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Large Eddy Simulation für turbulente, nicht vorgemischte Verbrennung

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Zusammenfassungen

SAM: Eine neuartige, multidimensionale Lagrange Transportmethode höherer Ordnung wurde entwickelt. Die neue Methode basiert auf der Beschreibung von Fluidelementen als Lagrange-Finite Volumen, welche transportiert und deformiert werden. Explizite, kardinale Interpolationenen werden gebraucht, für die Interpolation der Fluidelemente auf ein fixes Rechengitter.

Während den Untersuchungen wurde das komplette Set der orthogonalen Polynome mit einem Ooptimum an Approxiamations-Eigenschaften entwickelt. Die optimalen Eigenschaften sind Regulatität und „compact support".

LTNT: Als Teil des Projektes wurden LES Berechnungen an einer kalten „Bluff Body"-Strömung durchgeführt und die Resultate wurden mit denjenigen einer bestehenden U-RANS Berechnung verglichen.

Anschliessend wurde eine Literaturstudie zum Thema Kopplung von Flamelet-Modellen mit der LES-Strömungsberechnung durchgeführt. Die Modellierung der slalaren Dissipation erweist sich hier als Schlüsselgrösse, es bieten sich eine ganze Reihe von Möglichkeiten an, die in der nächsten Projektphase ausgetestet werden.

LAV: Das Problem der Smagorinksy Large-Eddy-Simulations (LES) Modelle, welche zur Beschreibung der Geschwindigkeitsfluktuationen Statistiken 2. Ordnung verwenden, ist die Erhöhung der räumlichen Auflösung mit zunehmender Reynolds-Zahl, proportional zu $Re^{8/4}$ (Direkte Numerische Simulation ~$Re^{9/4}$). Um den Anstieg der räumlichnen Auflösung von LES mit zunehmender Reynolds-Zahl zu reduzieren wurde eine Modell-Modifikation ("Intermittency Correction") vorgeschlagen. Die Modifikation wurde für inkompressible Kanalströmungen getestet. Die Resultate zeigen deutlich das Potenzial einer solchen Modifikation in Bezug auf die Reduktion der räumlichen Auflösung und daraus resultierend, der Rechenzeiten.

Das LES-Modell "Approximate Deconvolution Model", wurde in ein inkompressibles spektrales Element-Programm implementiert. Der Aspekt der Filterung wird im Bericht kurz erläutert.

1. Large Eddy Simulation of Non-premixed Combustion using a Truly Multidimensional Explicit Transport Method and High-resolution Stochastic Sub-grid Models

(**Part 1.** A Truly Multidimensional High-order Lagrangian Transport Method)

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Introduction

Large Eddy Simulation is a numerical tool where the large vortex structures in a fluid are solved explicitly over a coarse mesh. It is important that the numerical method used to simulate the dynamics of these structures produces very low numerical diffusion. Large numerical diffusion could dominate the diffusion process of the simulation and induce large errors into the sub-grid structures.

In Finite Volume methods one source of large numerical diffusion is the straightforward dimensional splitting of the equations in each coordinate direction. The cross derivatives are simply not taken into account in the numerical approximations and therefore the numerical errors are dependent on the flow direction. Even if one-dimensional high order schemes are used in each direction, the overall accuracy is still low due to the lack of fluxes through the corners. The finite character of the fluid elements and the discrete time steps force the schemes to include the multidimensionality in a coupled manner. The original idea of simple one-dimensional splitting of the equations is valid only in the analytic limit when the volume of the elements is zero.

It has been investigated at the Seminar of Applied Mathematics of the ETH-Zurich, that the spatial splitting of fluxes used in multidimensional finite volume codes is not truly multidimensional and produces large errors (numerical diffusion) when the main flow direction is not inline with the coordinate directions. A solution to this problem is the Method of Transport (MoT) [2], where truly multidimensional fluxes are computed. Unfortunately, this method contains complicated expressions if high order accuracy is to be achieved.

Following the same philosophy of the MoT, we propose the development of a compressible Lagrangian-transport method. In this method the equations are integrated along fluid element trajectories represented by Lagrangian Finite Volumes. In one discrete time step these volumes deform and an explicit algebraic mapping is used to interpolate the transported quantities back to a fixed Cartesian mesh.

During this research we have discovered the complete Orthonormal Spline Basis that we have named Z-splines. They are the unique piecewise polynomial solution to the general interpolation problem of minimum compact support, and successive maximum smoothness and accuracy.

All the fluid properties are represented by the Z-spline basis. The Z-splines provide a stable and highly accurate extension of the discrete fluid properties to the continuous space and therefore any source term given in integral or differential form is computable in perfect consistency with the numerical representation. In this context, the source terms are computed with multidimensional finite difference approximations and interpolated to the discrete positions along the trajectories. The same interpolation technique is used to reinitialise the fields at the end of a Runge-Kutta integration step in order to avoid further problems due to large Lagrangian-grid distortion. The mapping and the interpolation are achieved with the Z-spline functions. The Lagrangian Transport Method is truly multidimensional, local, explicit, high order in time and space, and produces negligible numerical diffusion. Domain decomposition for parallel processing with the MPI standard and immersed boundaries to represent complex geometries are straightforward.

The Lagrangian Transport Method

The Lagrangian Transport Method is based on the solution of the homogeneous transport equation

$$\frac{d}{dt}a(x,t)=\frac{\partial}{\partial t}a+u\cdot\nabla a=0$$

where the velocity field *u=u(x,t)* is used to integrate the Lagrangian trajectory of every point in the domain, given by the characteristic equations

$$\frac{d}{dt}x(x_0,t)=u(x,t)$$

The scalar function *a=a(x,t)* is conserved along the trajectory, no diffusion or waves are present.

