C²PAP – THE COMPUTATIONAL CENTER FOR PARTICLE AND ASTROPHYSICS

C2PAP

TUM

LMU

THE C²PAP NETWORK

The map shows the distribution of lead scientists of C²PAP proposals across the different partner institutions of the Excellence Cluster Universe.

ABOUT THE COMPUTATIONAL CENTER FOR PARTICLE AND ASTROPHYSICS

Progress in understanding the exciting scientific questions of the origin and evolution of the Universe requires considerable computational effort. This includes producing theoretical models as well as extracting and interpreting observational and experimental data. The resulting computing and developmental needs in astrophysics and particle physics therefore have increased significantly in recent years and will continue to increase in the future.

To meet these ever-growing demands, the Excellence Cluster Universe in the second period of the Excellence Initiative founded the Computational Center for Particle and Astrophysics (C²PAP). It is built around the collaboration with the Leibniz Rechenzentrum LRZ and allows the members of the Universe Cluster to keep pace and harvest the progress of the continuously broadening developments in the high-performance computing (HPC) domain.

C²PAP operates its own computing cluster with 2084 processor cores, which is essentially a smaller version of the supercomputer SuperMUC at LRZ with some modifications owing to the needs of the Universe Cluster scientists such as nodes with larger main memory or local disk storage. This provides computing resources to the members of the Universe Cluster enabling them to develop their tools for efficient usage of supercomputers like SuperMUC and cloud-computing facilities. Its own data storage system also provides 300 Terabytes for data intensive projects for members of the Universe Cluster.
By employing five full-time staff members, C²PAP provides key personnel with the expertise in all areas of scientific computing such as high-performance computing, parallelization, algorithm development and novel computing architectures as well as further aspects of large-scale computing like usage of modern software packages, database design, data preservation and visualization to allow members of the Universe Cluster to achieve their scientific goals.

Through yearly application rounds, the Center staff works in partnership with a large number of research groups within the Cluster, serving as a connector for the transfer of technical knowledge between the groups and across the different disciplines. Through regular meetings, C²PAP personnel monitors the progress of the individual projects and a governing committee with scientists representing the different research areas in the Universe Cluster oversees the operation of C²PAP. Throughout more than 100 project applications from Cluster scientists during the funding period 2012 to 2017, C²PAP supported different Cluster groups to conduct their research within the growing and vastly changing technological landscape of high performance computing, data processing and data management. They enable the research groups to integrate their research into the local high-performance computing centers and to proceed more rapidly and efficiently toward new discoveries.

THE C^{2}PAP TEAM

DIRECTORS

DR. KLAUS DOLAG (LMU)

works mainly on computational astrophysics and cosmology. He utilizes high-performance computing facilities to carry out forefront numerical simulations, especially focusing on the field of numerical treatment and modelling of various, highly complex and interacting physical processes, which need to be considered to understand in detail how galaxies and galaxy clusters emerge within the large-scale structure of the Universe.

DR. GÜNTER DUCKECK (LMU)

works as an experimental particle physicist. He has been involved for many years in the ATLAS experiment at LHC. In addition, he coordinates the participation of the German computing centers to the worldwide ATLAS distributed computing system.

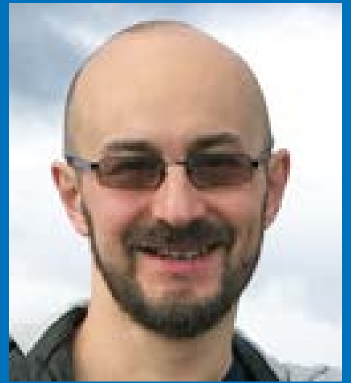
PROF. DR. JOSEPH MOHR (LMU)

is Chair for Cosmology and Structure Formation in the physics faculty. His focus is on observational cosmology and the use of multiwavelength survey data to map the emergence of structure in the Universe. He is also leading the development of the processing pipelines for Dark Energy Survey data within the context of the ESA Euclid mission. He was the founding director of C^{2}PAP and led it from 2012 – 2016.

STAFF

DR. FREDERIK BEAUJEAN (LMU)

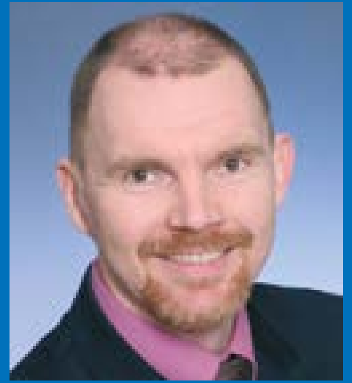
is the staff member for all questions regarding data analysis, statistical methods and numerical optimization. He did a PhD in particle physics and results of his work include numerous research articles and open-source software packages in C++ and python.



DR. DAVID HUBBER (LMU)

works on high-performance computing codes for astrophysical hydrodynamical simulations and has previously developed the GANDALF code for use on C^{2}PAP. His tasks include improving the parallel performance on multiple processors using OpenMP, MPI and new technologies such as OpenACC, and implementing new physics algorithms into the cosmological code GADGET. David fills in for Margarita during her maternity leave.

STAFF



DR. ALEXEY KRUKAU (LRZ)

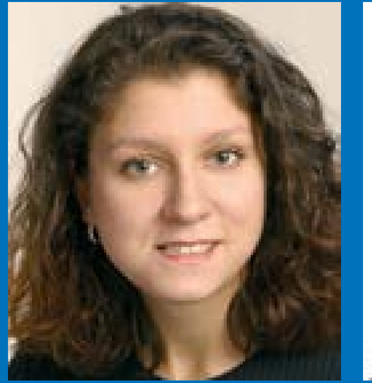
works on the parallelization of the scientific algorithms for the high-performance computing systems using OpenMP/MPI techniques as well as on the development and optimization of the parallel I/O (input/output). He is also administrating the C^{2}PAP computing facility and provides user support for the topics related to the usage of the computing cluster.

DR. MOHAMMAD MIRKAZEMI (LMU)

focuses on algorithm and software development for astrophysical application in C++, Python and R. He is involved in projects related to the calibration of the Dark Energy Survey (DES) photometry using Gaia space-telescope spectroscopic data. He also works on spectral object classification using machine learning methods as well as developing algorithms for measuring the distance of galaxy clusters.

DR. JOVAN MITREVSKI (LMU)

is a former ATLAS reconstruction group convener, currently a reconstruction and software sub-group convener for the e/gamma performance group. He is mainly focused on software for experimental particle physics, and is currently exploring applying machine learning to searches for new physics and to particle reconstruction.



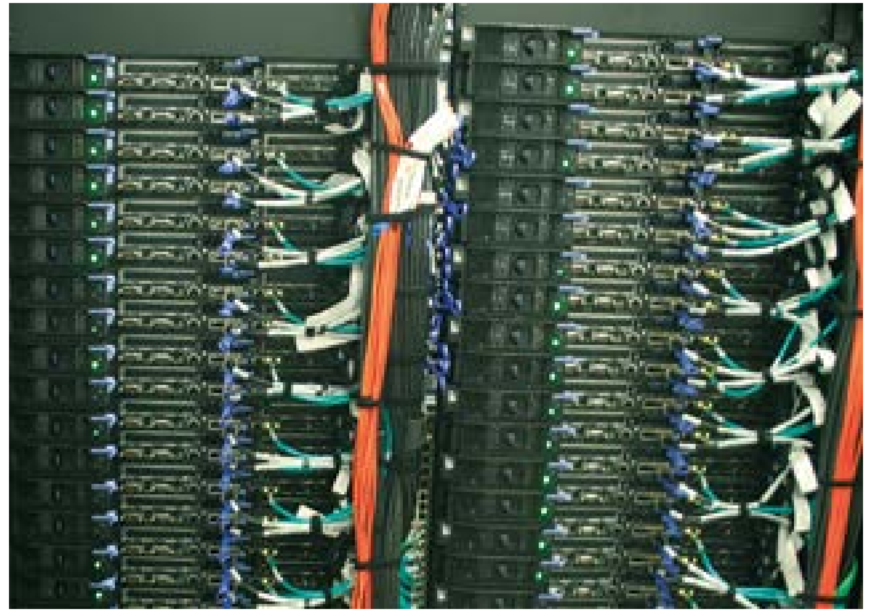
DR. MARGARITA PETKOVA (LMU)

is interested in HPC and numerical algorithms and previously worked as a developer of the astrophysical codes GADGET and AREPO. In C^{2}PAP she works on parallelization and optimization of various astrophysical codes, using MPI, OpenMP and OpenACC. She consults several groups about optimizing and developing their codes, among them the cosmological simulation code GADGET, the supernova code Prometheus and the spectral fitting code Lephare.

