Preliminary investigation of overlap coupling for hybrid LES/RANS

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ABSTRACT

The RANS and LES methods for computing turbulent flows perform well in different situations. The RANS method gives good results in anisotropic flows like shear-flows and boundary layers in wall-bounded flows. The LES method gives good results in isotropic regions like the free-stream. This results in the idea to combine both of these methods in one hybrid-method. However, proposed methods like blending (DES) and zonal methods are ad-hoc. And only give satisfying results in specific cases. Hence the overlap-method is proposed in an attempted to solve these problems.

In this method the LES model is used on the entire computational domain, however, in some regions an additional computational domain is also present for a separate RANS model. In the additional regions the RANS model is anticipated to provide a prediction superior to that of the LES model. The LES solution will be gently forced such that its average resembles the RANS-solution. This is achieved using a proportionalcontrol source term, the strength of the source depends on the difference between RANS and LES solution multiplied by a parameter which determines the strength of the coupling. The difference between RANS and LES is computed using two different functionals, resulting in two different overlap coupling method. First, the difference in conservative variables results in what is called variable coupling, and second, the difference in influx (flux-divergence) what is called flux-divergence coupling. In the attempt to let the small scales develop freely, without being influenced by the coupling, three types of VMS coupling are introduced:

- Type I separates wrt the test space
- Type II separates wrt the trail space
- Type III separates wrt both the test and trail space

Three test cases are studied to assess this newly introduced overlap coupling. For the first two test cases 1D convection-diffusion is the governing equation. This equation is chosen for its simplicity, it is linear. Analytic and numerical solutions can be easily obtained. In the third test case the non-linear convection-diffusion equation is used. The Time-discontinuous Galerkin method using spectral finite elements is used.

In the first test case the time rate of change of the coupled solution is completely governed by the coupling, the physical net-influx is completely ignored. The ability of the overlap coupling term to reproduce the reference solution is assessed. In the second test case the time rate of change of the coupled solution is computed from a combination of the physical net-influx and the coupling. The interaction between these terms is investigated. After this a numerical stability analysis is performed on all coupling methods. In the third test case the governing equation is the 1D Burgers equation. A comparison between VMS and normal overlap coupling can be made, as a n energy cascade is present. The expected improved representation of the small scales is checked. Using these test cases the following conclusions can be drawn.

It is possible to let a solution of one model resemble the solution of another model. This resemblance becomes better with increasing coupling parameter. The variable coupling has an advantage over flux-divergence coupling, as it always has a decaying homogeneous part. The flux-divergence coupling, in contrast, only has a decaying homogeneous solution when the physical model poses some diffusion. Analytical stability is satisfied for both methods when the coupling parameter is taken positive. Resonance can occur for flux-divergence coupling when the errors are canceled by the homogeneous part of the coupling. All normal coupling methods and VMS variants of variable coupling are numerically stable. While VMS variants of flux-divergence coupling can be numerically unstable. For these three reasons flux-divergence coupling is discarded as a satisfying coupling method.

Of the proposed VMS types type I and III give improvements in the small scales part of the solution. With Type-I VMS the small scales improve with increasing coupling parameter, while for Type-III VMS this is only
until a certain coupling parameter after which the small scales start deteriorating. VMS type II does not give a improvement in the small scales, but the large scales coupling deteriorated and singularity problems arise. Therefore VMS type II is recommended. The small scales might not be represented correctly in the overlapped region, however, they are at least as good as in the zonal approach. Therefore it is expected the overlap coupling method will outperform the zonal coupling. 2000 Mathematics Subject Classification: primary: 76F99, secondary: 65M60.

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Chapter 1
Introduction to the computation of turbulent flows

This chapter will give a short introduction to the computation of turbulent flows via the Navier-Stokes equations. It will also describe the motivation for and implementation of methods which couple solutions of the Reynolds-Averaged Navier-Stokes equations to Large-Eddy simulations.

1. The Navier-Stokes equations
The governing equations of fluid dynamics are the Navier-Stokes equations. These equations were obtained by M. Navier and G. Stokes independently. The differential form of these equations is [6]:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{T}
\]

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) = \mathbf{u} \cdot (\nabla \cdot \mathbf{T} - \nabla p)
\] (1.1)

Where \( \rho \) is the mass density, \( \mathbf{u} \) is the velocity, \( p \) is the pressure, \( E \) the total energy per unit mass and \( \mathbf{T} \) is the viscous stress tensor. These equation state mass, momentum and energy are conserved. To complete the system of equations, an equation of state and a constitutive equation is necessary. The most common equation of state is that of a perfect gas:

\[
p = (\gamma - 1)\rho(E - \frac{1}{2} \mathbf{u} \cdot \mathbf{u})
\] (1.2)

While the most common constitutive equation is that for a Newtonian fluid:

\[
\mathbf{T} = \nu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)
\] (1.3)

Where \( \gamma \) is the ratio of specific heats and \( \nu \) is the viscosity, usually both are taken to be constant. Due to non-linear nature of these equations and the irregular boundaries of realistic domains, an analytic solution is usually not available. To find solutions of equations (1.1) numerical methods can be deployed.

2. Direct Numerical Simulation
Direct Numerical Simulation (DNS) is the brute-force method of solving the Navier-Stokes equations. The concept is generally quite simple, however, the computational effort can be enormous. With this
method the equations are discretized using finite-difference, finite-volume, finite-element or spectral methods for example. The solution is found by choosing the discretization such that all relevant physics are adequately resolved.

In the case of turbulence, however, the relevant physics might include very small length and time scales. These scales are called the Kolmogorov-scales, and depend on the viscosity: the smaller the viscosity the smaller the Kolmogorov-scales. Hence high Reynolds-number turbulent flows, which contain a very wide range of relevant scales, are very expensive to calculate using DNS. In practice, such flows are common, especially in aeronautics. Fortunately there are means of circumventing this problem, namely RANS and LES techniques.

3. Large-Eddy Simulation

Large-Eddy Simulation (LES) is a method for computing turbulent flows which is gaining popularity due to the increase in available computing power. The field has recently been revolutionized by the Variational-MultiScale (VMS) method, introduced by Hughes [3, 4, 5] and Collis [1]. Traditionally, the separation between large and small scales is made by spatial filtering. This leads to all kinds of complications especially near walls where the filter is applied inconsistently.

The VMS approach to LES circumvents this problem by separating the scales apriori by means of variational projection. The large scales are associated with a specific function space, while the small scales are associated with another function space. This is concept is easily grasped in a Spectral-Finite-Element-Method context. The large and small scales are associated with specific shape functions and hence ad-hoc filtering techniques can be omitted. This leads to a more logical and clean formulation.

The effect of the neglected scales on the resolved scales has to be modeled. This is usually done using a (dynamic) Smagorinsky eddy-viscosity model. The strength of the VMS approach is that the model can be applied to only the smallest of the resolved scales. This results in better performance of this method, as it mimics the physics better than traditional methods. Due to the energy cascade, nearby scales influence each other the most. The neglected scales have a direct influence on the smallest resolved scales, while the influence on the large resolved scales is only indirect via the smallest resolved scales. Hence only the smallest resolved scales need a model to take into account the neglected scales.

The Smagorinsky model assumes isotropic turbulence. Hence the VMS method has difficulty finding the correct solution when the turbulence is anisotropic, like in wall-bounded flows. In these cases the resolved scales have to be very small to get to the correct answer. The resolution of the scheme then becomes dependent on the Reynolds-number. This goes against the goal of LES to have a resolution demand independent of the Reynolds-number.

4. Reynolds-Averaged Navier-Stokes

The Reynolds-Averaged Navier-Stokes (RANS) method is popular in practice, as it is relatively computational inexpensive and well-established. It decomposes the total solution in two parts: an ensemble average of the solution and superimposed fluctuations. The fluctuations are not solved for, but the effect of these fluctuations on the average solution are modeled. This is usually done with an eddy-viscosity model which increases viscosity locally. In other words, the complex unsteady turbulent flow is treated as a simple steady laminar flow with increased viscosity. This is why RANS is a relatively inexpensive method. It gives good results in shear-flows, like boundary layer and wall-bounded flows. A major drawback is that it is difficult to make turbulence models for arbitrary situations. Another drawback of this method is that hardly any information about the turbulence itself is known.

5. Hybrid RANS/LES

In the previous two sections, RANS and LES are briefly introduced. A quick conclusion is that both methods perform well in different situations. This results in the idea to combine both of these methods in one hybrid method. RANS can be used in anisotropic shear-flow regions (e.g. near walls), while using the VMS-LES can be used in the free stream (where the isotropic assumption is more valid).
5.1 Universal turbulence models
This is the most common variant of hybrid RANS/LES methods. Both the RANS and LES are formulated in a similar framework, allowing one to switch between LES and RANS where desired. Another option is blending where at the interface region there is a weighted mix of both LES and RANS. See for example the DES of Spalart [2] or the hybrid method of Speziale [9].

These methods have the disadvantage of being quite restrictive. The types of RANS and LES have to be compatible to be able to switch from one to the other when desired. This restriction in available RANS and LES types plus the ad-hoc character of the blending can lead to poor results.

5.2 Zonal methods
With this approach the domain is decomposed in LES and RANS regions. See figure 1.1. Complications arise at the interface of these regions. This problem can be split in two subproblems.