In the numerical method, the fields *a=a(x,t)* and *u=u(x,t)* are represented on a three-dimensional Cartesian mesh. The integration of the trajectory of every point on the mesh is done with an explicit Runge-Kutta method. After every time step the "moved" field *a=a(x,t)* has the be interpolated back to the original Cartesian mesh in order to avoid too much deformation of the fluid elements and therefore the divergence of the method. The elements are then re-initialized on the Cartesian mesh after every time step.

Interpolation from the deformed mesh

The interpolation from the "deformed" Lagrangian Finite Volumes is achieved through the inversion of a non-linear mapping. The Lagrangian Finite Volumes are defined by the coordinates of the *8* corner points (for a linear Z-spline Finite Volume), *64* neighboring points (for a cubic Z-spline Finite Volume), or more points for higher order Z-splines. The coordinates of the corners in the mapped space $\xi=(\xi,\eta,\zeta)$ are defined as integer numbers on a Cartesian mesh, such that, in order to represent a point *x=(x,y,z)* given $\xi=(\xi,\eta,\zeta)$, it is necessary to use the cardinal spline interpolation formula of order *2m-1*

$$x(\xi,\eta,\zeta)=\sum_i x(\xi_i,\eta_i,\zeta_i)Z_m(\xi-\xi_i)Z_m(\eta-\eta_i)Z_m(\zeta-\zeta_i)$$

where $x(\xi_i,\eta_i,\zeta_i)$ are the coordinates of the corners of the Lagrangian Finite Volumes.

Any point inside each Lagrangian Finite Volume can be represented in the coordinates $\Delta\xi=(\Delta\xi,\Delta\eta,\Delta\zeta)$ through the inversion of a non-linear mapping given by the Taylor series expansion around the local Lagrangian coordinates $\xi=(0,0,0)$

$$\begin{aligned}
\Delta x &= x_\xi\Delta\xi + x_\eta\Delta\eta + x_\zeta\Delta\zeta + x_{\xi\eta}\Delta\xi\Delta\eta + x_{\xi\zeta}\Delta\xi\Delta\zeta + x_{\eta\zeta}\Delta\eta\Delta\zeta + x_{\xi\eta\zeta}\Delta\xi\Delta\eta\Delta\zeta + \dots \\
\Delta y &= y_\xi\Delta\xi + y_\eta\Delta\eta + y_\zeta\Delta\zeta + y_{\xi\eta}\Delta\xi\Delta\eta + y_{\xi\zeta}\Delta\xi\Delta\zeta + y_{\eta\zeta}\Delta\eta\Delta\zeta + y_{\xi\eta\zeta}\Delta\xi\Delta\eta\Delta\zeta + \dots \\
\Delta z &= z_\xi\Delta\xi + z_\eta\Delta\eta + z_\zeta\Delta\zeta + z_{\xi\eta}\Delta\xi\Delta\eta + z_{\xi\zeta}\Delta\xi\Delta\zeta + z_{\eta\zeta}\Delta\eta\Delta\zeta + z_{\xi\eta\zeta}\Delta\xi\Delta\eta\Delta\zeta + \dots
\end{aligned}$$

The displacements $(\Delta x,\Delta y,\Delta z)$ are known. The derivatives at $\xi=(0,0,0)$, including all cross derivatives, are computed through the products of the derivatives of the corresponding multidimensional Z-splines.

The non-linear mapping given by the Taylor series expansion is inverted using Newton's method in three dimensions. The values of $\Delta\xi=(\Delta\xi,\Delta\eta,\Delta\zeta)$ are computed up to machine precision in a few iterations (typically four). The initial guess is given by the direct inversion of the linear problem without the cross derivatives.

The *routine* to compute $\Delta\xi=(\Delta\xi,\Delta\eta,\Delta\zeta)$ must check if the computed coordinates lie on the interval *[0,1)* and, if out of bound, the it computes them again inside the correct Lagrangian Finite Volume.

Results

The Orthonormal Piecewise Polynomial Basis: Z-splines

The complete family of orthonormal piecewise polynomials has been discovered as a sub-product of this research. The basis consists of Hermite-Birkhoff curves $Z_m=Z_m(x)$ of degree and order *2m-1* that represent explicit finite differences computed by Taylor series expansions. One-sided Z-splines and arbitrary-interval Z-splines have been also engineered such that the Z-splines are the explicit solution to the general interpolation problem.

A publication of the general theory of the Z-splines has been prepared for submission. In the paper a detailed analysis of their properties is achieved. The Z-splines are the unique piecewise polynomial solution to the general interpolation problem of minimum compact support and successive maximum accuracy and regularity (smoothness). It has been proven that the following properties are equivalent for the Z-splines:

1) They represent exactly polynomials of degree or equal than *2m-2*.
2) They conserve the first *2m-1* discrete moments of the interpolated data.
3) They have unity zero integral moment and *2m-2* vanishing higher integral moments.
4) They have *(2m-1)*-th order of accuracy.
5) Their Fourier transform is unity at wave number zero and has zeroes of order *2m-1* at the multiples of 2π.
6) They are the best piecewise polynomial approximation to the perfect reconstruction filter *sinc(x).*

The properties of the Z-splines have also been observed numerically. The easiest test is the vanishing moments property. A graphic representation of the theory of the orthonormal piecewise polynomial basis is presented in Fig. 1.