DR. MARION CADOLLE BEL (LMU)

is an astrophysicist. For C^{2}PAP, she has been working on testing and optimizing the Dark Energy Survey data processing software. She also contributed for a large concept to develop a public web portal service at C^{2}PAP and LRZ. Her expertise is parallel computing, Monte-Carlo methods, data archiving and processing or distributed computing. She is now working at the Max Planck Computing and Data Facility as a data scientist.

C²PAP'S HARDWARE



- 126 compute nodes: each 64 GB RAM, 250 GB HDD, 16 Intel Xeon CPU cores 2.7 GHz
- 3 login nodes: each 128 GB RAM, 300 GB HDD, 16 Intel Xeon CPU cores 2.7 GHz
- 1 "fat" node: 750 GB RAM, 15 TB HDD with 20 Intel Xeon CPU cores 2.7 GHz
- Network: Mellanox Infiniband (40 Gbit/s) Adapters
- IBM Storage system with total volume of 260 TB

C²PAP COMPUTE CLOUD

(Credit: shutterstock)

LRZ offers with the Compute Cloud an attractive new concept to acquire computing resources on demand. This service is also available for C²PAP projects. Based on virtualization the users can provide their own operating system images adapted to their application requirements. Different types of resources are available, ranging from standard worker nodes to high-memory nodes or highly parallel GPU clusters.

CONFERENCE ACTIVITIES

C²PAP staff members regularly participate at and contribute to numerous (more than 40 so far) national and international workshops, schools and conferences. Thereby the team members continuously gather experience and accumulate knowledge in the field of modern programming paradigms, hardware development, statistical and numerical methods as well as algorithm and optimization strategies on HPC platforms. In addition, the C²PAP staff actively supported different project teams on events like Hackathons or workshops (see picture gallery), where HPC centers guide project teams to improve their numerical tools for the next generation of HPC hardware. Furthermore, the C²PAP staff also contributes to the dissemination of the research results from the different projects by participation at national and international physics conferences and is also actively involved in co-organizing workshop and seminar series as well as giving lectures in schools covering the full range of C²PAP activities.

(Credit: Hackathon 2017)

(Credit: Fernanda Foertner)

(Credit: GridKa School Organizing team)

Fred Beaujean (left), Margarita Petkova (middle) and David Hubber (upper right) supporting different project teams making their first experience with GPU programming on various Hackathons organized by Europena HPC centers. Mohammad Mirkazemi (lower right) on the GridKaschool on advance computing techniques.

C²PAP HIGHLIGHT 1

COMPUTING THE UNIVERSE

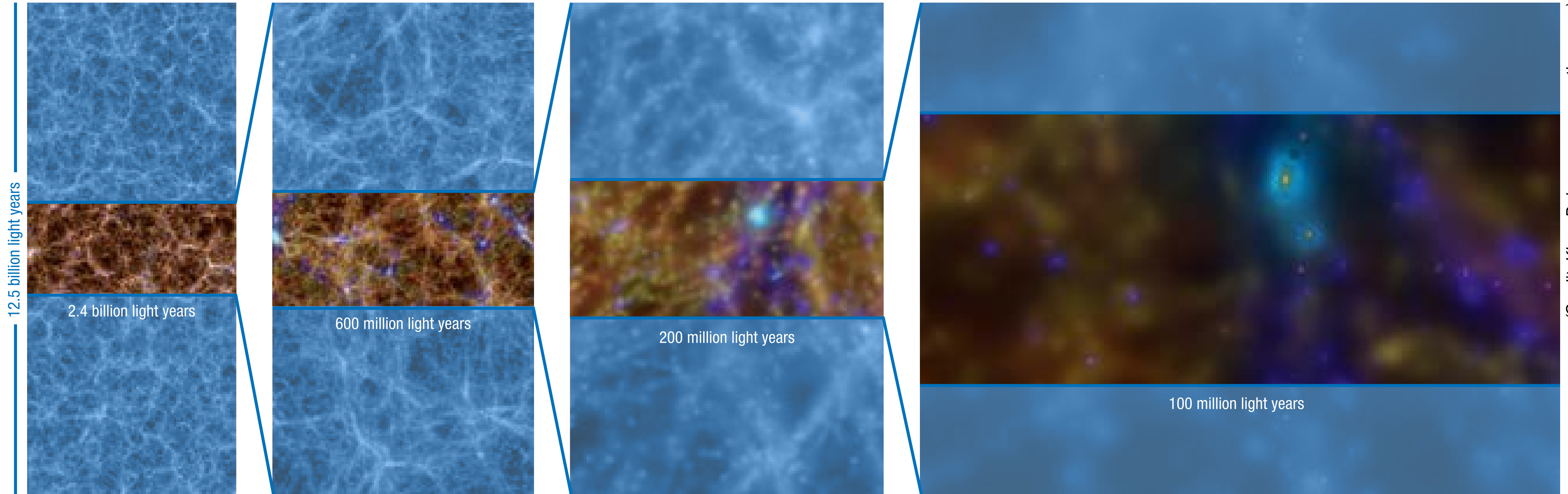
KLAUS DOLAG (LMU)

