ORDER BY ORDER OPTIMIZATION OF LOW-ENERGY CHIRAL NUCLEAR INTERACTIONS

Christian Forssén,
Dept. of Fundamental Physics, Chalmers, Sweden
and
Dept. of Physics and Astronomy, University of Tennessee,
Physics Division, Oak Ridge National Laboratory, USA

CHALMERS

STINT
The Swedish Foundation for International Cooperation in Research and Higher Education

European Research Council
erc

TRIUMF Theory Workshop *Progress in Ab Initio Techniques in Nuclear Physics*, Vancouver, Feb. 17, 2015

Acknowledgements

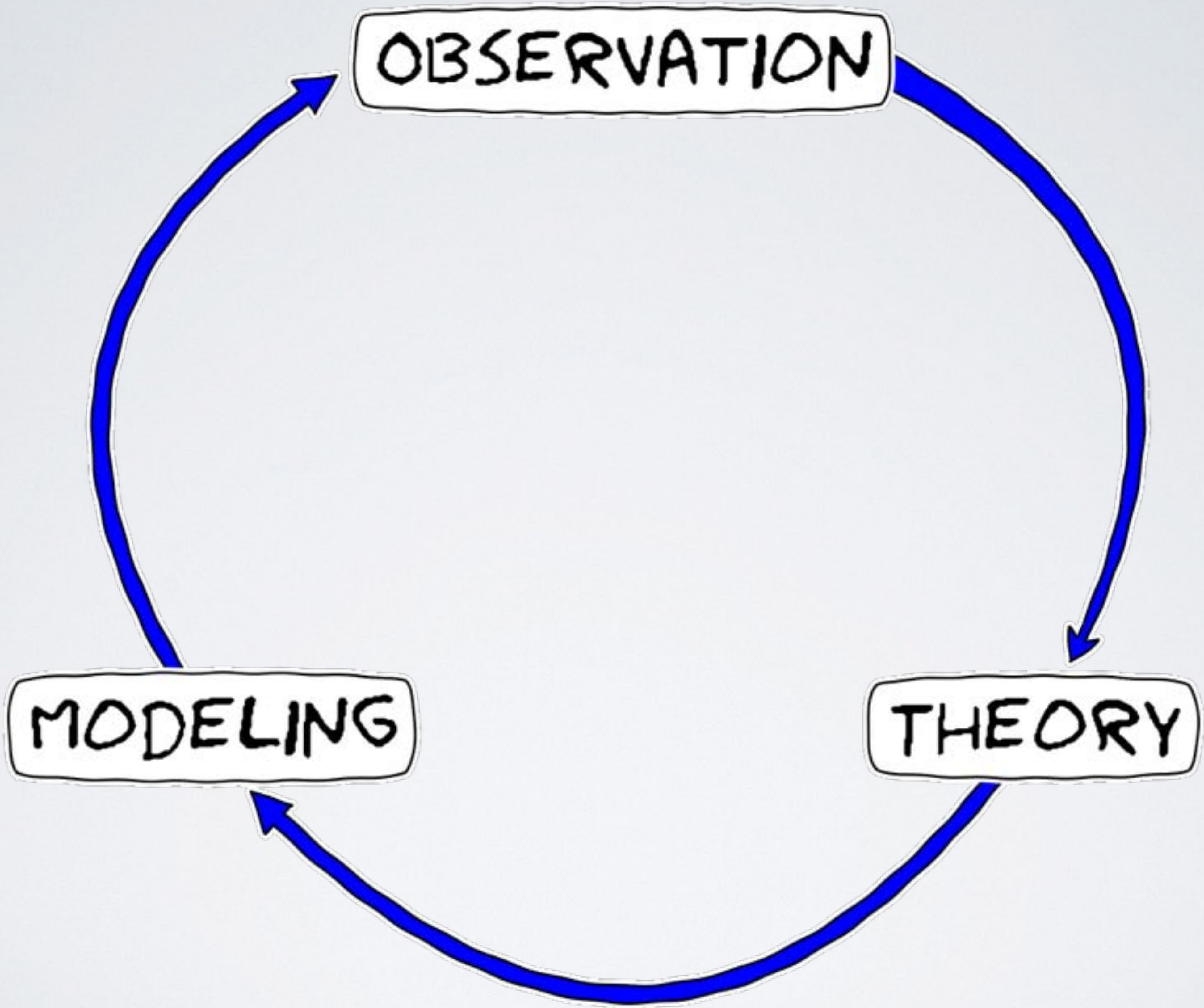
Many thanks to my collaborators

- **Boris Carlsson**, Jimmy Rotureau, Emil Ryberg, Daniel Sääf, Håkan Johansson (Chalmers),
- **D. Strömberg, O. Lilja, M. Lindby, B. Mattsson** (Chalmers),
- Petr Navrátil (TRIUMF), Robert Roth (Darmstadt),
- Morten Hjorth Jensen (UiO, MSU), Witek Nazarewicz (ORNL, MSU),
- **Andreas Ekström**, Gaute Hagen, Gustav Jansen, Thomas Papenbrock, **Kyle Wendt** (ORNL/UT), Lucas Platter (UT).

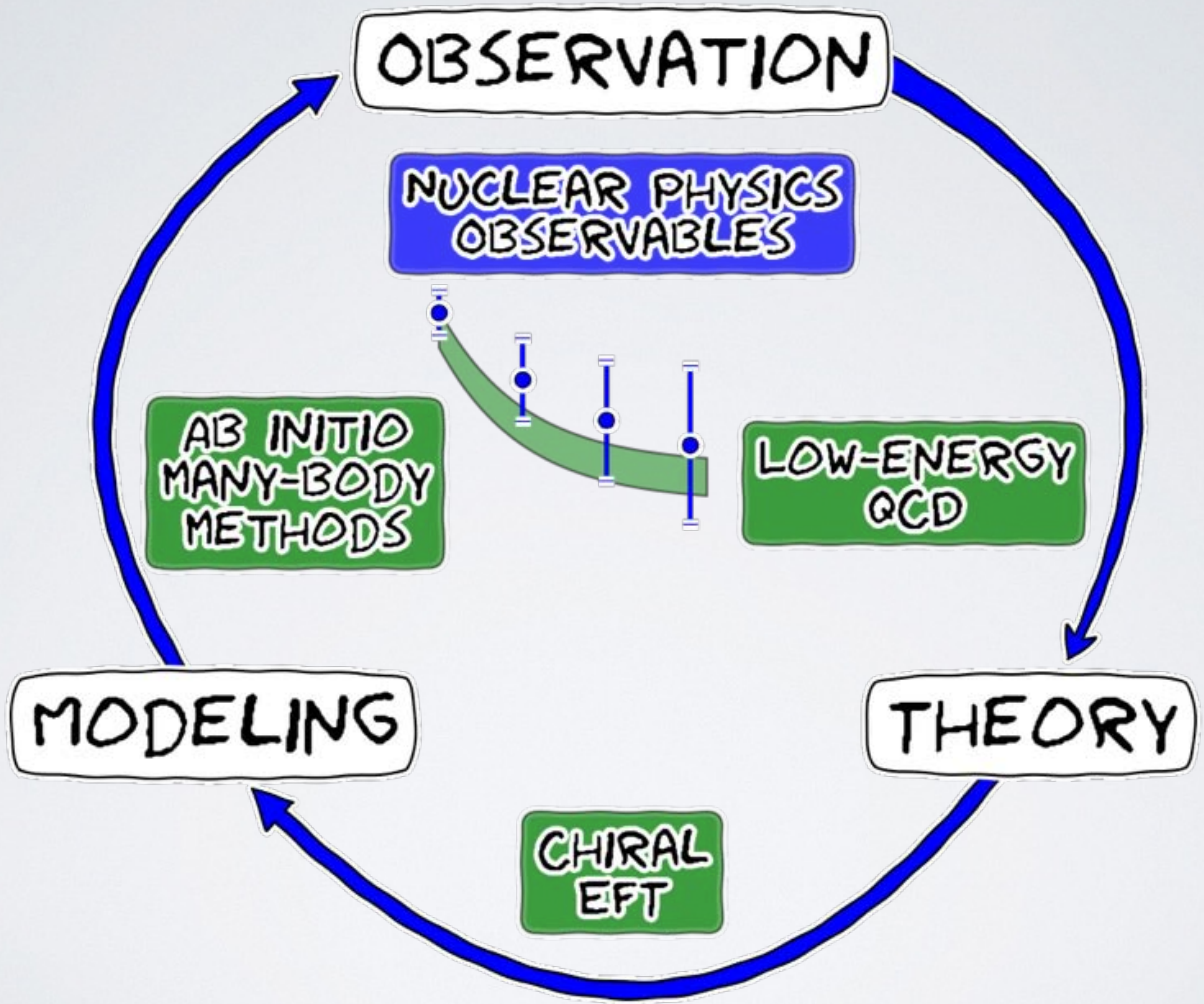
Research funded by:
- STINT
- European Research Council

