

# **NuMeriQS Retreat 2025**

## **Report of Contributions**

Contribution ID: **1**

Type: **not specified**

# Welcome

*Tuesday 16 September 2025 09:00 (15 minutes)*

**Presenter:** URBACH, Carsten (HISKP, Uni Bonn)

Contribution ID: 2

Type: **not specified**

## Machine learning for (theoretical) chemistry

*Tuesday 16 September 2025 09:15 (1 hour)*

**Presenter:** WESTERMAYR, Julia

Contribution ID: 3

Type: **not specified**

## **Simulating helical magnetic fields and chiral asymmetries in the early Universe**

*Tuesday 16 September 2025 10:45 (1 hour)*

**Presenter:** SCHOBER, Jennifer

Contribution ID: 4

Type: **not specified**

# The Coupled Cluster Algorithm

*Tuesday 16 September 2025 13:00 (1 hour)*

**Presenter:** NEESE, Frank

Contribution ID: 5

Type: **not specified**

## Lattice QCD for dummies

*Wednesday 17 September 2025 11:30 (1 hour)*

Contribution ID: 6

Type: **not specified**

## General Meeting and Discussion

*Thursday 18 September 2025 09:00 (1h 30m)*

Contribution ID: 7

Type: **not specified**

## Mitgliederversammlung

*Thursday 18 September 2025 11:00 (1h 30m)*

Contribution ID: 8

Type: **not specified**

## Departure Bus to Bonn

*Thursday 18 September 2025 14:00 (20 minutes)*

Contribution ID: 9

Type: **not specified**

## Breakfast

Contribution ID: **10**

Type: **not specified**

## Project A01

*Tuesday 16 September 2025 14:00 (5 minutes)*

**Presenters:** KIRCHNER, Barbara (Uni Bonn); URBACH, Carsten (HISKP, Uni Bonn); HAMAEEKERS, Jan (Fraunhofer SCAI)

**Session Classification:** Project Afternoon

Contribution ID: **11**

Type: **not specified**

## Project A03

*Tuesday 16 September 2025 14:05 (5 minutes)*

**Presenters:** KIRCHNER, Barbara (Uni Bonn); DÖLZ, Jürgen (University of Bonn)

**Session Classification:** Project Afternoon

Contribution ID: **12**

Type: **not specified**

## Project A04

*Tuesday 16 September 2025 14:10 (5 minutes)*

**Presenter:** OSTMEYER, Johann

**Session Classification:** Project Afternoon

Contribution ID: **13**

Type: **not specified**

## Project B01

*Tuesday 16 September 2025 14:15 (5 minutes)*

**Presenters:** LUU, Thomas C. (Helmholtz-Institut für Strahlen- und Kernphysik); LUU, Thomas (uni-bonn); MEISSNER, Ulf-G. (Helmholtz-Institut für Strahlen- und Kernphysik)

**Session Classification:** Project Afternoon

Contribution ID: 14

Type: **not specified**

## Project B03

*Tuesday 16 September 2025 14:20 (5 minutes)*

**Presenter:** FLAD, Heinz Juergen (Institut fuer Numerische Simulation)

**Session Classification:** Project Afternoon

Contribution ID: 15

Type: **not specified**

## Project B05

*Tuesday 16 September 2025 14:25 (5 minutes)*

**Presenters:** RÖNCHEN, Deborah (Forschungszentrum Jülich); RÖNCHEN, Deborah (Helmholtz-Institut für Strahlen- und Kernphysik); MEISSNER, Ulf-G. (Helmholtz-Institut für Strahlen- und Kernphysik)

**Session Classification:** Project Afternoon

Contribution ID: **16**

Type: **not specified**

## Project C01

*Tuesday 16 September 2025 14:30 (5 minutes)*

**Presenters:** URBACH, Carsten (HISKP, Uni Bonn); FUNCKE, Lena (University of Bonn)

**Session Classification:** Project Afternoon

Contribution ID: 17

Type: **not specified**

## Project C03

*Tuesday 16 September 2025 14:35 (5 minutes)*

**Presenter:** FUNCKE, Lena (University of Bonn)

**Session Classification:** Project Afternoon

Contribution ID: **18**

Type: **not specified**

## **Posters A01, A03, A04, B01, B03, B05, C01, C03**

*Tuesday 16 September 2025 14:40 (1h 20m)*

**Session Classification:** Project Afternoon

Contribution ID: **19**

Type: **not specified**

## Project A02

*Tuesday 16 September 2025 16:00 (5 minutes)*

**Presenters:** NEESE, Frank; NEESE, Frank (Max-Planck-Institut für Kohlenforschung)

**Session Classification:** Project Afternoon

Contribution ID: 20

Type: **not specified**

## Project A05

*Tuesday 16 September 2025 16:05 (5 minutes)*

**Presenters:** KIRCHNER, Barbara (Uni Bonn); SUAREZ, Estela (Forschungszentrum Juelich GmbH); SUAREZ, Estela (uni-bonn); MUTZEL, Petra (uni-bonn)

