bwHPC Symposium 2017 Editorial

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We had the great pleasure to host the bwHPC Symposium 2017 which brought together scientists from various disciplines and IT experts from the compute centers participating in the bwHPC project[1]. The event took place in Tübingen on October the 4th 2017. We were able to secure a very appealing event location, the 'Alte Aula' of the University of Tübingen. It is one of the oldest and most historic university buildings in Tübingen, offering an appropriate ambiance for our event. The main lecture hall gave us literally a great stage for the scientific talks from various disciplines. After a brief welcome to the some 70 participants, T. Walter, director of the IT Center of the University of Tübingen, gave an introduction to the bwHPC project. He highlighted the achievements of the past years as for example the specialization on certain disciplines by participating compute centers. By hosting specialized HPC resources in conjunction with support through competence centers, optimal research environments for different communities have been established. Currently there are four bwForClusters available in the state of Baden-Württemberg, namely the Justus cluster in Ulm supporting computational chemistry, the Nemo in Freiburg for neurosciences, micro systems engineering and particle physics, the MLS&WISO in Heidelberg/Mannheim for economics, social sciences, systems biology and structural biology, and the BinAC in Tübingen for bioinformatics and astrophysics. To offer an entry level and a generic platform to cope with the needs of smaller communities, the bwUniCluster is hosted by the KIT in Karlsruhe. A unique shareholder model is in place involving university and universities of applied science alike handling operation, maintenance and user support in a collaborative manner. Special emphasis was put on future developments as the actualization of the realization concept for bwHPC and the ambitious vision to establish a statewide data federation. The keynote speech was delivered by A. Brinkmann, head of the Zentrum für Datenverarbeitung and of the Efficient Computing and Storage Group of the Johannes Gutenberg University Mainz. He shared his experiences with supporting communities with high performance computing and storage needs such as bioinformatics. Of particular interest was the argumentation about scaling of compute centers with respect to required personnel per operated compute resource. Afterwards, J. Rosskopf from the Institute of Theoretical physics gave a lively presentation about numerical methods for handling many-body-systems, clearly demonstrating that quantum effects are not only relevant in physics, but also for biology and medicine. K. Rabbertz concluded the morning sessions with insights about high precision predictions for particle collisions calculated on the NEMO cluster. He has a double affiliation at the KIT and the Cern, the later the location of the Large Hadron Collider (LHC) for which these predictions are made. For the lunch break we took a little walk through the historic city center of the beautiful town of Tübingen to have our meals at the 'Prinz Karl' university canteen. It was a pleasure to watch how the participants of the bwHPC mixed and grouped, continuing there lively discussions about scientific and HPC related topics.

The first afternoon session was started by M. Orzechowski and J. Kitowski from PL-Grid who gave an overview about federated HPC and data handling in Poland. The federate approach of their ONEDATA project addressed some challenges also present for the anticipated data federation in Baden-Württemberg. D. Thorwarth from the University Clinic in Tübingen illustrated how simulations may help to reduce the damage to healthy tissue for cancer patients undergoing radiation therapy. A. Gorska from the Algorithms in Bioinformatics Group at the University of Tübingen gave a fascinating talk about the dynamics of the human gut phageome and how it is affected during an antibiotics therapy. J. Kratzke spoke about his fluid dynamics simulations of human blood vessels which provide valuable insight for the design of aortic medical prostheses. During the following coffee break all participants had the chance to discuss various topics with the authors of the more than 16 posters presented at the bwHPC symposium. A topic drawn from life was addressed by P. Saini from the Service Operations Management Group at the University of Mannheim. Using HPC resources she explored the optimal location for small businesses such as convenient stores. I. Witte from the University of Hohenheim assessed the impact of climate change on agro-ecosystems. She employed multi-model ensemble simulations on the bwUniCluster. The final afternoon session was concluded by P. Renze head of the Institute of Energy and Drive Technologies of the Ulm Univer-

[1] www.bwhpc.de

sity of Applied Sciences. His presentation about computational fluid dynamics addressed the impact of the surface structure of tubes and pipes for different cooling devices.

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We look forward meeting all of you again on the next bwHPC symposium in 2018 in Freiburg.