The contributions to the HLRS proceedings present the results of large scale simulations for elementary particle models, nano-systems, soft matter systems and astrophysics phenomena. Several important results have been achieved by the computer time granted at the HLRS, in several cases resulting in publications in prestigious journals like Nature and Physical Review Letters.

Z.Y. Meng, T.C. Lang, S. Wessel, F.F. Assaad, and A. Muramatsu (Stuttgart University and Würzburg University) have analyzed the Hubbard model of spin-1/2 fermions on the honeycomb lattice at half-filling using large-scale quantum Monte Carlo simulations. The authors find that the weak coupling semimetal and the antiferromagnetic Mott insulator at strong interaction are separated by an extended gapped phase in an intermediate coupling regime. Exploring excitation gaps, various correlation functions as well as probing for flux quantization, they conclude that a quantum spin liquid, lacking any conventional order, emerges with local charge and spin correlations, best described by a resonating valence bonds state.

J.H. Kühn, P. Marquard, M. Steinhauser and M. Tentyukov from the KIT Karlsruhe have investigated massive and massless four-loop integrals, the computations were mainly performed on the Landeshöchstleistungsrechner XC4000. The problems treated within their project aim for the evaluation of so-called Feynman diagrams which in turn lead to quantum corrections within a given quantum field theory like Quantum Electrodynamics or Quantum Chromodynamics but also supersymmetric theories. The typical CPU time reaches from several hours to several months depending on the concrete problem under consideration. In order to be able to manipulate huge expressions a special tool is necessary. The workhorse of the authors for such calculations is the computer algebra program FORM and its parallel versions ParFORM and TFORM. The parallelization concept for FORM is quite simple: The original expression is divided into several pieces which are then distributed to the individual processors or cores (workers). Once the workers have finished their job the resulting expressions have to be collected by one processor which combines the results. A computer architecture running ParFORM or TFORM
requires a fast connection to the (in general) local hard disks of the order of one terabyte per core.

Michael Walter from the University of Freiburg studied the properties of clusters by density functional theory (DFT). The DFT calculations used in his studies were performed at the RZ Karlsruhe with the real-space grid code GPAW using a generalized gradient approximation, and the Kohn-Sham states were represented via the projector-augmented wave method. The author shows in his contribution for two experimentally characterized clusters that the super-atom-picture found for pure Au clusters applies equally well to protected Au alloy clusters. The stability of these clusters is a consequence of the 8-electron shell closing, where the elements Ag and Au donate one and the elements Pd and Pt donate no electron to the set of delocalized electrons. The author proposes the stability of clusters similar to the stable thiol protected \( \text{Au}_{25}(\text{SR}_{3})_{18} \) via the replacement of one of the Au atoms by X=Pd, Ag and Cd, and he shows, that the stability of the well known carbonyl protected nickel-silver/gold clusters is governed by delocalized electronic shell closings. The clusters not only separate sterically, but also electronically into nickel-carbonyl and silver/gold subsystems.

Ph. de Forcrand from the ETH Zürich and O. Philipsen from the University of Münster have calculated the critical surface bounding the region featuring chiral phase transitions in the quark mass and chemical potential parameter space of quantum chromo dynamics (QCD) with three flavours of quarks. Their calculations are valid for small to moderate quark chemical potentials, \( \mu \leq T \). For their Monte Carlo simulations the authors used the standard Wilson gauge and Kogut-Susskind fermion actions. Configurations are generated using the Rational Hybrid Monte Carlo (RHMC) algorithm. The simulations have been performed on the NEC SX-8 at the HLRS in Stuttgart and the EEGE Grid at CERN. An estimate of the Binder cumulant for one set of mass values consisted of at least 200k trajectories, and the estimate of a critical point required at least 500k trajectories.

Jens Smiatek from the University of Münster and Friederike Schmid from the University of Mainz in their project focused on the DPD simulation of coupled electrohydrodynamic phenomena on the microscale like polyelectrolyte dynamics in microchannels in external electric fields. The effects of electroosmotic flow and slippage combined with polyelectrolyte electrophoresis have been investigated in detail by taking full account of hydrodynamic and electrostatic interactions. All simulations in this work have been carried out by extensions of the software package ESPResSo (An Extensible Simulation Package for Research on Soft matter). One of the programs advantages is its high performance MPI-parallelisation implemented for simulations on supercomputers. The simulations have been run on the NEC SX-8 Cluster at the HLRS. The authors show that the product of the inverse screening length and the slip length massively influences the electroosmotic flow and therefore the total mobility of the polyelectrolyte. An important result of their study is that the characteristics of the boundaries have to be taken into account for a proper de-
scription of the polyelectrolyte migration dynamics. Even a negative mobility for certain parameter sets can be achieved, which has been observed in recent experiments. The characteristics of the channel walls could be used to significantly enhance flow profiles, which offers the possibility to reduce the time which is needed for polymer migration or separation techniques. This could be an important aspect for future applications in microchannels or micropumps to accelerate the measuring time in experiments.

B. Müller, L. Hüdepohl, A. Marek, F. Hanke, and H.-Th. Janka from the MPI for Astrophysics in Garching have investigated two-dimensional (core collapse) supernova by simulations and give an overview on the relevant equations and the algorithm for its solution that are employed in their code, and report on their efforts to improve the physics in their supernova code VERTEX as well as its the computational efficiency. Recent results of simulations performed on the NEC SX-8 at the HLRS include the first multi-dimensional general-relativistic neutrino transport simulations conducted with a new extension of the VERTEX code as well as simulations of neutron star cooling over several seconds for different nuclear equations of state.

Philipp Gerhold, Karl Jansen, and Jim Kallarackal from the Humboldt University and DESY Zeuthen considered a chirally invariant lattice Higgs-Yukawa model based on the Neuberger overlap operator. The model is evaluated using PHMC-simulations and the authors present final results on the upper and lower Higgs boson mass bound. The question of a fourth generation of heavy quarks has recently gained attention and the authors illustrate preliminary results of the Higgs boson mass bounds within this framework. The authors as well discuss their progress on properties of the Higgs boson with respect to its unstable nature, such as the decay width and the resonance mass of the Higgs boson.

Markus Flaig and Patrick Ruoff from the University of Tübingen studied dust, chemistry and radiation transport in magneto-rotational instability (MRI)-turbulent protoplanetary discs. The authors aim at setting up 3D protoplanetary disc models that include all the physically relevant factors, namely magnetic fields, radiation transport, chemistry and dust, in a self-consistent manner. They present results from radiative models (neglecting dust and chemistry), where for the first time radiation transport has been included into a 3D turbulent protoplanetary disc model. Their models achieve a quasi-steady state of saturated turbulence, where the turbulent heating is balanced by cooling due to radiation transport. For sufficiently high resolution, the turbulent saturation level shows a trend to converge towards a value of $\alpha \sim 2$. 