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Massively Parallel Simulations of Lagrangian Plasma Turbulence

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Some of the outstanding problems in space- and astrophysical plasma systems include hydro- or magnetohydrodynamic (MHD) turbulence (e.g. in the interstellar medium). In many situations the region under consideration contains particles advected by the turbulent flow. The statistics of these particles (Lagrangian statistics) such as scaling behaviour or mass density distributions is an active field of research. Numerical simulations of fully developed turbulence demand for high resolution, an efficient parallel implementation and a powerful computational infrastructure. The main focus of this work lies on flows which can be considered as incompressible. Nevertheless, some comparisons to compressible turbulence will be drawn. We will describe the physics behind these problems and present the numerical frameworks for solving them on massive parallel computers, such as the IBM Blue-Gene architecture.

1 Introduction

In this paper we will present numerical simulations of turbulence in plasmas and neutral flows. The focus hereby is on the computation of the Lagrangian statistics, i.e. statistical properties of particles suspended in an incompressible turbulent flow.

Turbulence is one of the most important unsolved problems in classical physics. Coherent non-linear structures in turbulent flows, such as vortex filaments (see left part in Fig. 4) and current sheets play a crucial role for the subtle statistical properties. Understanding the statistics of particles advected by a turbulent flow is a challenging theoretical and numerical problem. Simulations of fully developed turbulence make great demands on the computational infrastructure and numerical methods, especially in the case of plasma turbulence.

The incompressible simulations are carried out using a pseudo-spectral solver, called LATU. This solver will be presented in detail in the following section and demands on the computational infrastructure will be discussed. Results obtained from high-resolution numerical simulations using the LATU solver will be presented in section 4. Although, most of the research on turbulence deals with incompressible flows, one encounters compressible flows in many physical circumstances. Simulations of compressible turbulence, which develop shocks (see right part in Fig. 4) need a completely different numerical solver. We use an adaptive mesh refinement framework for hyperbolic conservation laws, *racoon*. It will be presented in section 3 and results are summarized in section 4.

2 LATU: An Incompressible MHD Solver with Passive Particles

In this section a highly parallel pseudo-spectral solver, called LATU, will be presented. The code solves the magnetohydrodynamic (MHD) equations

$$\partial_t \vec{\omega} = \nabla \times \left[\vec{v} \times \vec{\omega} - \vec{b} \times (\nabla \times \vec{b})\right] + \mu \Delta \vec{\omega}, \qquad (1)$$

$$\partial_t \vec{b} = \nabla \times (\vec{v} \times \vec{b}) + \eta \Delta \vec{b}, \qquad (2)$$

$$\nabla \cdot \vec{v} = 0, \quad \nabla \cdot \vec{b} = 0, \qquad (3)$$

$\vec{v}$ denoting the velocity field, related to the vorticity by $\vec{\omega} = \nabla \times \vec{v}$, and $\vec{b}$ the magnetic field which is given in non-dimensional multiples of a reference Alfvén speed. μ, η are the kinematic viscosity, magnetic diffusivity, respectively. This set of equations regards a plasma as a conducting fluid, which is appropriate in many physical situations such as in the solar wind. The left equation of (3) establishes the condition of incompressibility.

Setting $\vec{b} = 0$ in the Equations (1) to (3) one obtains the Navier-Stokes equations, which describe the motion of a neutral fluid. These equations are commonly used for studying fully developed turbulence.

The set of equations (1)–(3) are solved using a pseudo-spectral method. The underlying equations are treated in Fourier-space, while convolutions arising from non-linear terms are computed in real-space. A Fast-Fourier-Transformation (FFT) is used to switch between these two spaces. The time scheme is a (low storage) Runge-Kutta of third order. The inter-process communication uses the Message Passing Interface (MPI). More than half of the computational time is spend on the FFTs. Therefore, an efficient implementation deserves attention. The LATU-code is able to use different implementations for the FFT-algorithm. First, it can use the MPI-parallel, portable FFTW library[1] (version 2.1.5). This library decomposes the entire domain via slab-geometry, depicted in the left part of Fig. 1. Every CPU processes an ensemble of 2D-slices. This FFT parallelizes very efficiently on mid-size computers, with up to several hundred CPUs. Apparently the number of used CPUs is limited to the number of grid points in each direction. To overcome this restriction, the LATU-code uses in addition to the FFTW the San-Diego P3DFFT library. This is a parallel interface to 1D-FFT routines. For these one dimensional FFTs one can use for example the ESSL library or the FFTW3 library. The P3DFFT permits a 2D-decomposition of the computational domain, depicted in the right part of Fig. 1. Hence, the limiting restriction concerning the number of used CPUs is weakened.