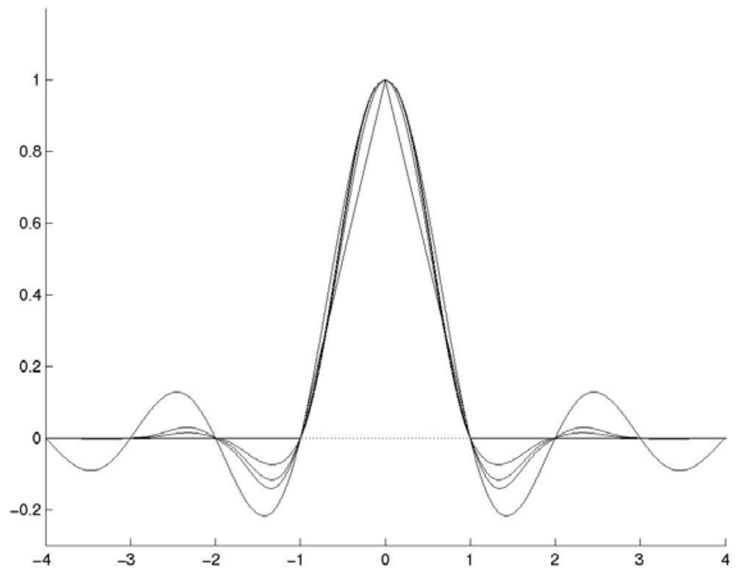

Figure 1: The first four z-splines and the sinc(x).

Convergence of the High-order Lagrangian Transport Method

The convergence of the high-order Lagrangian Transport Method has been observed numerically. The code has been named *LESReact* and it has been tested for the case of inviscid Green-Taylor vortices given by

$$u = -2\pi\cos(2\pi x)\sin(2\pi y)$$
$$v = 2\pi\sin(2\pi x)\cos(2\pi y)$$
$$w = 8\pi^2\cos(2\pi x)\cos(2\pi y)$$

where u and v are the horizontal and vertical velocity components and w is the vorticity. The convergence of the method is observed computing the L_2-error of the analytic solution (invariant of time) compared with the numerical solution after one time step for a fixed CFL = 0.5. The results are shown in Fig.2 for linear Finite Volumes (solid line) and cubic Finite Volumes (dashed line). Linear, cubic and fifth order interpolations are compared.

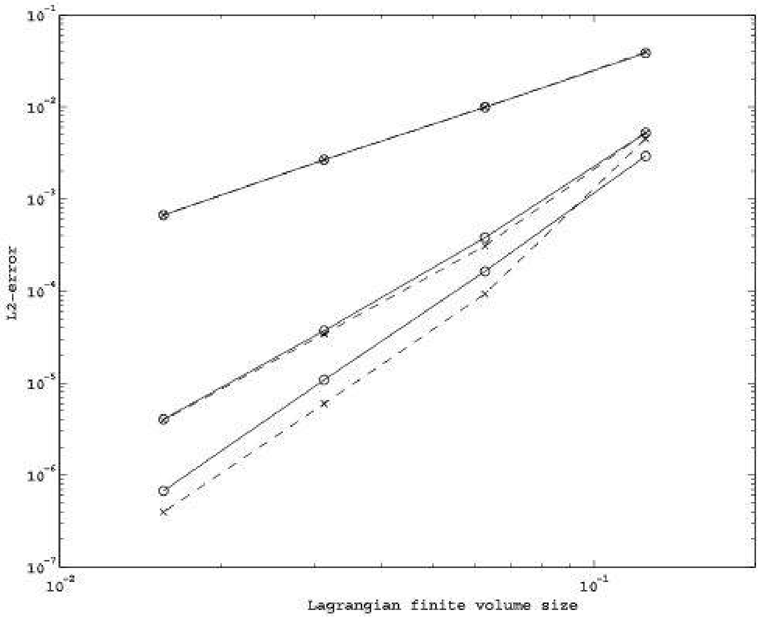

Figure 2: Convergence of the Lagrangian transport method for linear (solid line) and cubic (dashed line) elements.

Summary 2002 and Future Plans

The discovery of the orthonormal piecewise polynomial basis has allowed to construct a high-order, truly multidimensional, Lagrangian transport method. The low numerical diffusion of this method will be a strong basis for a Large Eddy Simulation code. The transformation of the actual code to a Navier-Stokes solver will be based on the analytic representation of the physical variables given by the Z-splines. Differentiation and integration can be done analytically, reducing to the application of convolution kernels.

In the near future the code will be extended to solve the Navier-Stokes equations and used to simulate the analytical asymptotic solutions found at the Seminar of Applied Mathematics for laminar triple point flames. During next year the code will be extended to do Large Eddy Simulation and high-resolution stochastic sub-grid models will be studied.

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2. Non-Premixed turbulent combustion modeling using large eddy simulation and unsteady flamelet models

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Project Target

The numerical simulation of turbulent combustion processes has developed to be a valuable tool for the development of combustion equipment like internal combustion engines or gas turbine burners. As mostly in engineering applications, for the calculation of the turbulent flow nowadays the Reynolds time averaged Naviers Stokes (RANS) equations are used with modelled turbulence. The dimension of recirculation zones, as present in most technical turbulent flows is badly predicted. Especially for combustion equipment such recirculation zones are of big importance for flame stabili.zation in stationary burners and NOx reduction due to flue gas recirculation. Turbulence models based on RANS employ turbulent approximations with an effective turbulent viscosity that is by orders of magnitude larger than the molecular viscosity. In particular if steady state versions of these equations are used, this tends to suppress large-scale instabilities, which occur in flows with combustion even more frequently than in nonreacting flows. If these instabilities are to be resolved in numerical simulations, it is necessary to resort more advanced, but computationally more expensive methods such as Direct Numerical Simulation (DNS) or Large Eddy Simulation (LES). The last research studies are shown that the fluctuations of the scalar dissipation rate can only be observed in LES type calculations, which implies that the level of accuracy obtained with LES cannot be achieved using Reynolds averaged methods[1,2,]. This investigation, which part of the directly calculated structure of turbulence can be used and what is the role of the subgrid model turbulence parameter for the coupling between flow and combustion model will be the major task of this project

