RWTH Aachen University

Project Thesis

Investigations on one-way coupling effects of particle-laden decaying isotropic turbulent flows

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2 Introduction

in Computational Methods for Multiphase Flow ist auf den Seiten 3-9 ein interessantes Beispiel.

3 Mathematical models

Sollen wir hier noch isotrope Turbulenz etc. erklaeren? Entdimensionierung erklären (Christain), Kolmogorov Skala (Steffen), Stokes-Zahl, ψ einführen als coupling rate einführen

3.1 Single-phase flow

In this section the mathematical basics for understanding and simulating turbulent flows are discussed. However, it should be pointed out that this is no complete treatise of the mathematical and physical basics. The reader can achieve further insight on this topic by looking at different books and papers, e.g. [7].

3.1.1 The Navier-Stokes equations

The Navier-Stokes-Equations are of great importance for understanding turbulent phenomena. This set of equations exists in forms for compressible and incompressible fluids. For an infinitesimal small volume element $\mathrm{d}\tau$ and using the cartesian coordinate system, they can be written in the so-called 'divergence form':

$$\frac{\partial \boldsymbol{Q}}{\partial t} + \boldsymbol{\nabla} \boldsymbol{H} = 0 \tag{3.1}$$

It should be noted by the reader that this work only contains investigations about chemically inert fluids and particles, and that the simulation results only fit under this condition. The vector $\boldsymbol{Q}$ contains all the variables which are conserved, i.e. the density ρ, the velocity $\boldsymbol{u}$ and the specific inner energy E:

$$\boldsymbol{Q} = \begin{pmatrix} \rho \\ \rho \boldsymbol{u} \\ \rho E \end{pmatrix} \tag{3.2}$$

$\boldsymbol{H}$ is the flux vector which stores all the floating variables and may be split up into two parts:

$$\boldsymbol{H} = \boldsymbol{H}^{\mathbf{i}} + \boldsymbol{H}^{\mathbf{v}} \tag{3.3}$$

The contents of the two vectors are displayed below:

$$\boldsymbol{H}^{\mathbf{i}} = \begin{pmatrix} \rho \boldsymbol{u} \\ \rho \boldsymbol{u}\boldsymbol{u} + p \\ \boldsymbol{u}(\rho E + p) \end{pmatrix} \tag{3.4}$$

$$\boldsymbol{H}^{\mathbf{v}} = -\frac{1}{Re} \begin{pmatrix} 0 \\ \boldsymbol{\tau} \\ \boldsymbol{\tau}\boldsymbol{u} + \boldsymbol{q} \end{pmatrix} \tag{3.5}$$

$\boldsymbol{H}^{\mathbf{i}}$ is called inviscid flux and contains only the variables that are independent of the fluids viscosity, it describes the way a fluid with zero viscosity would behave. In contrast, the viscous flux $\boldsymbol{H}^{\mathbf{v}}$ represents the effects of viscosity. The Reynolds number $Re = \frac{\rho v d}{\eta}$ is defined to be the ratio of inertia to tenacity, which makes it very valuable for understanding turbulent flows. This is also due

to the fact that two familiar objects with the same Reynolds number behave similar in turbulence. One can assume that flows with $Re << 1$ are laminar and flows with $Re >> 1$ are turbulent. To solve the Navier-Stokes-Equations, more information regarding some variables is required. For Calculating the specific inner Energy E and the heat conduction $\boldsymbol{q}$, the following equations are used:

$$E = e\frac{1}{2}|\boldsymbol{u}|^2 \tag{3.6}$$

$$\boldsymbol{q} = -\frac{\mu}{Pr(\gamma - 1)}\boldsymbol{\nabla} T \tag{3.7}$$

with

$$\gamma = \frac{c_p}{c_v} \tag{3.8}$$

and the Prandtl number

$$Pr = \frac{\mu_\infty c_p}{k_t} \tag{3.9}$$

using the specific heat capacities of the fluid c_v and c_p. If one could assume that the fluid is a newtonian fluid, the linear correlation between stress and the rate of strain results in:

$$\boldsymbol{\tau} = 2\mu\boldsymbol{S} - \frac{2}{3}\mu(\boldsymbol{\nabla} * \boldsymbol{u})\boldsymbol{I} \tag{3.10}$$

in which $\boldsymbol{S} = \frac{(\boldsymbol{\nabla u})(\boldsymbol{\nabla u})^T}{2}$ denotes the rate-of-strain-tensor. Additionally, the viscosity μ can be aprroximated through Sutherland's law, which is based on the ideal gas-theory:

$$\mu(T) = \mu_\infty(\frac{T}{t_\infty})^{3/2}\frac{T_\infty + S}{T + S} \tag{3.11}$$