Simulations of Navier-Stokes and MHD turbulence with 1024^3 collocation points each were performed using up to 512 CPUs on the IBM p690 machine of the John von Neumann Institute in Jülich. Results of scaling tests with collocation points ranging from 512^3 to 2048 on BlueGene/L using up to 16384 processors are depicted in the left part of Fig. 2. All tests were done in the virtual node mode, i.e. both cores are used for computation. By doubling the number of processes, the performance increases by 80%, the remainder is spend on the inter-process communication. A better scalability might be achieved in the communication mode. However, the overall performance of the virtual node mode is better.

A pseudo-spectral scheme is very accurate and produces negligible numerical dissipation. This is because derivatives are computed in Fourier-space and are therefore exact. Only the need for removing aliasing errors from convolutions sums and the time scheme

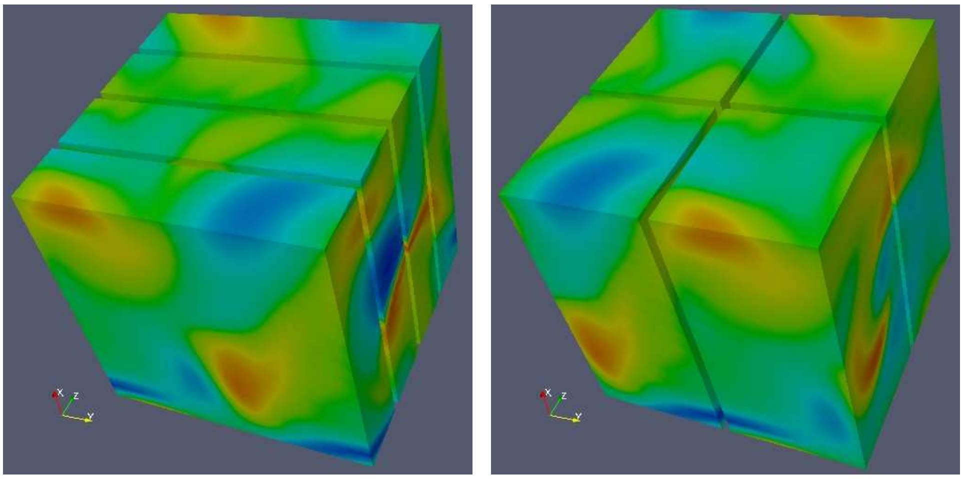

Figure 1. Partitioning of the domain for four processes. Left: slab-geometry (FFTW). Right: 2D-decomposition (P3DFFT).

yield a tiny source of dissipation. In order to choose the most adapted method of dealiasing for simulations of turbulence we compared three different strategies in the case of the Euler-equations[2]. These are obtained from the Navier-Stokes equations by neglecting viscosity and are very sensitive to the small scale accuracy of the numerical scheme. The main result is that a high-exponential cut-off is the most appropriate dealiasing strategy because it on the one hand suppresses almost all Gibbs-oscillations and on the other hand allows for significantly more physically relevant grid points than the classic 2/3-Rule.

