Optimization of chiral NN (and 3NFs)

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More Progress in Ab-Initio Techniques, TRIUMF, Vancouver

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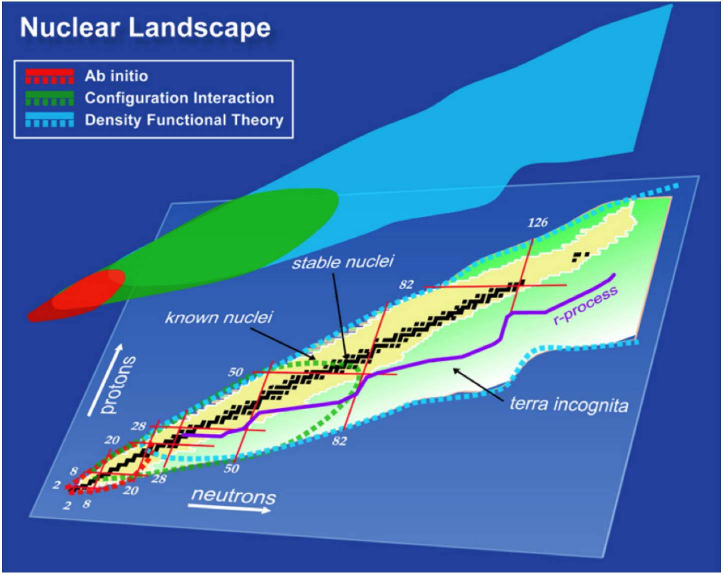
Physics Case



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effective Lagrangian

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi}(f_\pi, m_\pi) + \mathcal{L}_{\pi N}(f_\pi, M_N, g_A, c_i, d_i, ...) + \mathcal{L}_{NN}(C_i, \tilde{C}_i, D_i, ...) + \ldots$$

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- How much freedom do we have when choosing the parameters of our chiral Lagrangian?
- Important for assessing and understanding discrepancies with respect to experiment.
- Can we improve chiral forces?
- Keywords: sensitivity analysis, uncertainty quantification, parameter optimization

Overview

- Stay at NNLO and use an optimization algorithm to determine the parameters

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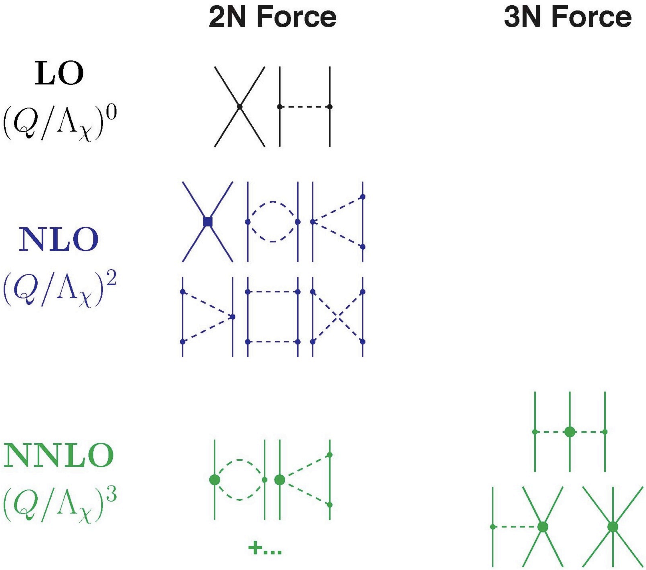
- Re-fitting the NNLO-3NF to the POUNDerS-NNLO.
- whats next?

Related talks at this workshop

- **Gaute Hagen** *Structure of neutron rich oxygen and fluorine isotopes*
- **Gustav Jansen** *Shell evolution in the neutron rich calcium isotopes*
- **Christian Forssén** *Clustering in light nuclei*

Chiral interactions



The parameters

[5+2+2] reagarded as constants

$m_{\pi^+}, m_{\pi^-}, m_{\pi^0}, m_n, m_p, g_A, f_\pi, \Lambda_{LS}, \Lambda_\chi$

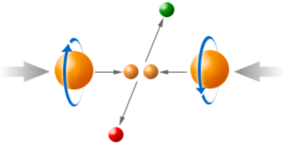
[14+2] Optimization parameters up to NNLO

$\tilde{C}^{pp}_{^1S_0}, \tilde{C}^{nn}_{^1S_0}, \tilde{C}^{np}_{^1S_0}, \tilde{C}_{^3S_1}$
$C_{^1S_0}, C_{^3P_0}, C_{^1P_1}, C_{^3P_1}, C_{^3S_1}, C_{^3S_1-^3D_1}, C_{^3P_2}$
$c_1, c_3, c_4, (c_D, c_E)$

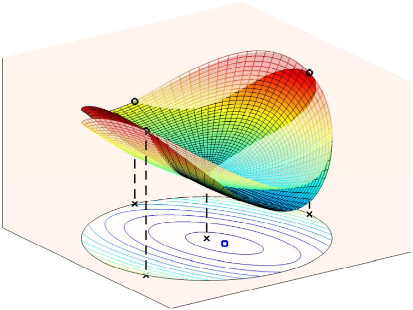
POUNDerS

Practical Optimization Using No Derivatives (Square/Structure)

function evaluation



POUNDerS step



- Optimize over computationally expensive, nonlinear functions arising in science and engineering
- Function values all you have, and derivatives are computationally expensive
- Use an interpolating quadratic

Optimization strategy

Initial study

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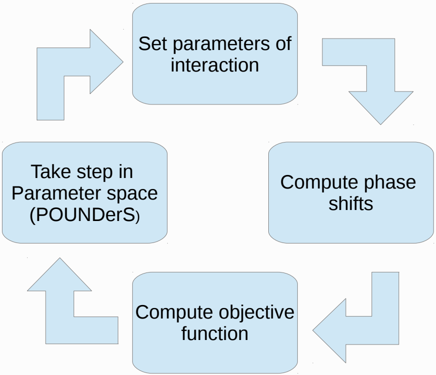