The Performed Work and Results

A cold case LES computation has been done with CFX-Tascflow and comparison of LES with U-RANS computation were completed. A part of these results were presented at The Joint Meeting of the Competence Centers on: Combustion and Pollutant Formation . Although LES computation was performed with a coarser grid (200x10E3), the results show that the predictions of the axial mean velocity and recirculation length are better than the U-RANS computations. In both cases autocorrelation function of the axial velocity component at different positions on the symmetry axis and inside the recirculation zone were calculated and existence of a main frequency was observed at around 7 Hz. But the experimental result for the cold flow done by Lars Blum doesn't show any periodicity in the flow.

Figure 1 is a skectch of the configuration of the annual jet geometry considered in the cold case LES computation. Figure 2 shows the streamlines on a plane through the symmetry axis. The values of axial velocity component w on the symmetry axis are shown in Figure 3 for comparison, together with C. Del Taglia's[3] RANS results experimental data of Stroomer[4] and Blum.

Detailed chemical information will be introduced with the implementation of transient laminar flamelet model developed at LTNT by Ferreira[5] as a next step in project. Depending on its strain rate, the common steady laminar model always assumes a flamelet in equilibrium. However, in highly strained flames an intense interaction of local extinction and re-ignition is observed. After re-ignition, the flamelet needs a certain time to reach its equilibrium state. The TLFM considers the time evolution of a non-equilibrium flamelet by a time constant, which was taken in the RANS calculation to be k/ε plus a variable describing the reaction progress. The LES calculation offers the possibility to evaluate such a time constant in a better way by considering the total vorticity and strain rate. The resulting code will be used for the simulation of the turbulent counterflow and jet burner experiments. The experimental results will be used for code validation.

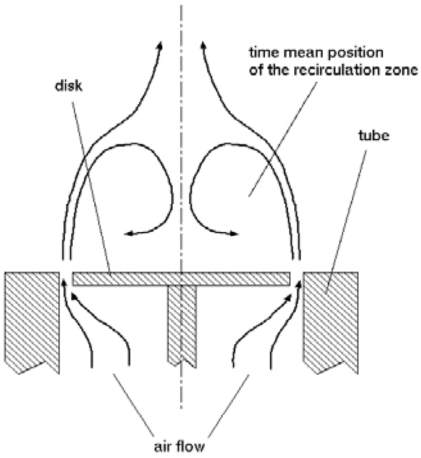

Figure 1

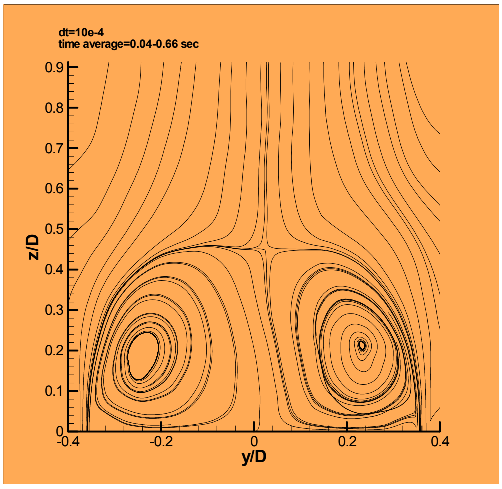

Figure 2

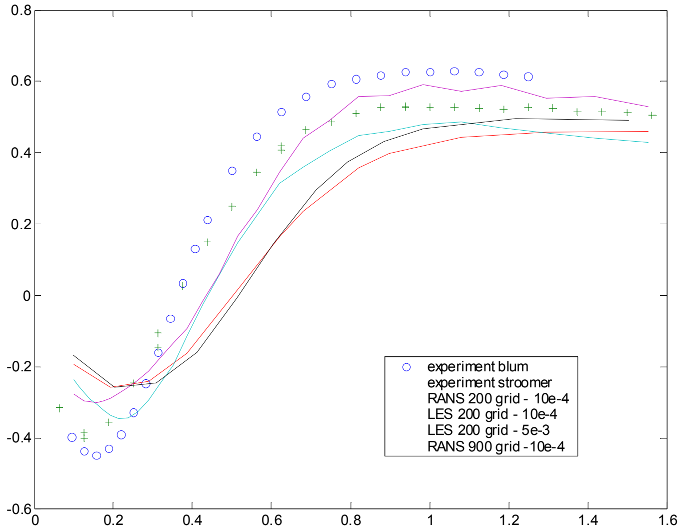

Figure 4

National Work Relations

This project is done in collaboration with the Aerothermochemistry and Combustion System Lab (LAV) of the Institute of Energy Technology, The Institute of Fluid Dynamics (IFD) and the Seminar für Angewandte Mathematik (SAM).

Valuation 2001 and Outlook 2002

The aim is to couple reaction and turbulence parameters by using LES and Flamelet models. This year as a part of this study LES computation has been done with cold flow and the results were compared with existing URANS results[8]. These results were presented at The Joint Meeting of the Competence Centers on: Combustion and Pollutant Formation. The results can be found previous section. The next step of the project is to couple LES code with Flamelet model. At this stage we propose some new ideas on this coupling procedure. The details and the theory of this new approach are explained in the following paragraphs.