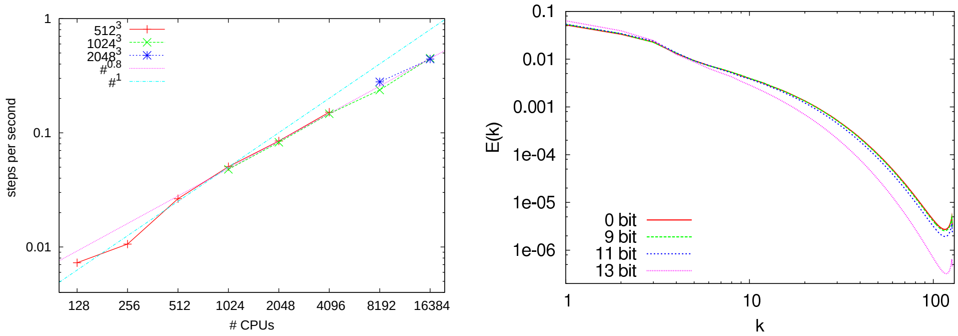

Figure 2. Left: Mixture of strong and weak scaling of the LaTu code on BlueGene/L. Right: energy-spectra for single floating-point precision simulations with an artificially reduced number of bits.

Because simulations of fully developed turbulence demand for the highest achievable computational resources, we analyzed the influence of the floating-point precision on the obtained statistical results. Therefore we artificially reduced the number of bits in the floating-point representation and compared the results to a double floating-point precision computation. It turns out[3] that single floating-point precision is sufficient up to 4096^3 collocation points (see right part of Fig. 2) and therefore allows for a larger number of grid points by a given amount of memory. In addition many super-computers process single-precision code faster than double-precision computations.

Besides solving the Navier-Stokes and MHD equations the LATU-code is able to advect a passive scalar field according to

$$\partial_t \Theta + \vec{v} \nabla \Theta = \kappa \Delta \Theta.$$

The passive scalar Θ streams according to the velocity field and is subject to diffusion with a constant parameter κ.

An important subject in the field of turbulence is the Lagrangian statistics. This statistics deals with quantities recorded along a trajectory of a fluid element (tracer particle) exposed to a turbulent flow. In order to sample the numerical domain homogeneously and to obtain reliable statistical result within a few large-eddy turn-over times, millions of particles have to be integrated. The LATU-code is able to advect tracers and particles lighter or heavier than the surrounding fluid. This provides the possibility to analyze the influence of inertia on certain statistical quantities with a single run. All particles are treated in a parallel way using MPI. We performed simulations with up to 10^7 particles on the IBM p690 machine.

The crucial point is the interpolation scheme needed in order to obtain the velocity field at the particle positions from the numerical grid. The code uses a tri-cubic interpolation scheme which on the one hand provides a high degree of accuracy[3] and on the other hand parallelizes efficiently.

In conclusion, the LATU-code provides the opportunity to gather a lot of important quantities with a single parallel high-resolution numerical simulation of fully developed turbulence both for neutral as for conducting flows. As state of art simulations demand for resolutions of 2048^3 and millions of advected particles in order to shed light on the subtle non-linear features of self-organization of turbulence, the Blue-Gene architecture provided by the John von Neumann Institute is a key infrastructure for such simulations.

3 The Framework *racoon*

All simulations of compressible turbulence use finite volume methods and are performed using the framework *racoon*[4]. Instead of taking into account the equation, $\nabla \cdot v = 0$ (in the incompressible case), in addition to the momentum equation one now solves

$$\partial_t \rho + \nabla \cdot \rho \vec{v} = 0.$$

The pressure p is given by an isothermal equation of state.

racoon is a computational framework for the parallel, mesh-adaptive solution[5] of systems of hyperbolic conservation laws like the time-dependent Euler equations in compressible gas dynamics or Magneto-Hydrodynamics (MHD) and similar models in plasma physics. Local mesh refinement is realized by the recursive bisection of grid blocks along each spatial dimension, implemented numerical schemes include standard finite-differences as well as shock-capturing central schemes[6], both in connection with Runge-Kutta type integrators. Parallel execution is achieved through a configurable hybrid of

