.838628	-28.664198	X
6	1.043801	-28.818533	-28.517725	X
7	0.591408	-28.800078	-28.629752	X
8	0.659596	-28.792894	-28.602977	X
9	0.617514	-28.788417	-28.610644	X
10	0.556563	-28.771409	-28.611278	X

1	15.274638	5.520E+08	6.363E+08	3.0000
2	6.365698	7.230E+06	7.690E+06	3.0000
3	19.162424	1.650E-04	1.966E-04	10.0000
4	207.786364	4.400E-01	1.354E+00	50.0000
5	86.667500	1.200E+05	2.240E+05	50.0000
6	72.293810	4.200E-01	7.236E-01	100.0000

nlamvar=5

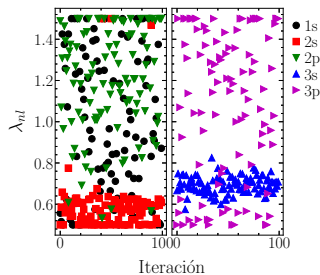
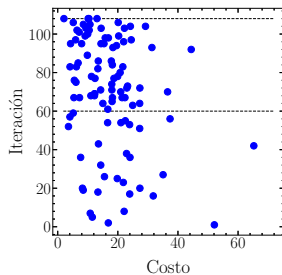
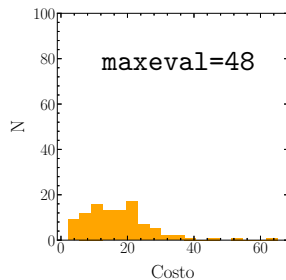
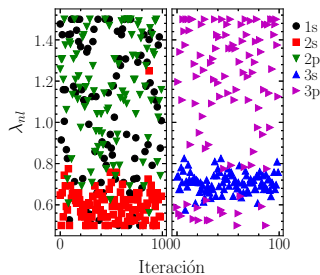
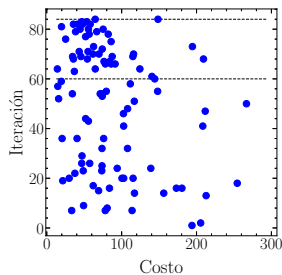
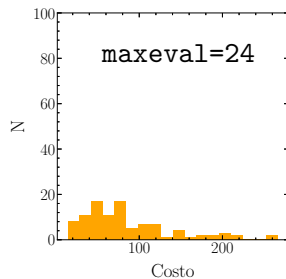


i	er%	observed	computed	acc
1	0.480494	-29.336884	-29.195922	0
2	0.433600	-29.136586	-29.010250	0
3	0.545566	-28.949000	-28.791064	0
4	0.352892	-28.862288	-28.760435	0
5	0.400973	-28.838628	-28.722993	0
6	0.834828	-28.818533	-28.577948	0
7	0.381467	-28.800078	-28.690215	0
8	0.459179	-28.792894	-28.660683	0
9	0.409399	-28.788417	-28.670557	0
10	0.349454	-28.771409	-28.670866	0

1	8.692E+00	5.520E+08	6.000E+08	3.0000
2	1.236E+01	7.230E+06	8.124E+06	3.0000
3	1.523E+01	1.650E-04	1.901E-04	10.0000
4	2.052E+02	4.400E-01	1.343E+00	50.0000
5	7.495E+01	1.200E+05	2.099E+05	50.0000
6	4.852E+01	4.200E-01	6.238E-01	100.0000

Minimización de t transiciones normalizadas:

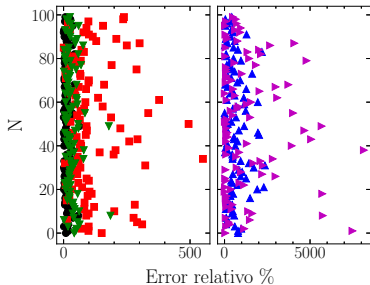
initer=60



Minimización de t transiciones normalizadas:

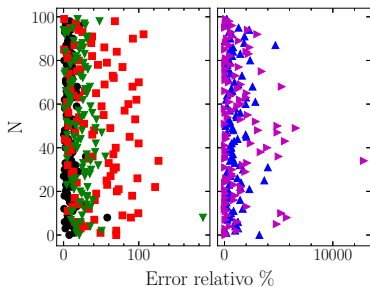
initer=60

maxeval=24



i	er%	observed	computed	acc
1	0.480494	-29.336884	-29.195922	0
2	0.433600	-29.136586	-29.010250	0
3	0.545566	-28.949000	-28.791064	0
4	0.352892	-28.862288	-28.760435	0
5	0.400973	-28.838628	-28.722993	0
6	0.834828	-28.818533	-28.577948	0
7	0.381467	-28.800078	-28.690215	0
8	0.459179	-28.792894	-28.660683	0
9	0.409399	-28.788417	-28.670557	0
10	0.349454	-28.771409	-28.670866	0
1	8.692E+00	5.520E+08	6.000E+08	3.0000
2	1.236E+01	7.230E+06	8.124E+06	3.0000
3	1.523E+01	1.650E-04	1.901E-04	10.0000
4	2.052E+02	4.400E-01	1.343E+00	50.0000
5	7.495E+01	1.200E+05	2.099E+05	50.0000
6	4.852E+01	4.200E-01	6.238E-01	100.0000

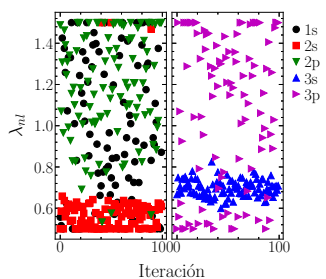
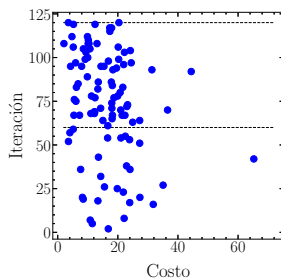
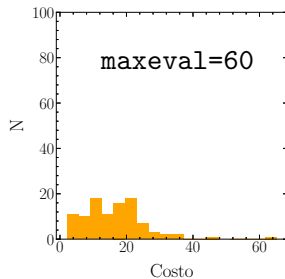
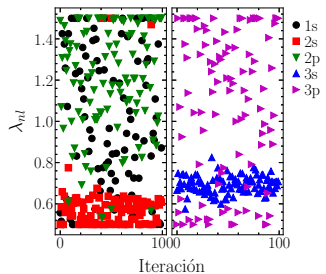
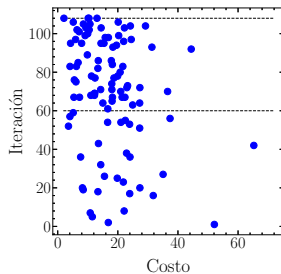
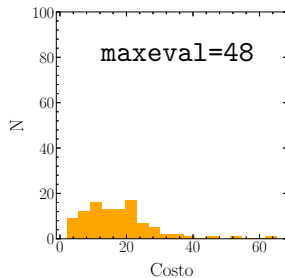
maxeval=48



i	er%	observed	computed	acc
1	0.555468	-29.336884	-29.173927	0
2	0.511340	-29.136586	-28.987599	0
3	0.557107	-28.949000	-28.787723	0
4	0.381486	-28.862288	-28.752182	0
5	0.446752	-28.838628	-28.709791	0
6	0.906490	-28.818533	-28.557296	0
7	0.403349	-28.800078	-28.683913	0
8	0.603200	-28.792894	-28.619215	0
9	0.443844	-28.788417	-28.660641	0
10	0.378886	-28.771409	-28.662398	0
1	1.512E+00	5.520E+08	5.603E+08	3.0000
2	7.999E-01	7.230E+06	7.172E+06	3.0000
3	1.865E+01	1.650E-04	1.958E-04	10.0000
4	2.168E+02	4.400E-01	1.394E+00	50.0000
5	1.459E+02	1.200E+05	2.951E+05	50.0000
6	2.533E+00	4.200E-01	4.306E-01	100.0000

Minimización de t transiciones normalizadas:

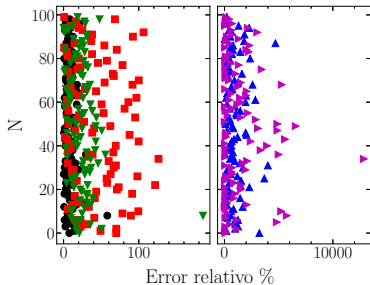
initer=60



Minimización de t transiciones normalizadas:

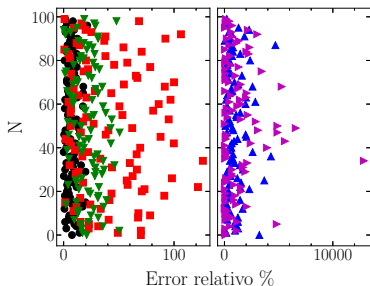
initer=60

maxeval=48



●	$2s^1S_0 \rightarrow 2p^1P_1$	i	er%	observed	computed	acc
		1	0.555468	-29.336884	-29.173927	0
■	$2s^1S_0 \rightarrow 3p^1P_1$	2	0.511340	-29.136586	-28.987599	0
▼	$2s^1S_0 \rightarrow 2p^3P_2$	3	0.557107	-28.949000	-28.787723	0
		4	0.381486	-28.862288	-28.752182	0
▲	$2s^1S_0 \rightarrow 3p^3P_1$	5	0.446752	-28.838628	-28.709791	0
		6	0.906490	-28.818533	-28.557296	0
►	$2s^1S_0 \rightarrow 4p^1P_1$	7	0.403349	-28.800078	-28.683913	0
		8	0.603200	-28.792894	-28.619215	0
		9	0.443844	-28.788417	-28.660641	0
		10	0.378886	-28.771409	-28.662398	0
		1	1.512E+00	5.520E+08	5.603E+08	3.0000
		2	7.999E-01	7.230E+06	7.172E+06	3.0000
		3	1.865E+01	1.650E-04	1.958E-04	10.0000
		4	2.168E+02	4.400E-01	1.394E+00	50.0000
		5	1.459E+02	1.200E+05	2.951E+05	50.0000
		6	2.533E+00	4.200E-01	4.306E-01	100.0000

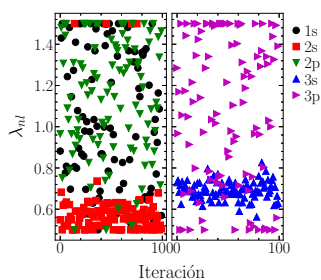
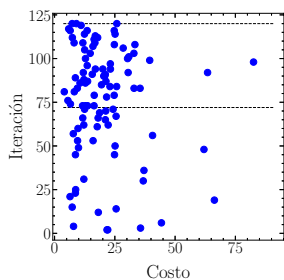
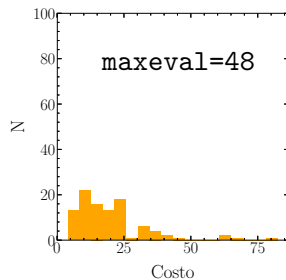
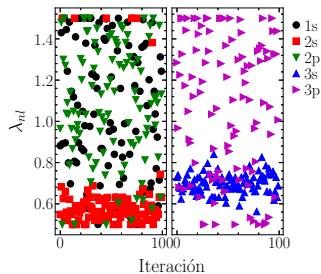
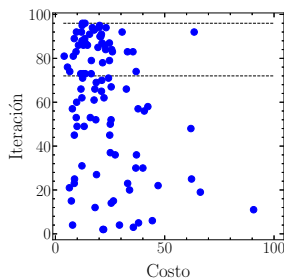
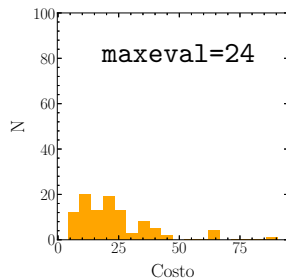
maxeval=60



		i	er%	observed	computed	acc
●	$2s^1S_0 \rightarrow 2p^1P_1$	1	0.555468	-29.336884	-29.173927	0
■	$2s^1S_0 \rightarrow 3p^1P_1$	2	0.511340	-29.136586	-28.987599	0
▼	$2s^1S_0 \rightarrow 2p^3P_2$	3	0.557107	-28.949000	-28.787723	0
▲	$2s^1S_0 \rightarrow 3p^3P_1$	4	0.381486	-28.862288	-28.752182	0
▶	$2s^1S_0 \rightarrow 4p^1P_1$	5	0.446752	-28.838628	-28.709791	0
		6	0.906490	-28.818533	-28.557296	0
		7	0.403349	-28.800078	-28.683913	0
		8	0.603200	-28.792894	-28.619215	0
		9	0.443844	-28.788417	-28.660641	0
		10	0.378886	-28.771409	-28.662398	0
		1	1.512E+00	5.520E+08	5.603E+08	3.0000
		2	7.999E-01	7.230E+06	7.172E+06	3.0000
		3	1.865E+01	1.650E-04	1.958E-04	10.0000
		4	2.168E+02	4.400E-01	1.394E+00	50.0000
		5	1.459E+02	1.200E+05	2.951E+05	50.0000
		6	2.533E+00	4.200E-01	4.306E-01	100.0000