INTRODUCTION:
Ab initio nuclear theory and nuclear forces

Scientific wheel of progress



Promising approach for nuclear physics

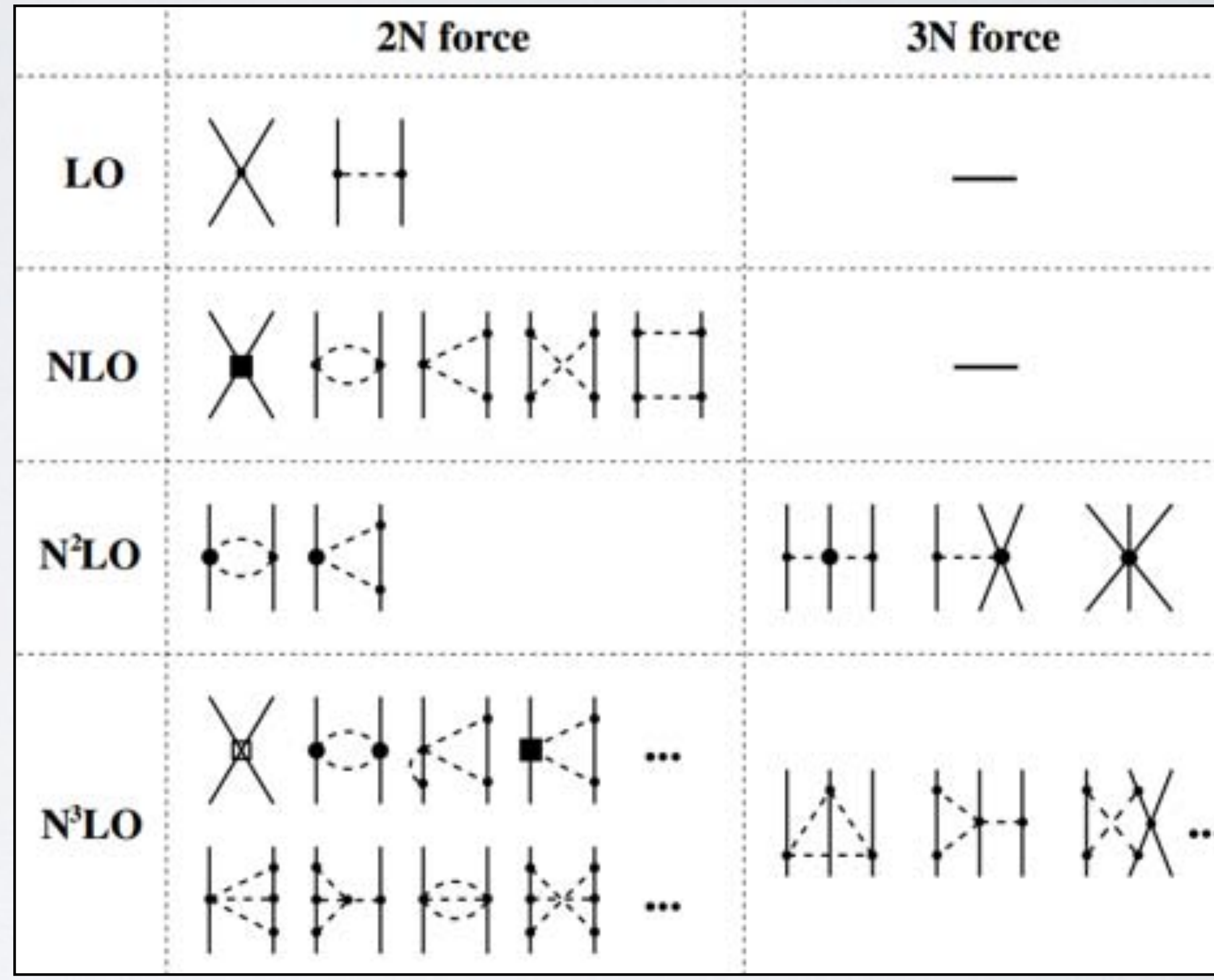


Chiral nuclear interactions

Chiral EFT

- Systematic low-energy expansion: $(q/\Lambda_\chi)^\nu$
- Connects several sectors: πN, NN, NNN, j_N
- Short-range physics included as contact interactions. LECs need to be fitted to data.

$$\chi^2(\vec{p}) = \sum_i \left(\frac{O_i^{\text{theo}}(\vec{p}) - O_i^{\text{exp}}}{\sigma_{\text{tot},i}} \right)^2$$

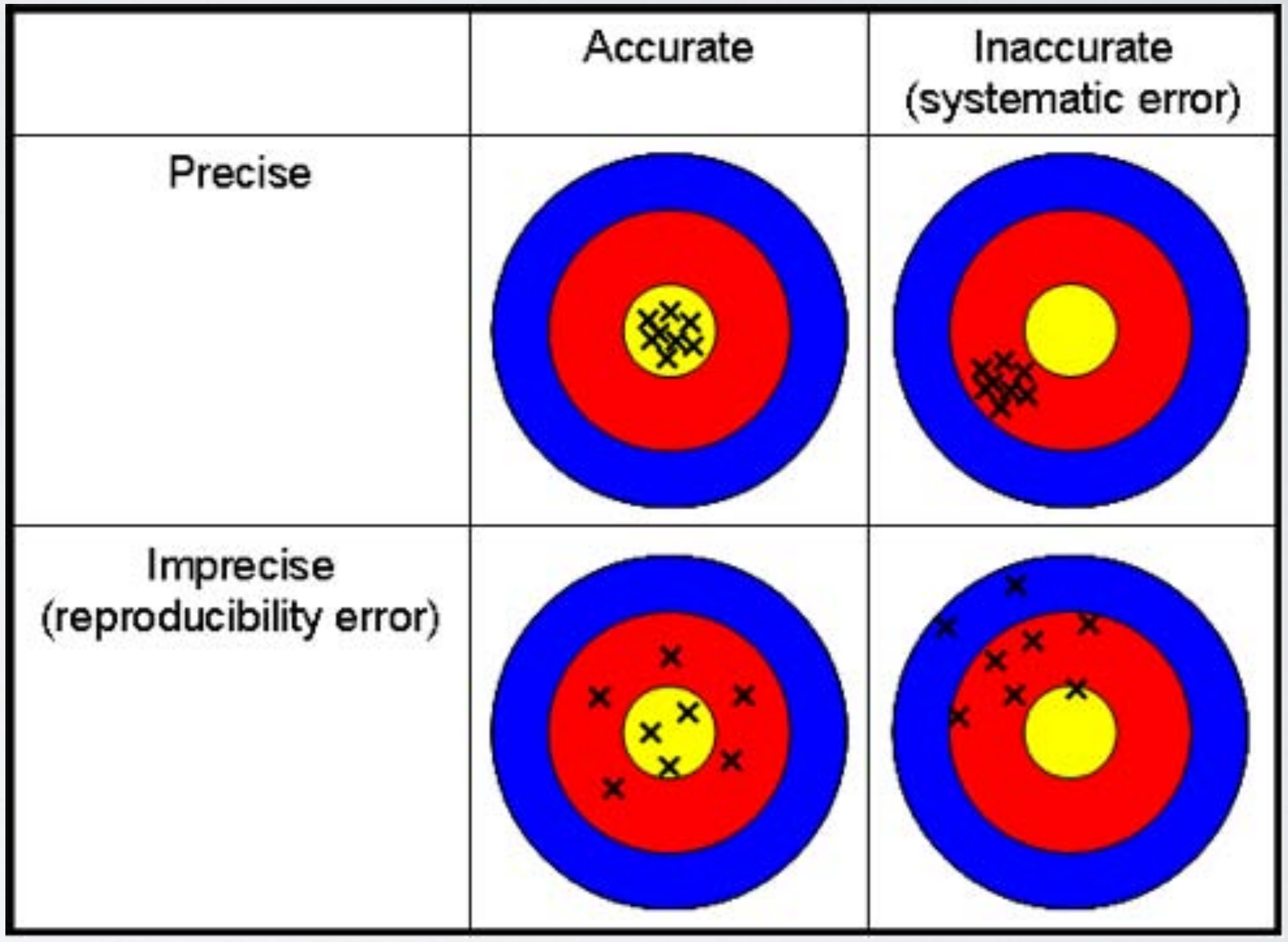


Chiral EFT
- E. Epelbaum, H. Hammer, U. Meissner Rev. Mod. Phys. **81** (2009) 1773
- R. Machleidt, D. Entem, Phys. Rep. **503** (2011) 1

Key science questions

What is the precision of nuclear-structure calculations in this approach?

What is the accuracy of nuclear-structure calculations in this approach?



Key science questions

What is the precision of nuclear-structure calculations in this approach?

$$O_{\text{calc}} = O_0 \pm \Delta O$$

Uncertainty should be possible to extract in chiral EFT + *ab initio* framework

What is the accuracy of nuclear-structure calculations in this approach?

See talks by:

- A. Ekström
- K. Wendt

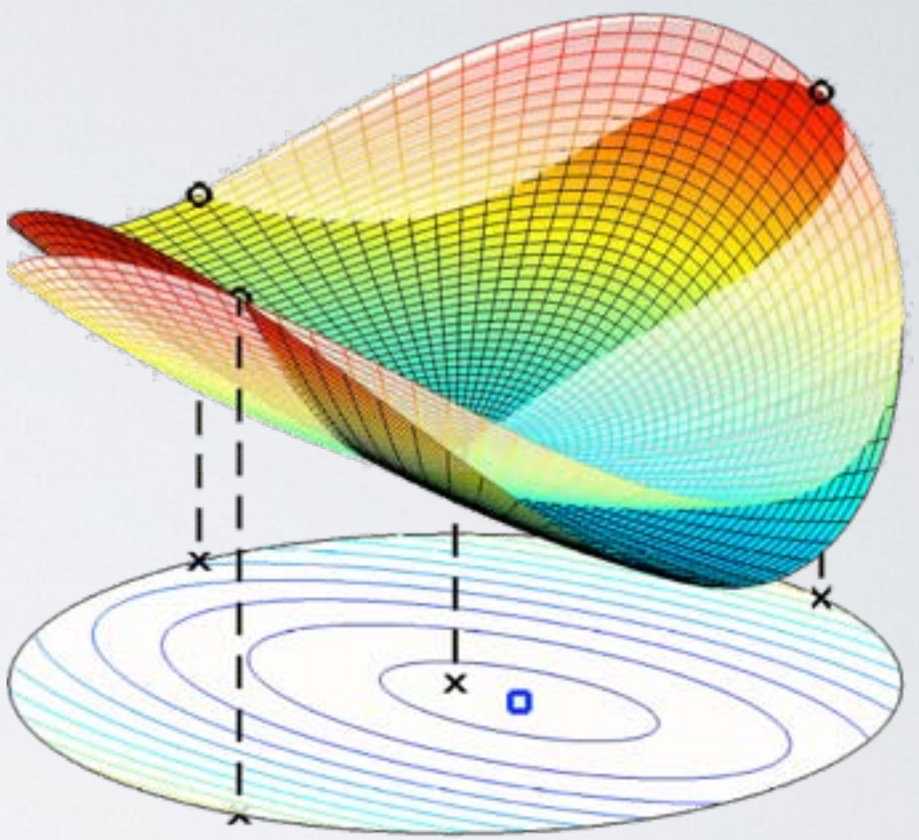
and recent preprint:

- arXiv:1502.04682 [nucl-th]

Chiral Forces: From NN to A=4 with error analysis

Statistical error analysis

- Aim for a good description of low-energy data within chiral EFT
  - NN- and πN-scattering
  - NNN structure properties
- Aim for a good understanding of low-energy data and of our model
  - What are the error bars on our calculations?
  - How sensitive is different data to different parts of the interaction?
  - What are the correlations between data? and between model parameters?



Optimization strategy

Low-energy constants (LECs) enter through contact interactions and need to be fitted to experimental data.

$$\chi^2(\vec{p}) \equiv \sum_i \left(\frac{O_i^{\text{theo}}(\vec{p}) - O_i^{\text{expr}}}{\sigma_{\text{tot},i}} \right)^2 \equiv \sum_i r_i^2(\vec{p})$$

Standard approach:

1. **πN LECs determined first** from Pion-Nucleon scattering phase shifts or from NN phase shifts in peripheral waves
2. **(NN-only) objective function based on Nijmegen phase shift analysis**
   - Chi-by-eye optimization
   - N^3LO needed for high-accuracy fit up to T_{lab}=290 MeV
3. **NNN LECs determined at the end** given the NN part. Usually at NNLO. First results at N^3LO are coming.