In non-premixed turbulent combustion, the rate of mixing is determined by the motions of the largest eddies. The size, orientation, and rate of rotation of these eddies depends on the particular flow configurations. Chemical occurs only if fuel and oxidizer are mixed at the molecular level. Although turbulent mixing is responsible for stirring the reactants at large scales, it contributes to the molecular scalar mixing only indirectly, increasing the scalar variances and thereby the scalar gradients. Molecular mixing essentially occurs at the smallest turbulent scales by removal of the scalar variance. The rate of molecular scalar mixing is represented by the scalar dissipation rate, which can be identified as the most important parameter in the description of non-premixed combustion. In the literature are some different types of scalar mixing definitions. However if local extinctions events start to become important (i.e. in highly strained flames), these methods can no longer be used[1]. Here, we present a method which proposes a new approach for definition of scalar dissipation by using total vorticity and subgrid scale strain rates.

$$\chi = C_{\chi}\left[\left(\vec{\Delta}\ \mathrm{x}\ \vec{V}\right)^2 + \left(\overline{Z''}_{SGS}\ \frac{\mu_t}{\ell^2}\right)^2\right]^{1/2}$$

The first term the in square bracket represents the macroscopic rate of strain, Hult et. al. showed that vortices impinging from the fuel side on the flame front were the dominating extinction mechanism. According to Takahashi[7] and Katta[8] the local extinction caused by the internal vortices is largely due to unsteady transport effects on chemical kinetics. When the vortex approaches the flame front it strains the front and the steep fuel concentration gradient ahead of its leading edge causes a large fuel flux into the reaction zone. This large flux of methane and also some performed methyl radicals into the reaction zone depletes the radical pool (OH, H and O) in the strained flame zone, and thus quenches the flame locally.

The second term represents the rate of strain of subgrid scale turbulence. The mixture fraction variance is given by following Pierce and Moin [9,10]

$$\widetilde{Z}''^2 = C_Z \Delta^2 \left(\widetilde{Z}\right)^2$$

The Smagorinsky coefficient and the coefficient C_Z are computed from solution of resolved scales by applying the dynamic procedure. The eddy viscosity is given by Smagorinsky[11] model as

$$\mu_t = C\Delta^2 |S|$$

In the new method approach; while local extinctions are defined by scalar dissipation rate, a distinct definition for flame evolution is proposed by

$$\tau_{residence} = \frac{\ell}{V}$$

Therefore flame evolution and its extinction are defined apart from each other. It is the first time will be implemented in a combustion flow solver.

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3. Diffusion Jet Flame Large Eddy Simulation with an Approximate Deconvolution Model (ADM)

(**Part1.** Incompressible flow-calculations without reactions)

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The Intermittency-modified LES

In this section we investigate a modification proposed by Yakhot [1] of the Approximate Deconvolution LES model ADM [2]. The model modification is applied to channel-flow calculations in the sense of very large eddy simulations (VLES).
The most prominent flow structures, observed in wall bounded flows, are the streaks having approximate dimensions 1000 x 100 x 10 in wall units (streamwise x spanwise x wall normal direction). These are the smallest “high” energy containing scales, which should be resolved in an LES. That means that for an LES around three discrete points should be in the streak intervall. Otherwise, the calculation is more a VLES.
The idea of the LES model correction has its origin in the fact that actual LES models are not able to generalize their success to higher Re-number flows without substantial increase of the resolution. This problem was investigated in [1] and [3]. Therefore [1] concludes, the computational work involved in LES for wall bounded flows, though giving substantial computational savings compared to the DNS, scales a bit less than Re^3.
The problem of the breakdown of the Smagorinsky-like approaches is addressed in [1] and an improvement of approaches based on second-order statistics (for example the second order structure function to estimate characteristic velocity fluctuations) is proposed. The proposal in general is that the expression for a physically plausible model for the effective viscosity, generated by the small-scale velocity fluctuations, must involve the combination of the Kolmogorov relaxation time $\Sigma \approx \varepsilon^{1/3}\, \Delta^{-2/3}$ in addition to the one determined by the local value of the rate of strain.

The idea behind the Approximate Deconvolution LES-model (ADM)

We consider the LES model developed by Stolz, Adams and Kleiser [2]. The primary filter operation is defined as:

$$\overline{u(x)} = G * u = \int_{x-\Delta_2}^{x-\Delta_1} G\left(\frac{x-x'}{\Delta}\right) u(x') \frac{dx}{\Delta} \tag{1}$$

where Δ = const is the filter width in the computational space and $\overline{u(x)}$ is the filtered field. Generalization of this expression to the three-dimensionsal case is straightforward. Assuming that the filter and differentiation operations commute, we obtain the equation:

$$\partial_t \bar{u}_i + \partial_j \bar{u}_i \bar{u}_j + \partial_i \bar{p} - \frac{1}{\mathrm{Re}} \partial_j^{\,2} \bar{u}_i = \partial_j \bar{u}_i \bar{u}_j - \overline{\partial_j u_i u_j} = \sigma \tag{2}$$

with the right-hand side to be modeled. Defining an approximate inverse filtering operator Q_N

$$Q_N = \sum_{\nu=0}^{N} (I-G)^{\nu} \approx G^{-1} \tag{2.1}$$

where I is the identity operator and $u_i^* = Q_N * \overline{u}_i$ gives:

$$\partial_t \overline{u}_i + \partial_j \overline{u_i^* u_j^*} + \partial_i \overline{p}_i - \frac{1}{\mathrm{Re}} \partial_j^2 \overline{u}_i = -\chi (I - Q_N * G) * \overline{u}_i \quad (3)$$

where the right-hand side of the equation accounts for the effect of the sub-grid modes and pressure is determined from the incompressibility condition $\partial_i \overline{u}_i = 0$. To complete the model, an expression for the „relaxation time" $\tau = 1/\chi$ is needed. The authors of the model [2] have chosen a relation based on a second-order structure function. The dynamical condition behind their choice was to preserve the energy flux from large to small scales.