![Figure 1.1: Schematic explanation of the zonal RANS/LES method](image)

First there are the auxiliary variables. In general both methods use different auxiliary variables to describe the turbulence. These have to be estimated based on the primary variables. This is not always as straightforward as expected, although solutions have been proposed yielding acceptable results.

Secondly, the LES has a high frequency content which is not present in the RANS. Hence the inflow of small scales into the LES-domain poses a serious problem. Approaches to circumvent this problem [8] are not entirely satisfying. An other option is just to ignore this issue and use a low frequency boundary condition for the LES. This leads to poorly excited small scales in the LES, while these are of major importance for correctly representing the energy decay.

5.3 Overlap methods
The proposed solution for the problems arising from the zonal approach is what we call the overlap method. In this method the LES model is used in the entire computational domain. However, in some regions an additional computational domain is also present for a separate RANS model.

![Figure 1.2: Schematic explanation of the overlap RANS/LES method](image)

In the additional regions the RANS model is anticipated to provide a prediction of the large-scale behavior superior to that of the LES model. Hence it is desired to gently force the LES solution such that its average resembles the RANS solution. This method can be seen as an extension of the zonal method: instead of a spatial interface there is a more abstract interface between two different 'realities'. See figures 1.1 and 1.2. The RANS solution is of lower resolution then the LES solution, the RANS model only computes the averages while the LES model also computes a portion of the fluctuations. This gives complications when the coupling of the RANS and LES solution is too rigid.
The LES solution will resemble the RANS solution too much and fluctuations will be forced to be zero just like in the RANS solution. This problem can be circumvented when only a part of the LES solution is coupled (the large scales) while the other part is unaffected (the small scales). This is what we call the Variational Multi Scale (VMS) approach to overlap coupling.

6. Thesis structure

First the numerical scheme will be introduced. This is split in two parts. The first part gives a brief introduction to the time-discontinuous galerkin method using spectral finite elements which is the numerical scheme which will be used throughout the thesis. The second part introduces coupling methods and their VMS implementation. Zonal coupling is explained while overlap is developed and pursued in the remaining sections.

After introducing candidate approaches to overlap coupling a sequence of analyses with increasing complexity are used to study their behavior. For the first two test cases 1D convection-diffusion is the governing equation. This linear equation is chosen for its simplicity. Analytic and numerical solutions can be easily obtained. In the third test case the non-linear convection-diffusion equation is used.

In the first test case the time rate of change of the coupled solution is completely governed by the coupling, the physical net-influx is completely ignored. The ability of the isolated overlap coupling term to reproduce the reference solution can be assessed. Limits on the coupling parameter are also determined, and coupling resonance solutions are investigated.

In the second test case, the time rate of change of the coupled solution is computed from a combination of the physical net-influx and the coupling. The interaction between these terms is investigated. A numerical stability analysis is performed on both coupling methods. This stability analysis is done for the all-scale approach as well as the three VMS approaches.

In the third test case the governing equation is the 1D Burgers equation. This equation is non-linear but it is the simplest equation with an energy cascade. With this cascade the comparison between VMS and all-scale overlap coupling can be made. The improved representation of the small scales obtained from VMS overlap coupling is demonstrated.
Chapter 2
Basic numerical scheme

In this chapter the numerical scheme used throughout the report is introduced. The numerical method used is based on a Galerkin-Least-Squares (GLS) Spectral-Finite-Element-Method (SFEM) using the Space-Time (ST) formulation. In section 1 the formulation of a general conservation law is described. After this the space-time framework is defined in section 2. In section 3 the Galerkin weak formulation is introduced including the GLS stabilization. The implementation of boundary conditions is discussed in section 3.1. The actual discretization and the shape functions will be discussed in the section 4.

1. General Conservation Laws
A general conservation law (CL) basically states: the time rate of change of a conservative variable equals the net spatial influx plus the source. In combined vector and tensor notation, using Einstein’s convention, this can be written as:

\[ \frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} = \mathbf{S} \tag{1.1} \]

Where \( \mathbf{u} \) is the vector of conservative variables, \( \mathbf{F} \) are the spatial fluxes, \( \mathbf{S} \) is the source and \( x \) are the spatial coordinates. The subscript \( i \) denotes the spatial direction. The conservative variables, \( u_i \), and array of fluxes, \( F_i \), are specific for each conservation law. The quasi-linear form of equation (1.1) is:

\[ u_i + \frac{\partial F_i}{\partial u} u_i = S \tag{1.2} \]

Where \( \frac{\partial F_i}{\partial u} \) are the flux Jacobians and \( u_i \) is a short-hand notation for \( \frac{\partial }{\partial x} \). In the space-time framework time is seen as just another (spatial) direction, so equation (1.2) reduces to:

\[ \frac{\partial F_i}{\partial t} u_i = S \tag{1.3} \]

Now \( F_i \) and \( x_i \) also contain the temporal flux and the temporal coordinate.

2. Space-Time framework
The spatial domain \( \Omega \) is a bounded and open region in \( \mathbb{R}^n \) with piecewise smooth boundary (Lipschitz continuous) \( \Gamma = \partial \Omega \). The time interval is \([0,T]\), with \( T > 0 \). Combining these gives the space-time domain \( Q = \Omega \times [0,T] \). The lateral boundary is denoted \( \Gamma = \Gamma \times [0,T] \), while the upper-time and lower-time boundaries are \( \Omega_1 \) and \( \Omega_0 \), respectively.
Figure 2.1: The space-time slab

Now several inner products can be defined:

\[(f, g)_Q = \int_Q f^T g \, dQ\]
\[(f, g)_P = \int_P f^T g \, dP\]
\[(f, g)_{\Omega} = \int_{\Omega} f^T g \, d\Omega\]  \hspace{1cm} (2.1)

The boundary integral around \( Q \) is:

\[(f, g)_{\partial Q} = (f, g)_{\partial_0} + (f, g)_{\partial_2} + (f, g)_P\]  \hspace{1cm} (2.2)

3. Galerkin formulation

The general conservation law (1.3) can be transformed into a weak formulation by multiplying it with a test function and integrating over the entire space-time domain, the problem then becomes.

Find \( u \in \mathcal{U} \) such that:

\[\left\langle \left( w, \frac{\partial F_i}{\partial u} u_i \right) \right\rangle_Q = (w, S)_Q \quad \forall \ w \in \mathcal{W} \]  \hspace{1cm} (3.1)

Where \( \mathcal{U} \) and \( \mathcal{W} \) are appropriate Hilbert spaces resulting in valid integrals. In some cases, like for CL’s with diffusion terms, it can be useful to transform equation (3.1) by means of integration by parts:

\[(w, n_i F_i)_Q - (w_i, F_i)_Q = (w, S)_Q \quad \forall \ w \in \mathcal{W} \]  \hspace{1cm} (3.2)

Evaluating the boundary integral gives:

\[ (w, u)_{\partial_1} - (w, u)_{\partial_0} + (w, n_i F_i)_P - (w_i, F_i)_Q = (w, S)_Q \quad \forall \ w \in \mathcal{W} \]  \hspace{1cm} (3.3)

Or in a different notation:

\[ B(w, u) = (w, S)_Q \quad \forall \ w \in \mathcal{W} \]  \hspace{1cm} (3.4)

Where \( B(\cdot, \cdot) \) is the operator defined as:

\[ B(w, u) = (w, u)_{\partial_1} - (w, u)_{\partial_0} + (w, n_i F_i)_P - (w_i, F_i)_Q \]  \hspace{1cm} (3.5)
3.1 Boundary conditions

There are basically three boundary conditions considered in this report.

First there is the periodic boundary condition. This directly relates the solution at one boundary to the solution at another boundary. The outflow at one part of the domain is the inflow at another part of the domain. Using this boundary condition for the time boundaries can result in a steady-state calculation. When the shape functions are linear in time they are forced to be constant by the periodic boundary condition. Hence the time derivative will be zero and a steady-state formulation is obtained. When higher-order shape functions are used, the periodic boundary condition doesn’t eliminate the time derivative, and the formulation will remain unsteady. However, the mean solution is still steady although periodic fluctuations are allowed. Using this boundary condition for the spatial boundaries results in a closed circular domain, without spatial boundaries.

The second is the strong Dirichlet boundary condition. This boundary condition is enforced by choosing the appropriate trial space for \( \mathbf{u} \) which \emph{a priori} satisfies the Dirichlet boundary conditions. Using this boundary condition for the time boundary, for each consecutive space-time slab, results in a Continuous-Galerkin time-marching method. In this case the initial condition is the solution on \( \Omega_1 \) of the previous space-time slab, see figure 2.2. Each space-time slab has to start with the same discretization as the previous slab has ended. Adaptation can only be done within a space-time slab in a continuous manner. The same argument can be given for the spatial boundaries. When the Dirichlet boundary condition is prescribed by the results from another computational domain the mesh and shape functions have to be the same on both sides of the interface. This is an unacceptable restriction if domains with different discretizations are coupled, like LES and RANS domains.

The third method weakly enforces the flux (a Neumann boundary condition) at the boundaries. This results in a method without the restrictions of the previous two boundary conditions.