Objective function

$$\chi^2(\vec{p}) \equiv \sum_i r_i^2(\vec{p}) = \sum_{j \in NN} r_j^2(\vec{p}) + \sum_{k \in \pi N} r_k^2(\vec{p}) + \sum_{l \in 3N} r_l^2(\vec{p})$$

Sector	Observable	LO	NLO	NNLO
NN	Scattering	X	X	X
2H	E_{gs}, r_{ch}, Q	X	X	X
πN	Scattering			X
3He	E_{gs}, r_{ch}			X
3H	E_{gs}, r_{ch}, $T_{1/2}$			X

NN

πN

3N

Sequential

Objective function

$$\chi^2(\vec{p}) \equiv \sum_i r_i^2(\vec{p}) = \sum_{j\in NN} r_j^2(\vec{p}) + \sum_{k\in\pi N} r_k^2(\vec{p}) + \sum_{l\in 3N} r_l^2(\vec{p})$$

Sector	Observable	LO	NLO	NNLO
NN	Scattering	X	X	X
2H	E_{gs}, r_{ch}, Q	X	X	X
πN	Scattering			X
3He	E_{gs}, r_{ch}			X
3H	E_{gs}, r_{ch}, $T_{1/2}$			X

NN

πN

3N

Simultaneous

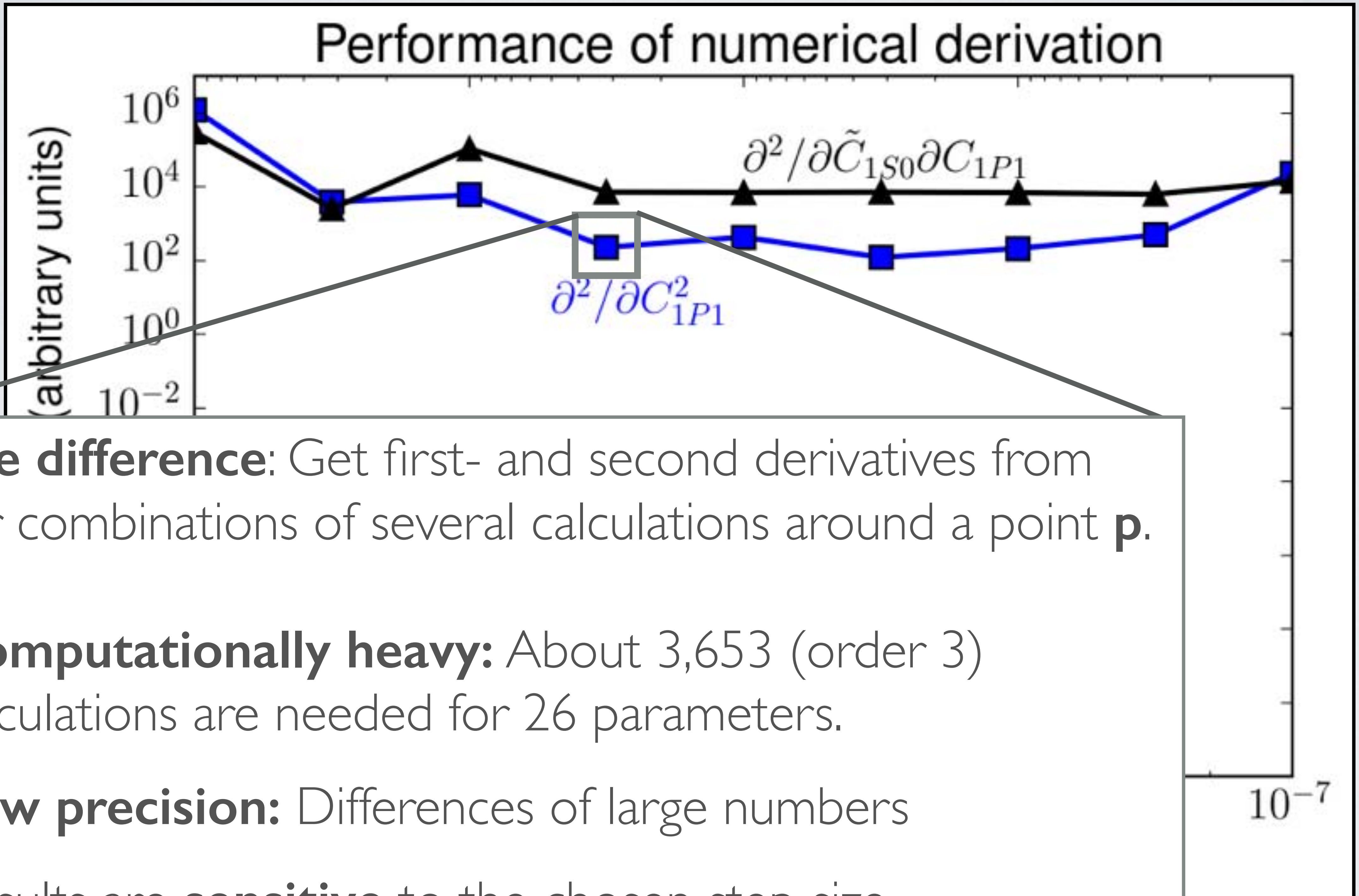
Optimization with derivatives

- First implementation used POUNDerS for optimization.
- More efficient algorithms (Levenberg-Marquardt, Newton), and statistical error analysis require **derivatives**

$$\frac{\partial r_i}{\partial p_j} \quad \text{and} \quad \frac{\partial^2 r_i}{\partial p_j \partial p_k}$$

- Numerical derivation using **finite differences** is plagued by **low numerical precision** and is **computationally costly.**
- Instead, we use **Automatic Differentiation** (AD)

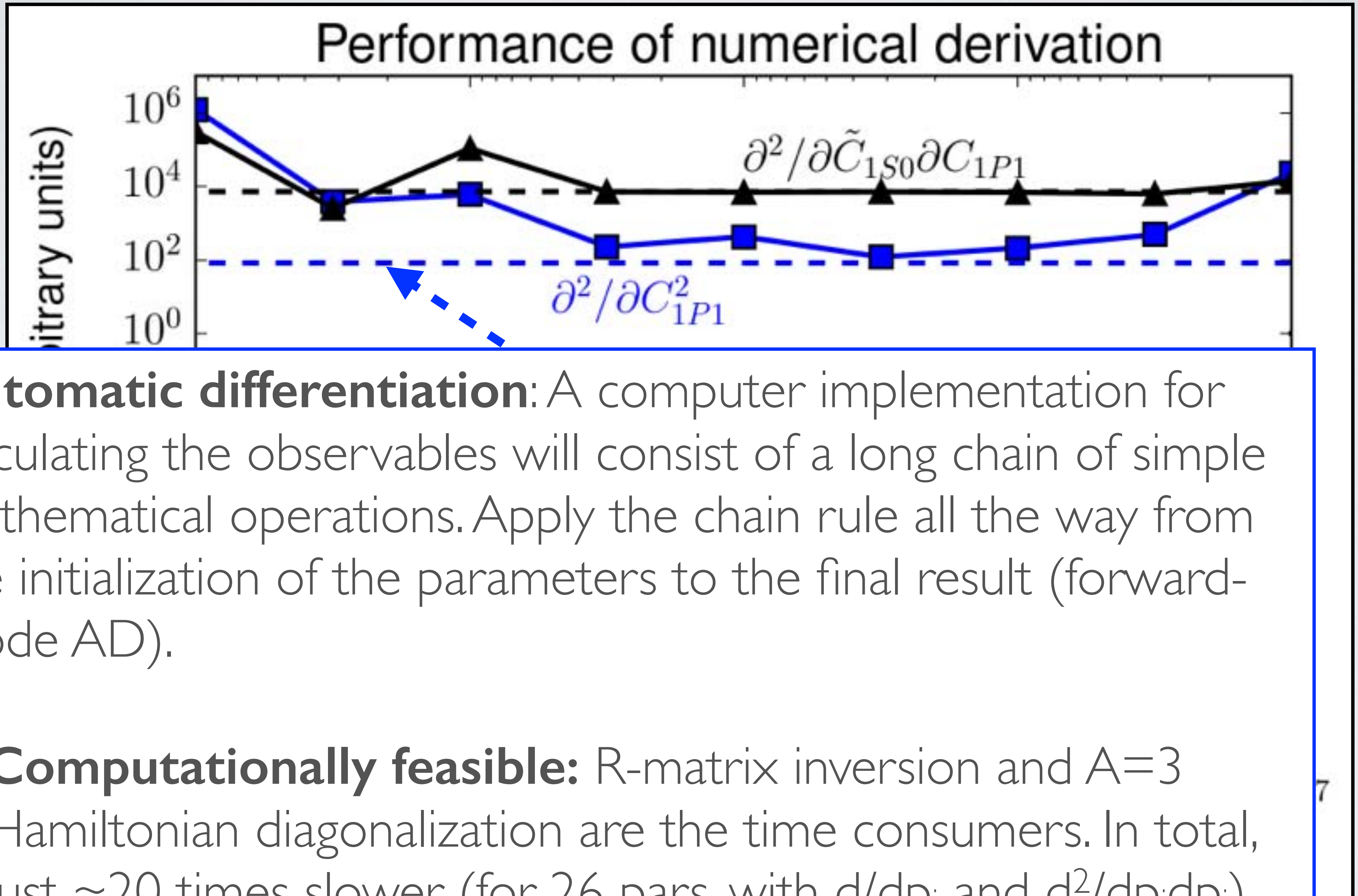
Numerical derivation: finite differences



Finite difference: Get first- and second derivatives from linear combinations of several calculations around a point **p**.

- **Computationally heavy:** About 3,653 (order 3) calculations are needed for 26 parameters.
- **Low precision:** Differences of large numbers
- Results are **sensitive** to the chosen step size.

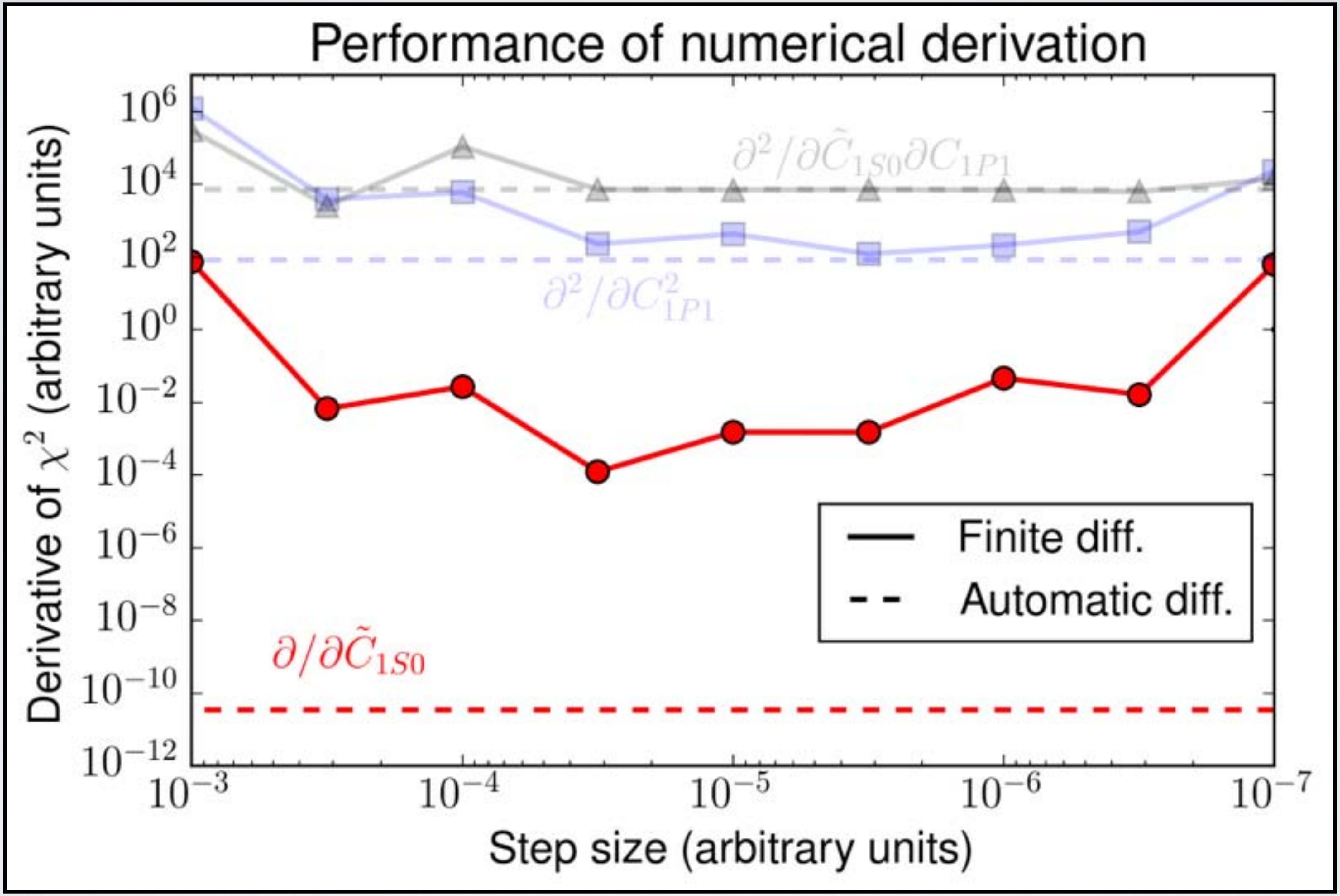
Numerical derivation: Automatic differentiation



Automatic differentiation: A computer implementation for calculating the observables will consist of a long chain of simple mathematical operations. Apply the chain rule all the way from the initialization of the parameters to the final result (forward-mode AD).