Intermittency-corrected LES

According to [1], we introduce a model giving correct asymptotics in the limit of both small and large values of the rate of strain S_{ij}:

$$\frac{1}{T} = \frac{\chi}{\left(1 + S_{ij}^2 \frac{L^2}{U_0^2}\right)^{1/2}} \quad (4)$$

where L the length scale and U_0 the velocity scale is. The rate of strain is defined as

$$S_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \quad (4.1)$$

In equation (3) the relaxation time T instead of $\tau = 1/\chi$ is used. We see that the effect of the rate of strain is to decrease this viscosity in the regions of strong fluctuations of S_{ij}.

The low Reynolds Number LES

The following calculations are done with the incompressible LES-channel flow code from the Institute of Fluid Dynamic (ETHZ), called TRANSIT. First, we investigate the effect of the intermittency correction (YKT) [1] on the performance of the Stolz-Adams-Kleiser (SAK) model [2]. The simulations were conducted on a 24x36x48 mesh spread over the 2πxπx2 domain. The results are summarized in Table 1 where we compare the computed friction velocity Reynolds number (Re_τ) and von Karman constant (KC).

Model	Re	Re_τ(calc)	Re_τ(DNS)	KC(calc)	KC(exp)
SAK	2800	180	180	2.5	2.5
YKT		186		2.4	
SAK	6874	361	395	2.17	2.5
YKT		395		2.5	
SAK	10934	517	586	2.15	2.5
YKT		549		2.5	

Table 1: Overview of YKT- and SAK-simulations in combination with the Re_τ from a Direct Numerical Simulation DNS [4]

The results are presented on Figs. 1-6. As we see, the results of the SAK model for *Re=2800*, giving $Re_*=180$ agree with the data very well. The results on a flow at *Re=6874* demonstrate some deviation from the law-of-the-wall and yield a low value for Re_τ. The disagreement with the DNS becomes more pronounced in the case of *Re=10934*, investigated earlier by the well-resolved DNS of Moser *et al.* [6] who obtained the well-developed logarithmic layer and $Re_\tau=586$. For this low resolution (24x36x48) the SAK model gives $Re_\tau=517$ leading to the 25% error in the 24x36x48-mesh- computed friction coefficient.
The results obtained with the YKT model based on (4) are presented on Figs. 4-6. In the low Reynolds number (*Re=2800*) case, the obtained $Re_\tau=186$ deviated from the DNS only by 2.7%, while the outcome of the simulation (*Re=6874*) agreed with both experimental data and analytic velocity profile. In the case *Re=10934*, a logarithmic velocity profile with the correct value of the von Karman constant was obtained.