MAGNETICUM

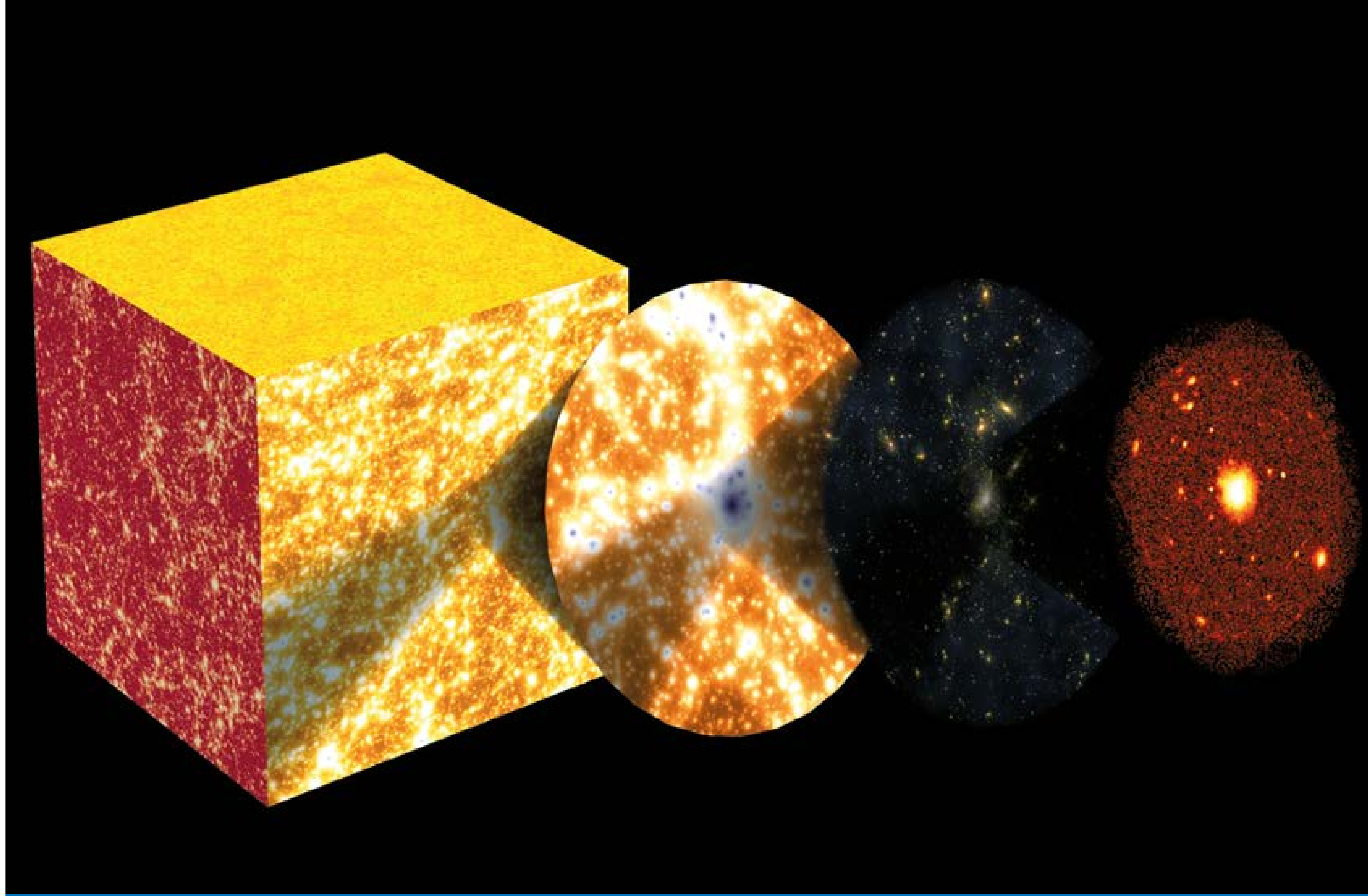
„Magneticum Pathfinder“ (www.magneticum.org) is the world‘s most elaborate cosmological simulation of the evolution of our Universe and has been accomplished by theoretical astrophysicists of the LMU in cooperation with C²PAP and LRZ. A group of theorists led by C²PAP director Klaus Dolag has performed a new, unique hydrodynamic simulation of the large-scale distribution of the Universe’s visible matter. The most recent results regarding the three most important cosmic ingredients of the Universe are taken into account – the dark energy, the dark matter and the visible matter. The researchers transform their knowledge about the physical processes forming our Universe into mathematical models and simulate the evolution of our Universe on high-performance computers over billions of years.

For the first time, these numerous characteristics make it possible to compare a cosmological simulation in detail with large-scale astronomical surveys. „Astronomical surveys from space telescopes like Planck or Hubble observe a large segment of the visible Universe while sophisticated simulations so far could only model very small parts of the Universe, making a direct comparison virtually impossible,“ says Klaus Dolag. „Thus, Magneticum Pathfinder marks the beginning of a new era in computer-based cosmology.“

These data are available for interested researchers worldwide. C²PAP researchers developed a new web interface called “Cosmowebportal” allowing access to the Magneticum Pathfinder data. Users can filter objects by size, mass or other properties and visualize them.



(Credit: Klaus Dolag, www.magneticum.org)



Visualizations of the simulated distributions of gas and stars in the Universe from data provided by Cosmowebportal. *(Credit: P. Baintner & H. Brüchle, LRZ)*

The South Pole Telescope during the long polar night. *(Credit: Keith Vanderlinde)*

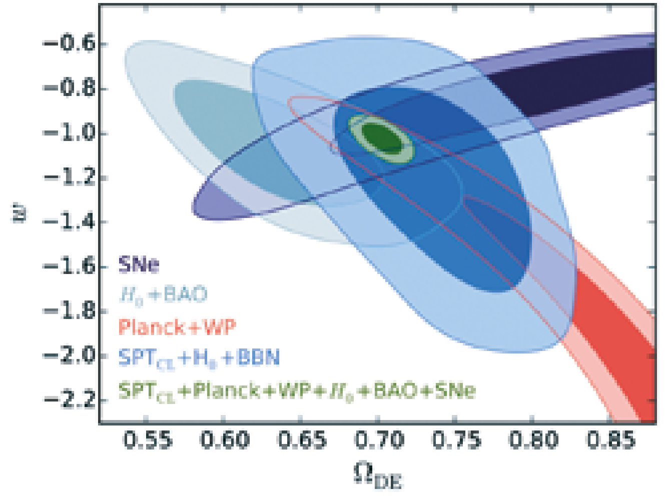
C²PAP HIGHLIGHT 2

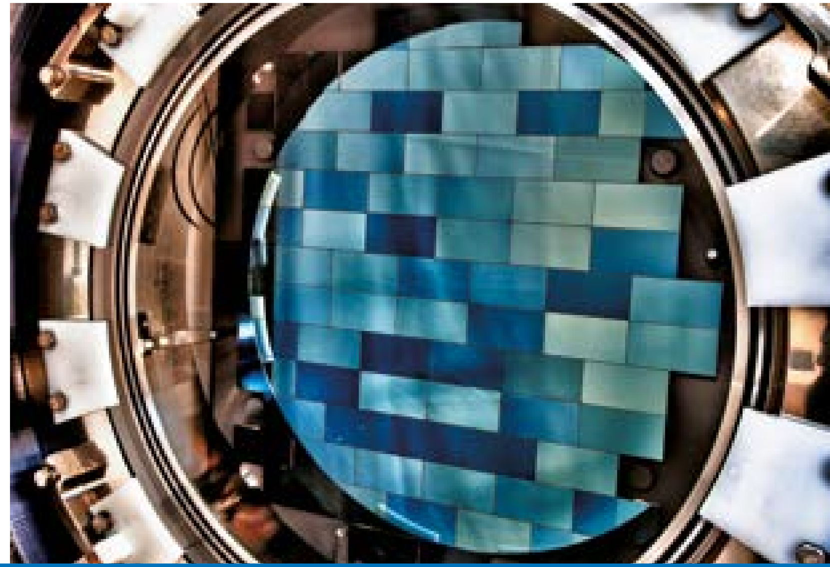
HUNTING DARK ENERGY WITH C²PAP

JOSEPH MOHR (LMU)

Since 1998 when it was discovered that the expansion of the Universe is accelerating, attention has turned to using the evolution of the large-scale structure such as voids, walls, filaments and galaxy clusters to understand whether this acceleration is driven by some new component of the Universe – termed "dark energy" – or whether our understanding of gravity is flawed. Two leading astronomical surveys – the South Pole Telescope (SPT) and the Dark Energy Survey (DES) – are designed to address these questions. The SPT is a high angular resolution cosmic microwave background mapping experiment in Antartica. We use these maps to identify galaxy clusters from the moment of their formation. The DES is a multiband optical imaging survey carried out from the Chilean Andes. We use the DES data to measure the distance or redshift to each SPT selected galaxy cluster.

Astronomers of the Universe Cluster have used C²PAP to validate processing pipelines that turn the 0.5 Giga-pixel exposures from the Dark Energy Camera (DECam) into science ready images and catalogs. In one demonstration run, these high efficiency pipelines were used to prepare an entire observing season (125 nights, 15 TB) of DES data for science analysis over a two week period. C²PAP has been used to run the cosmological analysis software on the SPT+DES galaxy cluster sample, producing the most sensitive constraints to date on the nature of dark energy. These results show that over the 10 billion years of evolution probed by the galaxy cluster sample, the dark energy has exhibited the properties of a constant energy density vacuum energy.





Constraints on nature of dark energy from an SPT analysis, DES image of SPT galaxy cluster (middle), and the Dark Energy Camera (right; *Credit: Dark Energy Survey*).