3.1.1 Initial conditions

The numerical implementation is as follows. First the Conservation Law (1.3) is augmented with an initial condition:

\[
\mathbf{u} = \mathbf{u}_0 \quad \text{ in } \Omega_0
\]

(36)

This \( \mathbf{u}_0 \) can be the true initial condition of the calculation, or the solution on \( \Omega_1 \) of the previous space-time slab, see figure 2.3. This results in a Discontinuous-Galerkin time-marching method. Equation (3.6) can be rewritten as:

\[
\mathbf{u} = (1 - \lambda_0)\mathbf{u} + \lambda_0\mathbf{u}_0 \quad \text{ in } \Omega_0
\]

(37)

If these identities are substituted in the Galerkin formulation (3.4) the equation becomes:

\[
(w, \eta_i \mathbf{F}_i)_P - (w, (1 - \lambda_0)\mathbf{u} + \lambda_0\mathbf{u}_0)_{\Omega_0} + (w, \mathbf{u})_{\Omega_0} - (w_i, \mathbf{F}_i)_Q = (w, \mathbf{S})_Q \quad \forall w \in \mathcal{W}
\]

(38)

By reordering a penalty formulation is obtained:

\[
B(w, \mathbf{u}) + \lambda_0 (w, \mathbf{u} - \mathbf{u}_0)_{\Omega_0} = (w, \mathbf{S})_Q
\]

(39)
This is the Galerkin formulation of equation (3.4) with an additional penalty term which weakly enforces the initial condition.

Choosing $\lambda_0 \to \infty$ results in a method which mimics the previously mentioned Continuous-Galerkin time-marching method as close as possible. No trade off is made between the errors made in the interior and at the lower time boundary. The error on the lower-time boundary is forced to be zero (in the weak sense), while the error on the interior is neglected for the Degrees Of Freedom (DOFs) which also affect the lower time boundary. When the mesh and shape functions are equal on both sides of the interface, the CG-method is obtained. Choosing $\lambda_0 = 0$ results in a method without initial conditions. Normally this will be an ill-posed method. So the parameter $\lambda_0$ can be used to tune the discretization. Choosing the penalty parameters to be $\lambda_0 = 1$ the well-known traditional Time-Discontinuous-Galerkin formulation is obtained:

$$B_{TDC}(w, u) = (w, S)_Q + (w, u_0)_{\Omega_0} \quad \forall \ w \in W \tag{3.10}$$

With $B_{TDC}(\cdot, \cdot)$ defined as:

$$B_{TDC}(w, u) = (w, u)_{\Omega} + (w, n_{\Omega} F_i)_P - (w_i, F_i)_Q \tag{3.11}$$

This method is discretely conservative. In this method a trade off is made between errors in the interior of the domain and errors on the boundaries. As this method is known to give good results, this will be the time boundary conditions used from now on.

### 3.1.2 Spatial boundary conditions

The numerical implementation is as follows. First the Conservation Law (1.3) is augmented with a boundary condition:

$$n_{\Omega} F_i = F_P \quad \text{in } P \tag{3.12}$$

This can be rewritten as:

$$n_{\Omega} F_i = (1 - \lambda_p) n_{\Omega} F_i + \lambda_p F_P \quad \text{in } P \tag{3.13}$$

If these identities are substituted in the Galerkin formulation (3.4) the equation becomes:

$$- (w_i, F_i)_P - (w, F_P)_P - (w_i, F_i)_Q = (w, S)_Q \quad \forall \ w \in W \tag{3.14}$$

By reordering a penalty formulation is obtained:

$$B(w, U) + \lambda_p (w, F_P - n_{\Omega} F_i)_P = (w, S)_Q \quad \forall \ w \in W \tag{3.15}$$

This is the Galerkin formulation (3.4) with an additional penalty term which weakly enforces the spatial boundary condition. As with the initial condition, the parameter $\lambda_p$ can be used to tune the method. The penalty parameters can be used for making a trade off between errors in the interior of the domain and errors on the boundaries. Choosing a large penalty makes the errors at the boundaries more dominant, hence the boundary error will be relatively small. Choosing the penalty to be small, however, will result in a dominant internal error resulting in a relatively large boundary error.
4. Discretization

Proceeding from a weak formulation of a conservation law, like 3.5 or 3.8, to a numerical discretization is a small step. Restricting the infinite-dimensional function spaces $\mathcal{U}$ and $\mathcal{V}$ to finite-dimensional subspaces $\mathcal{U}^h$ and $\mathcal{V}^h$ will do the trick. In this work, the finite-dimensional subspaces are generated with spectral finite elements. This method combines the flexibility of finite-element methods with the high-order accuracy of spectral methods. Space and time are discretized simultaneously, leading to a so-called space-time formulation. All variables are discretized using the same approximate subspace.

The space-time domain is divided into several subdomains (elements). On each element the solution is represented by a sum of polynomials. Due to the restrictions on the infinite function space, and hence the finite subspace, the discretization should be $C^0$ continuous over the element interfaces. The VMS-formulation as discussed in section 3 demands the use of a hierarchical basis. Hence a modal expansion based on orthogonal Jacobi polynomials, as discussed in [7], is used. It is important to notice that the basis is not entirely orthogonal with respect to the $L_2$-inner product due to the linear component in each shape function.

The numerical approximation of $u$ will be denoted as $u^h$ and can be represented by:

$$u^h = a_j w_j$$ (4.1)

Where $w_j$ are the shape functions which span $\mathcal{U}^h$ and $\mathcal{V}^h$ and $a_j$ are the DOFs. For simplicity assume the weak formulation is equation (3.10). The discretized equation then becomes:

$$B_{TDCG}(w_k, a_j w_j) = (w_k, S)_{Q} + (w_k, u_0)_h \quad \forall \ k$$ (4.2)

Which is an algebraic system of equations in the unknowns $a_j$.

Discretizations like these can give poor results with convection-dominated problems, with solutions which possess spurious oscillations. Another problem is the incompatibility of trial spaces in case of the Euler or Navier-Stokes equations for example. Stabilization terms can be added to circumvent these problems. A commonly-used stabilization is Least-Squares (LSQ) stabilization:

$$B_{TDCG}(w, u) + B_{lsq}(w, u) = (w, S)_{Q} + (w, u_0)_h \quad \forall \ w \in \mathcal{V}$$ (4.3)

Where $B_{lsq}(\ldots)$ is the LSQ-stabilization term, defined as:

$$B_{lsq}(w, u) = \left( \frac{\partial F_i}{\partial u} w_j, \tau \frac{\partial F_i}{\partial u} u_j \right)_Q$$ (4.4)

Where $\tau$ is a matrix which can be chosen to tune the discretization. For reasons of simplicity, $\tau$ will be set to zero which results in the normal Galerkin weak formulation.

5. Solution strategy

At each time step the solution of the space-time slab is found using equation (4.2). This is an algebraic system of equations in the unknowns $a_j$. The Jacobian, used for solving the algebraic system of equations, is:

$$A_M = \frac{\partial}{\partial a_j} B_{TDCG}(w_k, u^h + u_k w_l)|_{u_k=0}$$

$$= (w_k, I w_l)_h + \left( w_k, u_l \frac{\partial F_i}{\partial u} u_l \right)_P - \left( w_k, \frac{\partial F_i}{\partial u} u_l \right)_Q$$ (5.1)

5.1 Linear case

When the original conservation law is linear, $\frac{\partial F_i}{\partial u}$ and hence $A_M$ will not depend on $u^h$. Defining the right-hand-side:

$$b_k = (w_k, S)_{Q} + (w_k, u_0)_h$$ (5.2)
Algorithm

1. Choose initial guess $a_0$ and set $n = 0$
2. Compute the Jacobian $A_{kl}$ and residual $r_k$ based on $a_k$
3. Solve linear system of equations: $A_{kl} \Delta a = r_k$
4. Update solution: $a_{k+1}^h = a_k^h + \Delta a^h$
5. Check convergence: $\epsilon = \frac{\|\Delta a^h\|}{\|a^h\|}$
6. When $\epsilon > \epsilon_{tol}$: set $n = n + 1$ and goto step 2
7. Solution is converged

Figure 2.4: The Newton-Raphson solution strategy

Now equation (4.2) will result in the following linear system of equations:

$$A_{kl} \Delta a = b_k$$  \hspace{1cm} (5.3)

With this relation the solution on a space-time slab can be determined based on the upper-time trace of the previous solution and the source term. This can be computed with direct solver like sparse LU, or iterative solvers like GMRes.

5.2 Non-linear case
When the original conservation law is non-linear, $\frac{\partial F}{\partial u}$, and hence $A_{kl}(u^h)$ will depend on $u^h$. In this case a solution can be found using the Newton-Raphson iteration method. Defining the residual:

$$r_k = (u_k, S)_Q + (w, u_0)_{\partial Q} - B_{TDG}(w_k, u^h)$$  \hspace{1cm} (5.4)

The solution of equation (4.2) can be found using the following algorithm: The Newton-Raphson iterations are incremental, in that each new solution is a correction on the previous solution (see step 4). However, when the magnitude of $\Delta a$ becomes much smaller then the magnitude of $a$ this increment does not have any effect. This is due to the finite accuracy of both vectors. Therefore it is straightforward to choose the convergence criteria as the ratio of the magnitudes of these two vectors, see 5. The tolerance $\epsilon_{tol}$ can be chosen larger than the numerical accuracy limit.

This Newton-Raphson iteration method can also be used for linear systems of equations. In this case the correct solution will be found after only one iteration step.
Chapter 3
Coupling methods

In this chapter two different coupling methods are presented. First the zonal coupling method is introduced in section 1. This method is only mentioned as an alternative to overlap coupling, it will not considered further. The overlap-coupling method is then introduced in section 2. This method will be developed and evaluated in the remainder of the report.