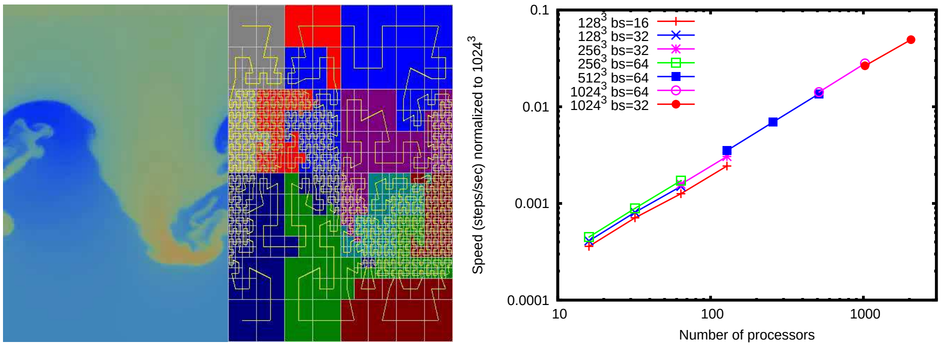

Figure 3. Left: Simulation of a Rayleigh-Taylor instability. Load balancing is based on a Hilbert curve distribution, Right: Strong scaling for different block sizes (bs) varying from 16^3 to 64^3.

POSIX-multithreading and MPI distribution with dynamic load balancing based on space-filling Hilbert curves[7] (see left part of Fig. 3).

Incompressible flows are conveniently solved using pseudo-spectral codes. Neutral incompressible flows develop coherent vortex filaments shown in the left part of Fig. 4. The formation of strong shocks in compressible gas dynamics (see right part of Fig. 4) needs a shock capturing central scheme and allows the application of adaptive mesh refining techniques (AMR)[9], so this problem is predestined to the *racoon* framework (see below). With this we examined isothermal Euler turbulence up to an effective resolution of 1024^3 cells. The right part of Fig. 4 shows the vorticity of a high Mach number compressible simulation.

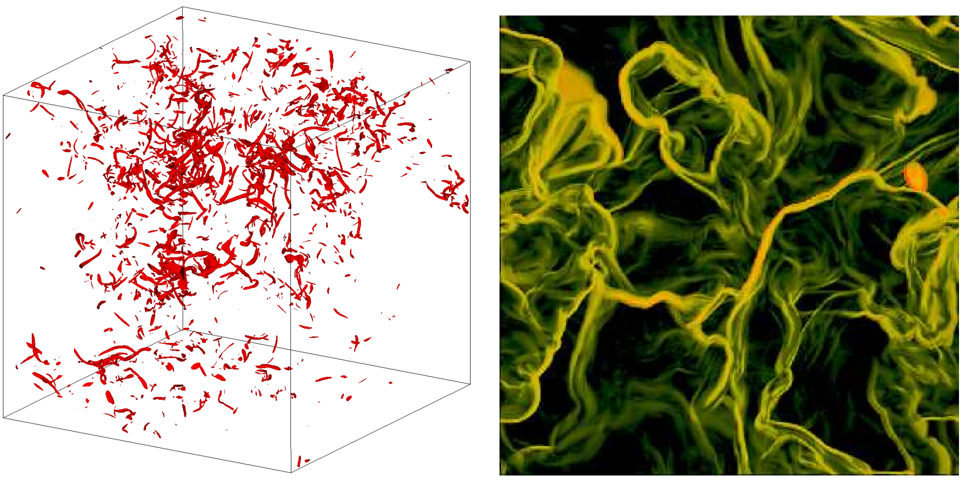

Figure 4. Dissipative structures in turbulent flows Left: Isosurface of vorticity showing vortex filaments. Right: Volume rendering of vorticity of compressible turbulence showing shock-like structures.

In compressible MHD simulation an additional problem is to assure $\nabla \cdot \vec{b} = 0$. A proper way to do this seems to be the constraint transport method[10] on a staggered grid in combination with divergence-free reconstruction[11] for the AMR.

racoon also has the ability to advect tracer particles with the flow using the same parallelization strategy as for the blocks. The main numerical work for the particle integration is spent in the interpolation routines from cell values to the actual particle positions.

Benchmarks on IBM p690 machines with 32 CPUs show that the hybrid concept in fact results in performance gain over a pure MPI parallelization, which, however requires a careful optimization of the multi-threaded implementation.

On very massively parallel machines such as the IBM BlueGene, a MPI only version is used. Scaling tests on the BlueGene/L JUBL at the FZ Jülich reveal linear scaling up to 2048 processors (see left part of Fig. 3).