The data

V. G. J. Stoks *et al.* Phys. Rev. **C** 48, 792 (1993)

Phase shifts

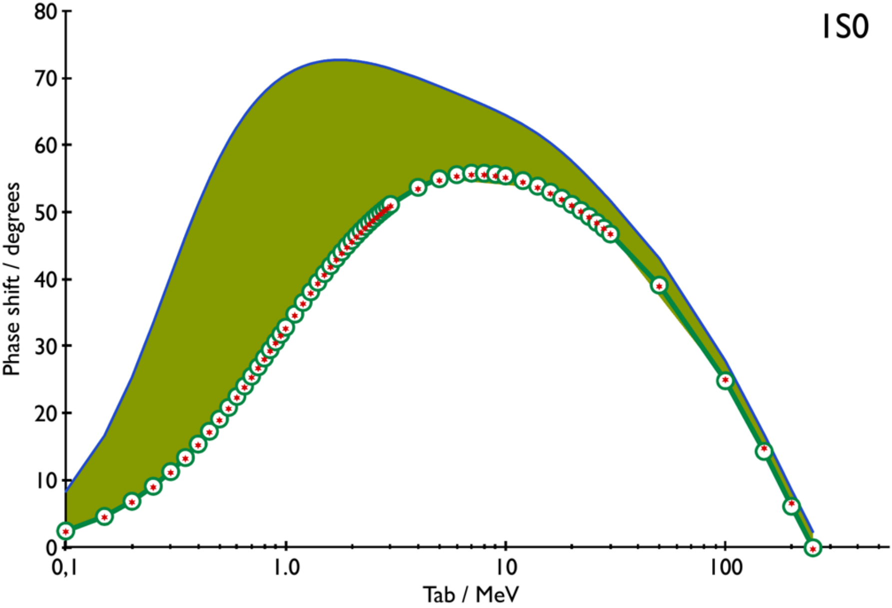
They are not observables. Obtained from a partial wave analysis (PWA) of various scattering cross sections (Nijmegen). Thus, phase shifts parametrize the actual scattering data.

- Given phase shifts, it is trivial to compute observables
- The reverse procedure is *not* trivial, since the equations are transcendental.

TABLE IV. *pp* isovector phase shifts and their multienergy error in degrees as obtained in the multienergy *pp* analysis. Errors smaller than 0.0005° are not shown. The lower part lists the phase shifts as obtained in the combined $pp + np$ analysis.

T_{lab}	$^1S_0$	$^1D_2$	$^1G_4$	$^3P_0$	$^3P_1$	$^3F_3$	$^3P_2$	ϵ_2	$^3F_2$	$^3F_4$	ϵ_4	$^3H_4$
1	32.684 ±0.005	0.001	0.000	0.134	−0.081	−0.000	0.014	−0.001	0.000	0.000	−0.000	0.000
5	54.832 ±0.017	0.043	0.000	1.582 ±0.006	−0.902 ±0.001	−0.005	0.214 ±0.001	−0.052	0.002	0.000	−0.000	0.000
10	55.219 ±0.025	0.165	0.003	3.729 ±0.017	−2.060 ±0.002	−0.032	0.651 ±0.002	−0.200	0.013	0.001	−0.004	0.000
25	48.672 ±0.039	0.696 ±0.001	0.040	8.575 ±0.053	−4.932 ±0.008	−0.231	2.491 ±0.008	−0.810 ±0.001	0.105	0.020	−0.049	0.004
50	38.899 ±0.049	1.711 ±0.004	0.152	11.47 ±0.09	−8.317 ±0.017	−0.690	5.855 ±0.016	−1.712 ±0.004	0.338	0.108 ±0.001	−0.195	0.026
100	24.97 ±0.08	3.790 ±0.018	0.418 ±0.001	9.45 ±0.11	−13.258 ±0.032	−1.517 ±0.003	11.013 ±0.025	−2.659 ±0.017	0.817 ±0.004	0.478 ±0.007	−0.539	0.108
150	14.75 ±0.13	5.606 ±0.033	0.700 ±0.003	4.74 ±0.14	−17.434 ±0.045	−2.100 ±0.010	13.982 ±0.039	−2.873 ±0.029	1.197 ±0.014	1.032 ±0.022	−0.849	0.211
200	6.55 ±0.16	7.058 ±0.045	0.993 ±0.010	−0.37 ±0.17	−21.25 ±0.07	−2.487 ±0.025	15.63 ±0.052	−2.759 ±0.037	1.424 ±0.034	1.678 ±0.039	−1.108	0.321
250	−0.31 ±0.18	8.27 ±0.06	1.272 ±0.024	−5.43 ±0.21	−24.77 ±0.12	−2.724 ±0.049	16.59 ±0.07	−2.542 ±0.046	1.47 ±0.06	2.325 ±0.051	−1.314	0.428
300	−6.15 ±0.25	9.42 ±0.08	1.503 ±0.048	−10.39 ±0.33	−27.99 ±0.19	−2.84 ±0.11	17.17 ±0.10	−2.34 ±0.09	1.34 ±0.11	2.89 ±0.06	−1.47	0.526
350	−11.13 ±0.46	10.69 ±0.14	1.64 ±0.08	−15.30 ±0.57	−30.89 ±0.27	−2.87 ±0.13	17.54 ±0.15	−2.21 ±0.11	1.04 ±0.16	3.30 ±0.11	−1.588 ±0.001	0.608
100	24.97 ±0.08	3.782 ±0.017	0.418	9.55 ±0.09	−13.245 ±0.030	−1.518 ±0.002	11.013 ±0.021	−2.654 ±0.016	0.816 ±0.003	0.471 ±0.006	−0.539	0.108
200	6.55 ±0.16	7.039 ±0.043	0.993 ±0.008	−0.27 ±0.17	−21.18 ±0.06	−2.499 ±0.021	15.65 ±0.05	−2.731 ±0.035	1.414 ±0.029	1.656 ±0.034	−1.107	0.321
300	−6.22 ±0.23	9.42 ±0.08	1.501 ±0.040	−10.44 ±0.29	−27.80 ±0.16	−2.89 ±0.07	17.15 ±0.09	−2.27 ±0.06	1.30 ±0.09	2.95 ±0.05	−1.473	0.526