1. Zonal coupling
The weak Neumann boundary condition, as discussed in the previous section, can be used to couple two computational domains. The flux prescribed at the interface should be based on the states at both sides of the interface. The Riemann flux seems the most logical choice, as this is the flux which would be expected in reality.

Recall equation (3.15), where $F_P$ is the Riemann flux and $u_c$ is the solution of the neighboring domain:

$$F_P = F_r(u, u_c, n_i)$$  \hfill (1.1)

This yields:

$$B(w, u) + \lambda_P C_z(w, u, u_c) = (w, S)_Q \quad \forall \ w \in \mathcal{W}$$

With $C_z(w, u, u_c)$ the zonal operator defined as:

$$C_z(w, u, u_c) = (w, F_r(u, u_c, n_i) - n_i F_i)_P$$  \hfill (1.2)

Recall the definition of $B(w, u)$ from equation (3.5) and undo the partial integration step:

$$\left( w, \frac{\partial F_i}{\partial u} u_i \right)_Q + \lambda_P (w, F_r(u, u_c, n_i) - n_i F_i)_P = (w, S)_Q \quad \forall \ w \in \mathcal{W}$$  \hfill (1.3)

Transforming the $P$-integral into a $Q$-integral using the Dirac-delta function:

$$\left( w, \frac{\partial F_i}{\partial u} u_i \right)_Q + \lambda_P (w, \delta_P(F_r(u, u_c, n_i) - n_i F_i))_Q = (w, S)_Q \quad \forall \ w \in \mathcal{W}$$  \hfill (1.4)

Transforming this weak formulation back into the strong from yields:

$$\frac{\partial F_i}{\partial u} u_i + \lambda_P \delta_P(F_r(u, u_c, n_i) - n_i F_i) = S \quad \forall \ w \in \mathcal{W}$$  \hfill (1.5)
From this equation it can be seen the weak zonal coupling is just a proportional control on the flux boundary.

For nonlinear conservation laws, like the Euler equations, the exact solution of the Riemann problem is not always available explicitly. For such cases it can only be found iteratively. This is computationally expensive, but more importantly, the Jacobian of the Riemann flux with respect to the left or right state is not available. This is a problem when Newton-Raphson iterations are used for solving the non-linear system of equations. Fortunately, a wide range of explicit approximate Riemann solvers are available. These have mainly been developed for finite-volume methods.

When the discretization on both sides of the interface is identical, one might expect a continuous solution if \( \lambda_p \to \infty \). This is not necessarily the case, although the method is discretely conservative. For \( \lambda_p \to \infty \), \( B_2(w, u, u_c) = 0 \), so that:

\[
n_i F_i(u) = F_i(u, u_c, n_i)
\]  \hspace{1cm} (1.6)

However this relation holds on both sides of the interface, hence:

\[
n_i F_i(u_{left}) = n_i F_i(u_{right}) = F_i(u_{left}, u_{right}, n_i)
\]  \hspace{1cm} (1.7)

This relation proves the statement the coupling method is discretely conservative. Depending on the flux formulation and the Riemann flux the solution might be discontinuous. The method does not mimic the normal Continuous-Galerkin (CG) method as might be expected. This is because the internal error of on these boundaries is not taken into account due to the large penalty formulation. Hence the the DOFs near the boundary are only effected by this boundary and not by the internal error.

Choosing \( \lambda_p = 1 \) is the most natural and most common choice. This also leads to a conservative coupling. But with a better balance between interior and boundary errors.

Zonal coupling with \( \lambda_p = 1 \) provides a simple and natural method for coupling RANS and LES domains. When information is flowing from the RANS to the LES regions, however, an exact Riemann solver will provide a zero boundary condition for the smaller scales. For the remainder of the report we therefore consider a new approach based on overlap coupling.

2. **Overlap coupling**

\( u_c \) represents the solution obtained by a different method incorporating superior modeling characteristics. It is desired that the solution \( u \) resembles the solution \( u_c \) in the overlapping region, as this solution is considered to be more accurate. Although \( u_c \) is considered to be accurate, it has a low level of resolution.

The solution \( u \) is in a larger function space then \( u_c \). However, the function space of \( u_c \) might not be completely inside the function space of \( u \). This might be due to different meshes or different shape functions in both function spaces. Therefore \( u \) is required to be equal to \( u_c \) in a weak sense. This will be achieved with a proportional control source term. The strong form of the conservation law of equation (1.2) with the additional source term is:

\[
u_t = -\frac{\partial F_i}{\partial u_i} u_i + S + \lambda c(u, u_c)
\]  \hspace{1cm} (2.1)

Where \( c(u, u_c) \) is some functional relating \( u \) and \( u_c \). The weak formulation of equation (2.1), adding the source term to the Galerkin formulation of equation (3.4) results in:

\[
B(w, u) = (w, S) + \lambda c_0(w, u, u_c) \quad \forall w \in \mathcal{W}
\]  \hspace{1cm} (2.2)

With the overlap coupling operator \( c_0(\cdot, \cdot, \cdot) \), is defined as:

\[
C_0(w, u, u_c) = (w, c(u, u_c))_Q
\]  \hspace{1cm} (2.3)

From equation (2.1), it is clearly seen the time change of conservative variables is not only governed by the net-influx and source but also by the additional proportional-control term. The parameter \( \lambda \) gives the possibility to choose the the "strength" of the coupling.
2.1 Source functionals
The functional \( C(u, u_c) \) should be zero if \( u = u_c \) and monotonic (in some sense) with respect to the difference between \( u \) and \( u_c \). A larger deviation between \( u \) and \( u_c \) should result in a stronger source term. Numerous options for this functional are available, including non-linear variants, however only two options will be discussed:

- Difference in Conservative Variables
- Difference in Flux Divergence

These functionals are both relatively simple to analyze. A combination of both functionals is also a valid option. This option is not considered for reasons of simplicity.

2.1.1 Difference in conservative variables
In this case the functional is simply:

\[
c(u, u_0) = u - u_0
\]  
(24)

This type of overlap coupling will be referred to as conservative variable coupling. To be able to relate the coupling term to the net-influx term (the flux divergence \( F_{\nu_i} \)), the penalty parameter \( \lambda \) should be made dimensionless.

\[
\lambda = \lambda_0 \kappa
\]  
(25)

with:

\[
\kappa = \mathcal{O} \left( \frac{\partial F_i}{\partial u} \frac{\partial}{\partial x_i} \right) \quad \text{or} \quad \kappa = \mathcal{O} \left( \frac{\partial F_i}{\partial u_j} \frac{\partial^2}{\partial x_i \partial x_j} \right)
\]  
(26)

Usually the first term will be used, if present. This term is also used to scale the second term (the diffusion term), resulting in the definition of the Reynolds number. For the 1D linear convection-diffusion problem, for example, this results in:

\[
\kappa = \frac{2 \pi a}{L}
\]  
(27)

Where \( L \) is the domain length and \( a \) is the convection speed

2.1.2 Difference in flux divergence
The penalty term can also be chosen such that the scaling is incorporated in the formulation. This can be done by including the gradient and the flux explicitly in the coupling term. This is the case when the functional is chosen to be the difference in flux divergence:

\[
c(u, u_c) = F_{s,i} - F_{c_{s,i}}
\]  
(28)

Where \( i \) are only the spatial directions. This type of overlap coupling will be referred to as flux-divergence coupling. Using the chain rule of differentiation:

\[
F_{s,i} = \frac{\partial F_i}{\partial u} u_{i,i} + \frac{\partial F_i}{\partial u_j} u_{i,j}
\]  
(29)

yields:

\[
c(u, u_c) = \left( \frac{\partial F_i}{\partial u} (u) \cdot u_{i,i} + \frac{\partial F_i}{\partial u_j} (u) \cdot u_{i,j} \right) - \left( \frac{\partial F_i}{\partial u} (u_c) \cdot u_{i,i} + \frac{\partial F_i}{\partial u_j} (u_c) \cdot u_{i,j} \right)
\]  
(2.10)

In the case the of a linear conservation law this results in:

\[
c(u, u_c) = \frac{\partial F_i}{\partial u} \cdot (u_{i,i} - u_{c_{i,i}}) + \frac{\partial F_i}{\partial u_j} \cdot (u_{i,j} - u_{c_{i,j}})
\]  
(2.11)
For non-linear conservation laws, it seems reasonable to assume the Jacobians based on \( \mathbf{u} \) or \( \mathbf{u}_c \) will be quite equal as \( \mathbf{u} \) and \( \mathbf{u}_c \) should be fairly equal. This assumption yields the same equation as the linear case. Evaluating the Jacobians at \( \mathbf{u}_c \) yields a coupling term linear in \( \mathbf{u} \).