Minimización de t transiciones normalizadas:

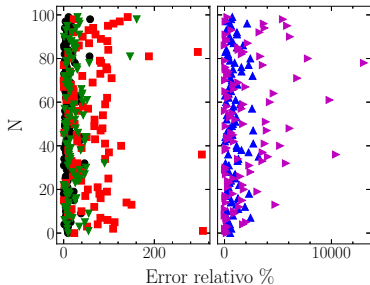
initer=72



Minimización de t transiciones normalizadas:

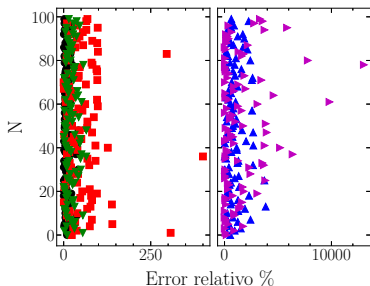
initer=72

maxeval=24



i	er%	observed	computed	acc
1	0.923759	-29.336884	-29.065882	0
2	0.873219	-29.136586	-28.882160	0
3	1.048568	-28.949000	-28.645450	0
4	0.883695	-28.862288	-28.607233	0
5	1.217316	-28.838628	-28.487571	0
6	1.050870	-28.818533	-28.515688	0
7	1.071750	-28.800078	-28.491413	0
8	0.864181	-28.792894	-28.544071	0
9	1.055618	-28.788417	-28.484521	0
10	1.108145	-28.771409	-28.452580	0
1	8.837E+00	5.520E+08	5.032E+08	3.0000
2	1.466E-02	7.230E+06	7.231E+06	3.0000
3	9.116E+00	1.650E-04	1.500E-04	10.0000
4	6.724E+02	4.400E-01	3.398E+00	50.0000
5	4.527E+01	1.200E+05	1.743E+05	50.0000
6	8.739E+02	4.200E-01	4.090E+00	100.0000

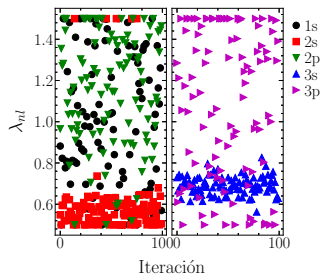
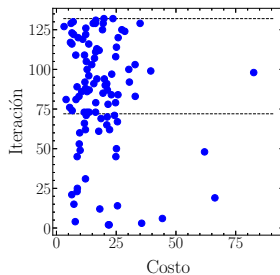
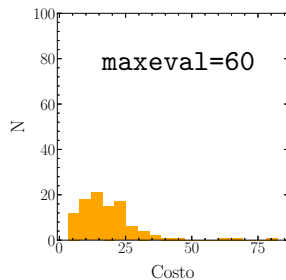
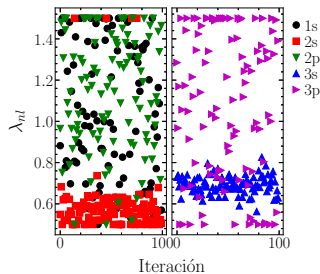
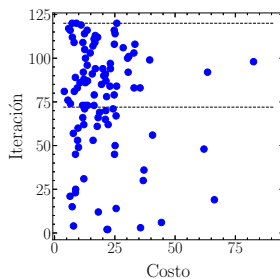
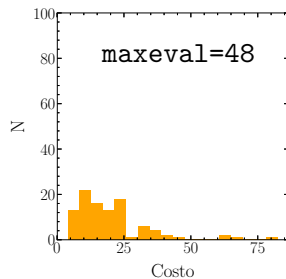
maxeval=48



i	er%	observed	computed	acc
1	0.923759	-29.336884	-29.065882	0
2	0.873219	-29.136586	-28.882160	0
3	1.048568	-28.949000	-28.645450	0
4	0.883695	-28.862288	-28.607233	0
5	1.217316	-28.838628	-28.487571	0
6	1.050870	-28.818533	-28.515688	0
7	1.071750	-28.800078	-28.491413	0
8	0.864181	-28.792894	-28.544071	0
9	1.055618	-28.788417	-28.484521	0
10	1.108145	-28.771409	-28.452580	0
1	8.837E+00	5.520E+08	5.032E+08	3.0000
2	1.466E-02	7.230E+06	7.231E+06	3.0000
3	9.116E+00	1.650E-04	1.500E-04	10.0000
4	6.724E+02	4.400E-01	3.398E+00	50.0000
5	4.527E+01	1.200E+05	1.743E+05	50.0000
6	8.739E+02	4.200E-01	4.090E+00	100.0000