$^1S_0$ proton-proton Nuclear + Coulomb interaction



Objective function

$$f(\vec{x}) = \sum_{q=1}^{N_q} \left(\frac{\delta_q^{\mathrm{NNLO}}(\vec{x}) - \delta_q^{\mathrm{Nijm93}}}{w_q} \right)^2$$

πN

The πN contacts c_1, c_3, c_4 were optimized simultaneously using the peripheral $(L \geq 2)$ waves ${}^1D_2, {}^3D_2, {}^3F_2, E_2, {}^3F_3, {}^1G_4$, and ${}^3F_4$

NN-contacts

The NN contacts $\tilde{C}^{pp}_{^1S_0}$ $\tilde{C}^{nn}_{^1S_0}$ $\tilde{C}^{np}_{^1S_0}$ $C_{^3P_0}$ $C_{^1P_1}$ $C_{^1S_0}$ $\tilde{C}_{^3S_1}$ $C_{^3S_1}$ $C_{^3S_1-^3D_1}$ $C_{^3P_2}$ were optimized in the respective partial wave.

χ^2/datum, *np* scattering data (1999 database)

The previous picture...

T_{lab} bin (MeV)	N3LO	NNLO[1]	NLO[1]	AV18
0-100	1.06	1.71	5.20	0.95
100-190	1.08	12.9	49.3	1.10
190-290	1.15	19.2	68.3	1.11
0-290	**1.10**	**10.1**	**36.2**	**1.04**

[1] E. Epelbaum et al., Eur. Phys. J. A19, 401 (2004)

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... changes with POUNDerS

T_{lab} bin (MeV)	POUNDerS-NNLO(500)
0-35	0.85
35-125	1.17
125-183	1.87
183-290	6.09
0-290	**2.95**

χ^2/datum, *pp* scattering data (1999 database)

The previous picture...

T_{lab} bin (MeV)	N3LO	NNLO[1]	NLO[1]	AV18
0-100	1.05	6.66	57.8	0.96
100-190	1.50	28.3	62.0	1.31
190-290	1.93	66.8	111.6	1.82
0-290	**1.50**	**35.4**	**80.1**	**1.38**

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0-35	1.11
35-125	1.56
125-183	23.95 (4.35[a])
183-290	29.26
0-290	**17.10 (14.03)**[2]

[2] Total (0-290) MeV *pp* χ^2/datum when excluding two low-uncertainty data sets.

POUNDerS-NNLO optimized parameter values

'empirical' values

πN LEC	πN-scattering[1]	NN-PWA[2]	NNLO[3]	N3LO
c_1 [GeV^{-1}]	-0.81±0.15	-0.76±0.07	-0.81	-0.81
c_3 [GeV^{-1}]	-4.69±1.34	-4.78±0.10	-3.40	-3.20
c_4 [GeV^{-1}]	+3.40±0.04	+3.96 ±0.22	+3.40	+5.40

[1] πN Fit 1, in P. Büttiker, U-G. Meißner Nucl. Phys. A **668**, 97 (2000)
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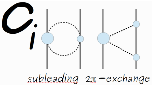

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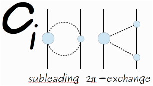

POUNDerS

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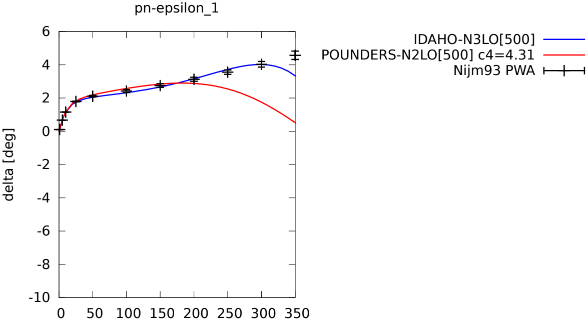

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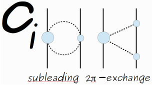

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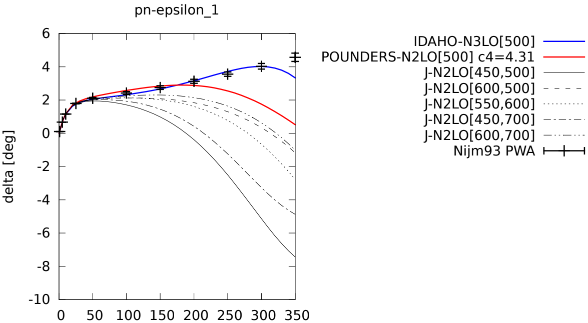
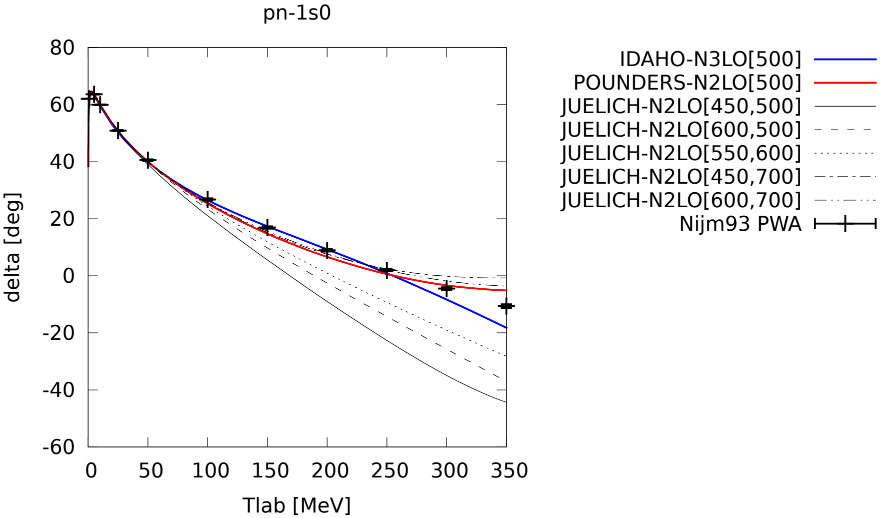