4 Turbulence

Turbulence is an important and wide spread matter in today's research. From gas in molecular clouds to blood streaming through a heart valve one has to deal with turbulent flows and their properties. Although their generation is based on different forces and although they are enclosed by specific boundaries, there are features which all turbulent flows have in common.

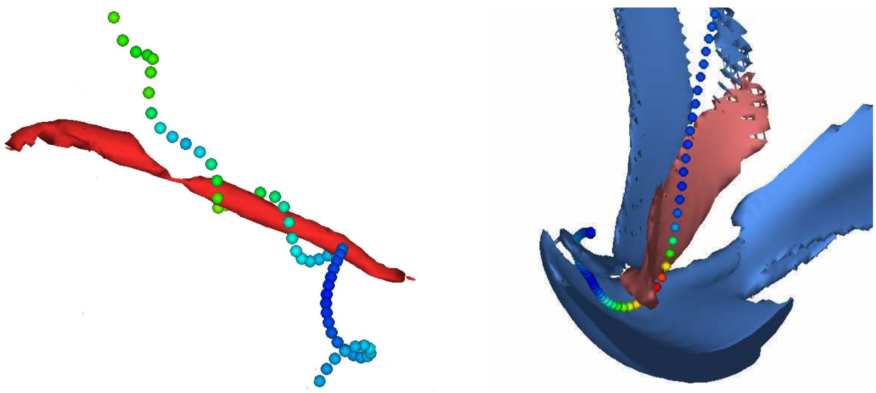

Figure 5. Particle trajectories near singular events (left: Navier-Stokes, right: MHD)

The forces and boundaries naturally act on the large scales of the motion. From these scales turbulence generates a whole range of structures of different sizes down to the smallest scales where the dissipation transforms the kinetic energy into heat. The universality sets in at scales smaller than the boundary or forcing scale down to scales larger than the dissipation scales. Here the information of the geometry and the specific dissipation mechanism of the flow is lost and the motion is completely determined by the non-linear inertial interaction of the eddies. This range is called inertial range. Physical theories often deal with fundamental features such as scaling behaviour and intermittency of this range of scales. In order to analyze its properties numerically it is necessary to provide a large amount of scales. Numerical simulations of Euler- and Navier-Stokes-turbulence revealed that a resolution of at least 512^3 collocation points is needed to obtain an inertial range of scales within a turbulent flow.

Lagrangian statistics of turbulent neutral and magnetohydrodynamic flows has undergone a rapid development in the last 6 years to enormous progress in experimental techniques measuring particle trajectories[12]. Lagrangian statistics is not only interesting for obtaining a deeper understanding of the influence of typical coherent or nearly-singular structures in the flow but also of fundamental importance for understanding mixing, clustering and diffusion properties of turbulent astrophysical fluid and plasma flows.

Concerning the incompressible case we computed the Lagrangian statistics of MHD- and neutral turbulence. The comparison revealed the intriguing and differing influence of the flow structures on the Eulerian and Lagrangian statistics[13] (see Fig. 5). The issue of intermittency was addressed by the computation of probability density functions (PDFs) and structure functions and comparison to a multifractal model[14].

An up to now poorly understood problem in the measured Lagrangian statistics is the absence of a clear scaling range. Even the largest numerical simulations, which do show a spatial scaling range in the Eulerian framework, lack of a temporal scaling range. We addressed this issue by introducing a new time increment[15], which shows a clear scaling range (see left part in Fig. 6) and identified the large scale sweeping as a possible cause of the spoiled scaling range of the standard increment.