Minimización de t transiciones normalizadas:

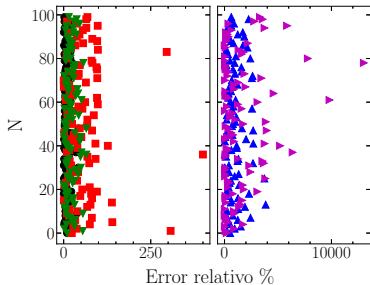
initer=72



Minimización de t transiciones normalizadas:

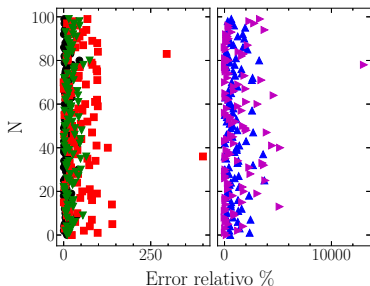
initer=72

maxeval=48



●	$2s^1S_0 \rightarrow 2p^1P_1$	i	er%	observed	computed	acc
		1	0.923759	-29.336884	-29.065882	0
■	$2s^1S_0 \rightarrow 3p^1P_1$	2	0.873219	-29.136586	-28.882160	0
▼	$2s^1S_0 \rightarrow 2p^3P_2$	3	1.048568	-28.949000	-28.645450	0
▲	$2s^1S_0 \rightarrow 3p^3P_1$	4	0.883695	-28.862288	-28.607233	0
▶	$2s^1S_0 \rightarrow 4p^1P_1$	5	1.217316	-28.838628	-28.487571	0
		6	1.050870	-28.818533	-28.515688	0
		7	1.071750	-28.800078	-28.491413	0
		8	0.864181	-28.792894	-28.544071	0
		9	1.055618	-28.788417	-28.484521	0
		10	1.108145	-28.771409	-28.452580	0
		1	8.837E+00	5.520E+08	5.032E+08	3.0000
		2	1.466E-02	7.230E+06	7.231E+06	3.0000
		3	9.116E+00	1.650E-04	1.500E-04	10.0000
		4	6.724E+02	4.400E-01	3.398E+00	50.0000
		5	4.527E+01	1.200E+05	1.743E+05	50.0000
		6	8.739E+02	4.200E-01	4.090E+00	100.0000

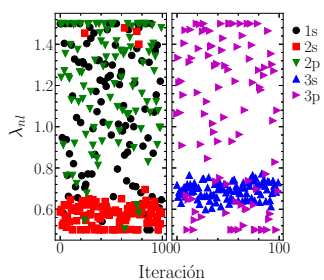
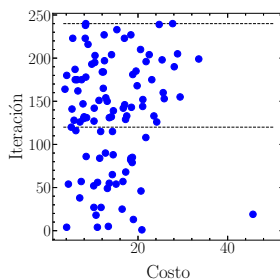
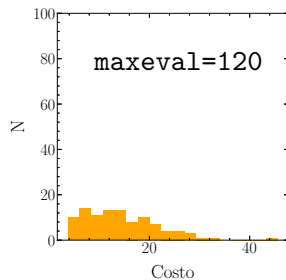
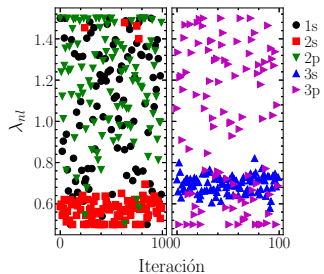
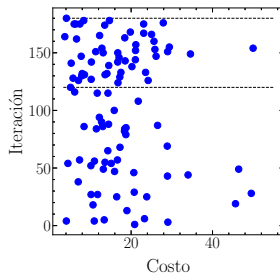
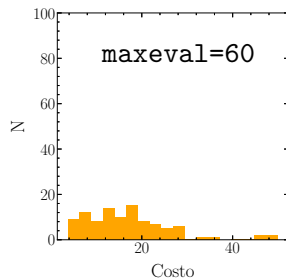
maxeval=60