- **Computationally feasible:** R-matrix inversion and A=3 Hamiltonian diagonalization are the time consumers. In total, just ~20 times slower (for 26 pars, with d/dp_i and $d^2/dp_i dp_j$).
- **High precision:** derivatives calculated are about as exact as the value of the observable itself.

Numerical derivation: Automatic differentiation



Total error budget

- The total error budget is

E.g., NCSM → $\sigma^2_{\mathrm{method}}$; Neglected → σ^2_{num}

$$\sigma^2_{\mathrm{tot}} = \sigma^2_{\mathrm{exp}} + \sigma^2_{\mathrm{theo}} + \sigma^2_{\mathrm{method}} + \sigma^2_{\mathrm{num}}$$

- At a given chiral order ν, the omitted diagrams should be of order

$$\mathcal{O}\left((Q/\Lambda_\chi)^{\nu+1}\right)$$

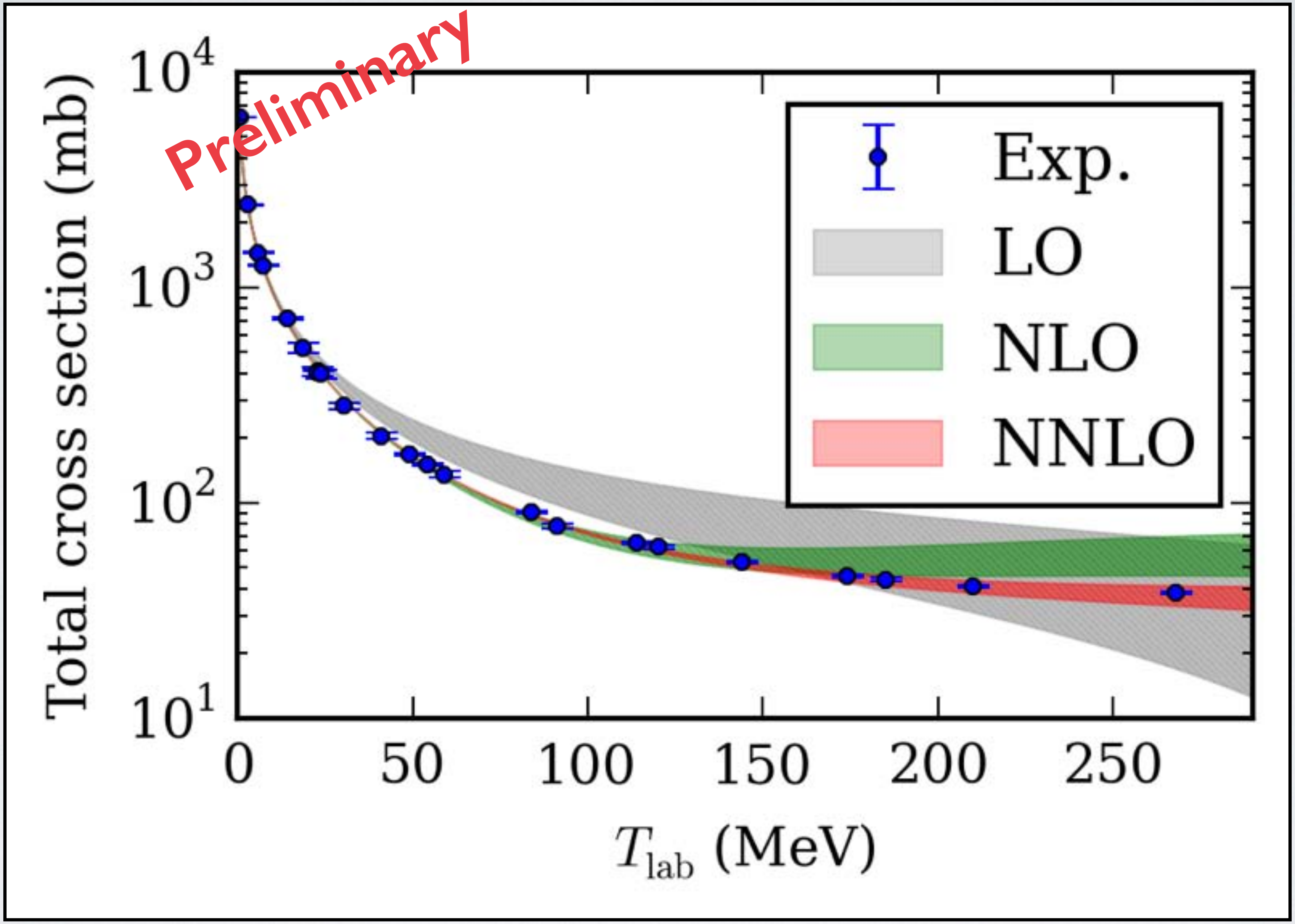
- Still needs to be converted to actual numbers σ_{theo}

- We translate this into an error in the scattering amplitudes

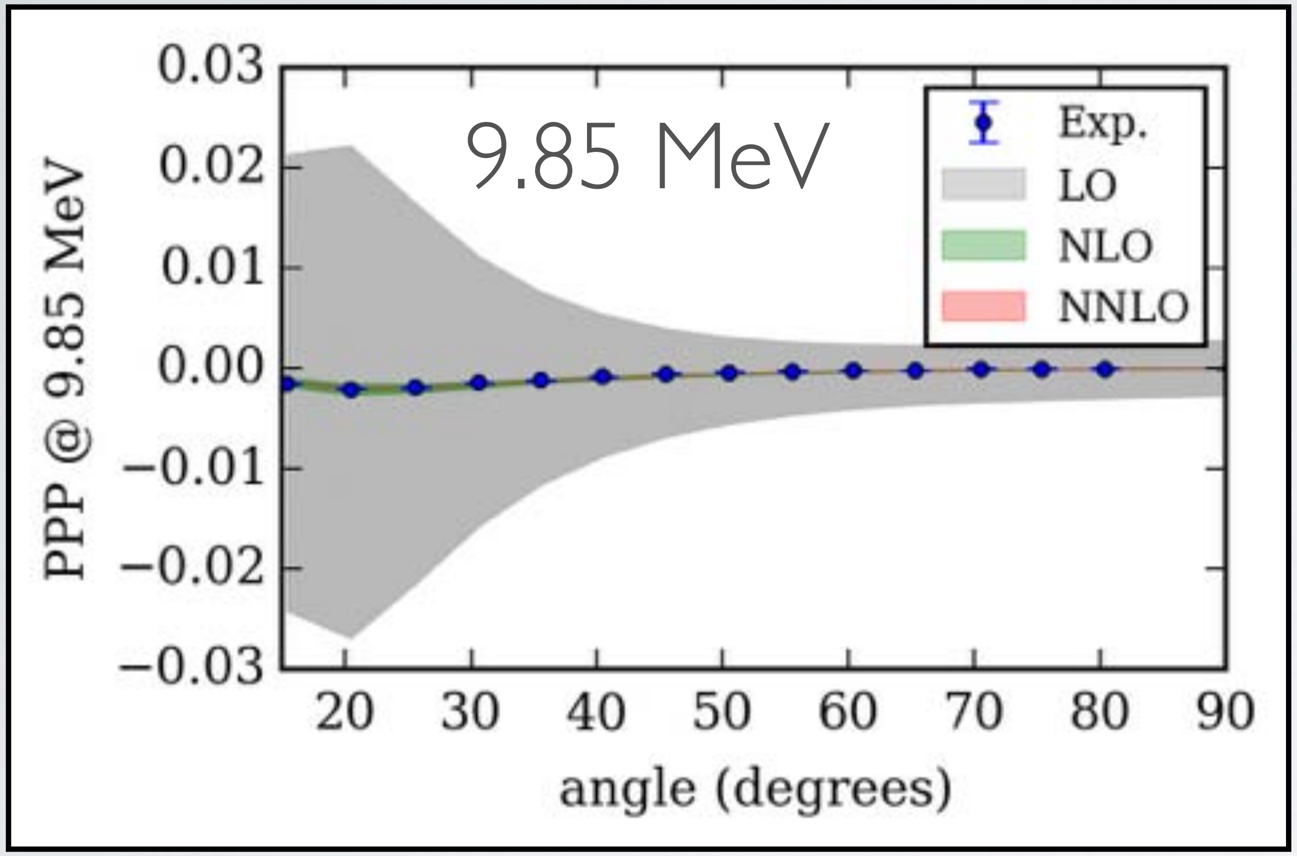
$$\sigma^{(\mathrm{amp})}_{\mathrm{theo,x}} = C_x \left(\frac{Q_{\mathrm{cm}}}{\Lambda_\chi}\right)^{\nu+1} \quad , \quad x \in \{\mathrm{NN}, \pi\mathrm{N}\}$$