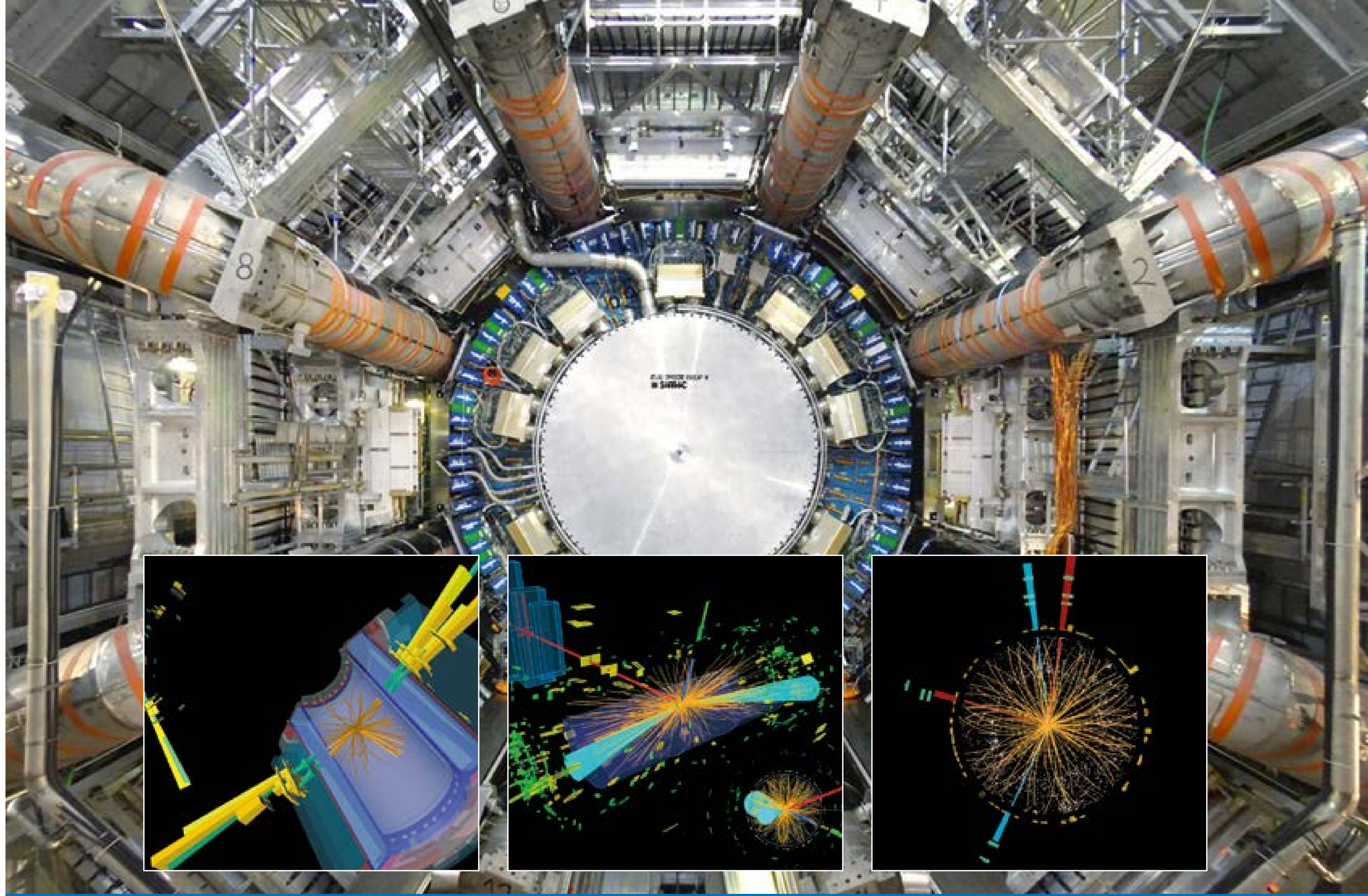
C^{2}PAP HIGHLIGHT 3

PARTICLE COLLISIONS IN A SUPERCOMPUTER

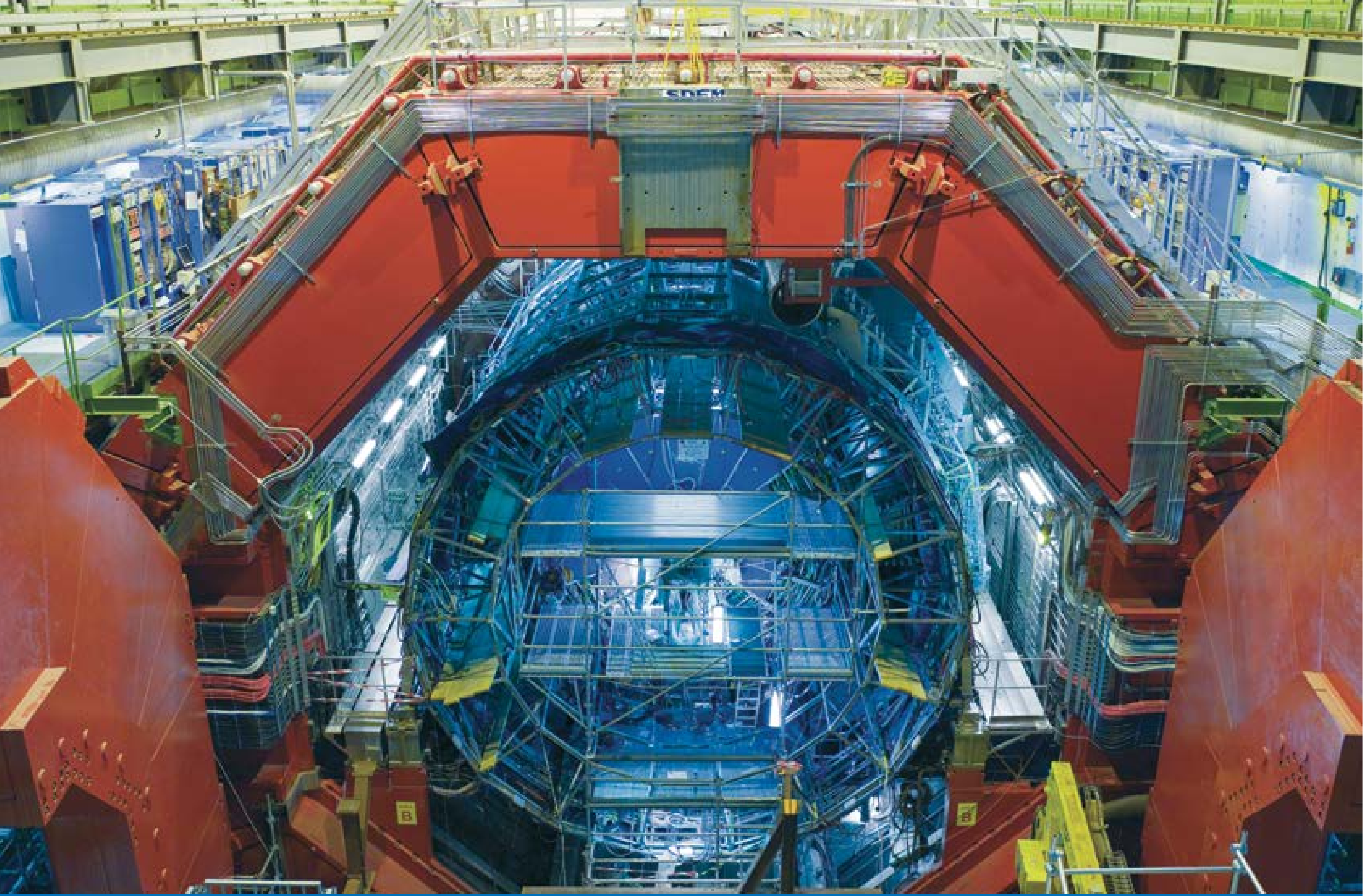
GÜNTER DUCKECK (LMU)

The ATLAS experiment is one of two multi-purpose experiments at the world's largest particle accelerator, the Large Hadron Collider (LHC) at CERN, designed to record large numbers of proton-proton collision events. The ATLAS collaboration has already published more than 500 journal articles including the celebrated discovery of the Higgs boson. The 2nd phase of LHC run-2 is ongoing since 2015 at a center-of-mass energy of 13 tera-electronvolts. For identifying new phenomena within the recorded data, simulations of proton-proton collisions, based on theoretical predictions combined with detailed modelling of the detector response, are indispensable. Simulating a single complex collision event is computationally expensive and can take up to 1,000 seconds on a single CPU core. The ATLAS experiment records about 10 billion collision events per year. The detailed analysis of this data requires at least the same amount of simulated events for standard processes in order to perform the baseline optimizations and background corrections and in addition requires many extra samples to perform searches for "New Physics" processes – the main purpose of the LHC program. This simulation production is part of a worldwide effort, involving more than 100 computing centers in all ATLAS member states. Besides the substantial amount of dedicated resources for ATLAS/LHC, this effort also relies to a large extent on the opportunistic use of temporarily available resources at the associated institutions.