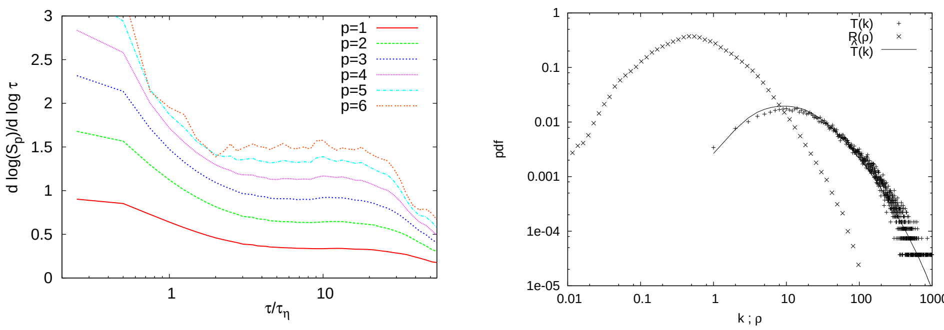

Figure 6. Left: Logarithmic derivative of structure functions of the novel time increment showing plateau and therefore a clear scaling range in incompressible turbulence, Right: The mass density PDF $R(\rho)$ (x), the measured particle distribution T (+) and the theoretical prediction $\hat{T}$ (solid line) in compressible turbulence.

A significant difference in the Lagrangian statistics between the incompressible and compressible case is found for the mass distribution of the tracers. While one finds Poisson-distributions resembling homogeneity for incompressible flows, tracers cluster in compressible flows. We found an explanation[16] for the PDF of the spatial particle distribution as a counterpart of the mass density field (see right part in Fig. 6).

References

1. FFTW library, `http://www.fftw.org`.
2. T. Grafke and H. Homann and J. Dreher and R. Grauer, *Numerical simulations of possible finite time singularities in the incompressible Euler equations: comparison of numerical methods*, to appear in Physica D, doi:10.1016/j.physd.2007.11.006.
3. H. Homann and R. Grauer, *Impact of the floating-point precision and interpolation scheme on the results of DNS of turbulence by pseudo-spectral codes*, Comp. Phys. Comm. **177**, 560–565 (2007).
4. J. Dreher and R. Grauer, *Racoon: A parallel mesh-adaptive framework for hyperbolic conservation laws*, Parallel Comp. **31**, 913–932 (2005).
5. M.J. Berger, P. Colella, *Local adaptive mesh refinement for shock hydrodynamics*, J. Comp. Phys. **82**, 64–84 (1989).
6. A. Kurganov, E. Tadmor, *New high-resolution central schemes for nonlinear conservation laws and convectiondiffusion equations*, J. Comp. Phys. **160**, 241–282 (2000).
7. G.W. Zumbusch, *On the quality of space-filling curve induced partitions*, Z. Angew. Math. Mech. **81**, 25–28 (2001).
8. R. Rabenseifer, *Hybrid Parallel Programming on HPC Platforms*, Fifth European Workshop on OpenMP, Aachen (2003).
9. A. Kritsuk, M. L. Norman, P. Padoan, *Adaptive mesh refinement for supersonic molecular cloud turbulence*, The Astrophysical Journal **638**, L25-L28 (2006).
10. U. Ziegler, *A central-constrained transport scheme for ideal magnetohydrodynamics*, J. Computat. Phys. **196**, 393–416 (2004).
11. D. S. Balsara, *Second-Order-accurate Schemes for Magnetohydrodynamics with Divergence-free Reconstruction*, The Astrophysical Journal Supplement Series **151**, 149–184 (2004).
12. A. La Porta, G. A. Voth, A. M. Crawford, J. Alexander and E. Bodenschatz, *Fluid particle accelerations in fully developed turbulence*, Nature **409**, 1017–1019 (2001).
13. H. Homann, R. Grauer, A. Busse and W.C. Müller, *Lagrangian Statistics of Navier-Stokes- and MHD-Turbulence*, J. Plasma Phys. **73**, 821–830.
14. L. Biferale, G. Boffetta, A. Celani, B. J. Devenish, A. Lanotte and F. Toschi, *Multifractal Statistics of Lagrangian Velocity and Acceleration in Turbulence*, Phys. Rev. Lett. **93**, 064502 (2004).
15. R. Friedrich, R. Grauer, H. Homann and O. Kamps, *A Corrsin-type approximation for Lagrangian Fluid Turbulence*, submitted to Phys. Rev. Lett. (2007), arXiv:0705.3132v1 [physics.flu-dyn].
16. Ch. Beetz, Ch. Schwarz, J. Dreher, and R. Grauer, *Density-PDFs and Lagrangian Statistics of highly compressible Turbulence*, submitted to Physics Letters A, arXiv:0707.1798v1 [physics.flu-dyn].