POUNDerS-NNLO Phase shifts



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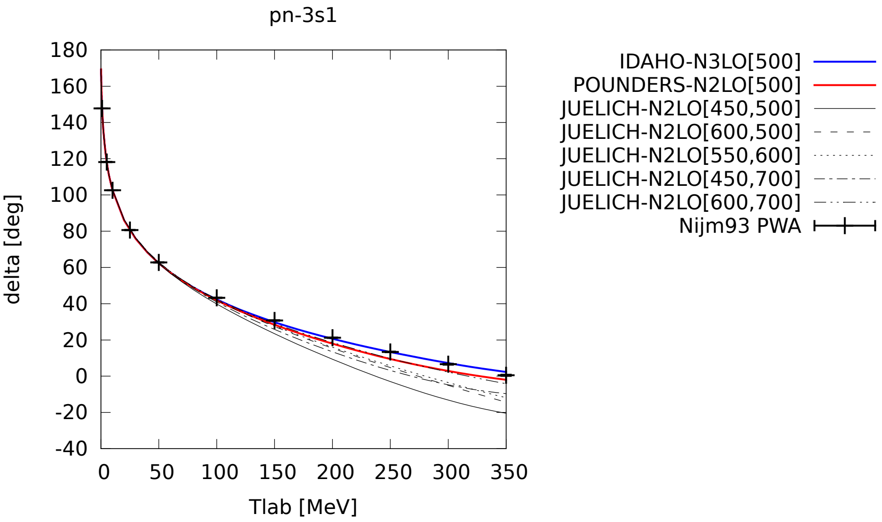

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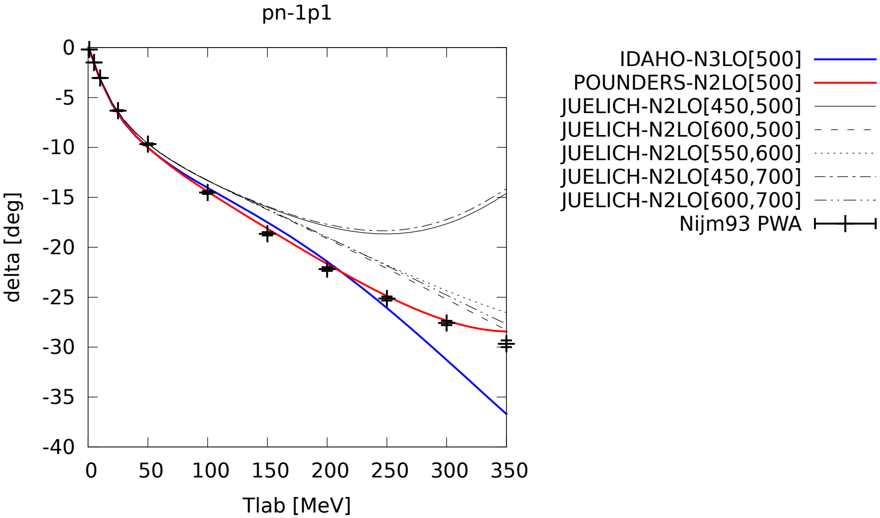

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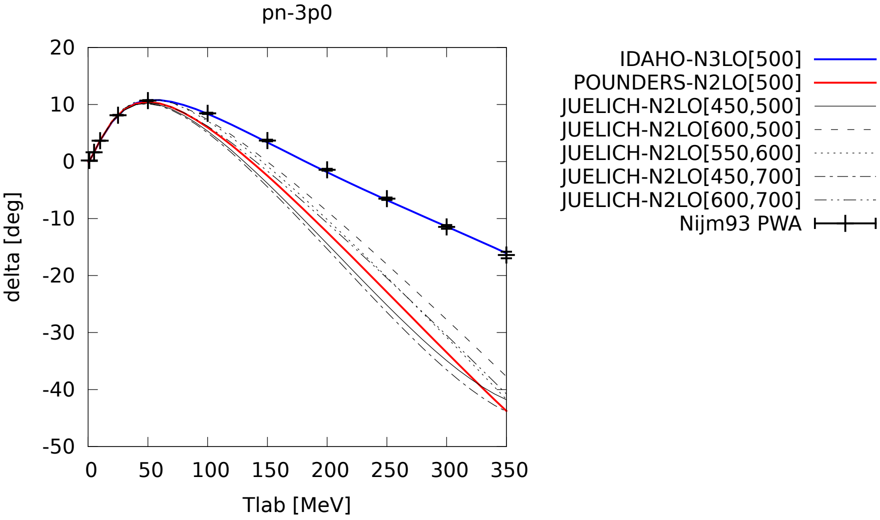
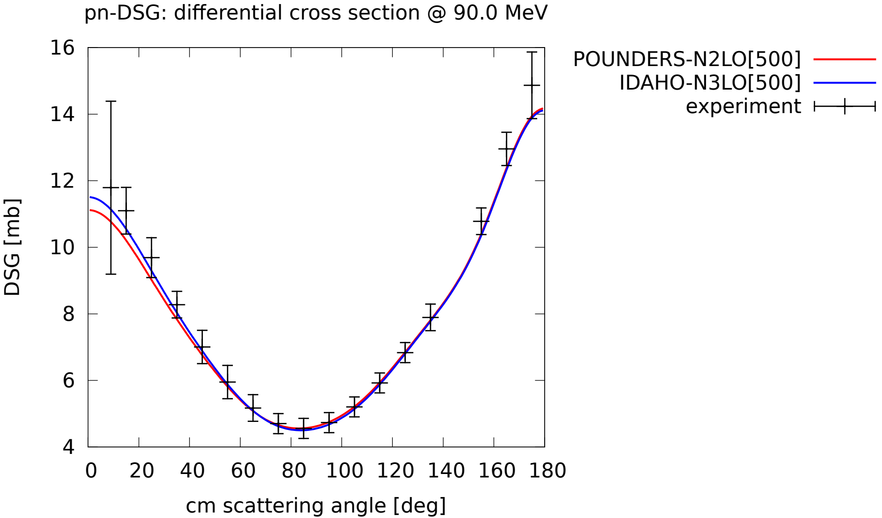
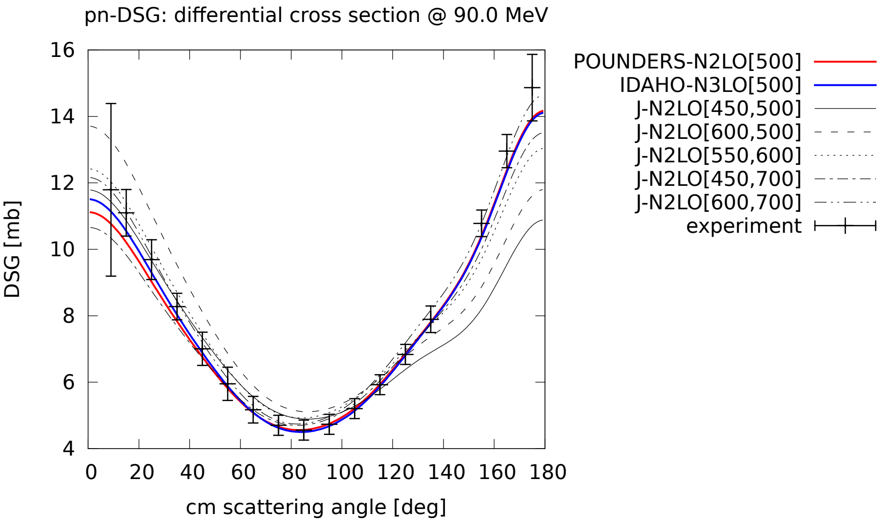



