C²PAP – THE COMPUTATIONAL CENTER FOR PARTICLE AND ASTROPHYSICS
THE CYPAP NETWORK

ABOVE 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 development needs in astrophysics and particle physics therefore have increased significantly in recent years and will continue to increase in the future.

To meet these growing demands, the Excellence Cluster Universe is in the second period of the Excellence Initiative toward the Computational Center for Particle and Astrophysics (CYPAP). It is built around the collaboration with the Leibniz Supercomputing Centre (LRZ) and enables 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.

CYPAP operates its own computing cluster with 1084 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 and local disk storage. This provides computing resources to the members of the Universe Cluster enabling them to develop 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 the full-time staff members, CYPAP provides key personnel with 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 contact for the transfer of technical knowledge between the groups and across the different disciplines. Through regular meetings, CYPAP 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 CYPAP.

Throughout more than 100 project applications from Cluster scientists during the funding period 2012 to 2017, CYPAP 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 map shows the distribution of CYPAP proposals across the different partner institutions of the Excellence Cluster Universe.
C²PAP’S HARDWARE

- 136 compute nodes: each 64 GB RAM, 276 GB SSD
- 18 Intel Xeon CPU: 2.7 GHz
- 3 high nodes: each 128 GB RAM, 160 GB SSD, 16 Intel Xeon CPU: 2.7 GHz
- 1 “test” node: 76 GB RAM, 15 TB SSD with 20 Intel Xeon CPU: 2.7 GHz
- Network: Mellanox Infiniband 100 GbE/16 Adapters
- IBM Stratacluster system with total volume of 288 TB

C²PAP COMPUTE CLOUD

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 visualization the user 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. This allows 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 supports 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.
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 CIPAP and LKZ. A group of theorists led by CIPAP director Klaus Dolag has performed a new, unique hydrodynamical 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. CIPAP 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.
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 Antarctica. We use these maps to identify galaxy clusters from the moment of their formation. The DES is a multi-band optical imaging survey carried out from the Chilean Atacama. We use the DES data to measure the distance or redshift to each SPT selected galaxy cluster.

Measurements of the Universe Cluster have used CSPAP to validate processing pipelines that turn the 0.5-Gigapixel exposures from the Dark Energy Camera (DECam) into science-ready images and catalogs. In one demonstration run, these high efficiency pipelines were used to process an entire observing season (335 nights, 15 TBS) of DES data for science analysis over a two week period. CSPAP 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 predicted by the galaxy cluster sample, the dark energy has exhibited the properties of a constant energy density vacuum energy.
The ATLAS experiment is one of two multipurpose 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 100 journal articles including the unambiguous discovery of the Higgs boson. The 2nd phase of the LHC run-2 is ushering in 13 TeV 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 realistic predictions combined with detailed modeling of the detector responses, 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 16 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 so-called “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.

CITAP makes very valuable contributions in two ways: on the one hand we could use CITAP resources to contribute effectively to this simulation production, but more importantly, since CITAP 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 DRMAD at the Max Planck Computing and Data Facility (MPCDF), and have integrated them into the ATLAS work-flows effort significantly extending the available CPU resources. In addition, CITAP staff strongly contributed to the optimization of the ATLAS reconstruction software in order to operate it on multi-threaded or parallel computer architectures.
How does matter behave at the highest temperatures and highest densities? These questions have been investigated since 2010 by the newly formed TUNLUC collaboration led by Prof. Dr. Nora Bancelinck (CERN). They have studied hot nuclear matter through simulations on the computing clusters C’PAP and SuperHE. 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 billion degrees – which is 160,000 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-Institut für Plasma-Physik and Technik Universität München. However, collisions of ultra-relativistic heavy ions (i.e., lead) at large particle accelerators are used in order to create quark-gluon plasmas experimentally. The local group of the ALICE experiment at CERN’s Lapps Hadron Collider is committed to experimental research in this field. Such heavy ion collisions are extraordinarily complex and last for less than 10⁻²⁹ seconds. These analyses require a thorough understanding of the underlying theory. In the numerical lattice QCD simulations of the TUNLUC 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 C’PAP architecture allows simulations with either only a few or many cores, C’PAP is well-suited for studies of QGP.

One of the merits of such simulations was the determination of the temperature for lifting confinement.
DUST EVOLUTION IN PROTOPLANETARY DISKS

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, CIPAP staff provided guidance to ESO researchers Marcin Tarnok 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 observatories from millimeters to submillimeters 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 virtual collaboration, a software package named GALARIO was created and released that can compare observations to model predictions in milliseconds what previously would have required several seconds. With this speedup, much more thorough scientific analyses are now possible and the astrophysicists can again focus on the modeling rather than the computing times. The initial development of GALARIO took place at a GPU hackathon in Dresden where the participants worked up to 15 hours in a stimulating atmosphere.
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.universecluster.de/c2pap

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

<table>
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<th>YEAR</th>
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* Papers as of October 2017

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

- A: How 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?
- G: C²PAP

One project can belong to multiple research areas.
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 colored-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.

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 of 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 coauthors but have not contributed directly.
EPilogue
WHY C³PAP IS SO IMPORTANT FOR THE UNIVERSE CLUSTER

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 Bavarian Cluster Universe performs state-of-the-art scientific research and the Labe- ria 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 storing machines at all performance levels in the Top 10 in the world (SuperMAX ranked #4 in the TOP500 at commissioning).

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

C³PAP personal 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, C³PAP 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 technology together with rapidly changing technologies will make concepts like C³PAP even more essential in the future.

With the renewal of the Universe Cluster in 2013, C³PAP has been established in the close neighbourhood of the LRZ in Munich/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 C³PAP has exceeded our expectations, spawning a large number of scientific developments and publications, partially uncompleted.

Due to its importance and success C³PAP is also a pillar of our new cluster program DURASH. We congratulate the very active team and the management board for this success.

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