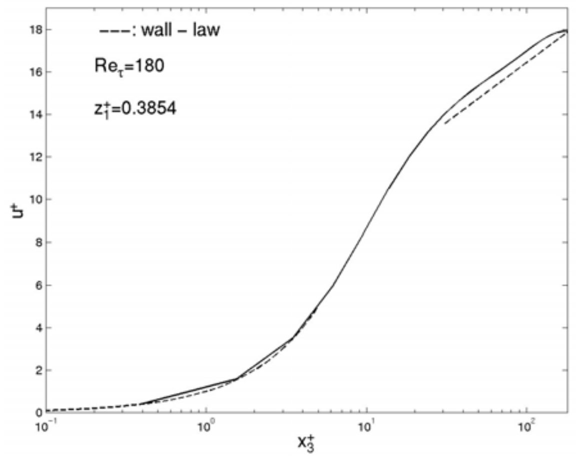

Figure 1: Re=2800, SAK, 24x36x48

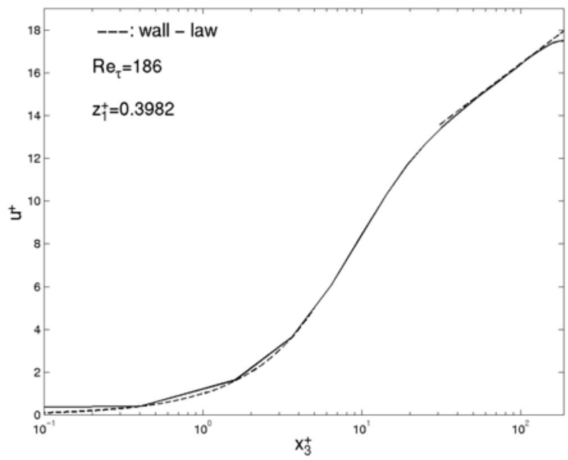

Figure 4: Re=2800, YKT, 24x36x48

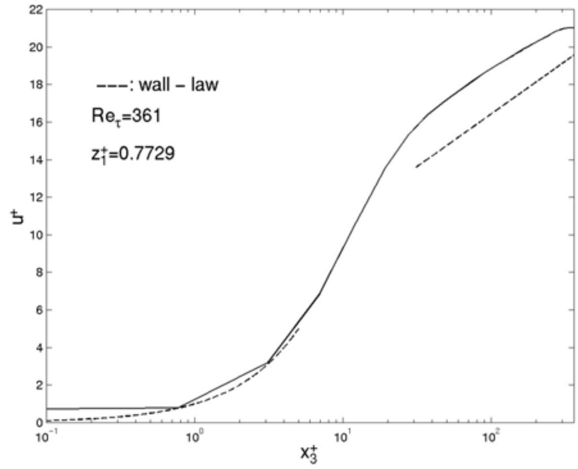

Figure 2: Re=6874, SAK, 24x36x48

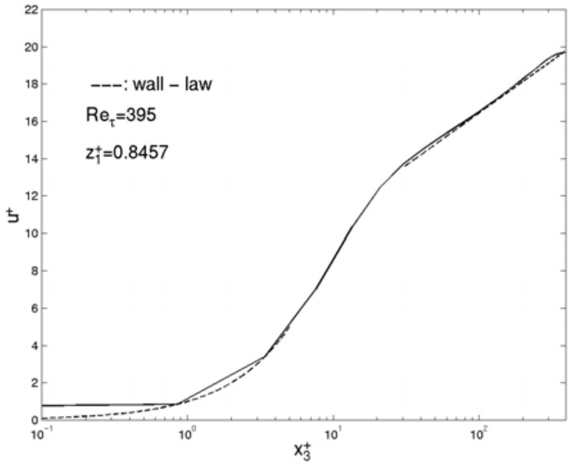

Figure 5: Re=6874, YKT, 24x36x48

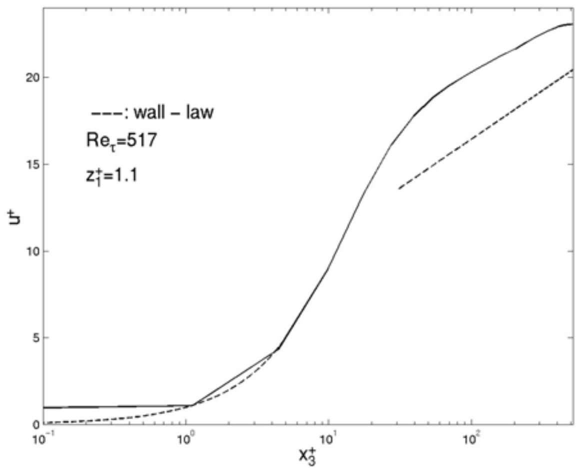

Figure 3: Re=10934, SAK, 24x36x48

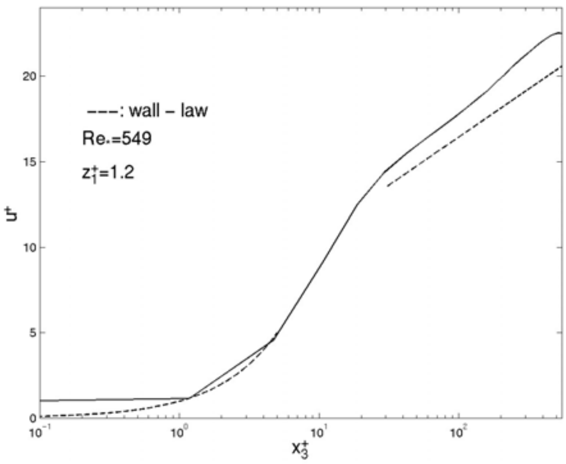

Figure 6: Re=10934, YKT, 24x36x48

To understand the reasons for this discrepancy, we repeated this simulation on a finer (24x36x96) grid. The result is shown on the Fig. 7. The velocity profile is close to the law-of-the-wall with Re_τ*=592*. It is interesting to note that the results did not improve upon further increasing the resolution to 24x36x192. The fact that the original ADM-model [2] gave similar results only on a 72x96x97 grid, demonstrate the potential of the „intermittency correction“ (4) to an order–of–magnitude savings in computational cost.

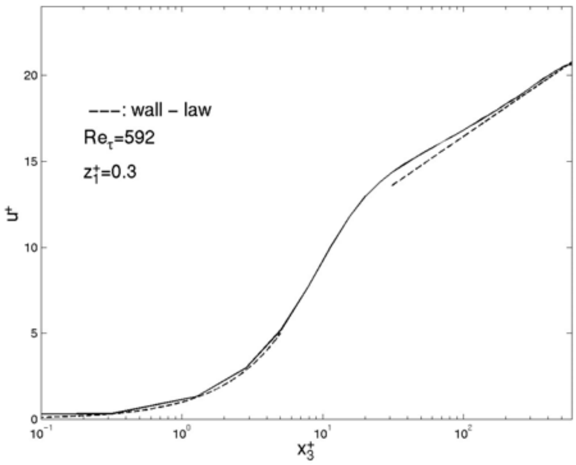

Figure 7: Re=10934, YKT, 24x36x96

The preliminary conclusion from these tests is that the streak resolution may not be too important after all: the precise presentation of the flow features in the wall normal direction, especially in the vicinity of the maxima of energy and rate of strain distributions in the channel, are more crucial.
One result deserves some attention. Trying to establish the role of the proportionality coefficient in front of S_{ij}^2 in the model expression (4), we found that doubling the coefficient did not lead to any modifications of main results except for the mild increase of the wall-stress fluctuations.

ADM-implementation in the incompressible spectral element code and preliminary results

ADM [2] was implemented in an incompressible spectral element code. The code uses Legendre-Lagrangian interpolants in combination with the Uzawa method to decouple the pressure and velocity field. For the time integration a mixed implicit/explicit scheme is used ([5], [6]). The original incompressible DNS spectral element code was modified to solve the filtered incompressible equations (3) and $\partial_i \overline{u}_i = 0$.