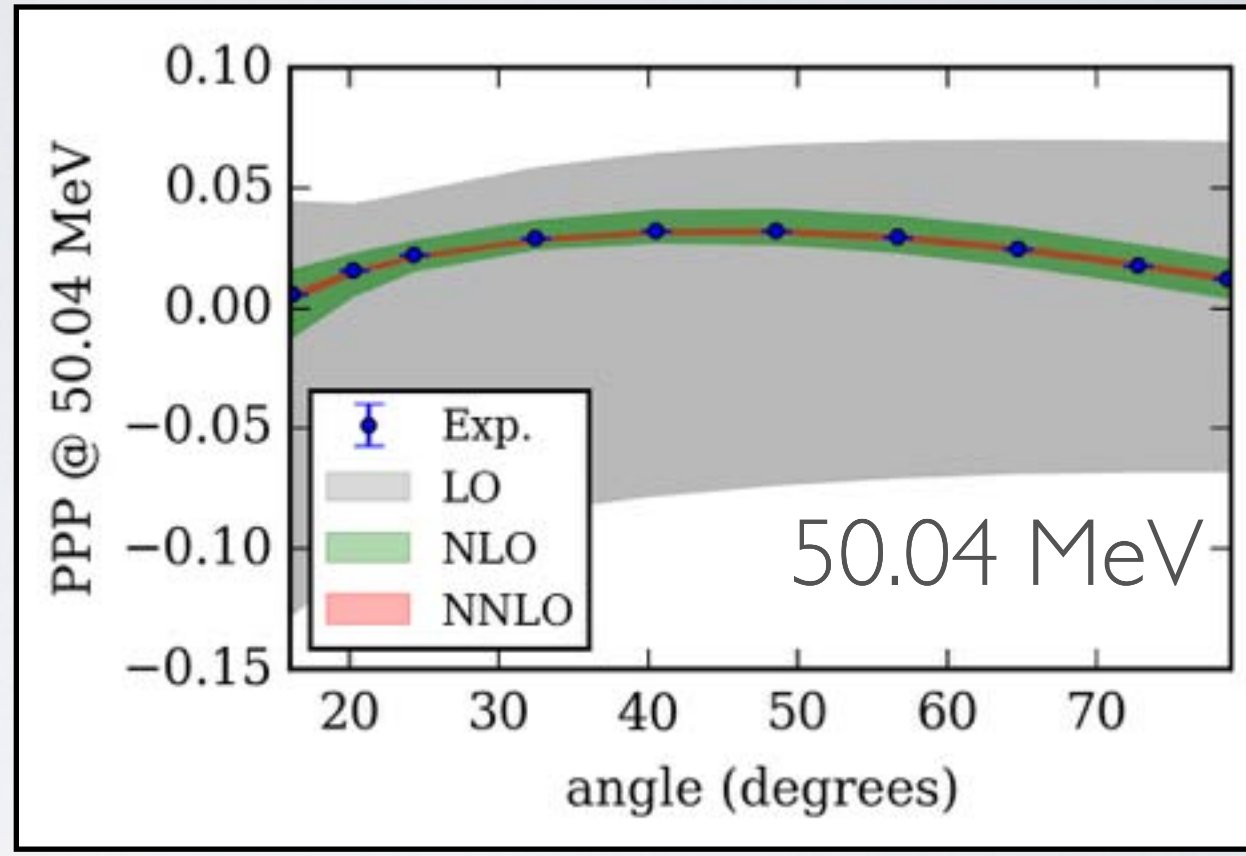
- which is then propagated to an error in the observable.