S is in this case the Sutherland temperature. To achieve closure the caloric state equation $e = c_v T$ and the state eqaution for an ideal gas $p = \rho RT$ are used. The specific gas constant is determined by $R = c_p - c_v$. These equations form a set of partial differential equations, so for solving them starting values are needed. These are initialized at the first timestep of the simulation. To achieve physical solutions, 150 timesteps are computed before the particles are initialized, so the turbulence can evolve from the synthetic values to a natural flow field.
Christoph Siewert: -2.1 bis 2.6 Stephan Fritz: -Navier-Stokes-Gleichungen (Anhang B) Randbedingungen?

3.2 Particle dynamics

Siewert: -3.1a-3.14 (spherical particles) OHNE GRAVITATION Stokes Drag/Stokes Coefficient Filterung (Fritz) -¿Viskositaet durch numerischen Fehler, Smagorinksy nicht benutzen

To get a usefull equation of motion for the particles in the flow, we use the Euler Lagrangian approach, as it is common in Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES). In this work we deal with small and heavy particles, that have a spherical shape. Their radius r_p is even smaller than the Kolmogorov scale η, but also large enough to neglect the Brownian motion. The density of the particles ρ_p is much higher than that of the fluid ρ_f . In addition due to the very low particle concentration we can neglect the influence of the particles on the mean flow and on each other. This simplification is called one-way coupling. That means that the particles can cross each other without any effect. That means particle collisions are neglected. After all this simplifications we obtain a simplified version of the Maxey-Riley equations.

$$\frac{\partial \boldsymbol{x_\mathrm{p}}}{\partial t} = \boldsymbol{v_\mathrm{p}} \tag{3.12}$$

$$\frac{\partial \boldsymbol{v_\mathrm{p}}}{\partial t} = \frac{f_\mathrm{D}}{\tau_\mathrm{p}}(\boldsymbol{u(x_\mathrm{p})} - \boldsymbol{v_\mathrm{p}}) \tag{3.13}$$

It shows that the particle motion is only depending on the the hydrodynamical drag force which results out of the actual difference between the fluid velocity $\boldsymbol{u(x_\mathrm{p})}$ at particle position $\boldsymbol{x_p}$ and the particle velocity $\boldsymbol{v_p}$. τ_p is the particle response time and a factor to obtain the drag force in Stokes flow conditions. To take the case of an Reynolds number $\Re$ of order 1 into account the correction factor

$$f_D = 1 + 0.15 Re_p^{0.687} \tag{3.14}$$

is used. The biggest simplification of this Lagrangian approach is that the interaction of particles coming close together is neglected.

4 Numerical methods

To simulate flows like those described above we have two options. The direct numerical simulation (DNS) is the easier one to understand, although it is numerically very expensive. The Large-eddy simulation (LES) is numerically more capable, still we must accept certain inaccuracies. These two numerical methods are now discussed in the following chapter.

4.1 Direct numerical simulation

The basis of the direct numerical simulation (DNS) are the Navier-Stokes equations as described above. The idea is that the computer is very good at calculating and solves these equations completely. This provides a very accurate result, as all scales of motion are being resolved. Still it requires an immense level of comptational resources which increases rapidly with the Reynolds number. These computational resources were not available until the 1970s. Even though it is not advisable to resolve every scale of motion, if only the contained energy is of greatest interest. With the large-eddy simulation, as described below, the comptational effort is 99.98 % less compared to DNS, which indeed is the fraction of the dissipative scale. This leaves 0.02 % of the flow, which is correlative with the fraction of the energy-containing larger-scale [7].

4.2 Large-eddy simulation

Due to the fact that DNS is effortful and wasting resources if a fully resolved resolution is not required, large-eddy simulation (LES) was created to save time and resources. This is especially efficient if mainly the temproal energy trend is considered, because the energy containing larger-scale motion is completely resolved and the indeed small effects of the expensive smaller-scale motion are just modelled. Otherwise in DNS resolving the small dissipative scale would require most of the computational resources.
Simulating only the larger-scale motions is also called filtering, which means that the smaller-scale motions are filtered out. To model the filtered smaller-scale motions ususally a subgrid-scale (SGS) model is used. According to Hickel (2007) the interference between explicit SGS and the trunctation error can be exploited, i.e. the trunctation error can serve as model of the effects of unresolved scales, which is therefore an implicit SGS model. Thus we call it implicit LES (ILES) [5].