**Session Classification:** Project Afternoon

Contribution ID: **21**

Type: **not specified**

## Project A06

*Tuesday 16 September 2025 16:10 (5 minutes)*

**Presenters:** KOLLATH, Corinna (Uni Bonn); LUITZ, David (uni-bonn)

**Session Classification:** Project Afternoon

Contribution ID: 22

Type: **not specified**

## Project B02

*Tuesday 16 September 2025 16:15 (5 minutes)*

**Presenters:** KOSTRZEWA, Bartosz (Helmholtz-Institut für Strahlen- und Kernphysik); KOSTRZEWA, Bartosz (Helmholtz-Institut für Strahlen- und Kernphysik); SUAREZ, Estela (Forschungszentrum Juelich GmbH); SUAREZ, Estela (uni-bonn); KRIEG, Stefan; KRIEG, Stefan (JSC, Forschungszentrum Jülich & HISKP, Bonn University)

**Session Classification:** Project Afternoon

Contribution ID: **23**

Type: **not specified**

## Project B04

*Tuesday 16 September 2025 16:20 (5 minutes)*

**Presenters:** DUHR, Claude; DÖLZ, Jürgen (University of Bonn)

**Session Classification:** Project Afternoon

Contribution ID: 24

Type: **not specified**

## Project B06

*Tuesday 16 September 2025 16:25 (5 minutes)*

**Presenters:** SCHWEITZER, Marc Alexander (Institut für Numerische Simulation & Fraunhofer SCAI); KRIEG, Stefan; KRIEG, Stefan (JSC, Forschungszentrum Jülich & HISKP, Bonn University)

**Session Classification:** Project Afternoon

Contribution ID: 25

Type: **not specified**

## Early Career Q&A with Julia Westermayr

*Monday 15 September 2025 11:00 (1 hour)*

**Presenters:** WESTERMAYR, Julia; FROEMGEN, Tom (MCTC)

Contribution ID: 26

Type: **not specified**

## Project C02

*Tuesday 16 September 2025 16:30 (5 minutes)*

**Presenters:** LUU, Thomas (uni-bonn); URBACH, Carsten (HISKP, Uni Bonn); LUU, Thomas C. (Helmholtz-Institut für Strahlen- und Kernphysik); NEESE, Frank (Max-Planck-Institut für Kohlenforschung); NEESE, Frank; LUITZ, David (uni-bonn)

**Session Classification:** Project Afternoon

Contribution ID: 27

Type: **not specified**

## Project Z02

*Tuesday 16 September 2025 16:35 (5 minutes)*

**Presenters:** KOSTRZEWA, Bartosz (Helmholtz-Institut für Strahlen- und Kernphysik); KOSTRZEWA, Bartosz (Helmholtz-Institut für Strahlen- und Kernphysik); SUAREZ, Estela (Forschungszentrum Juelich GmbH); SUAREZ, Estela (uni-bonn)

**Session Classification:** Project Afternoon

Contribution ID: **28**

Type: **not specified**

## Eifel Hike

*Monday 15 September 2025 14:00 (3h 30m)*

Please bring your hiking shoes and appropriate clothes

Contribution ID: 29

Type: **not specified**

## **Posters A02, A05, A06, B02, B04, B06, C02, Z02**

*Tuesday 16 September 2025 16:40 (1h 20m)*

**Session Classification:** Project Afternoon

Contribution ID: **30**

Type: **not specified**

## Tensor Networks

*Wednesday 17 September 2025 09:00 (15 minutes)*

**Presenter:** LUITZ, David (uni-bonn)

**Session Classification:** Methods Session

Contribution ID: **31**

Type: **not specified**

## Machine Learning

*Wednesday 17 September 2025 09:15 (15 minutes)*

**Presenters:** LUU, Thomas C. (Helmholtz-Institut für Strahlen- und Kernphysik); LUU, Thomas (uni-bonn)

**Session Classification:** Methods Session

Contribution ID: **32**

Type: **not specified**

## **HPC and Co-Design**

**Presenters:** SUAREZ, Estela (Forschungszentrum Juelich GmbH); SUAREZ, Estela (uni-bonn)

**Session Classification:** Methods Session

Contribution ID: 33

Type: **not specified**

## Quantum Computing

*Wednesday 17 September 2025 09:30 (15 minutes)*

**Presenter:** FUNCKE, Lena (University of Bonn)

**Session Classification:** Methods Session

Contribution ID: 34

Type: **not specified**

## Uncertainty Quantification

*Wednesday 17 September 2025 09:45 (15 minutes)*

**Presenter:** DÖLZ, Jürgen (University of Bonn)

**Session Classification:** Methods Session

Contribution ID: 35

Type: **not specified**

## Molecular Dynamics

*Wednesday 17 September 2025 10:30 (15 minutes)*

**Presenter:** KIRCHNER, Barbara (Uni Bonn)

**Session Classification:** Methods Session

Contribution ID: 36

Type: **not specified**

## Multilevel Methods

*Wednesday 17 September 2025 10:45 (15 minutes)*

**Presenter:** SCHWEITZER, Marc Alexander (Institut für Numerische Simulation & Fraunhofer SCAI)

**Session Classification:** Methods Session

Contribution ID: 37

Type: **not specified**

# Graph Algorithms and Learning

*Wednesday 17 September 2025 11:00 (15 minutes)*

**Presenter:** ROSSI, Aurora

**Session Classification:** Methods Session

Contribution ID: 38

Type: **not specified**

## Effective Field Theory

**Presenter:** MEISSNER, Ulf-G. (Helmholtz-Institut für Strahlen- und Kernphysik)

**Session Classification:** Methods Session

Contribution ID: 39

Type: **not specified**

## Numerical Quadrature

*Wednesday 17 September 2025 11:15 (15 minutes)*

**Presenter:** FLAD, Heinz Juergen (Institut fuer Numerische Simulation)

**Session Classification:** Methods Session