Total np cross section

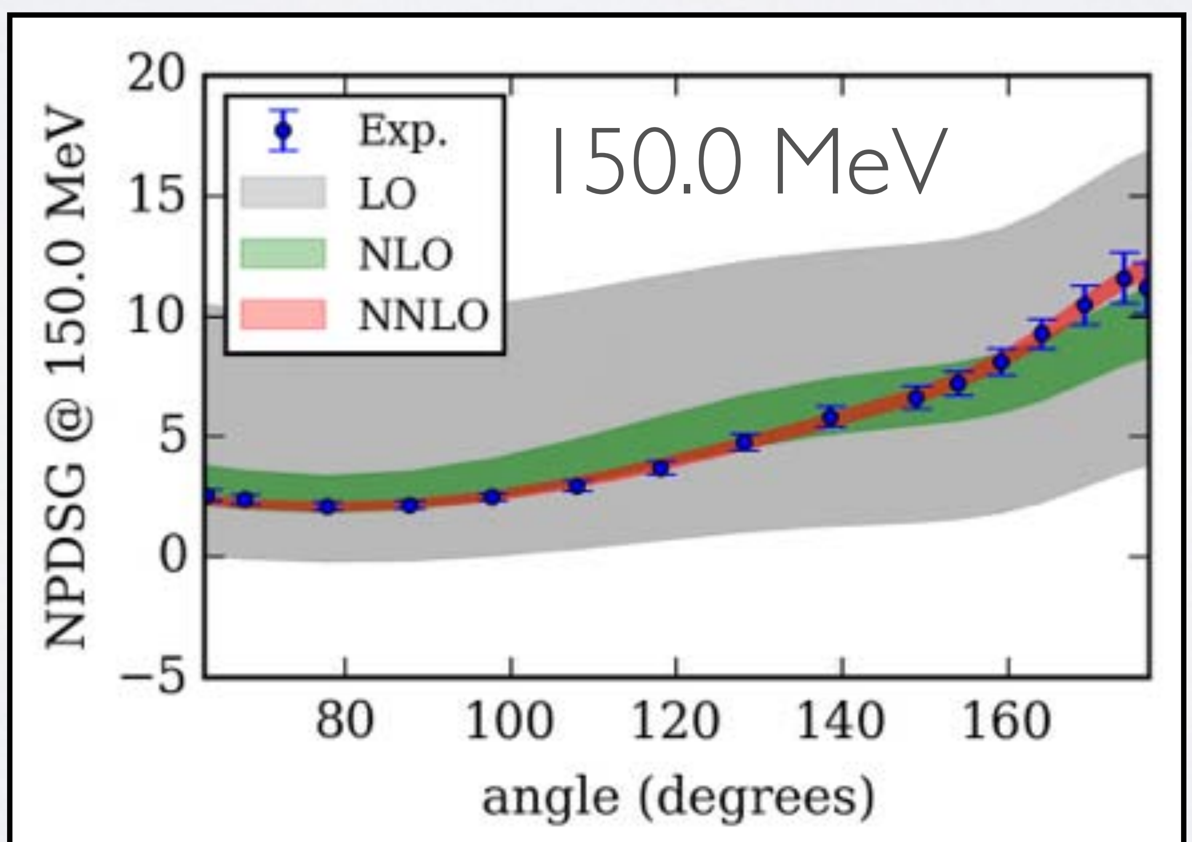


Differential scattering observables

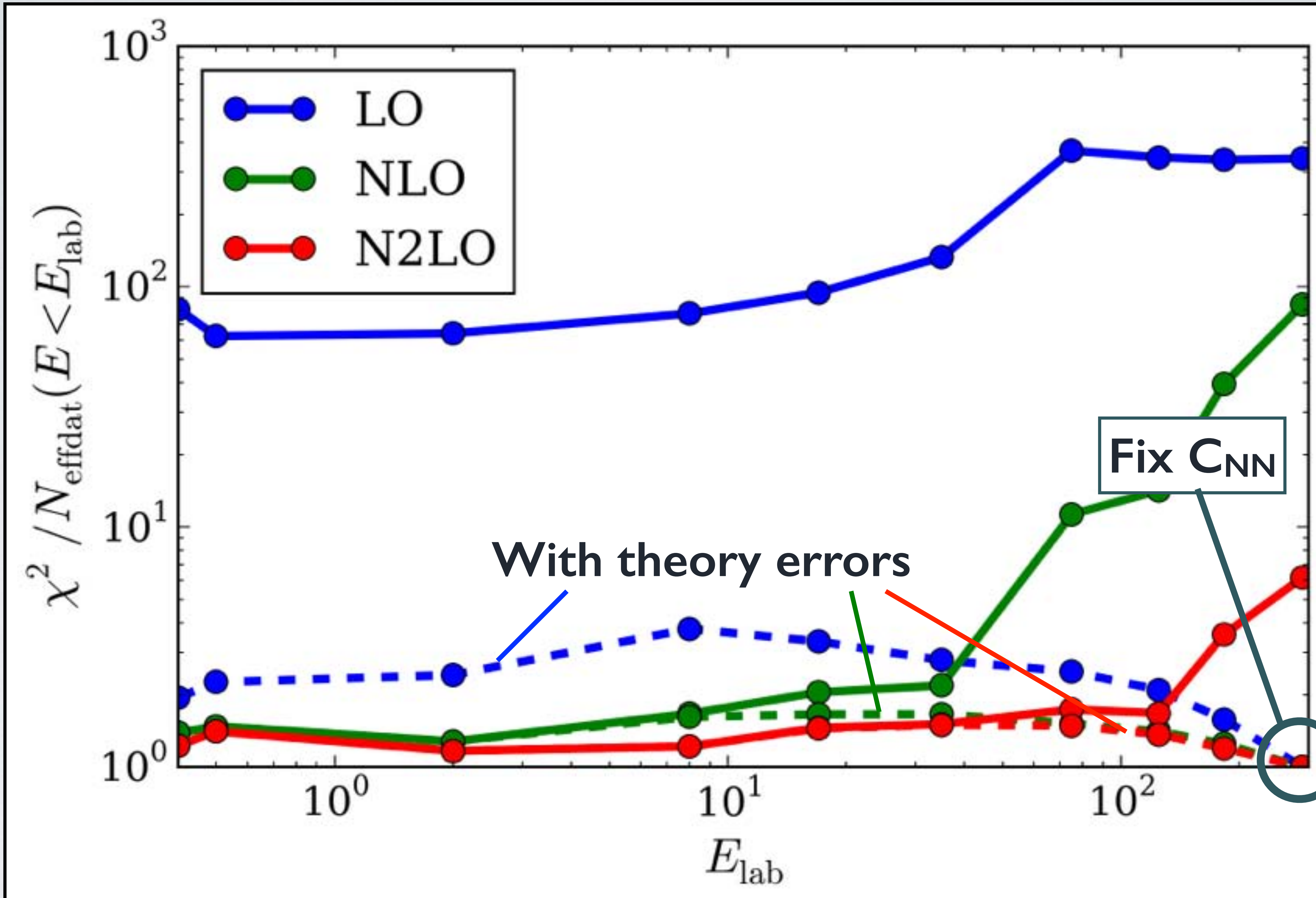




Preliminary

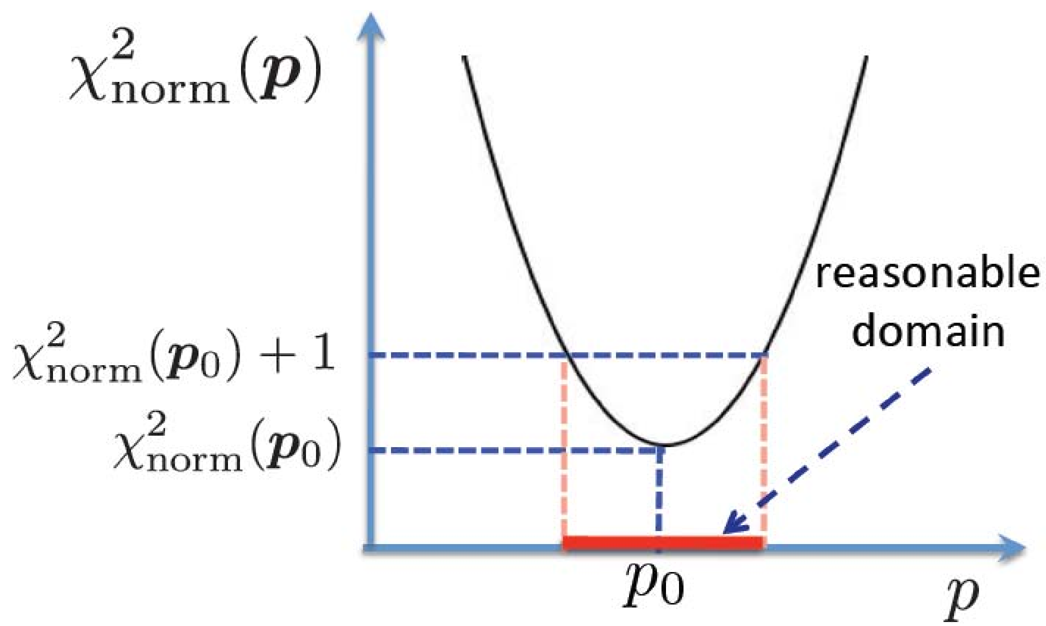


Chi-squared per energy bin



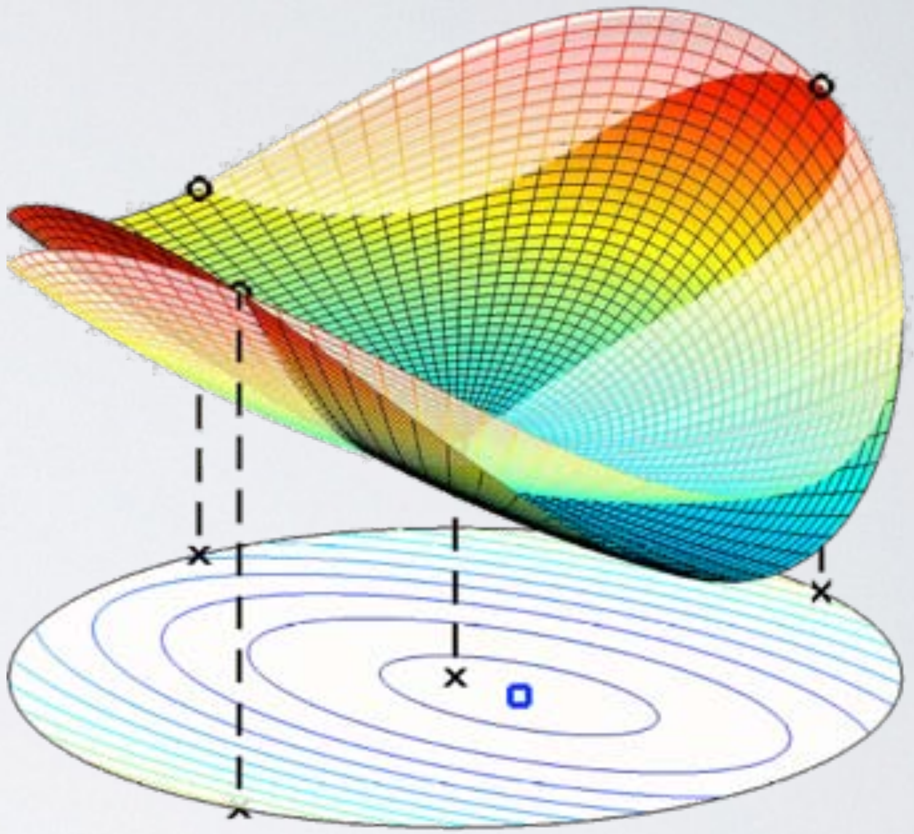
Statistical error analysis

- In a minimum there will be an **uncertainty in the optimal parameter values $\mathbf{p}_0$** given by the χ^2 surface.[1]



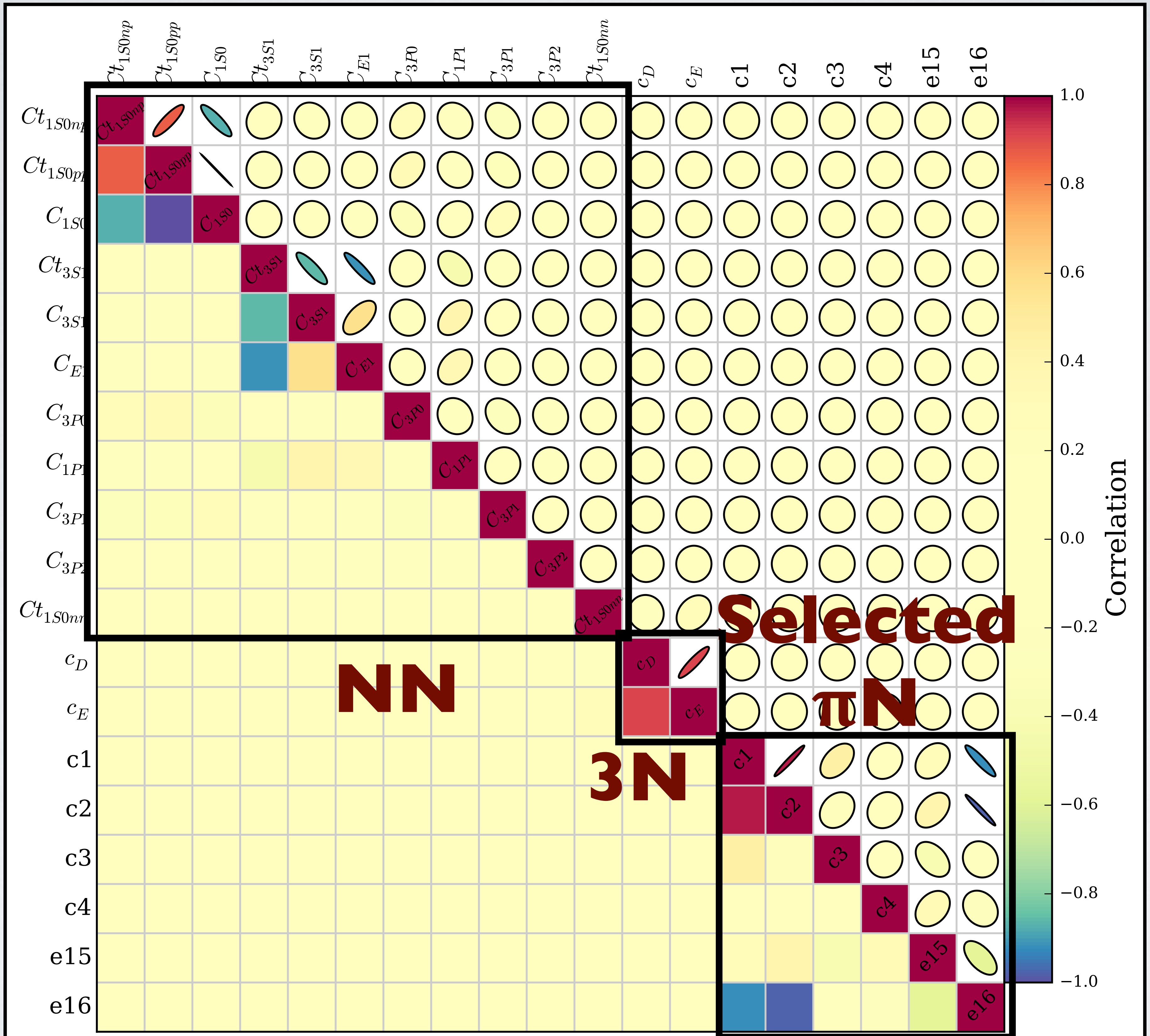
- From the hessian at $\mathbf{p}_0$ we can calculate a **covariance matrix** and from that a **correlation matrix**.

[1] J Dobaczewski et al 2014 J. Phys. G: Nucl. Part. Phys. 41 074001

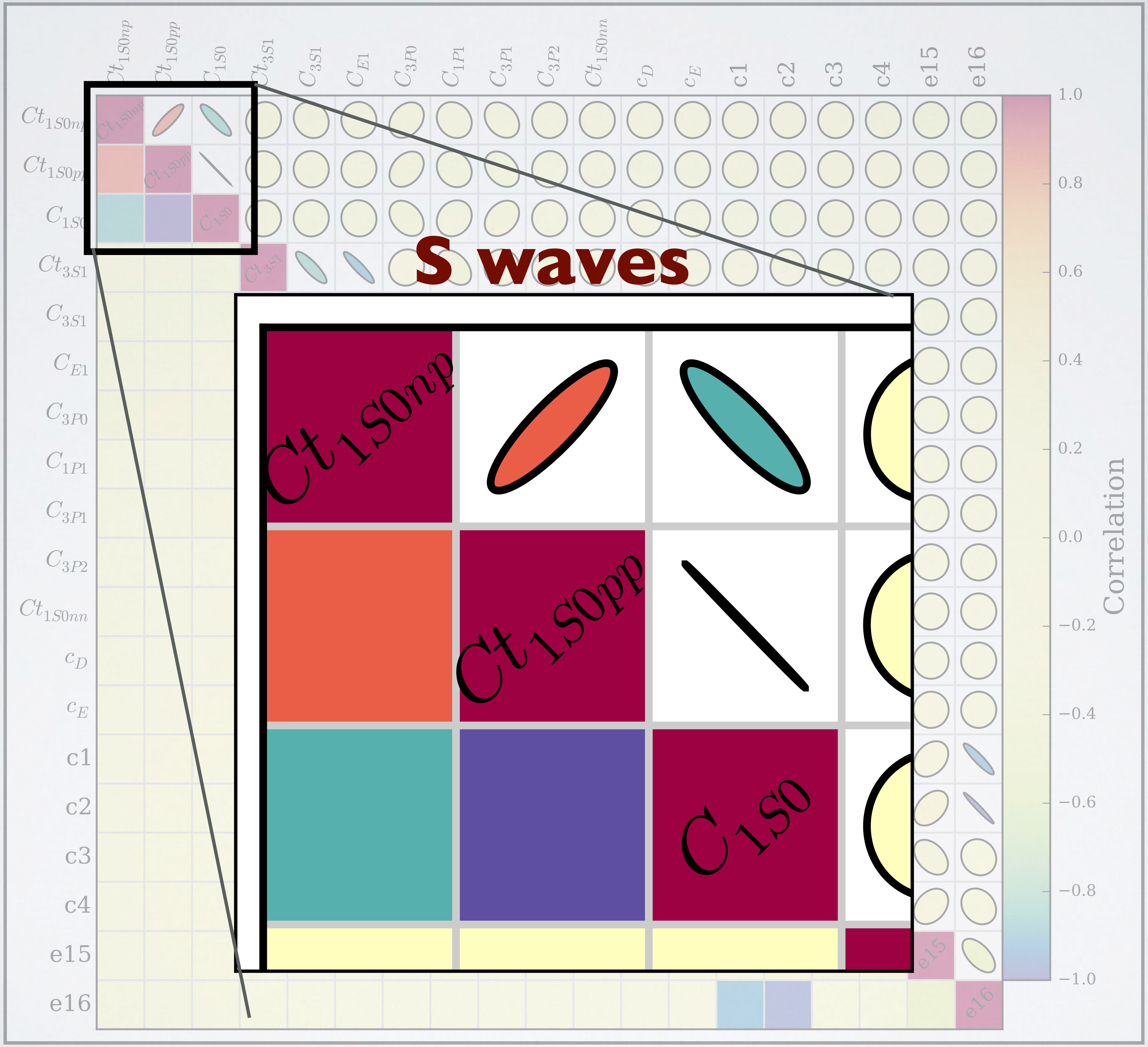


HESSIAN	COVARIANCE MATRIX	CORRELATION MATRIX
$H_{ij} = \frac{1}{2} \frac{\partial^2 \chi^2}{\partial x_i \partial x_j}\Big\vert_{\mathbf{x}=\mathbf{x}_\mu}$	$\mathbf{\Sigma} = \frac{\chi^2}{N_{df}} \mathbf{H}^{-1}$	$R_{ij} = \frac{\Sigma_{ij}}{\sqrt{\Sigma_{ii}\Sigma_{jj}}}$