pn-DSG: differential cross section @ 90.0 MeV
16
14
12
10
8
6
4
0 20 40 60 80 100 120 140 160 180
DSG [mb]
cm scattering angle [deg]
POUNDERS-N2LO[500]
IDAHO-N3LO[500]
experiment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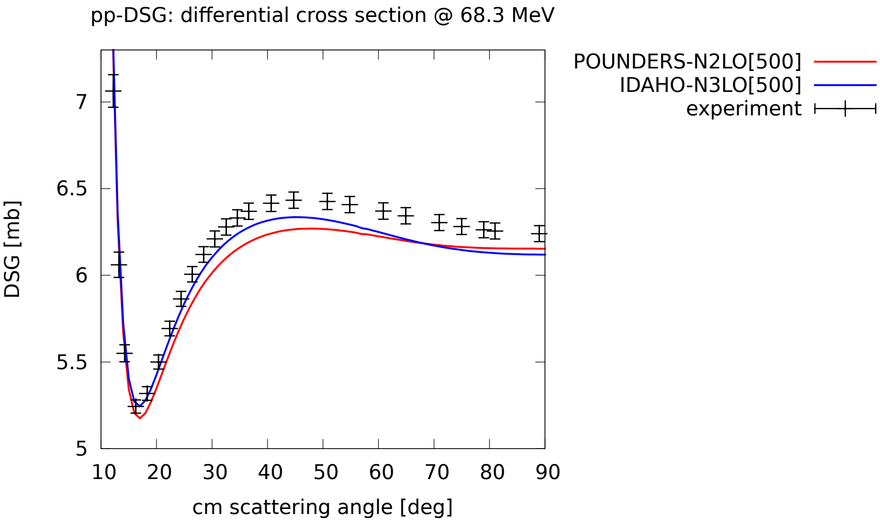
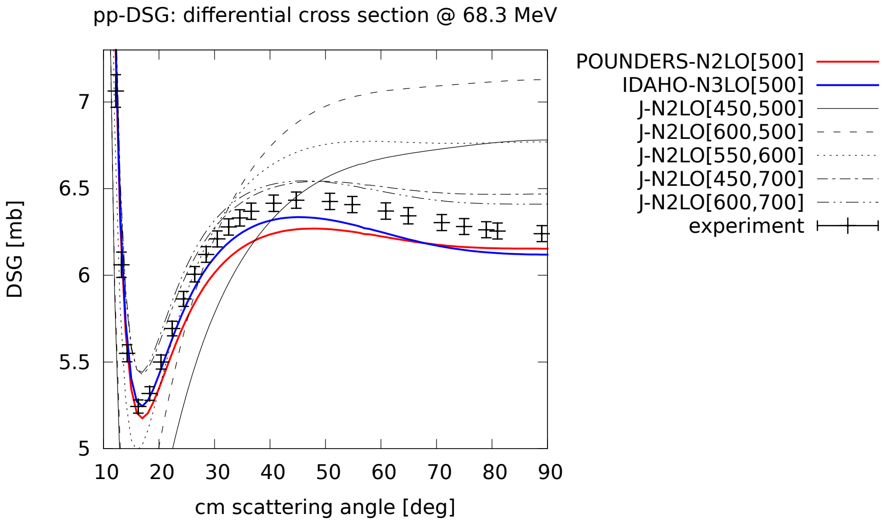
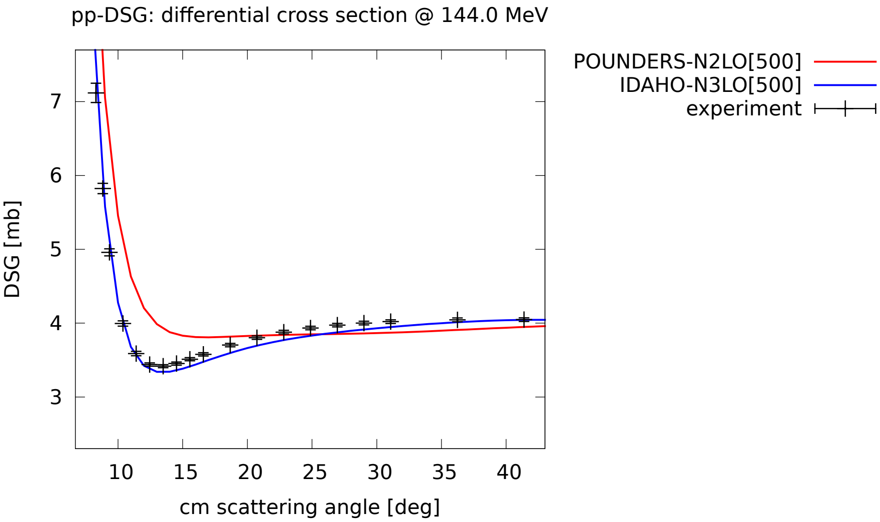