		er%	observed	computed	acc	
●	$2s^1S_0 \rightarrow 2p^1P_1$	i				
		1	1.010734	-29.336884	-29.040366	0
■	$2s^1S_0 \rightarrow 3p^1P_1$	2	0.929341	-29.136586	-28.865808	0
		3	1.116498	-28.949000	-28.625785	0
▼	$2s^1S_0 \rightarrow 2p^3P_2$	4	0.965109	-28.862288	-28.583735	0
▲	$2s^1S_0 \rightarrow 3p^3P_1$	5	1.289597	-28.838628	-28.466726	0
		6	1.026777	-28.818533	-28.522631	0
		7	1.165264	-28.800078	-28.464481	0
►	$2s^1S_0 \rightarrow 4p^1P_1$	8	0.836734	-28.792894	-28.551974	0
		9	1.142288	-28.788417	-28.459570	0
		10	1.191738	-28.771409	-28.428529	0
		1	6.723E+00	5.520E+08	5.149E+08	3.0000
		2	2.437E+00	7.230E+06	7.406E+06	3.0000
		3	2.168E+01	1.650E-04	1.292E-04	10.0000
		4	2.452E+01	4.400E-01	5.479E-01	50.0000
		5	2.353E+02	1.200E+05	4.024E+05	50.0000
		6	3.820E+02	4.200E-01	2.024E+00	100.0000

Minimización de t transiciones normalizadas:

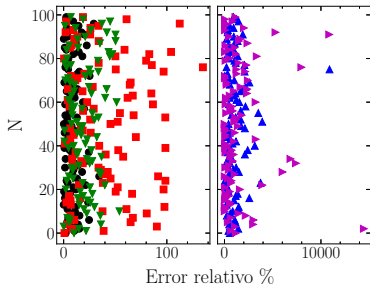
initer=120



Minimización de t transiciones normalizadas:

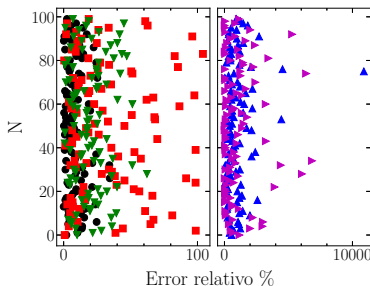
initer=120

maxeval=60



i	er%	observed	computed	acc
1	0.556828	-29.336884	-29.173528	0
2	0.499599	-29.136586	-28.991020	0
3	0.610063	-28.949000	-28.772393	0
4	0.416459	-28.862288	-28.742088	0
5	0.463122	-28.838628	-28.705070	0
6	0.894210	-28.818533	-28.560835	0
7	0.434603	-28.800078	-28.674912	0
8	0.507392	-28.792894	-28.646801	0
9	0.474526	-28.788417	-28.651808	0
10	0.415120	-28.771409	-28.651973	0
1	4.679E+00	5.520E+08	5.778E+08	3.0000
2	4.083E-01	7.230E+06	7.200E+06	3.0000
3	3.339E+00	1.650E-04	1.705E-04	10.0000
4	4.665E+02	4.400E-01	2.493E+00	50.0000
5	4.628E+02	1.200E+05	6.754E+05	50.0000
6	4.171E+01	4.200E-01	5.952E-01	100.0000

maxeval=120

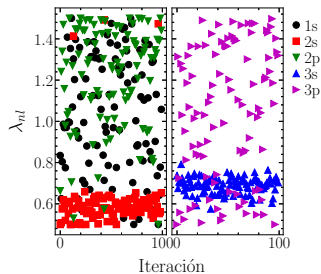
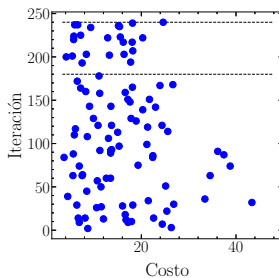
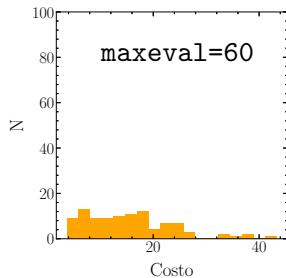


i	er%	observed	computed	acc
1	0.556828	-29.336884	-29.173528	0
2	0.499599	-29.136586	-28.991020	0
3	0.610063	-28.949000	-28.772393	0
4	0.416459	-28.862288	-28.742088	0
5	0.463122	-28.838628	-28.705070	0
6	0.894210	-28.818533	-28.560835	0
7	0.434603	-28.800078	-28.674912	0
8	0.507392	-28.792894	-28.646801	0
9	0.474526	-28.788417	-28.651808	0
10	0.415120	-28.771409	-28.651973	0
1	4.679E+00	5.520E+08	5.778E+08	3.0000
2	4.083E-01	7.230E+06	7.200E+06	3.0000
3	3.339E+00	1.650E-04	1.705E-04	10.0000
4	4.665E+02	4.400E-01	2.493E+00	50.0000
5	4.628E+02	1.200E+05	6.754E+05	50.0000
6	4.171E+01	4.200E-01	5.952E-01	100.0000