C^{2}PAP made very valuable contributions in two ways: on the one hand we could use C^{2}PAP resources to contribute effectively to this simulation production, but more importantly, since C^{2}PAP has a similar setup and architecture as large HPC clusters, we could tune and optimize the ATLAS production work-flows for such systems. Based on these developments we obtained access to two large HPC systems, SuperMUC at the LRZ and DRACO at the Max Planck Computing and Data Facility (MPCDF), and have integrated them into the ATLAS worldwide effort significantly extending the available CPU resources. In addition, C^{2}PAP staff strongly contributed to the optimization of the ATLAS reconstruction software in order to operate it on multi-threaded or parallel computer architectures.



View of the ATLAS detector and example pictures of particle collisions. *(Credit: CERN)*



The ALICE detector. *(Credit: CERN)*

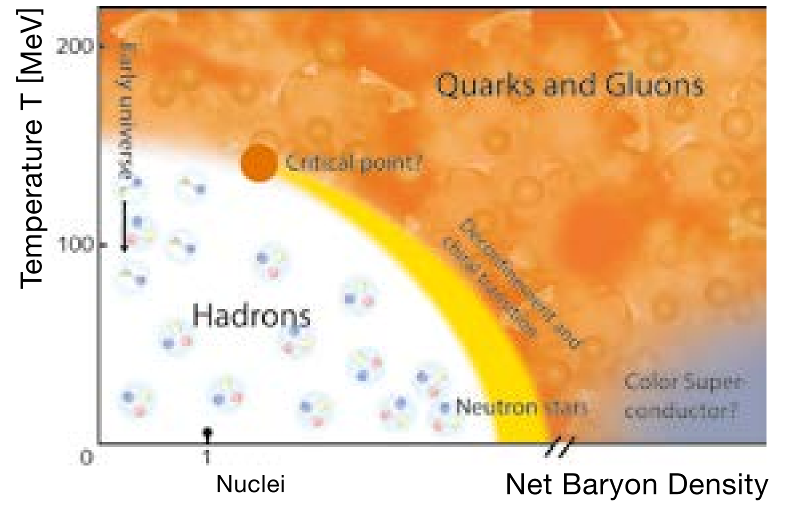
C²PAP HIGHLIGHT 4

HOTTEST AND DENSEST MATTER IN C²PAP

NORA BRAMBILLA (TUM)

How does matter behave at the highest temperatures and highest densities? These questions have been investigated since 2014 by the newly formed TUMQCD collaboration lead by Prof. Dr. Nora Brambilla (TUM). They have studied hot nuclear matter through simulations on the computing clusters C²PAP and SuperMUC. The interior of atomic nuclei consists of so-called nuclear matter and can be described using a highly non-linear theory called quantum chromodynamics (QCD). Using this theory, it is possible to simulate hot and dense matter on computers.

If nuclear matter is heated to temperatures beyond one trillion degrees – which is 100,000 times hotter than the center of our Sun –, then the particles basically break apart into their building blocks, i.e. quarks and gluons. The new aggregate state is called quark-gluon plasma (QGP). In many respects this aggregate state is similar to electromagnetic plasmas, which are studied experimentally at the Max-Planck-Institute for Plasma Physics and Technische Universität München. However, collisions of ultra-relativistic heavy ions (i.e. lead) at large particle accelerators are needed in order to create quark-gluon plasma experimentally. The local group of the ALICE experiment at CERN's Large Hadron Collider is committed to experimental research in this field. Such heavy-ion collisions are extraordinarily complex and last for less than 10^{-22} seconds. Their analysis requires a thorough understanding of the underlying theory. In the numerical lattice QCD simulations of the TUMQCD collaboration, they use finite elements- and Monte-Carlo-methods, putting the full quantum field theory on a space-time lattice without approximations. These simulations require massively parallelized computations, often using hundreds of CPUs. Many different lattice sizes are required to vary the temperature and achieve realistic physical results in the limit of infinite volume and vanishing lattice step. Since the C²PAP architecture enables simulations with either only a few or many cores, C²PAP is well-suited for studies of QGP. One of the results of such simulations was the determination of the temperature for lifting confinement.



(Credit: GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt/Germany)

C²PAP HIGHLIGHT 5

DUST EVOLUTION IN PROTOPLANETARY DISKS

LEONARDO TESTI (ESO)

The growth of solids from micrometer particles to planetesimals is a critical stage in the formation of rocky planets like Earth. Observations at millimeter and submillimeter wavelengths are sensitive probes of the solids in the disk midplane where planets are expected to form. In the course of three years, C²PAP staff provided guidance to ESO researchers Marco Tazzari and Leonardo Testi on efficient Monte Carlo sampling to perform the Bayesian analysis of models of grain growth in protoplanetary disks. The computational effort grows tremendously because the resolution of observations from interferometers such as ESO's ALMA is rapidly increasing and it becomes necessary to consider multiple wavelengths to cross-correlate information between physical phenomena on different scales. The required image manipulations can be accelerated by orders of magnitude when executed on a graphics card (GPU). In a fruitful collaboration, a software package named GALARIO was created and released that can compare observations to model predictions in milliseconds in what previously would have required several seconds. With this speed-up, much more thorough scientific analyses are now possible and the astrophysicists can again focus on the modeling rather than the computing time. The initial development of GALARIO took place at a GPU hackathon in Dresden where the participants worked up to 15 h/day in a stimulating atmosphere.