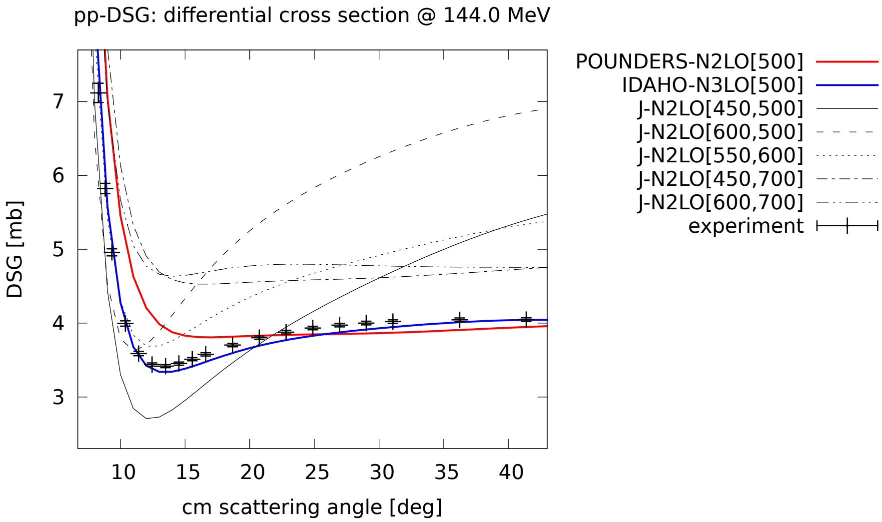
pp-DSG: differential cross section @ 68.3 MeV
POUNDERS-N2LO[500]
IDAHO-N3LO[500]
experiment
DSG [mb]
cm scattering angle [deg]
5
5.5
6
6.5
7
10
20
30
40
50
60
70
80
90



pp-DSG: differential cross section @ 68.3 MeV
DSG [mb]
cm scattering angle [deg]
5
5.5
6
6.5
7
10
20
30
40
50
60
70
80
90
POUNDERS-N2LO[500]
IDAHO-N3LO[500]
J-N2LO[450,500]
J-N2LO[600,500]
J-N2LO[550,600]
J-N2LO[450,700]
J-N2LO[600,700]
experiment



pp-DSG: differential cross section @ 144.0 MeV
DSG [mb]
cm scattering angle [deg]
3
4
5
6
7
10
15
20
25
30
35
40
POUNDERS-N2LO[500]
IDAHO-N3LO[500]
experiment



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3
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15
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J-N2LO[600,700]
experiment

$^1S_0$ scattering observables

	N^3LO	POUNDerS-NNLO	Empirical
a_{pp}^C	-7.8188	-7.8174	-7.8196(26)
			-7.8149(29)
r_{pp}^C	2.795	2.755	2.790(14)
			2.769(14)
a_{pp}^N	-17.083	-17.825	
r_{pp}^N	2.876	2.817	
a_{nn}^N	-18.900	-18.889	-18.95(40)
r_{nn}^N	2.838	2.797	2.75(11)
a_{np}	-23.732	-23.749	-23.740(20)
r_{np}	2.725	2.684	2.77(5)

The deuteron

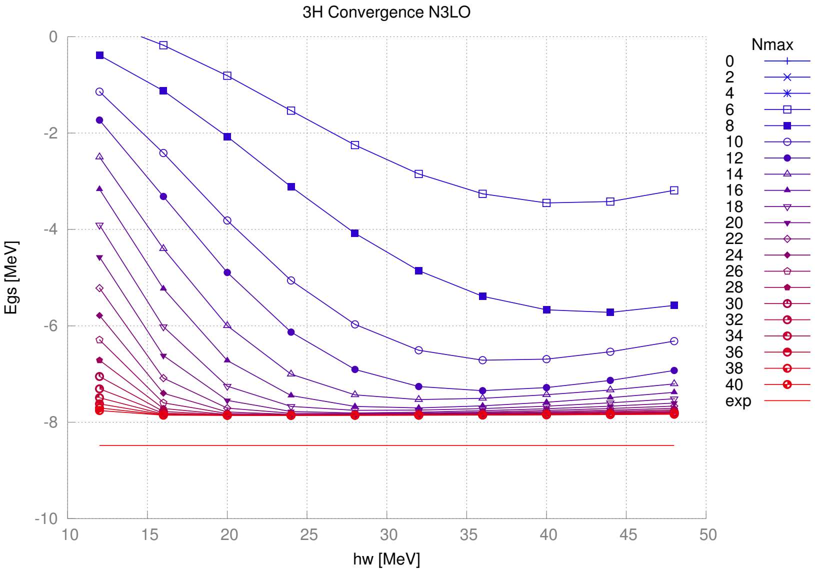
	N^3LO	POUNDerS-NNLO	Empirical
B_D (MeV)	2.224575	2.224582	2.224575(9)
r_D (fm)	1.975	1.967	1.97535(85)
Q_D (fm^2)	0.275	0.272	0.2859(3)
P_D	**4.51**	**4.05**	