**Weak formulation**

The weak formulation of the flux-divergence overlap coupling is:

\[
C_0(w, \mathbf{u}, \mathbf{u}_c) = (w, \mathbf{F}_i - \mathbf{F}_{ci})
\]

In the case of diffusion problems, or other problems involving second-order derivatives, this formulation leads to strict continuity demands on the trial space. Hence one partial integration step (Gauss law) is needed to reduce the order of the derivatives involved in the formulation. This eases the continuity demand. By doing so, this equation (2.12) is transformed in:

\[
C_0(w, \mathbf{u}, \mathbf{u}_c) = (w, n_i (\mathbf{F}_i - \mathbf{F}_{ci}))_E - (w, i_i (\mathbf{F}_i - \mathbf{F}_{ci}))_Q
\]

Assuming the conservation law is linear or at least obeys the homogeneity property, like the Euler-equations, this can be written as:

\[
C_0(w, \mathbf{u}, \mathbf{u}_c) = \left( w, n_i \left( \frac{\partial \mathbf{F}_i}{\partial \mathbf{u}} \cdot (\mathbf{u} - \mathbf{u}_c) + \frac{\partial \mathbf{F}_i}{\partial \mathbf{u}_i} \cdot (\mathbf{u}_i - \mathbf{u}_c) \right) \right)_E
- \left( w, i_i \left( \frac{\partial \mathbf{F}_i}{\partial \mathbf{u}} \cdot (\mathbf{u} - \mathbf{u}_c) + \frac{\partial \mathbf{F}_i}{\partial \mathbf{u}_i} \cdot (\mathbf{u}_i - \mathbf{u}_c) \right) \right)_Q
\]

(2.14)

2.2 Variational-Multi-Scale overlap coupling

At the beginning of this section it was stated the solution \( \mathbf{u}_c \) has low resolution. It only contains large scales, small scales are absent. Hence it is desired that only the large scales are coupled while the small scales are allowed to develop freely. The overlap-coupling methods introduced before don’t differentiate between scales, both large and small scales are coupled. The Variational-Multi-Scale (VMS) approach to overlap coupling is introduced in this subsection, in the hope to circumvent this problem.

Just like the turbulence-modeling variant of VMS, a separation between large and small resolved scales is made. This is done by means of a variational projection:

\[
\bar{w} \in \bar{W} \quad \bar{\mathbf{u}} \in \bar{U}
\]

\[
\bar{w} \in \bar{W} \quad \bar{\mathbf{u}} \in \bar{U}
\]

(2.15)

The finite spaces \( \mathcal{W}^h \) and \( \mathcal{U}^h \) are completely spanned by the subspaces:

\[
\mathcal{W}^h = \bar{W} \oplus \bar{\mathcal{W}}
\]

\[
\mathcal{U}^h = \bar{U} \oplus \bar{\mathcal{U}}
\]

(2.16)

Where \( \bar{W} \) and \( \bar{U} \) are function spaces containing the large scales, while \( \bar{\mathcal{W}} \) and \( \bar{\mathcal{U}} \) are function spaces containing the small scales. The spaces \( \bar{W} \) and \( \bar{U} \), on one side, and \( \bar{\mathcal{W}} \) and \( \bar{\mathcal{U}} \), on the other side, are identical except at Dirichlet boundaries. For simplicity it can be assumed \( \mathbf{u}_c \in \bar{U} \).

Based on this scale separation, three options for the VMS implementation of overlap coupling are considered:

- Separate wrt the test space
- Separate wrt the trial space
- Separate wrt both the test and trial space

Each will be treated separately in the next subsections.
2.2.1 Separate wrt the test space (type-I)
In this case the weak formulation of the coupling term is:

\[ C_o(\overline{w}, \mathbf{u}, \mathbf{u}_c)_Q \]  
(2.17)

And the resulting governing equation becomes:

\[ B(\overline{w}, \mathbf{u}) + \lambda_o C_o(\overline{w}, \mathbf{u}, \mathbf{u}_c)_Q = (\overline{w}, \mathbf{S}) \]
\[ B(\overline{w}, \mathbf{u}) = (\overline{w}, \mathbf{S}) \]  
(2.18)

Choosing \( \lambda_o \to \infty \) yields:

\[ C_o(\overline{w}, \mathbf{u}, \mathbf{u}_c)_Q = 0 \]
\[ B(\overline{w}, \mathbf{u}) = (\overline{w}, \mathbf{S}) \]  
(2.19)

2.2.2 Separate wrt the trial space (type-II)
In this case the weak formulation of the coupling term is:

\[ C_o(w, \mathfrak{u}, \mathfrak{u}_c)_Q \]  
(2.20)

And the resulting governing equation becomes:

\[ B(w, \mathfrak{u}) + \lambda_o C_o(w, \mathfrak{u}, \mathfrak{u}_c)_Q = (w, \mathbf{S}) \]  
(2.21)

Choosing \( \lambda_o \to \infty \) yields:

\[ C_o(w, \mathfrak{u}, \mathfrak{u}_c)_Q = 0 \]  
(2.22)

This formulation does not state anything with respect to \( \mathfrak{u} \), it is undetermined. This results in singular Jacobian. In practice there will be a limit on the maximum coupling parameter \( \lambda_o \).

2.2.3 Separate wrt both the test and trial space (type-III)
In this case the weak formulation of the coupling term is:

\[ C_o(\overline{w}, \mathfrak{u}, \mathfrak{u}_c)_Q \]  
(2.23)

And the resulting governing equation becomes:

\[ B(\overline{w}, \mathfrak{u}) + \lambda_o C_o(\overline{w}, \mathfrak{u}, \mathfrak{u}_c)_Q = (\overline{w}, \mathbf{S}) \]
\[ B(\overline{w}, \mathfrak{u}) = (\overline{w}, \mathbf{S}) \]  
(2.24)

Choosing \( \lambda_o \to \infty \) yields:

\[ C_o(\overline{w}, \mathfrak{u}, \mathfrak{u}_c)_Q = 0 \]
\[ B(\overline{w}, \mathfrak{u}) = (\overline{w}, \mathbf{S}) \]  
(2.25)

In case of orthogonal subspaces \( \overline{\mathcal{W}} \perp \widehat{\mathcal{W}} \) and \( \mathfrak{U} \perp \mathfrak{U} \). Or more importantly, \( \overline{\mathcal{W}} \perp \mathfrak{U} \) and \( \mathfrak{U} \perp \widehat{\mathcal{W}} \). The previous two VMS-types might become similar to this type, depending on the source functional.

3. Solution strategy
The coupled multi-model setup results in a large system of equations, like the example in equation 3.1.

\[ B_1(w^1, \mathbf{u}^1) + C_{12}(w^1, \mathbf{u}^1, \mathbf{u}^2) + C_{13}(w^1, \mathbf{u}^1, \mathbf{u}^3) = 0 \quad \forall \, w^1 \in \mathcal{W}^1 \]
\[ B_2(w^2, \mathbf{u}^2) + C_{21}(w^2, \mathbf{u}^2, \mathbf{u}^1) + C_{23}(w^2, \mathbf{u}^2, \mathbf{u}^3) = 0 \quad \forall \, w^2 \in \mathcal{W}^2 \]
\[ B_3(w^3, \mathbf{u}^3) + C_{31}(w^3, \mathbf{u}^3, \mathbf{u}^1) + C_{32}(w^3, \mathbf{u}^3, \mathbf{u}^2) = 0 \quad \forall \, w^3 \in \mathcal{W}^3 \]  
(3.1)
Due to the coupling terms $C_{ij}(w^j, u^i, u^j)$ there are cross dependencies between the models: the solution of one model depends on the solution of another model. Discretizing the monolithic system will eventually lead to a linear system of equations, as given in figure 3.1. In this figure $a^m_i$ is the vector of unknowns and $r^m_k$ is the residual of model $m$. $A^m_{kl}$ are the different parts of the Jacobian, which can be calculated using:

$$A^m_{kl} = \frac{\partial}{\partial u^k} B_m(w^m_k, u^i + u^l_i)|_{u^k=0}$$

$$A^m_{kl} = \frac{\partial}{\partial u^k} C_m(u^k_i, u^m_i, u^n_i + u^l_i)|_{u^k=0} \quad m \neq n$$

(3.2)

The Jacobians of the coupling terms $C_{ij}(w^j, u^i, u^j)$ are difficult to implement in the numerical code, as information from both models is necessary for their assembly.

A solution to this problem is to solve the monolithic system of equations with a block Gauss-Seidel iteration method. The solution of each model is updated separately, leaving the solutions of all other models unaffected. This is done sequentially for all models. The loop continues until all models are converged. In other words, the large monolithic system is replaced with a series of smaller partitioned systems. With this solving strategy there is no need to assemble the cross-dependent terms in the Jacobian, as the dependencies between the models are shifted to the residual.

See the algorithm in figure 3.2 for a schematic explanation of the partitioned solution strategy.

Step 3 is basically identical to the algorithm explained in section 5: a better approximation of the numerical solution is found using a Newton iteration step. Also the convergence check is similar. However, when the algorithm loops through the other models, the solutions of these models might be altered considerably. This can influence a model which was considered to be converged. Hence it is desired to check if the models are still converged. The check at step 3.e is not appropriate, as it demands the calculation $\Delta a^m_i$. This is requires a big effort which should be avoided.

To circumvent this problem the residual norm is calculated $\rho^m$ when the model is considered converged. Each consecutive loop the convergence is checked at the beginning of step 3. If the current residual norm does not deviate too much from the residual norm $\rho^m$ when the model was considered converged, the model is still considered to be converged. This margin is governed by $\gamma$. When the model is still considered converged, the algorithm will skip this model and the solution will not be updated.