4.3 Discretisation

To integrate the Lagrangian particle tracking equations, discussed above, a predictor-corrector scheme based on the trapezoidal rule for numerical integration

$$f(t+\delta t) \approx f(t) + \frac{\delta t}{2}\left[\frac{\partial f(t)}{\partial t} + \frac{\partial f(t+\delta t)}{\partial t}\right] \tag{4.1}$$

is used.
The first step is the prediction of the new particle position $\boldsymbol{x}_{n+1}^{(\mathrm{p})}$ using a Taylor

expansion for a small time step δt

$$\boldsymbol{x}_{n+1}^{(\mathrm{p})} = \boldsymbol{x}_n + \delta t \boldsymbol{v}_n + \frac{1}{2}\delta t^2 \boldsymbol{a}_n. \tag{4.2}$$

Due to the computational effort we will put $\boldsymbol{u}_{n+1}^{(\mathrm{p})}$ on the level of the nearest cell fluid velocity.
The updated velocity and acceleration are calculated as

$$\boldsymbol{v}_{n+1} = \frac{\boldsymbol{v}_n + \frac{1}{2}\delta t \left(\boldsymbol{a}_n + \frac{f_\mathrm{D}}{\tau_\mathrm{p}} \boldsymbol{u}_{n+1}^{(\mathrm{p})} + \boldsymbol{g}\right)}{1 + \frac{1}{2}\frac{f_\mathrm{D}}{\tau_\mathrm{p}}\delta t}, \tag{4.3}$$

$$\boldsymbol{a}_{n+1} = \frac{\frac{f_\mathrm{D}}{\tau_\mathrm{p}} \left(\boldsymbol{u}_{n+1}^{(\mathrm{p})} - \boldsymbol{v}_n - \frac{1}{2}\delta t \boldsymbol{a}_n\right) + \boldsymbol{g}}{1 + \frac{1}{2}\frac{f_\mathrm{D}}{\tau_\mathrm{p}}\delta t}. \tag{4.4}$$

The updated particle position must be corrected by an additional term according to the trapezoidal rule

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \frac{1}{2}\delta t \left(\boldsymbol{v}_{n+1} + \boldsymbol{v}_n\right) + \frac{1}{12}\delta t^2 \left(\boldsymbol{a}_{n+1} - \boldsymbol{a}_n\right). \tag{4.5}$$

4.4 Particle clustering

The high number of point particles require even more computational resources for the particle-laden simulation. The main idea to reduce this requirement is to create clusters of point particles, meaning that a new variable m_c is introduced. We consider a cluster of m_c point particles as one larger point particle, i.e. the programm has less particles to simulate. To compensate this lack of particles, the coupling force is multiplied by m_c, due to the m_c-fold mass of the (cluster-)particles. In chapter 5 (results) we evaluate the legitimacy of particle clustering and the maximum acceptable value of m_c.

Projektion (noComputationalParticles), Diskretisierung implizite LES (Motivation fuer LES - Pope Chapter 9, Bild 9.4), DNS

5 Results

5.1 Boundary conditions and simulation properties

The simulations where carried out using ZFS, the simulation tool developed and implemented at the Institute of Aerodynamics at RWTH Aachen University [1] [2]. The tool is capable of simulating finite-volume flows of compressible fluids. In this case the turbulence was simulated on a cubic grid using 64^3,96^3,128^3 and 256^3. The first three cases where simulated using LES, the case in which 256^3 cells where used is carried out as DNS. Futher information can be gained by looking at [7, p.344-357 for DNS and p. 558-639 for LES]. For simplification, the special case of isotropic turbulence was used. For this idealised flow form the statistical velocities are invariant in all directions of the grid. It follows that the flows velocity are invariant for rotations and reflections. The turbulence was initialised using a seed-based random generator. To achieve physical results, the simulation was carried out to timestep 150, at which a restart file was written out. This procedure insures a fully developed turbulent flow, which has emancipated from the initialisation. In this flow field, a specific number of spherical particles were injected. The velocties of the fluid were interpolated for each particle to match the velocities of particles and fluid as accurately as possible.

Parameter der Simulationen Coupling Rate in Zusammenhang mit den unterscheidlichen noComputationalParticles

boundary conditions, for example Reynolds number?

Graphen (particleFree rot, Laden gruen)

6 Conclusion

7 References

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