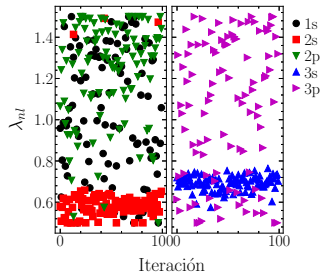
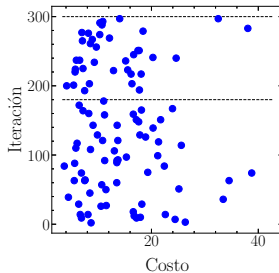
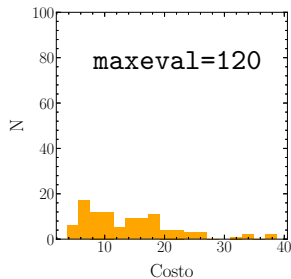
Minimización de t transiciones normalizadas:

initer=180

maxeval=60



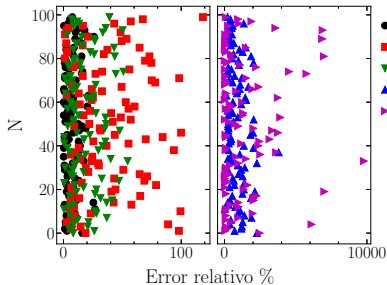
maxeval=120



Minimización de t transiciones normalizadas:

initer=180

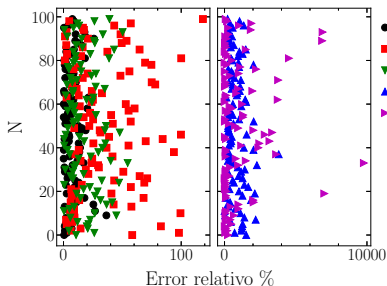
maxeval=60



i	er%	observed	computed	acc
1	0.544904	-29.336884	-29.177026	0
2	0.494355	-29.136586	-28.992548	0
3	0.546105	-28.949000	-28.790908	0
4	0.372862	-28.862288	-28.754671	0
5	0.437077	-28.838628	-28.712581	0
6	0.891236	-28.818533	-28.561692	0
7	0.378044	-28.800078	-28.691201	0
8	0.565406	-28.792894	-28.630097	0
9	0.439262	-28.788417	-28.661960	0
10	0.373826	-28.771409	-28.663854	0

1	6.533E-01	5.520E+08	5.484E+08	3.0000
2	1.219E+00	7.230E+06	7.318E+06	3.0000
3	1.003E+01	1.650E-04	1.815E-04	10.0000
4	5.531E+02	4.400E-01	2.874E+00	50.0000
5	5.075E+02	1.200E+05	7.290E+05	50.0000
6	9.948E+00	4.200E-01	3.782E-01	100.0000