The algorithm is also applicable when the models are linear. However, the convergence check at steps 3.e and 3.f can be omitted as the model will be converged after only one step. The residual after the correction of the solution will be machine zero. Hence the convergence criterium at the beginning of step 3 should not be chosen too strict, i.e. $\gamma$ should not be chosen too small.
Algorithm

1. Choose an initial guess $[\mathbf{a}_1, ..., \mathbf{a}_M]$ for each model
2. Set $\hat{r}^m = 0$ for each model
3. Loop over all models: $m = [1, ..., M]$
   - Compute residual $r_k^m$ based on $[\mathbf{a}_1, ..., \mathbf{a}_M]$
   - When $1 - \frac{r_k^m}{\| r_k^m \|} > \gamma$ then update $\mathbf{a}^m$:
     a. Set $\hat{c}^m = \text{false}$
     b. Compute the Jacobian $A_k^{mm}$ based on $[\mathbf{a}_1, ..., \mathbf{a}_M]$
     c. Solve linear system of equations: $A_k^{mm} \Delta \mathbf{a}_k^m = r_k^m$
     d. Update solution: $\mathbf{a}_k^m = \mathbf{a}_k^m + \Delta \mathbf{a}_k^m$
     e. Check convergence: $\epsilon = \frac{\| \Delta \mathbf{a}_k^m \|}{\| \mathbf{a}_k^m \|}$
     f. When $\epsilon < \epsilon_k^m$:
        - Recompute $r_k^m$ based on $[\mathbf{a}_1, ..., \mathbf{a}_M]$
        - Set $\hat{r}^m = \| r_k^m \|$ and $\hat{c}^m = \text{true}$
4. When not for each model $c = \text{true}$ goto 3
5. All solutions are converged

Figure 3.2: The partitioned solution strategy
Chapter 4
Pure overlap coupling

In this chapter the basic behavior of the overlap-coupling method developed in the previous section will be assessed, by considering the coupling terms in isolation. This allows us to set some limits on the value for the coupling parameter, $\lambda$, and provides preliminary insight into the difference between variable coupling and flux-divergence coupling.

The coupling terms in isolation means that the time rate of change of the solution is only governed by the difference between the solution $u$ and the reference solution $u_c$:

$$u_t = \lambda e(u_t, u)$$  \hspace{1cm} (0.1)

To simplify the analysis the reference solution will be based on solutions of the convection-diffusion equation. This is a linear equation making it simple to analyze and inexpensive to compute numerically. The length of the domain, $L$, is chosen to be unity for simplicity. A periodic boundary condition is chosen to circumvent problems at the boundary.

Two different initial conditions will be used for the analysis:

- A single Sine wave
- A Burgers shock

The difference between these initial conditions is their spectrum. The single Sine wave has a spectrum containing only one wavelength (equal to the length of the domain), while the Burgers shock has a spectrum containing all possible wavelengths.

This solution of equation (0.1) will be discussed for variable coupling in section 1 and for flux-divergence coupling in section 2. In both sections the analytic solution will be derived first. This is done by splitting the solution into a particular and homogeneous part. The particular solution is the part of the solution which depends on the reference solution. This part generally does not match with the given initial condition. Therefore the homogeneous part is added to the solution. This is a weighted sum of the Eigenfunctions of the homogeneous equation. This sum is chosen such that the total solution, the sum of particular solution and homogeneous solution, matches with the initial condition. When the assumed solutions for the homogeneous and particular part have the same temporal behavior resonance might occur. This can lead to unbounded growth of the solution.

After presenting the analytic solutions, some limit cases will be discussed to get some basic understanding of both coupling methods.
1. Variable coupling
With this type of overlap coupling the governing equation is:

\[ \mathbf{u}_k = \lambda (\mathbf{u}_c - \mathbf{u}) \]  
(1.1)

1.1 Analytic solution
1.1.1 Particular solution
The particular solution of equation (1.1) is computed using the decompositions given in appendix II. Substitution yields:

\[ \mathbf{b}_k (\omega \mathbf{i} a - \nu \alpha^2 k^2) = \lambda (\mathbf{a}_k - \mathbf{b}_k) \quad \forall k \]  
(1.2)

Reordering yields:

\[ \mathbf{b}_k = T^\text{par}_k \mathbf{a}_k \quad \forall k \]  
(1.3)

With the transfer coefficients:

\[ T^\text{par}_k = \frac{\lambda}{\omega \mathbf{i} a - \nu \alpha^2 k^2 + \lambda} \]  
(1.4)

This complex number can be split into real and imaginary parts:

\[ \text{Re}(T^\text{par}_k) = \frac{\lambda (\lambda - \nu \alpha^2 k^2)}{(\omega \mathbf{i} a)^2 + (\lambda - \nu \alpha^2 k^2)^2} \]
\[ \text{Im}(T^\text{par}_k) = \frac{\lambda \omega \mathbf{i} a}{(\omega \mathbf{i} a)^2 + (\lambda - \nu \alpha^2 k^2)^2} \]  
(1.5)

Resonance

Resonance occurs when \( T^\text{par}_k \) becomes singular. This happens when convection is absent (\( a = 0 \)) and the penalty parameter is exactly \( \lambda = \nu \alpha^2 k^2 \). In the general case, when all wave numbers are present in the solution, resonance will always occur. This specific wave number at which resonance occurs is called the critical wavenumber:

\[ k_r = \sqrt{\frac{\lambda}{\nu \alpha^2}} \]  
(1.6)

At this wavenumber, the particular solution is anticipated to evolve in a manner similar to the homogeneous solution (the temporal behavior is anticipated to be identical) hence both solutions will resonate. Instead of the decomposition given in equation .2 the decomposition given in .4 is used. Substitution in equation 1.1 yields equations 1.3 and 1.4 for all non-critical wave numbers and for the critical wavenumber:

\[ \mathbf{b}_k (1 + \nu \alpha^2 k^2) + 1 = \nu \alpha^2 k^2 (\mathbf{a}_k - \mathbf{b}_k (1 + t)) \]  
(1.7)

This simplifies to:

\[ \mathbf{b}_k = \nu \alpha^2 k^2 \mathbf{a}_k = \lambda \mathbf{a}_k \]  
(1.8)

Hence:

\[ T^\text{par}_{k_r} = \lambda \]  
(1.9)

1.1.2 Homogeneous solution
The homogeneous part of equation 1.1 is:

\[ \mathbf{u}_t = -\lambda \mathbf{u} \]  
(1.10)

Which has a solution of the form:

\[ \mathbf{u}_\text{hom} = \sum c_k e^{i \omega_{k_r} t} e^{-\lambda t} \]  
(1.11)
Form this homogeneous solution we can easily conclude the method is stable if $\lambda \geq 0$. Using the transfer coefficients for the particular solution $T_k^\text{par}$, the transfer coefficients for the homogeneous solution can be derived. These are simply $T_k^\text{hom} = 1 - T_k^\text{par}$, (see appendix III):

$$\begin{align*}
Re(T_k^\text{hom}) &= \frac{(aka)^2 - \nu\alpha^2k^2(\lambda - \nu\alpha^2k^2)}{(aka)^2 + (\lambda - \nu\alpha^2k^2)^2} \\
Im(T_k^\text{hom}) &= \frac{-\lambda\nu\alpha a}{(aka)^2 + (\lambda - \nu\alpha^2k^2)^2}
\end{align*} \tag{1.12}$$

For the case where convection is not present, the transfer coefficient for the critical wave number $k_r$ is:

$$\begin{align*}
Re(T_{kr}^\text{hom}) &= 1 - \lambda \\
Im(T_{kr}^\text{hom}) &= 0 \tag{1.13}
\end{align*}$$

1.1.3 Total solution

The total solution is the sum of the particular and homogeneous solution:

$$u = \sum_k T_k^\text{hom}a_k e^{-\lambda t} + \sum_k T_k^\text{par}a_k e^{i\omega_k x - \nu\alpha^2k^2 t}$$

$$= \sum_k (T_k^\text{hom} e^{-\lambda t} + T_k^\text{par} e^{-\nu\alpha^2k^2 t})a_k e^{i\omega_k x} \tag{1.14}$$

Or in case of resonance, hence $\omega = 0$, then $u$ becomes:

$$\begin{align*}
u &= (1 - \lambda)a_k e^{-\lambda t} + \lambda(1 + t)a_k e^{-i\alpha^2k^2 t} + \sum_{k \neq k_r} (T_k^\text{hom} e^{-\lambda t} + T_k^\text{par} e^{-\nu\alpha^2k^2 t})a_k e^{i\omega_k x} \\
&= (1 - \lambda)a_k e^{-\lambda t} + \lambda(1 + t)a_k e^{-\nu\alpha^2k^2 t} \tag{1.15}
\end{align*}$$

1.2 Limit cases

In this subsection the limit cases of pure convection and pure diffusion will be discussed. This assumption makes analysis of the results easier.