No-Core Shell-Model

- Following P. Navrátil *et al.* Phys. Rev. **C** 61, 044001 (2000) we solve the $A = 3, 4$-body problem in a Jacobi-HO basis up to $N_{\mathrm{max}} = 40, 20$, respectively
- $H_A^\omega = \sum_{i=1}^{A} \left[\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 r_i^2 \right] + \sum_{i<j}^{A} \left[V_{NN,ij} - \frac{1}{2A} m\omega^2 (\vec{r}_j - \vec{r}_j)^2 \right] + \sum_{i<j<k} V_{NNN,ijk}$
- We could transform to m-scheme (A. Nogga *et al.* Phys. Rev. **C** 73, 064002 (2006), but it is more efficient to stay in relative coordinates for $A < 5$.
- Use only bare forces

NNLO softness

^{3}H ground state ($N_{\mathrm{max}}, \hbar\omega$) - plot



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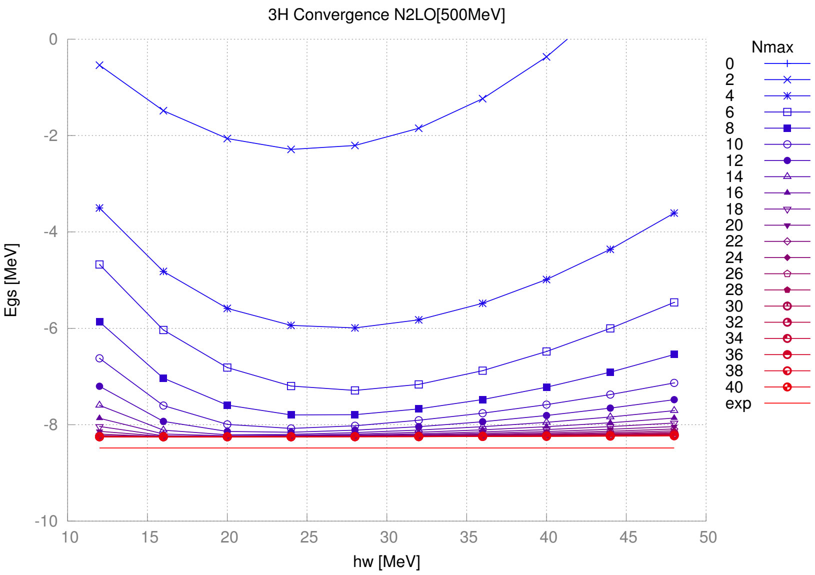


Chiral NNN interactions @NNLO

P. Navrátil Few Body Syst 41, 117 (2007), Regulator $F(q^2, \Lambda) = \exp[-q^4/\Lambda^4]$

$$V_{ijk}^{2\text{PE}} = \sum_{i \neq j \neq k} \frac{1}{2} \left(\frac{g_A}{f_\pi} \right)^2 \frac{(\vec{\sigma}_i \cdot \vec{q}_i)(\vec{\sigma}_j \cdot \vec{q}_j)}{(\vec{q}_i^{\,2} + m_\pi^2)(\vec{q}_j^{\,2} + m_\pi^2)} F_{ijk}^{\alpha\beta} \tau_i^\alpha \tau_j^\beta ,$$

where q_i denotes the momentum transfer associated with nucleon i, and

$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta} \left[-\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} \vec{q}_i \cdot \vec{q}_j \right] + \sum_\gamma \frac{c_4}{f_\pi^2} \epsilon^{\alpha\beta\gamma} \tau_k^\gamma \vec{\sigma}_k \cdot [\vec{q}_i \times \vec{q}_j] .$$

For this diagram, no new parameters are introduced since the c_1, c_3, c_4 appear already in the 2PE two-nucleon interaction. The remaining two three-body terms are given by

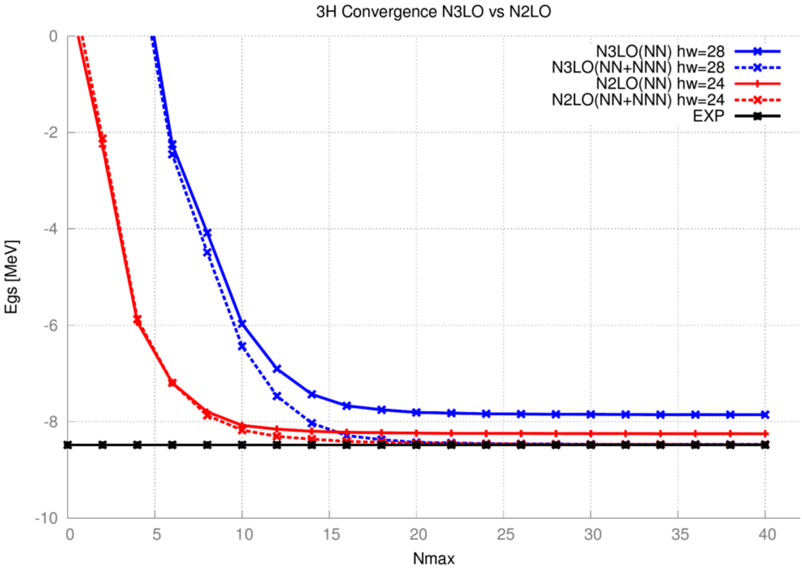
$$V_{ijk}^{1\text{PE}} = -\sum_{i \neq j \neq k} \frac{g_A}{8 f_\pi^2} \frac{c_D}{f_\pi^2 \Lambda_\chi} \frac{(\vec{\sigma}_j \cdot \vec{q}_j)}{(\vec{q}_j^{\,2} + m_\pi^2)} (\tau_i \cdot \tau_j)(\vec{\sigma}_i \cdot \vec{\sigma}_j)$$

and

$$V_{ijk}^{\text{CNT}} = \frac{1}{2} \sum_{i \neq j \neq k} \frac{c_E}{f_\pi^4 \Lambda_\chi} (\tau_i \cdot \tau_j)$$