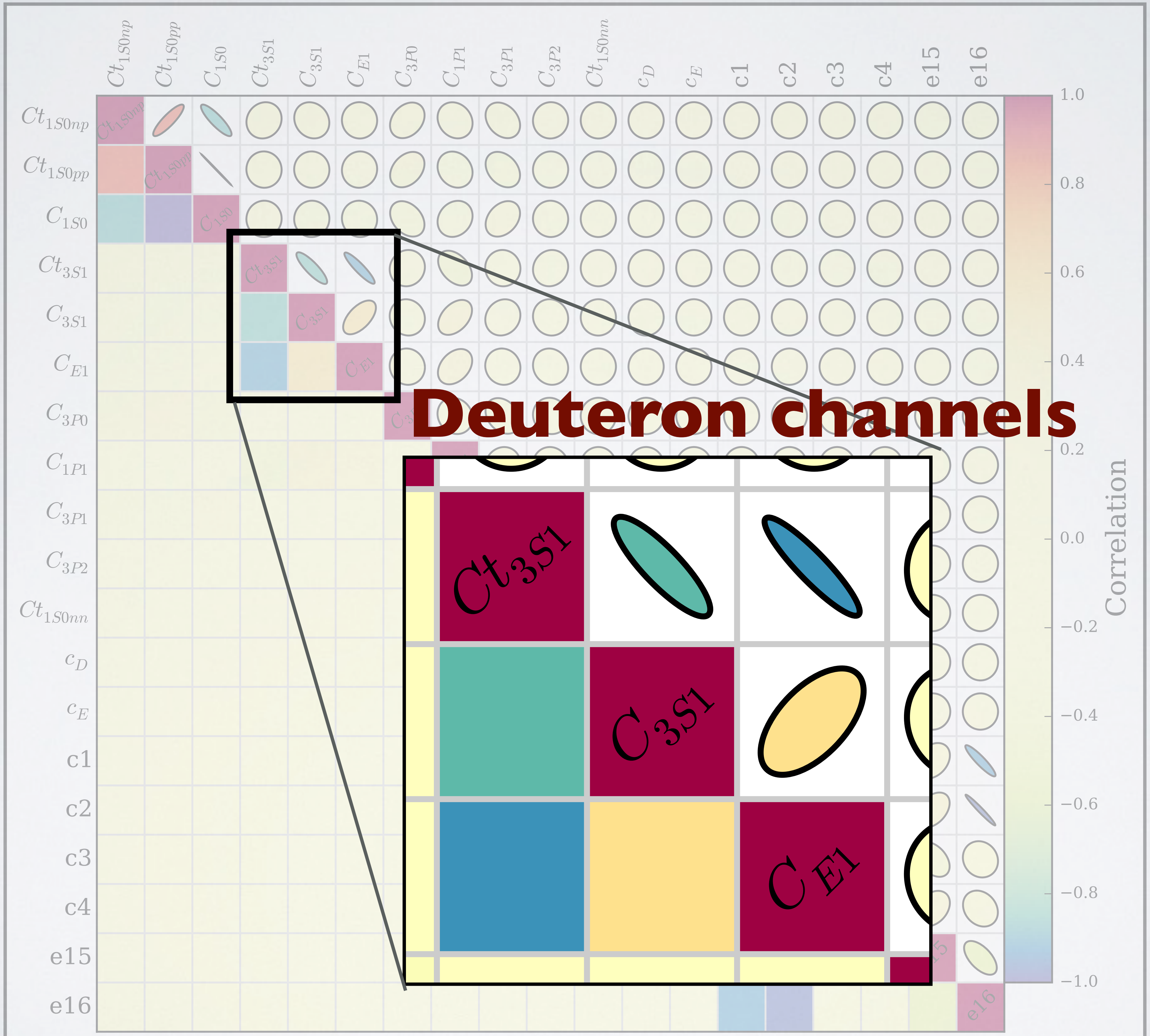
Correlations - sequential fits



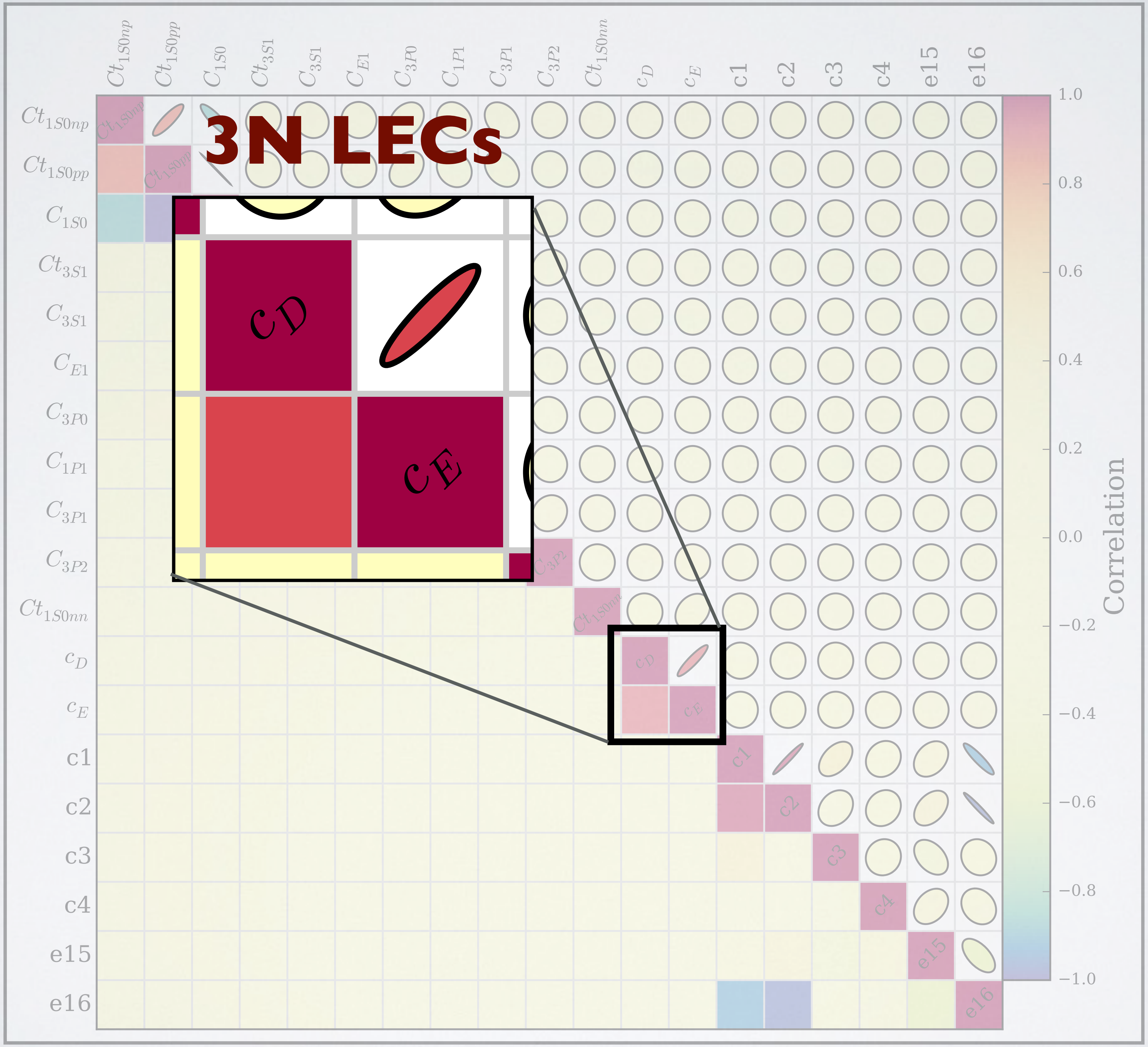
Correlations - sequential fits



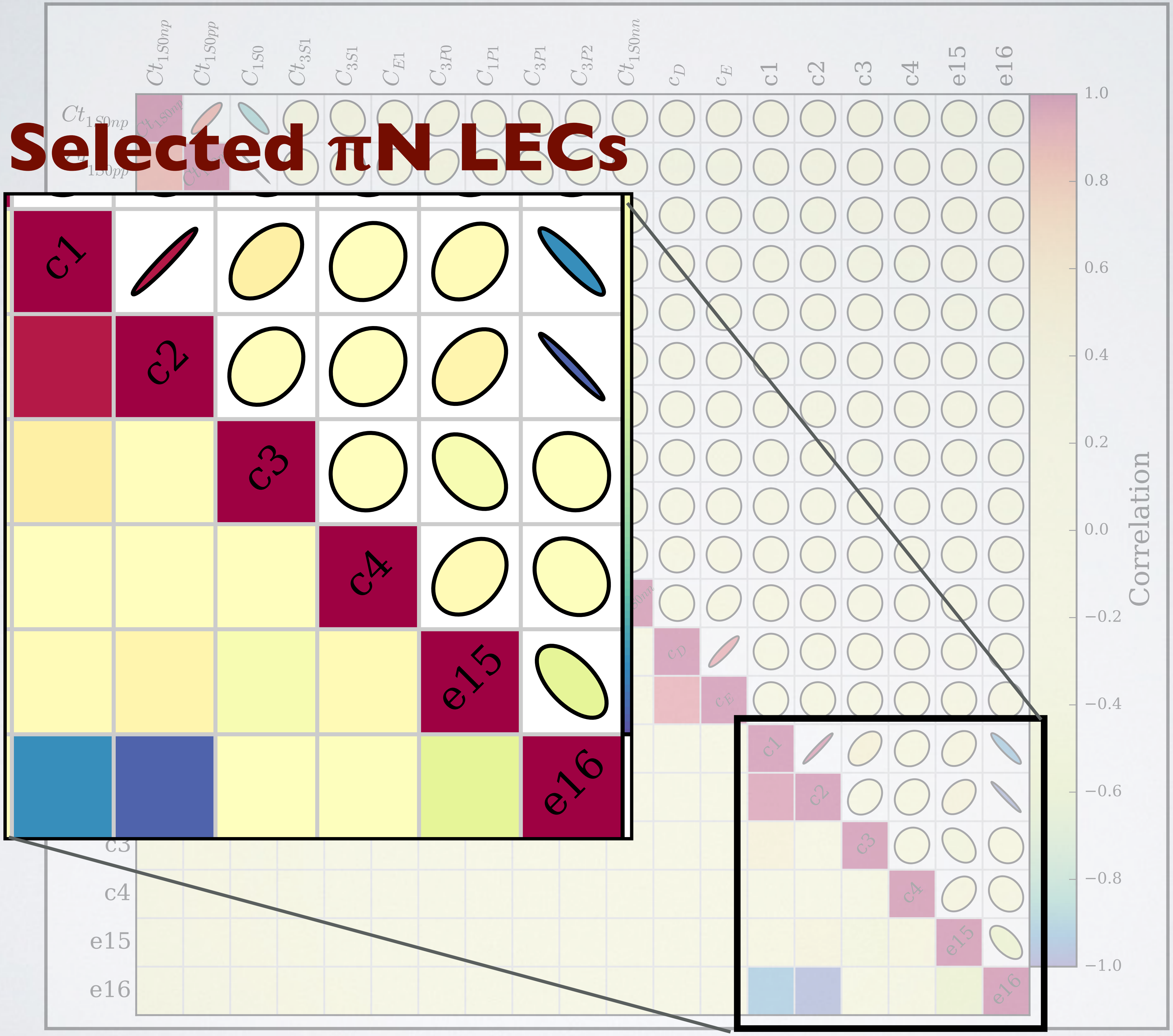
Correlations - sequential fits



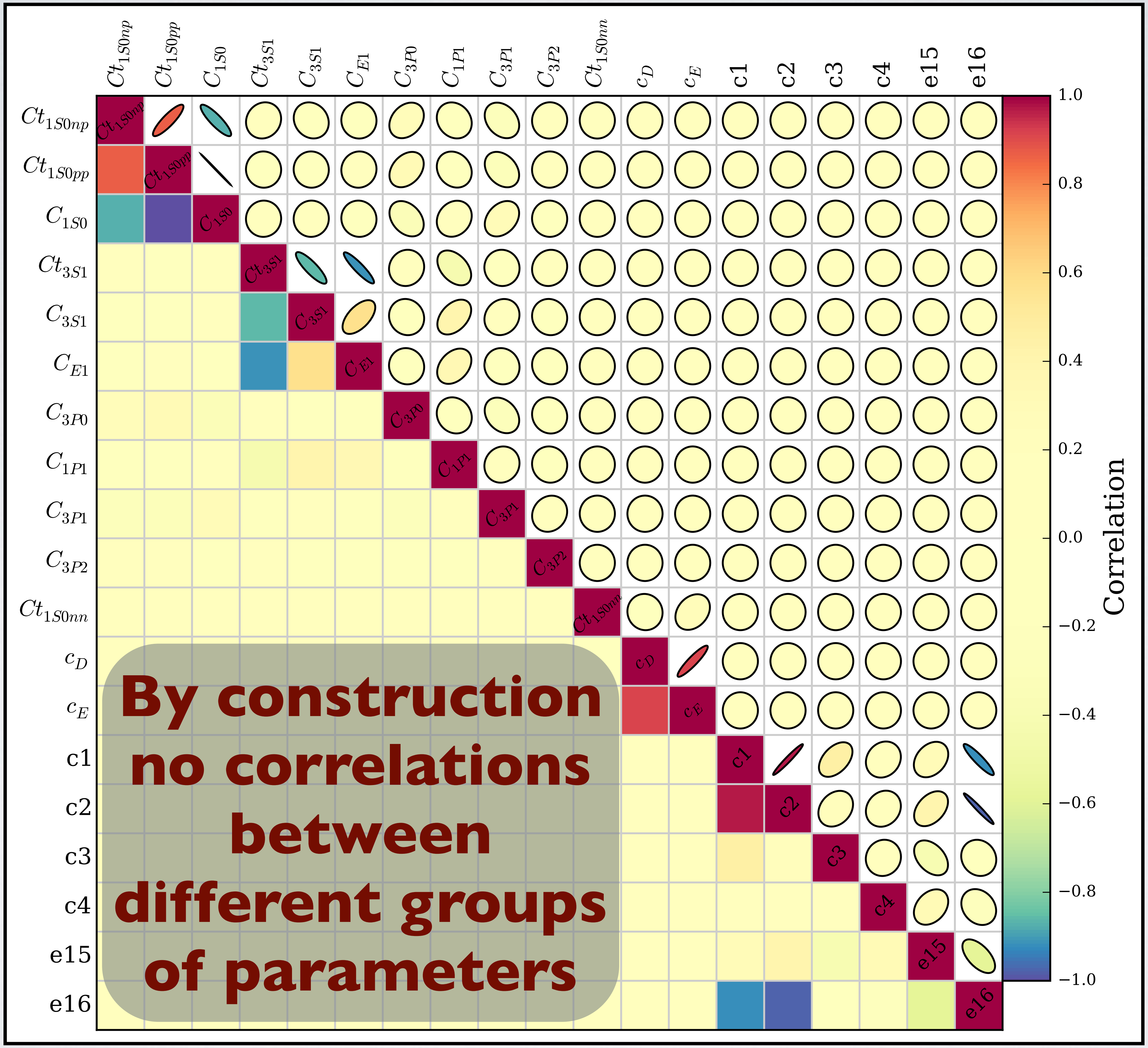
Correlations - sequential fits



Correlations - sequential fits

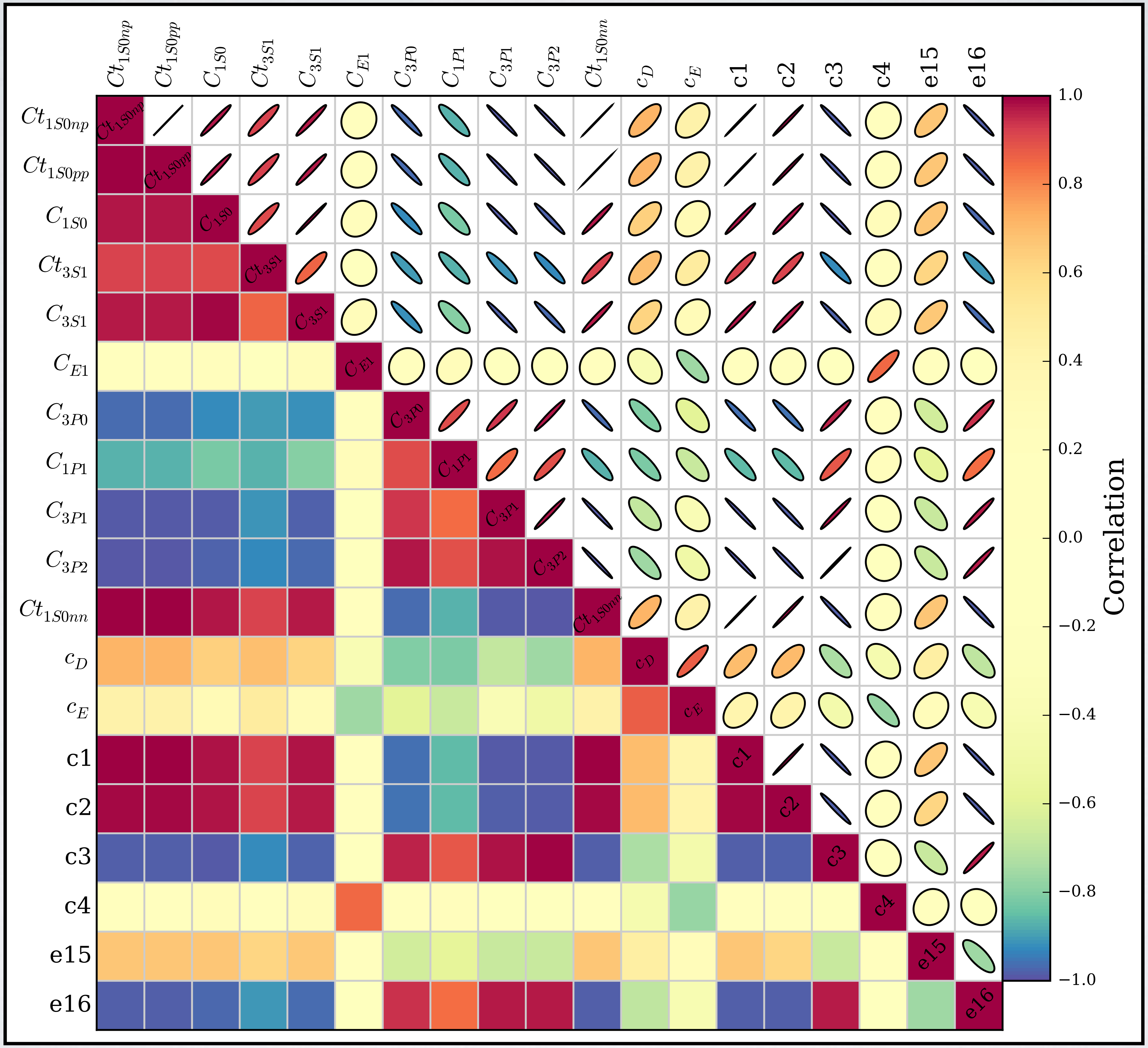


Correlations - sequential fits



By construction no correlations between different groups of parameters

Correlations - simultaneous fit



Error propagation: bound states

Predictions

Preliminary

Sector	Observable	LO	NLO	NNLO	Exp
2H	E_{gs}	-2.225	-2.225^{+1}_{-6}	-2.225(1)	-2.225
3H	E_{gs}	-11.44	-8.268^{+27}_{-38}	-8.482^{+2}_{-5}	−8.482(3)
3H	$T_{1/2}$ (ME)			0.6848(11)	0.6848(11)
4He	r_{ch}	1.080	1.482^{+3}_{-4}	1.445(2)	1.467(40)
4He	E_{gs}	-40.39	-27.44^{+13}_{-15}	-28.26^{+4}_{-5}	-28.30

$$O(\mathbf{p}) \approx O(\mathbf{p}_0) + J_O \Delta\mathbf{p} + \frac{1}{2}\Delta\mathbf{p}^T H_O \Delta\mathbf{p}$$

Asymmetric erors due to quadratic error propagation

Error propagation: bound states

Predictions

Preliminary

Sector	Observable	LO	NLO	NNLO	Exp
2H	E_{gs}	-2.225	-2.225^{+1}_{-6}	-2.225(1)	-2.225