1.2.1 Pure convection

In the case of pure convection, $\nu = 0$, the real and imaginary parts transfer coefficients of the particular solution become:

$$\begin{align*}
Re(T_k^\text{par}) &= \frac{\lambda^2}{(aka)^2 + \lambda^2} = \frac{\lambda_0^2}{k^2 + \lambda_0^2} = \frac{(\frac{\mu}{k})^2}{1 + (\frac{\mu}{k})^2} \\
Im(T_k^\text{par}) &= \frac{-\lambda\nu\alpha a}{(aka)^2 + \lambda^2} = \frac{-\lambda\omega_k}{k^2 + \lambda_0^2} = \frac{-\lambda}{1 + (\frac{\mu}{k})^2}
\end{align*} \tag{1.16}$$

The transfer coefficients for the homogeneous solution:

$$\begin{align*}
Re(T_k^\text{hom}) &= \frac{(aka)^2}{(aka)^2 + \lambda^2} = \frac{1}{1 + (\frac{\mu}{k})^2} \\
Im(T_k^\text{hom}) &= \frac{-\lambda\nu\alpha a}{(aka)^2 + \lambda^2} = \frac{-\lambda}{1 + (\frac{\mu}{k})^2} \tag{1.17}
\end{align*}$$

Where the normalized penalty is defined as $\lambda_0 = \frac{\lambda}{\mu}$. The real and imaginary parts of the transfer coefficients as function of the penalty parameter are given in plot $a$ of figure 4.1.
These can be translated into the magnitude and the argument of the complex transfer coefficients which are directly related to the magnitude and argument:

\[
||T_k^{\text{par}}|| = \sqrt{\text{Re}(T_k^{\text{par}})^2 + \text{Im}(T_k^{\text{par}})^2} = \sqrt{\left(\frac{\lambda_0}{\lambda_k}\right)^4 + \left(\frac{\lambda_0}{\lambda_k}\right)^2} = \sqrt{\frac{\lambda_0^2}{\lambda_k^2 + 1}}
\]

\[
\text{arg}(T_k^{\text{par}}) = \arctan\left(\frac{\text{Im}(T_k^{\text{par}})}{\text{Re}(T_k^{\text{par}})}\right) = \arctan\left(\frac{\lambda_0}{\lambda_k}\right) = \arctan\left(\frac{1}{\lambda_k}\right)
\]  

(1.18)

and:

\[
||T_k^{\text{hom}}|| = \sqrt{\frac{1 + \left(\frac{\lambda_0}{\lambda_k}\right)^2}{\left(1 + \left(\frac{\lambda_0}{\lambda_k}\right)^2\right)^2}} = \sqrt{\frac{1}{\lambda_k^2 + 1}}
\]

\[
\text{arg}(T_k^{\text{hom}}) = \arctan\left(\frac{\lambda_0}{1}\right) = \arctan\left(\frac{-\lambda_0}{\lambda_k}\right)
\]  

(1.19)

The magnitude and argument as function of the coupling parameter are given in plot b and c of figure 4.1. As \(\lambda_0 \rightarrow \infty\):

\[
\lim_{\lambda_0 \rightarrow \infty} ||T^{\text{par}}|| = 1 \quad \lim_{\lambda_0 \rightarrow \infty} \text{arg}(T^{\text{par}}) = 0
\]

\[
\lim_{\lambda_0 \rightarrow \infty} ||T^{\text{hom}}|| = 0 \quad \lim_{\lambda_0 \rightarrow \infty} \text{arg}(T^{\text{hom}}) = -\frac{\pi}{2}
\]  

(1.20)
Figure 4.2: The sine wave solution for pure convection with variable coupling

**Single sine wave**

For the single sine wave the analytic solution is easily constructed, as only the \( k = 1 \) wavenumber is present in the solution. Hence the transfer coefficients become:

\[
T_{\text{par}} = \frac{\lambda_0^2}{1 + \lambda_0^2} + i\frac{\lambda_0}{1 + \lambda_0^2}, \\
T_{\text{hom}} = \frac{1}{1 + \lambda_0^2} + i\frac{-\lambda_0}{1 + \lambda_0^2}
\]  

(1.21)

Resulting in the following solution:

\[
u = \left( \left( \frac{1}{1 + \lambda_0^2} + i\frac{-\lambda_0}{1 + \lambda_0^2} \right) e^{-\lambda t} + \left( \frac{\lambda_0^2}{1 + \lambda_0^2} + i\frac{\lambda_0}{1 + \lambda_0^2} \right) e^{-i\omega t} \right) a_1 e^{i\omega x} + \left( \frac{1}{1 + \lambda_0^2} \sin(\omega x) - \frac{\lambda_0}{1 + \lambda_0^2} \cos(\omega x) \right) e^{-\lambda t}
\]

\[
+ \left( \frac{\lambda_0^2}{1 + \lambda_0^2} \sin(\omega(x - at)) + \frac{\lambda_0}{1 + \lambda_0^2} \cos(\omega(x - at)) \right)
\]

(1.22)

These results are given in figure 4.2, where the DNS solution is the exact solution. It can be clearly seen the lag of the solution becomes larger with smaller coupling parameters. While the amplitude of the solution is decreased.

**Burgers shock**
Figure 4.3: The solution for the burgers shock with pure convection with variable coupling

For the burgers shock the analytic solution is as given in equations 1.14 and 1.15 with the appropriate $a_k$. The results are given in figure 4.3. Just like the sine wave, the lag of the solution becomes larger with smaller coupling parameters. Reducing the coupling parameter also leads to a more blunt shock, due to the coupling term which behaves differently for all wave numbers. Low coupling parameters, like $\lambda_0 = 1.0$, result in highly-deformed shock shapes.

1.2.2 Pure diffusion
In the case of pure diffusion, hence $a = 0$, the real and imaginary part of the transfer coefficients become:

$$
Re(T_{k}^{\text{par}}) = \frac{\lambda}{\lambda - \nu \alpha^2 k^2} = \frac{\lambda_0}{\lambda_0 - k^2} = \frac{\lambda_0}{\frac{\lambda_0}{k^2} - 1}
$$

$$
Im(T_{k}^{\text{par}}) = 0
$$

and the transfer coefficients for the homogeneous solution:

$$
Re(T_{k}^{\text{hom}}) = \frac{-\nu \alpha^2 k^2 (\lambda - \nu \alpha^2 k^2)}{(\lambda - \nu \alpha^2 k^2)^2} = \frac{-\nu \alpha^2 k^2}{\lambda - \nu \alpha^2 k^2} = \frac{-1}{\lambda - \frac{1}{\nu \alpha^2 k^2}} - 1
$$

$$
Im(T_{k}^{\text{hom}}) = 0
$$

(1.23)

where the normalized coupling parameter are defined as $\lambda_0 = \frac{\lambda}{\nu \alpha^2}$. The real and imaginary parts of the transfer coefficients as function of the coupling parameter are given in plot a figure 4.1.

This can be translated in the magnitude and the argument of the complex transfer coefficients which are directly related to the magnitude and argument:
\[ ||T_{k}^{\text{par}}|| = \sqrt{\text{Re}(T_{k}^{\text{par}})^2 + \text{Im}(T_{k}^{\text{par}})^2} = \frac{(\lambda_0)}{|(\lambda_0) - 1|} \]
\[
\text{arg}\ T_{k}^{\text{par}} = \arctan \frac{\text{Im}(T_{k}^{\text{par}})}{\text{Re}(T_{k}^{\text{par}})} = 0
\]  

(1.25)

And:

\[ ||T_{k}^{\text{hom}}|| = \frac{1}{|(\lambda_0) - 1|} \]
\[
\text{arg}\ T_{k}^{\text{hom}} = 0
\]  

(1.26)

The amplitude and phase errors as function of the penalty parameter are given in the second part of figure 4.4.

**Single sine wave**

For the single sine wave the transfer coefficients become:

\[ T_{1}^{\text{par}} = \frac{\lambda_0}{\lambda_0 - 1} \]
\[ T_{1}^{\text{hom}} = \frac{-1}{\lambda_0 - 1} \]  

(1.27)

Resulting in the following solution:

\[ u = \left( \frac{-1}{\lambda_0 - 1} e^{-\lambda x} + \frac{\lambda_0}{\lambda_0 - 1} e^{-\nu x^2 t} \right) a_1 e^{i\omega x} \]
\[
= \left( \frac{-1}{\lambda_0 - 1} e^{-\lambda x} + \frac{\lambda_0}{\lambda_0 - 1} e^{-\nu x^2 t} \right) \sin \alpha x
\]  

(1.28)

In case of resonance when \( \lambda = \nu x^2 \), the transfer coefficients become:

\[ T_{1}^{\text{par}} = \lambda = \nu x^2 \]
\[ T_{1}^{\text{hom}} = 1 - \lambda = 1 - \nu x^2 \]  

(1.29)
Figure 4.5: The sine wave solution for pure diffusion with variable coupling

Hence $u$ becomes:

$$ u = \frac{\lambda_0}{\lambda_0 - \lambda_0^2} + \frac{1}{\lambda_0 - \lambda_0^2} \ln \frac{1}{1 - \lambda_0^2} $$

Equation 1.30

The ratio of solution over exact solution now becomes:

$$ r = \frac{u}{u_0} = 1 + \nu \alpha^2 t $$

Equation 1.32

The results given in equation 1.28 and 1.30 are plotted in figure 4.5. It can be seen the solution always lags the true solution. This lag decreases when the coupling parameter is increased.

Burgers shock

For the burgers shock results are given in figure 4.6. In this case, the shock shape of the reference solution changes due to the diffusion. This shape change is quite accurately reproduced by the coupled solution. However, as for the sine wave, the solution always lags the true solution. This lag also decreases when the coupling parameter is increased.