Filtering

The filter implemented in the code is a 1-D filter, which is applied in each spatial direction and each spectral element separately. For simplicity we will discuss only the filtering of a 1-D function *u(x)*. For filtering *u(x)* at points x_i, we write *u(x)* in terms of Legendre-Lagrangian interpolants $h_j(x_i)$

$$u(x_i) = \sum_{j=0}^{N} \widetilde{u}_j h_j(x_i) = u_i \qquad (6)$$

(6) is unfavorable for filtering because the coefficients do not decrease with increasing order *j*. Therefore we intend to transform (6) in a space where the coefficients of the expansion decrease with increasing order *j*. Such a space is for example the Legendre-space [7].

$$u_N(x_i) = \sum_{k=0}^{N} \hat{u}_k L_k(x_i) \qquad (7)$$

where L_k is the *k-th* Legendre polynomial. Unfortunately, filtered quantities does not satisfy boundary conditions anymore. For example, $u_N(\pm 1)=0$ but the filtered function is not zero at both endpoints exept in special cases. According to Boyd [8] we rewrite $u_N(x_i)$ in terms of new basis functions $\phi_m(x)$ which individually satisfy homogeneous boundary conditions and then apply the filter to modify the coefficients $\breve{u}_m$ of this new basis. The filtered sum can then be transformed back into the original basis. We consider Dirichlet boundary conditions:

$$\begin{aligned} u_N(-1) &= \alpha \\ u_N(1) &= \beta \end{aligned} \qquad (8)$$

If the basis functions are choosen to satisfy homogeneous Dirichlet boundary conditions, i.e.

$$\phi_m(\pm 1) = 0, \tag{9}$$

then one may write

$$u_N(x) = \frac{\alpha+\beta}{2} + \frac{\beta-\alpha}{2}x + \sum_{m=2}^{N} \breve{u}_m \phi_m(x) = \sum_{m=0}^{N} \breve{u}_m \phi_m(x) \tag{10}$$

For the basis function $\phi_j(x)$ we choose

$$\phi_m(x) = \begin{cases} L_0(x); m = 0 \\ L_1(x); m = 1 \\ L_m(x) - L_{m-2}(x); m > 1 \end{cases} \tag{11}$$

For each specific Legendre-Gauss-Lobatto point x_i (10) can be written as

$$u_N(x_i) = \sum_{m=0}^{N} \breve{u}_m \phi_m(x_i) = \sum_{m=0}^{N} \breve{u}_m \phi_{im} = \underline{\underline{\Phi}}\,\underline{\breve{u}} \tag{12}$$

with the transformation-matrix $\underline{\underline{\Phi}} = \phi_{im}$. The filter does touch only the coefficients $\breve{u}_m$ (m > 1) and the filter-operation is done with a diagonal matrix $\underline{\underline{D}}_F$. The filtered vector $\underline{\breve{u}}$ is then

$$\underline{\bar{\breve{u}}} = \underline{\underline{D}}_F\,\underline{\breve{u}}, \tag{13}$$

and with (12)

$$\bar{u}_N(x_i) = \underline{\bar{u}}_N = \underline{\underline{\Phi}}\,\underline{\bar{\breve{u}}} \tag{14}$$

with (12), (13) and (14)

$$\underline{\bar{u}}_N = \underline{\underline{\Phi}}\,\underline{\underline{D}}_F\,\underline{\underline{\Phi}}^{-1}\underline{u}_N \tag{15}$$

Equation (15) was implemented as the filtering operation.

The filter operation (15) does not change the geometric boundary conditons. But note that with (15) the values at the spectral element boundaries are not changed as well. We do not have any information yet about the influence on LES calculations.

Filter Function

The diagonal elements of the filter diagonal Matrix $\underline{\underline{D}}_F$ are discrete values of a filter function *G(n)*, where *n* is the order in the spectral space. We prefer differentiable filter functions for which the following cutoff number κ_{cut} can be defined:

$$\kappa_{cut} : G\left(\frac{n}{N} = \kappa_{cut}\right) = 0.5 \tag{15.1}$$

where *N* is the maximal order of polynomials in the spectral space. Such functions are for example trigonometric frunctions. We are using for the filter function the following function, which is presented in Figure 8 as well.

$$G\left(\frac{n}{N}\right) = \begin{cases} 1; 0 \le \frac{n}{N} \le 1 - 2\kappa_{cut} \\ \frac{1}{2}\left[\cos\left(\left(\frac{n}{N} + 1 - 2\kappa_{cut}\right)\frac{\pi}{2(1-\kappa_{cut})}\right) + 1\right]; 1 - 2\kappa_{cut} < \frac{n}{N} \le 1 \\ 0; \frac{n}{N} \ge 1 \end{cases} \tag{15.2}$$

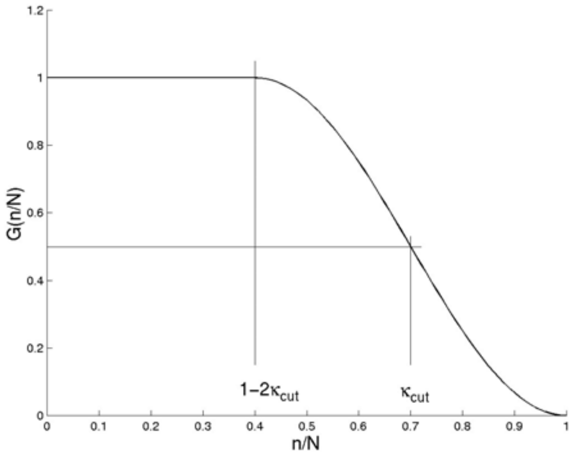

Figure 8: normalized filter function; n is the order in spectral space, N is the maximal order and κ_{cut} is the cutoff number

Future Objectives and planning update

During the next 6 months of the project we plan to perform following tasks:

1. Incompressible LES-channel flow calculations for Re=2800, 6875 and 10935
2. Favre averaged LES-formulation of the compressible low-Mach-number code
3. Non-isothermal free jet DNS
4. Non-isothermal free jet LES
5. Literature review on existing experimental data

Objectives during the 18-24 month period:

1. Existing literature data with additional measurments, if necessary
2. Comparison of the non-isothermal free jet DNS and LES
3. Implementation of the Combustion model

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