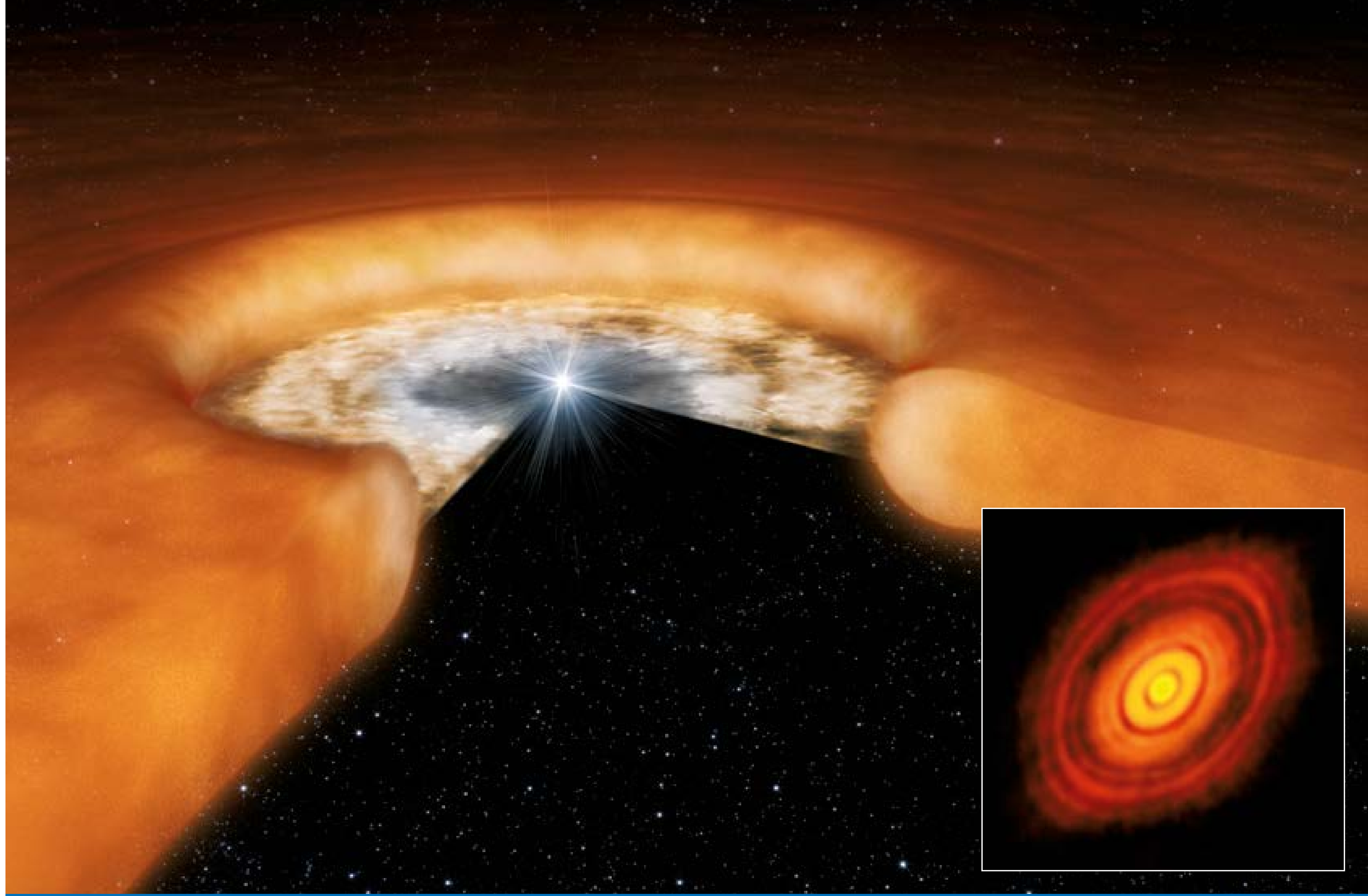
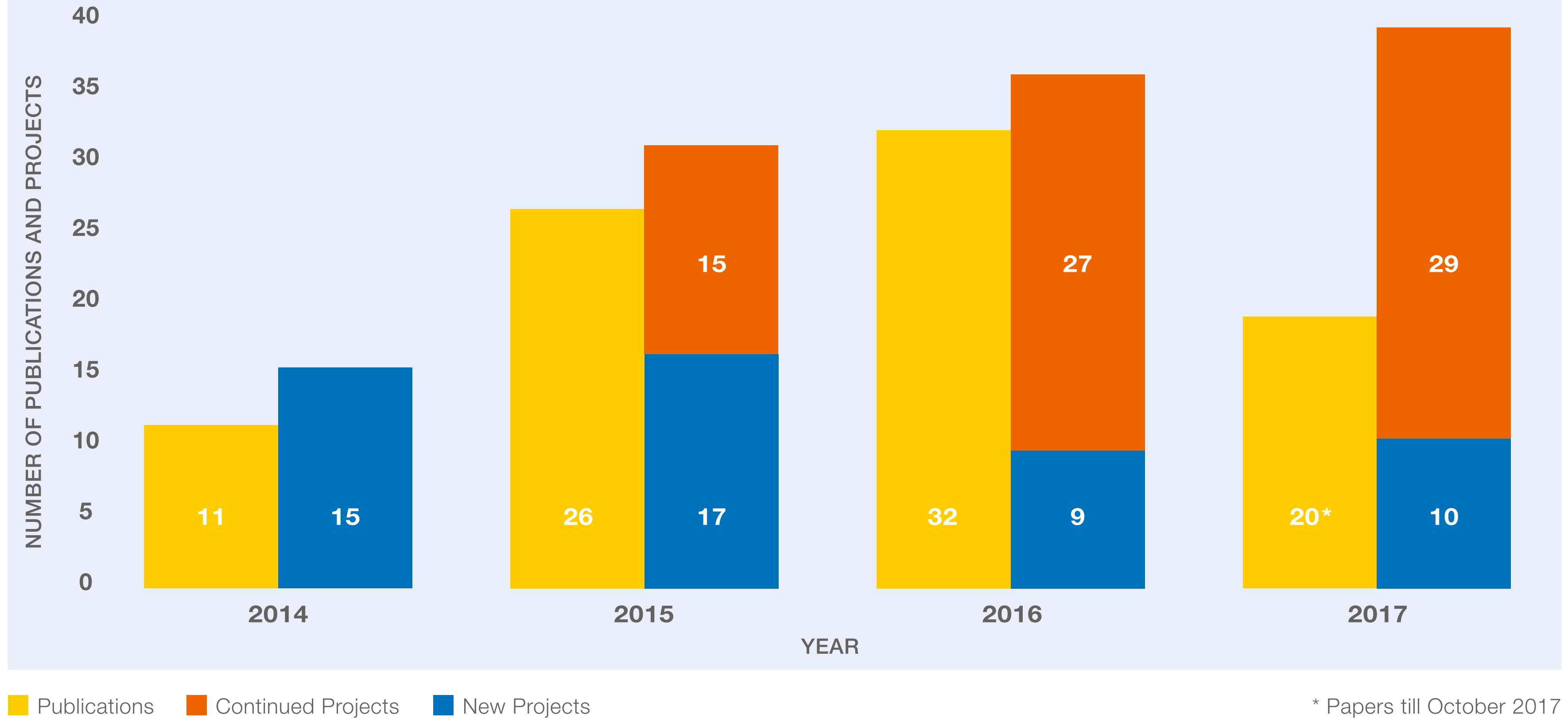


Illustration of a protoplanetary disk (left) and an ALMA image of such a disk (right) in the HL Tau system. *(Credit: ESO)*

C²PAP STATISTICS

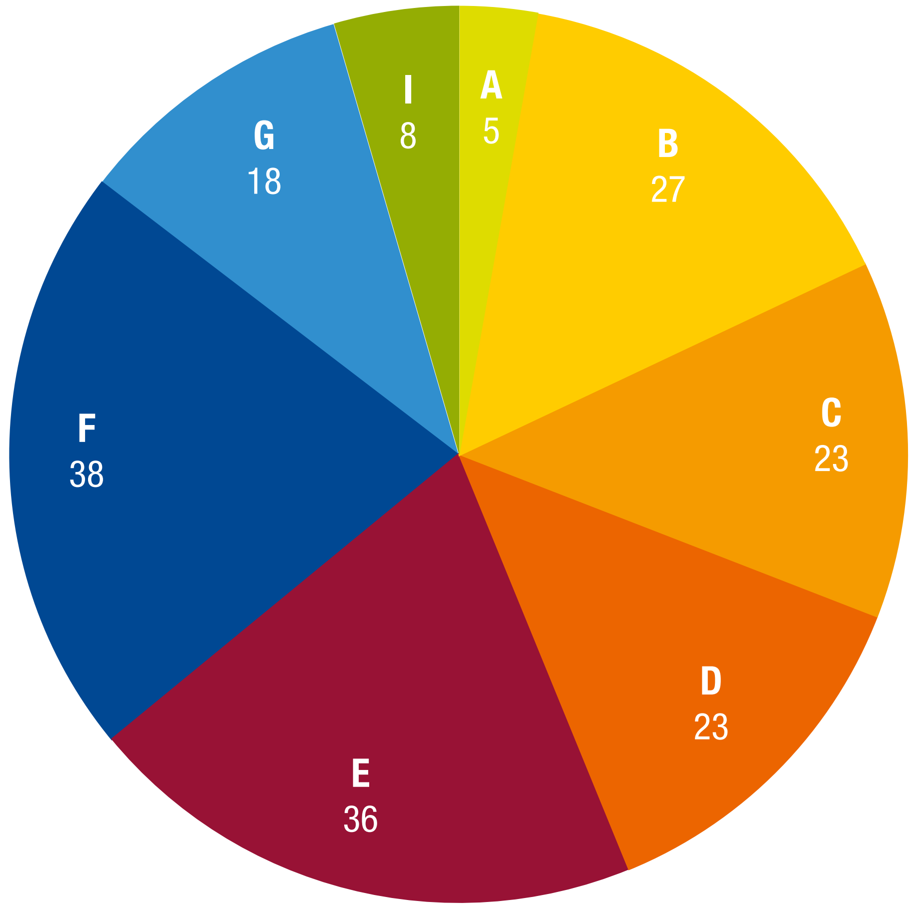
After the start of C²PAP the number of C²PAP projects have grown significantly over the years. A list of all C²PAP projects and about 100 associated publications can be accessed on the C²PAP website: www.universe-cluster.de/c2pap/

GROWTH OF THE NUMBER OF PUBLICATIONS AND PROJECTS SUBMITTED TO THE C²PAP



* Papers till October 2017

NUMBER OF C²PAP PROJECTS IN EACH RESEARCH AREA ACROSS ALL PROJECTS 2014 – 2017



A: What do matter and forces behave at the highest energies?

