Turbulence research since the days of Leonardo da Vinci, Leonhard Euler and their successors has continuously triggered the advancement of basic science and has contributed to or even laid the foundations of various theoretical concepts like dynamical systems theory, statistical physics of systems far from equilibrium, bifurcation theory and chaos, to name but a few. Apart from being a fascinating theoretical and mathematical problem in its own right, any progress in this field is appreciated in a variety of scientific disciplines ranging from astrophysics over climate system theory to civil engineering and medicine. Still, the statistical description of fully developed turbulence remains one of the most challenging problems of classical physics. In comparison with other fields of science, like e.g. high energy physics, where field theoretical methods allow for calculations of many central quantities with incredible precision, derivations of fundamental statistical properties of turbulent fields directly from the fluid dynamical equations are, with few exceptions, still far ahead of us. The main reason for this is the non-linear and non-local character of the governing equation of motion, the Navier-Stokes equation. These properties are on the one hand responsible for the highly complex spatio-temporal patterns observable in Direct Numerical Simulations (DNS), see Figure 1. On the other hand, the same properties are also the origin of the major obstacle on the way to a statistical description from first principles, namely the closure problem: when deriving evolution equations for moments or probability density functions (PDFs) from the Navier-Stokes equation, the statistical equations contain unclosed terms, which necessitate information from higher-order moments or more points in space. When tackling the problem by analytical means only, the validity of the results depends sensitively on the approximations made, and a too crude approximation can lead to unphysical results. This is one reason why turbulence simulations on modern supercomputers have become an indispensable tool to understand the nature of turbulent flows. Hence one of the goals of the current project is to supplement the analytical treatment of the statistical problem with results from direct numerical simulations. Moreover, temporal correlations of the flow are studied along fluid particle trajectories with special respect to the acceleration acting on the particles.

Figure 1: Volume rendering of the magnitude of vorticity (left) and velocity (right) from a simulation with 512^3 grid points. The vorticity tends to organize into thin filaments forming an entangled global structure. The velocity appears less clearly structured but displays long-range correlations. Volume rendering produced by VAPOR: www.vapor.ucar.edu

Numerical Details and conducted Simulations

For the direct numerical simulations we make use of the vorticity formulation of the incompressible Navier-Stokes equation. The method used is a standard pseudospectral method [1], in which most of the computations (evaluation of derivatives etc.) are performed in Fourier space. The nonlinear term is treated in real space, reducing the computational efforts from $O(N^2)$, due to the otherwise arising convolution sums, to $O(N \log N)$ needed for the Fourier transforms. Here $N$ is the total number of grid points. Adaptive time stepping is implemented employing a third-order Runge-Kutta scheme [2]. We conduct highly resolved simulations with up to $1024^3$ grid points on a periodic domain, integrated for up to tens of thousands of time steps. Our code is MPI parallelized and employs a slab domain decomposition, enabling us to effectively use up to 1,024 cores at a resolution of 1,024 grid points. Parallel IO is incorporated by the use of MPI-IO. The Fourier transforms are performed by the freely available library FFTW [3]. Additionally, we have implemented the possibility to follow trajectories of (so-called Lagrangian) tracer particles, where relevant quantities along the tracer trajectories are interpolated from the turbulent fields with a tricubic interpolation scheme. The HLRB II at LRZ turns out to be an optimal platform for the currently implemented parallelization scheme as the individual cores are comparably performant. The results of a scaling test are presented in figure 2.

A typical simulation basically consists of two stages. First, an artificial large-scale initial condition decays for some large-eddy turnover times, during
which a turbulent flow develops. Then an external forcing is applied, and the system eventually approaches statistical stationarity. After this preparation of proper initial conditions, the actual simulation is performed. Here, the flow field is advanced in the statistically stationary state. During this period fields (velocity, vorticity, velocity gradients etc.) are stored with a sampling rate sufficient to form a statistical ensemble. The statistical analysis is performed during the post-processing stage. Optionally tracer particles are advected with the flow and stored frequently. In total, a typical 1024^3 run requires several tens of thousands of CPU hours and easily produces a terabyte of data. Within the ongoing project runs with resolutions between 256^3 and 1024^3 grid points with Taylor-based Reynolds numbers ranging from about 75 to 250 have been performed, giving insight into the Reynolds number dependence of the statistical quantities under consideration as well as resolution issues. It has turned out that long simulation durations are important for the constitution of a proper statistical ensemble. Hence, we have performed simulations for more than 100 large-eddy turnover times at a resolution of 512^3 grid points, where special emphasis has been put on an adequate resolution of the small-scale features of turbulence.

Scientific Results
Within the ongoing project a number of scientific questions have been addressed so far. The first question on the agenda has been to investigate the statistics of the single-point velocity and vorticity probability density functions within the framework of the Lundgren-Monin-Novikov hierarchy [4,5,6], a theoretical framework for the statistical description of turbulent flows introduced in the late sixties of the last century. By exploiting statistical symmetries, it has been possible to derive relations that express the single-point statistics in terms of local correlations. For example, it has been shown that the single-point velocity PDF may be expressed in terms of the conditional statistics of the pressure gradient, the external forcing and the rate of energy dissipation. For the case of the vorticity statistics, a relation expressing the PDF in terms of vortex stretching and enstrophy dissipation has been established. DNS results then have been used to assess this conditional statistics. Thereby a physical discussion of the unclosed terms has been achieved, finally explaining the often discussed slightly sub-Gaussian shape of the velocity PDF as well as the super-Gaussian shape of the vorticity PDF [7,8]. A comparison between directly estimated PDFs and the results of a consistency check of the theoretical framework is presented in figure 3. Also two-point statistics has been investigated, especially focusing on the interaction of different spatial scales. Furthermore, the simulations have been used to gather acceleration data along Lagrangian tracer particle trajectories. Here, we have analyzed the multi-time PDFs of the acceleration with respect to Markovian properties. As a result, we have found that only for very long time lags the acceleration along the trajectory can be approximated by a Markov process. This especially has implications for the modeling of Lagrangian tracer particle trajectories, which is, for example, relevant in the context of mixing and dispersion.

Outlook
By joint numerical and theoretical efforts the current project has led to a comprehensive characterization of the single-point statistics of the velocity and vorticity field, and insights into the temporal correlations in terms of the Lagrangian acceleration statistics have been gained. One of the goals for future research is to obtain deeper insights into the multi-point statistics of turbulence. This is related to one of the most challenging questions of theoretical turbulence research, namely which aspects of the fine-scale structure of turbulence are responsible for the energy and enstrophy transfer across scales. Furthermore, we aim for a deeper understanding of the Lagrangian description of fully developed turbulence with respect to the origin of Lagrangian intermittency and implications for stochastic models for particle trajectories. Direct numerical simulations of fully developed turbulence on modern supercomputers undoubtedly will continue to foster new theoretical ideas.

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References

Applications

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