The POUNDerS-NNLO: NN+3NF

^{3}H and ^{4}He binding energies



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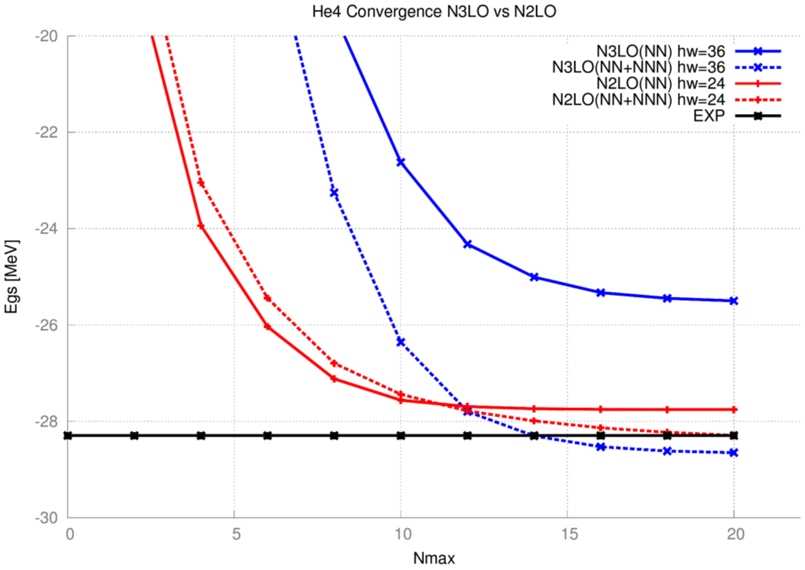


POUNDerS-NNLO: NN+3NF

$A = 3, 4$-systems

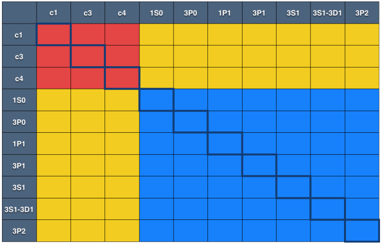
$$c_D = 0.50$$
$$c_E = -0.210$$

	^3H	^3He	^4He
NNLO	-8.249	-7.501	-27.759
NNLO+NNN	-8.470	-7.723	-28.290
Experiment	-8.482	-7.717	-28.296

Parameters re-fitted to $A = 3, 4$ binding energies only.

Ongoing work with POUNDerS

Optimization wrt observables, sensitivity analysis (SA), uncertainty quantification (UQ)



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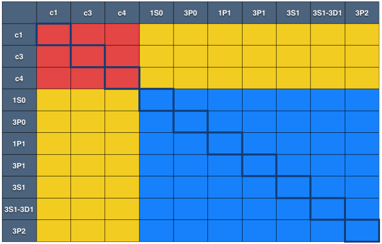

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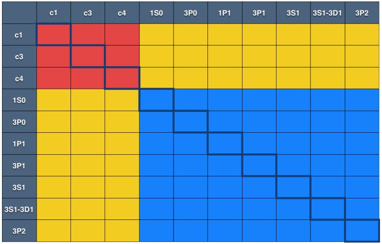

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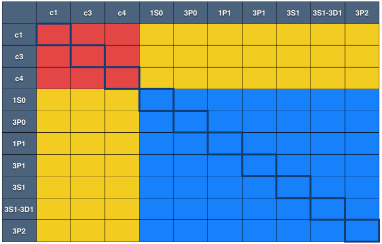
- Extract correlations and uncertainties for the LECs



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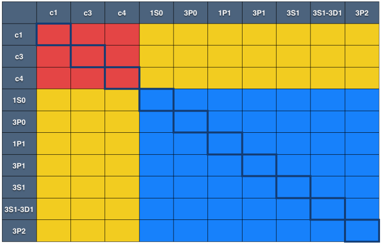

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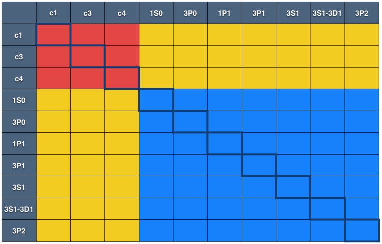

- Optimize *all* LECs at NNLO simultaneously
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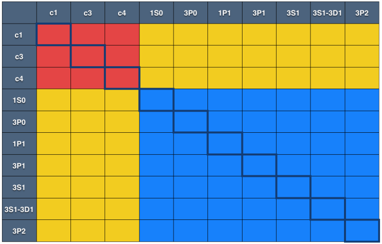

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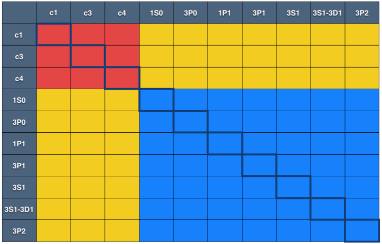

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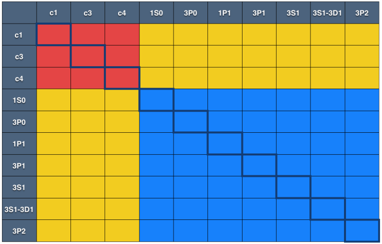

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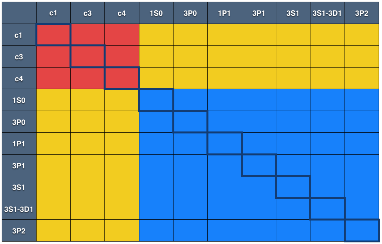

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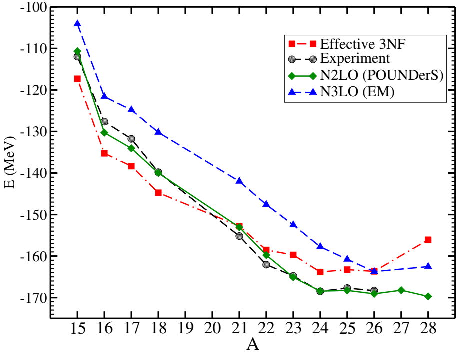
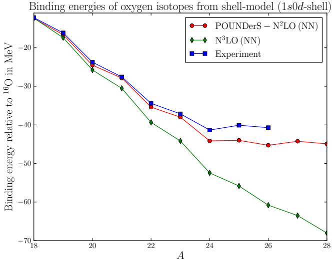


Coupled-Cluster

MBPT(3), Shell-Model



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