B: What are the symmetries in the early Universe?

C: What is the origin of particle flavour and mass?

D: What are the phase transitions in the early Universe?

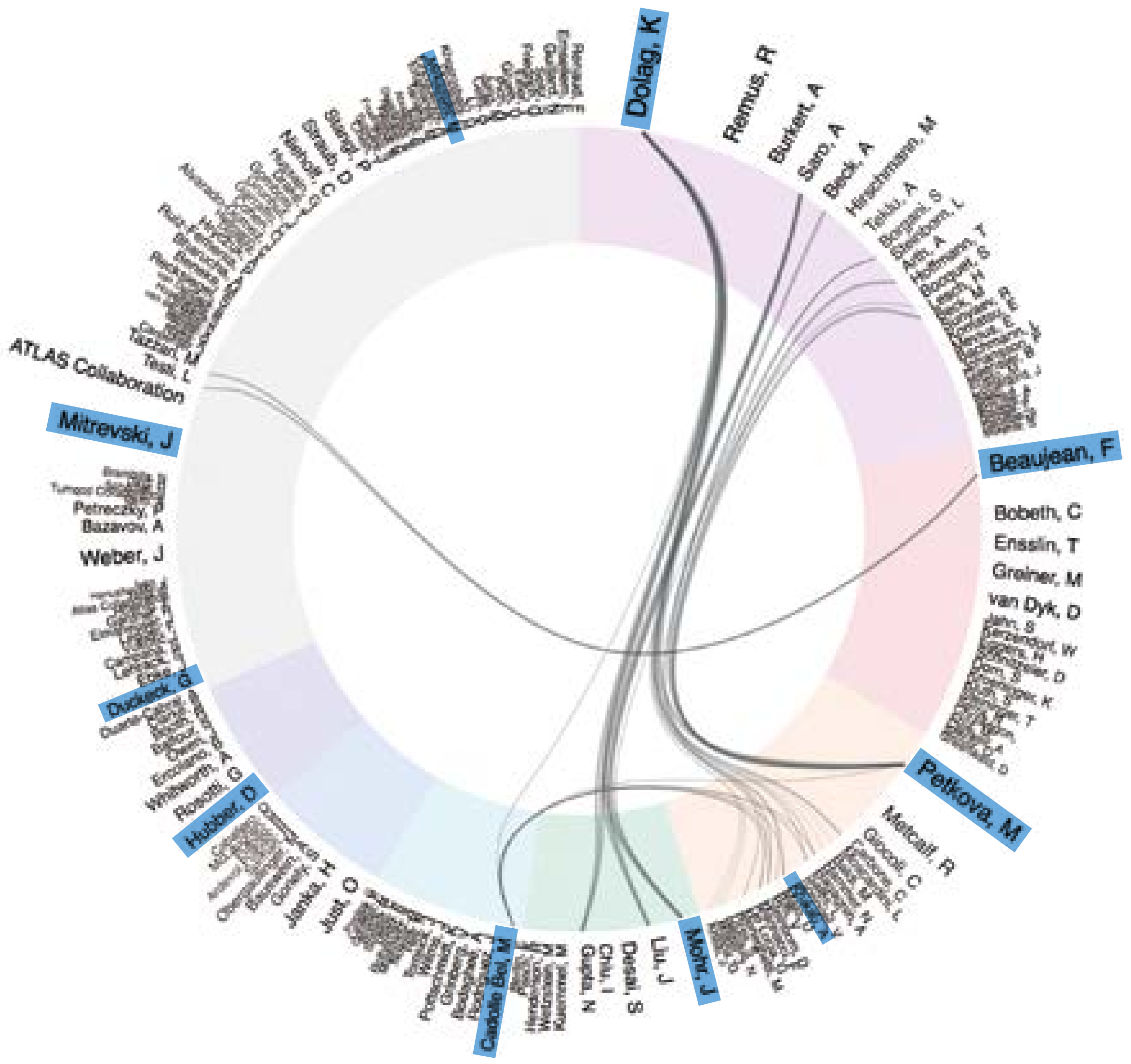
E: What is the nature of dark matter and cosmic acceleration?

F: What processes drive the building of the visible structures in the Universe?

I: C²PAP

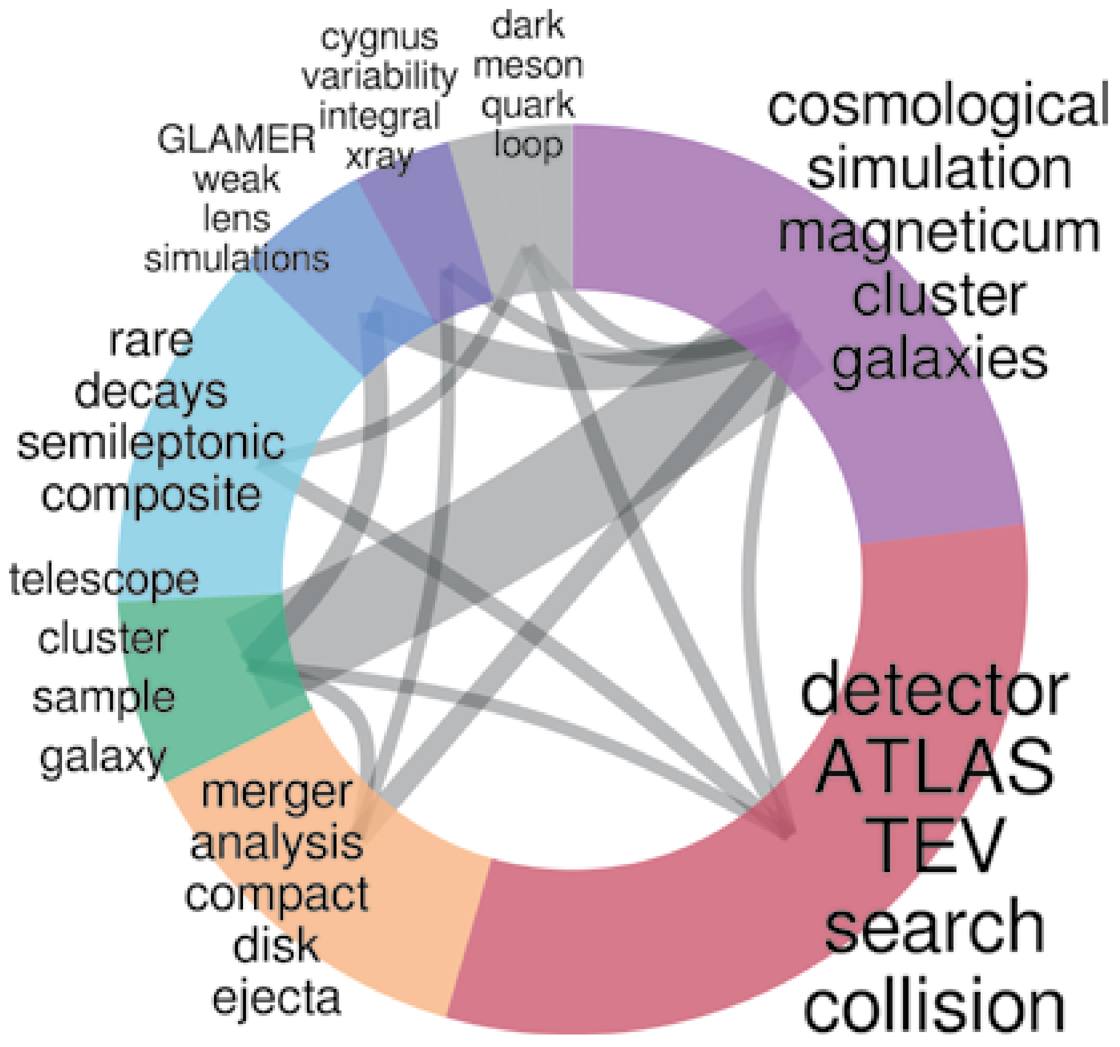
One project can belong to multiple research areas.