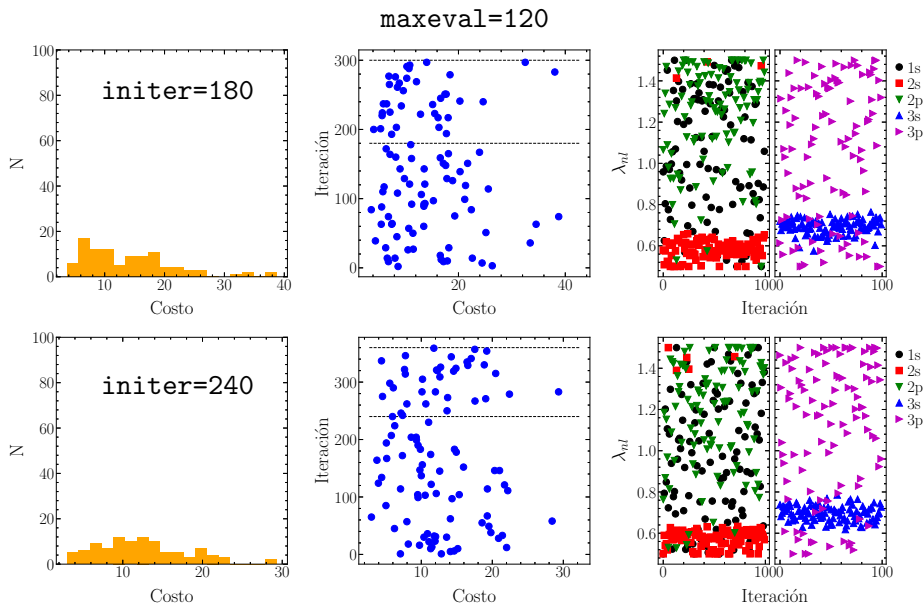
maxeval=120



i	er%	observed	computed	acc
1	0.544904	-29.336884	-29.177026	0
2	0.494355	-29.136586	-28.992548	0
3	0.546105	-28.949000	-28.790908	0
4	0.372862	-28.862288	-28.754671	0
5	0.437077	-28.838628	-28.712581	0
6	0.891236	-28.818533	-28.561692	0
7	0.378044	-28.800078	-28.691201	0
8	0.565406	-28.792894	-28.630097	0
9	0.439262	-28.788417	-28.661960	0
10	0.373826	-28.771409	-28.663854	0

1	6.533E-01	5.520E+08	5.484E+08	3.0000
2	1.219E+00	7.230E+06	7.318E+06	3.0000
3	1.003E+01	1.650E-04	1.815E-04	10.0000
4	5.531E+02	4.400E-01	2.874E+00	50.0000
5	5.075E+02	1.200E+05	7.290E+05	50.0000
6	9.948E+00	4.200E-01	3.782E-01	100.0000

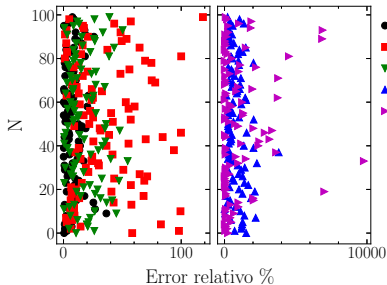
Minimización de t transiciones normalizadas:



Minimización de t transiciones normalizadas:

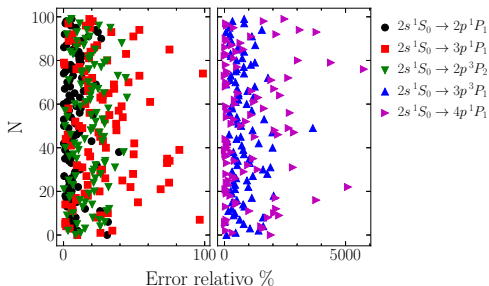
maxeval=120

initer=180



i	er%	observed	computed	acc
1	0.544904	-29.336884	-29.177026	0
2	0.494355	-29.136586	-28.992548	0
3	0.546105	-28.949000	-28.790908	0
4	0.372862	-28.862288	-28.754671	0
5	0.437077	-28.838628	-28.712581	0
6	0.891236	-28.818533	-28.561692	0
7	0.378044	-28.800078	-28.691201	0
8	0.565406	-28.792894	-28.630097	0
9	0.439262	-28.788417	-28.661960	0
10	0.373826	-28.771409	-28.663854	0
1	6.533E-01	5.520E+08	5.484E+08	3.0000
2	1.219E+00	7.230E+06	7.318E+06	3.0000
3	1.003E+01	1.650E-04	1.815E-04	10.0000
4	5.531E+02	4.400E-01	2.874E+00	50.0000
5	5.075E+02	1.200E+05	7.290E+05	50.0000
6	9.948E+00	4.200E-01	3.782E-01	100.0000

initer=240



i	er%	observed	computed	acc
1	0.849606	-29.336884	-29.087636	0
2	0.806574	-29.136586	-28.901578	0
3	0.880752	-28.949000	-28.694031	0
4	0.691444	-28.862288	-28.662721	0
5	0.753552	-28.838628	-28.621314	0
6	1.202900	-28.818533	-28.471875	0
7	0.706078	-28.800078	-28.596727	0
8	0.862410	-28.792894	-28.544581	0
9	0.760280	-28.788417	-28.569544	0
10	0.692854	-28.771409	-28.572065	0
1	3.596E+00	5.520E+08	5.718E+08	3.0000
2	1.533E+00	7.230E+06	7.119E+06	3.0000
3	1.496E+01	1.650E-04	1.897E-04	10.0000
4	4.964E+02	4.400E-01	2.624E+00	50.0000
5	4.070E+01	1.200E+05	7.117E+04	50.0000
6	1.387E+01	4.200E-01	4.782E-01	100.0000