3H	E_{gs}	-11.44	-8.268^{+27}_{-38}	-8.482^{+2}_{-5}	−8.482(3)
3H	$T_{1/2}$ (ME)			0.6848(11)	0.6848(11)
4He	r_{ch}	1.080	1.482^{+3}_{-4}	1.445(2)	1.467(40)
4He	E_{gs}	-40.39	-27.44^{+13}_{-15}	-28.26^{+4}_{-5}	-28.30
4He	E_{gs}	−40.27(13)	-27.56^{+14}_{-18}	-28^{+8}_{-18}	-28.30

Sequential approach with propagated errors

In this optimization, the ci:s were fitted separately to piN data, thus ignoring correlations and increasing errors.

Conclusion

Summary

❖ **Chiral EFT with error analysis**

- **Simultaneous optimization of all LECs** at LO, NLO, NNLO using NN, NNN and piN data is critical in order to:
  - capture all correlations between the parameters, and
  - reduce the statistical errors.
- We find that **statistical errors** are small ($\lesssim$1%), and the total error budget is dominated by **theoretical errors.** Statistical errors increase dramatically for sequentially optimized potentials.
- **Automatic differentiation** allows efficient and accurate computation of derivatives and allows a statistical error analysis.
- First results for correlations, parameter uncertainties and **error propagation in the few-body sector.**