C²PAP AUTHOR NETWORK



The author network of C²PAP publications created by ADS Bumblebee. This is based on the most frequently appearing authors and measures the frequency of collaboration between them, displaying color-coded groups of authors. The connecting lines are meant to illustrate the collaborative nature of some of the C²PAP publications and show cooperation between authors from different groups. There would be many more connecting lines between authors within the different groups, but these are not shown for clarity. C²PAP staff members are highlighted.

C²PAP SCIENCE NETWORK



The network for science topics of C²PAP publications created by ADS Bumblebee. This network is created by grouping papers that share a significant number of references, assuming that papers on the same subject have a significant overlap of their references. The names to the groups are then given by looking for shared, unique words in their titles. Connecting lines then link common authors across the different groups.

For clarity, we exclude all collaboration papers where C²PAP staff members formally are co-authors but have not contributed directly.

EPILOGUE

WHY C²PAP IS SO IMPORTANT FOR THE UNIVERSE CLUSTER


(Credit: Andreas Heddergott / TU München)

PROF. DR. ARNDT BODE

Particle and astrophysics have significant requirements for IT services in general and more specifically in the use of high performance supercomputers and archiving for numerical simulations. The Excellence Cluster Universe performs state-of-the-art scientific research and the Leibniz-Supercomputing Center of the Bavarian Academy of Sciences and Humanities (LRZ) offers the best IT services for science, especially in the field of supercomputing by running machines at all performance levels up to the Top 10 in the world (SuperMUC ranked #4 in the TOP500 at commissioning).

For its specific scientific requirements, the Universe Cluster decided to procure a HPC cluster compatible with SuperMUC but exclusively reserved for its scientists, professionally operated and administered by LRZ personnel in the energy-efficient environment of the purpose-built compute center.

C²PAP personnel supports program development, optimization and data curation for new discoveries in cosmology, particle physics and the evolution of cosmic structures. This supports the smooth transition of scientific software from the desktop to the most powerful supercomputers. In summary, C²PAP is an excellent example of the optimal combination of fundamental science research and professional IT support.

Growing numerical demands which are accompanied by growing HPC facilities together with rapidly changing technologies will make concepts like C²PAP even more essential in the future.

Prof. Dr. Arndt Bode, Chairman
of the Board of Directors of the LRZ (2008-2017)

C²PAP – A SUCCESS STORY


(Credit: Andreas Heddergott)

PROF. DR.
STEPHAN PAUL (TUM)


(Credit: Astrid Eckert)

PROF. DR.
ANDREAS BURKERT (LMU)

With the renewal of the Universe Cluster in 2012, C²PAP has been established in the close neighbourhood of the LRZ in München/Garching. It resolves a problem that is becoming more and more critical in numerical physics: providing computational groups with professional software developing expertise in order to run their codes efficiently and reliably on modern supercomputers. It also serves as computational support structure and provides key computing power not present for individual research groups on the campus. The success of C²PAP has exceeded our expectations, spurring a large number of scientific developments and publications, partially unexpected.

Due to its importance and success C²PAP is a key pillar of our new cluster proposal ORIGINS. We congratulate the very active team and the management board for this success.

Prof. Dr. Stephan Paul (TUM) Prof. Dr. Andreas Burkert (LMU)
Coordinators of the Excellence Cluster Universe

The supercomputer SuperMUC at the Leibniz-Supercomputing Center. *(Credit: Johannes Naumann / LRZ)*

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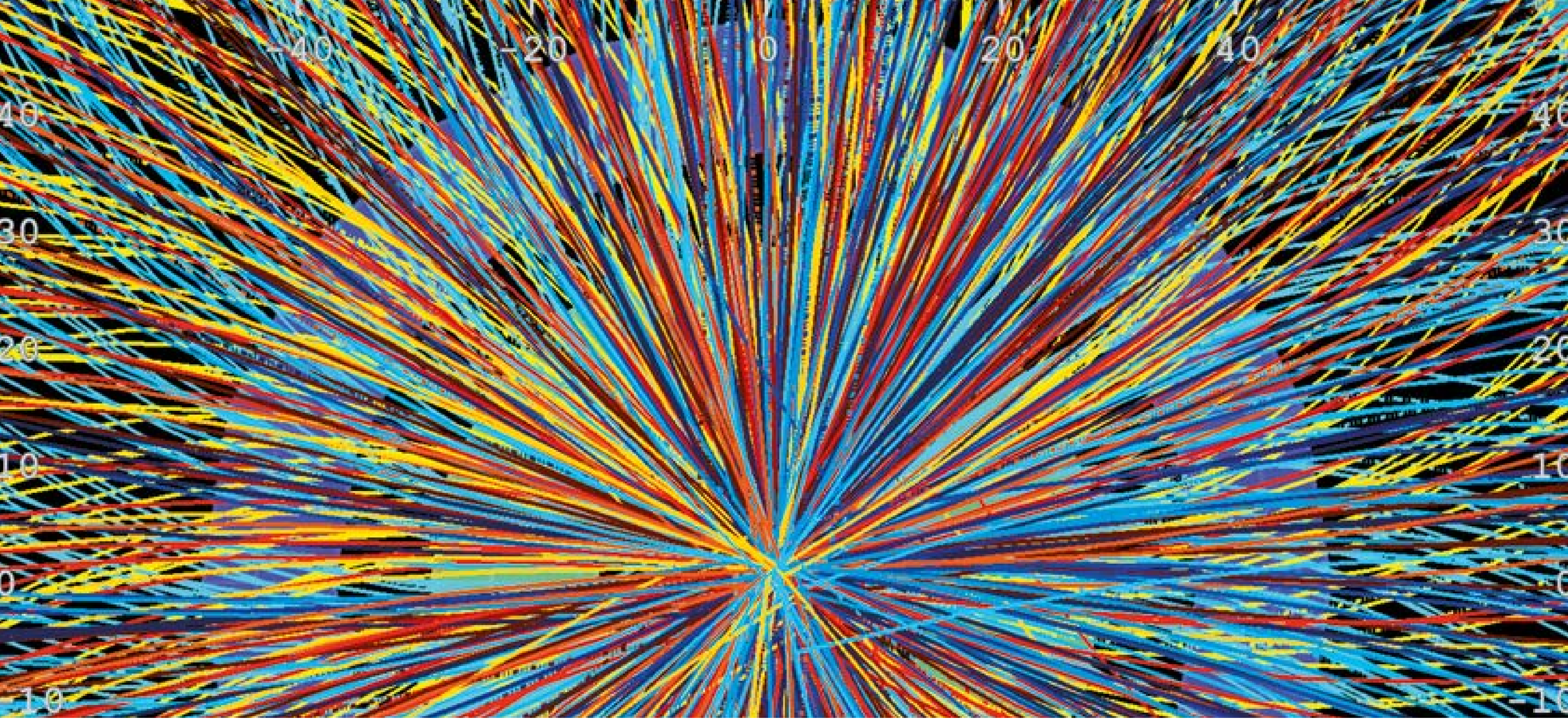

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