2. Flux-divergence coupling

The governing equation for flux-divergence coupling is:

$$ \mathbf{u}_c = \lambda (F_{0c} - \mathbf{F}_x) $$

Equation 2.1
For the 1D convection-diffusion equation this becomes:

\[ u_k = \lambda((\alpha u_{0x} - \nu u_{0xx}) - (\alpha u_x - \nu u_{xx})) \]  

(22)

2.1 Analytic solution

2.1.1 Particular solution

Substituting the decompositions of the solutions given in appendix II into equation (2.1) yields:

\[ b_k(-\alpha \omega^2 + \nu \omega^2 k^2) = \lambda((\omega \omega^2 + \nu \omega^2 k^2)a_k - (\omega \omega^2 + \nu \omega^2 k^2)b_k) \quad \forall k \]  

(23)

Reordering:

\[ b_k = T_k^{par}a_k \quad \forall k \]  

(24)

with the coupling coefficients:

\[ T_k^{par} = \frac{\lambda(\omega \omega^2 + \nu \omega^2 k^2)}{-\omega \omega^2 - \nu \omega^2 k^2 + \lambda(\omega \omega^2 + \nu \omega^2 k^2)} = \frac{\lambda}{\lambda - 1} \]  

(25)

There is no difference between pure convection (\( \nu = 0 \)) and pure diffusion (\( \alpha = 0 \)). And there is no need to normalize the penalty. The transfer coefficient is a real number since it has no imaginary part:

\[ Re(T_k^{par}) = \frac{\lambda}{\lambda - 1} \]

\[ Im(T_k^{par}) = 0 \]  

(26)
Figure 4.7: Transfer coefficient for both convection and diffusion with flux-divergence coupling

Translating this into the magnitude and the argument is trivial:

\[
\|T_k^{\text{par}}\| = \sqrt{\text{Re}(T_k^{\text{par}})^2 + \text{Im}(T_k^{\text{par}})^2} = \frac{\lambda}{\lambda - 1}
\]
\[
\arg T_k^{\text{par}} = \arctan \frac{\text{Im}(T_k^{\text{par}})}{\text{Re}(T_k^{\text{par}})} = 0
\]

(2.7)

The real and imaginary part as function of the coupling parameter are given in the plot a of figure 4.7, while the amplitude as function of the coupling parameter is given in plot b of the figure.

Resonance

Choosing the penalty to be \(\lambda = 1\) will result in resonance. This can be observed in both \(T_k^{\text{par}}\) and \(T_k^{\text{hom}}\) which become singular at this point. Hence the previously mentioned particular solution is no longer valid.

In the case of resonance the equation 2.1 becomes:

\[
u_t + F_x = F_{0x}
\]

(2.8)

Substitution of the decomposed solution as in equation 3 yields:

\[
((1 + t)(-\nu\alpha^2k^2) + 1 + a(1 + t)(\alpha k) + \nu(1 + t)(\alpha k)^2)\mathbf{b}_k = (a(\alpha k) + \nu(\alpha k)^2)\mathbf{a}_k \quad \forall k
\]

(2.9)

This simplifies to:

\[
\mathbf{b}_k = (a\alpha k + \nu\alpha^2k^2)\mathbf{a}_k \quad \forall k
\]

(2.10)

Hence:

\[
T_k^{\text{par}} = a\alpha k + \nu\alpha^2k^2
\]

(2.11)

2.1.2 Homogeneous solution

The homogeneous part of equation 2.1 is

\[
u_t = -\lambda(\alpha u_x - \nu u_{xx})
\]

(2.12)

Which has a solution of the form:

\[
u = \sum c_k e^{\alpha_k(x - \lambda at) - \nu\alpha^2k^2t}
\]

(2.13)
Form this homogeneous solution it can be concluded that the stability of the method depends on the presence of diffusion. In the case there is no diffusion the method is unconditionally stable. In the case diffusion is present, however, the method is stable only if $\lambda \geq 0$. With a negative coupling parameter the diffusion will be reversed and hence add energy to the system.

Using the transfer coefficients for the particular solution $T_k^{par}$ the transfer coefficients for the homogeneous solution can be derived. These are simply $T_k^{hom} = 1 - T_k^{par}$ (for an explanation see appendix III):

$$
Re(T_k^{hom}) = \frac{-1}{\lambda - 1}
$$

$$
Im(T_k^{hom}) = 0
$$

(2.14)

Or in case $\lambda = 1$ and the solution resonates:

$$
Re(T_k^{hom}) = 1 - \nu \alpha^2 k^2
$$

$$
Im(T_k^{hom}) = -a \omega k
$$

(2.15)

The real and imaginary part as function of the penalty parameter are given in the first part of figure 4.7, while the amplitude as function of the penalty parameter is given in the second part of the figure.

2.1.3 Total solution

The total solution is the sum of the particular and homogeneous solution:

$$
u = \sum \left( \frac{-1}{\lambda - 1} a_k e^{i k(\omega t - \omega t)x - \nu \alpha^2 k^2 t} + \frac{\lambda}{\lambda - 1} a_k e^{i k(\omega t + \omega t)x - \nu \alpha^2 k^2 t} \right)
$$

$$
= \sum \left( \frac{-1}{\lambda - 1} e^{-a \omega k \omega t - \nu \alpha^2 k^2 t} + \frac{\lambda}{\lambda - 1} e^{-a \omega k \omega t + \nu \alpha^2 k^2 t} \right) a_k e^{i k \omega t}
$$

(2.16)

Or in case of resonance, $\nu$ becomes:

$$
u = \sum \left( -a \omega k + (1 - \nu \alpha^2 k^2) a_k e^{i k(\omega t + \omega t)x - \nu \alpha^2 k^2 t} \right)
$$

$$
+ \sum \left( a \omega k + \nu \alpha^2 k^2) a_k (1 + t) e^{i k(\omega t - \omega t)x - \nu \alpha^2 k^2 t} \right)
$$

$$
= \sum \left( -a \omega k + (1 - \nu \alpha^2 k^2) + (a \omega k + \nu \alpha^2 k^2) (1 + t) a_k e^{i k(\omega t + \omega t)x - \nu \alpha^2 k^2 t} \right)
$$

$$
= \sum \left( 1 + (a \omega k + \nu \alpha^2 k^2) t \right) a_k e^{i k(\omega t + \omega t)x - \nu \alpha^2 k^2 t}
$$

(2.17)

For the case where the solution only contains one frequency $k$: the ratio solution over reference solution becomes:

$$
\frac{\nu}{\nu_0} = (a \omega k + \nu \alpha^2 k^2) (1 + t)
$$

(2.18)

Hence the ratio of solutions will diverge in time. When diffusion is absent this will give rise to algebraic instability.

2.2 Limit cases

In this subsection the limit cases of pure convection and pure diffusion will be discussed.

2.2.1 Pure convection

In the case of pure convection, hence $\nu = 0$ the total solution is:

$$
u = \sum \left( \frac{-1}{\lambda - 1} e^{-a \omega k \omega t} + \frac{\lambda}{\lambda - 1} e^{-a \omega k \omega t} \right) a_k e^{i k \omega t}
$$

(2.19)

Or in case of resonance:

$$
u = \sum (1 + a \omega k i t) a_k e^{i k(\omega t + \omega t)}
$$

(2.20)
Figure 4.8: The sine wave solution for pure convection with flux-divergence coupling

**Single sine wave**

For the single sine wave the analytic solution is easily constructed. As only the $k = 1$ wavenumber is present in the solution,

$$
\begin{align*}
\mathbf{u} &= \left( \frac{-1}{\lambda - 1} e^{-\alpha \lambda at} + \frac{\lambda}{\lambda - 1} e^{-\alpha \lambda at} \right) a_1 e^{\alpha \chi x} \\
&= \frac{-1}{\lambda - 1} \sin (\alpha (x - \lambda at)) + \frac{\lambda}{\lambda - 1} \sin (\alpha (x - at))
\end{align*}
$$

Or in case of resonance:

$$
\begin{align*}
\mathbf{u} &= (1 + a \alpha i t) a_1 e^{\alpha i (x - at)} \\
&= \sin (\alpha (x - at)) + a \alpha t \cos (\alpha (x - at))
\end{align*}
$$

The equations 2.21 and 2.22 are plotted in figure 4.8.

From these equations it can already be seen that the resonance case, $\lambda = 1$, will produce a growing solution. At $t = 1.0$ the solution is practically useless. The other coupling parameters give interesting results. From equation 2.21 it can be seen the particular and homogeneous part of the solution will convect at different speeds. However when the difference between the convected distance is an integer number of wavelengths, both solutions coincide and hence the coupled solution is identical to the reference solution.

**Burgers shock**
Figure 4.9: The shock solution for pure convection with flux-divergence coupling

For the burgers shock the analytic solution is as given in equations 2.16 and 2.17 with the appropriate \( a_k \). These results are given in figure 4.9. The same effect is observed as for the sine wave: the particular and homogeneous part of the solution will convect at different speeds, and when the difference between the convected distance is an integer number of wavelengths this component of the solution is identical to the component of the reference solution. This results in small wavelengths which are more often coinciding. These have a smaller contribution to the total solution, as \( a_k \) decreases rapidly with increasing \( k \).

2.2.2 Pure diffusion
In the case of pure diffusion, hence \( a = 0 \), the total solution is:

\[
\mathbf{u} = \sum \left( \frac{-1}{\lambda - 1} e^{-\lambda \alpha^2 t} + \frac{\lambda}{\lambda - 1} e^{-\alpha^2 t} \right) a_k e^{i k x} \tag{2.23}
\]

Or in case of resonance:

\[
\mathbf{u} = \sum (1 + \nu \alpha^2 k^2 t) a_k e^{i k x - \nu \alpha^2 t} \tag{2.24}
\]

Single sine wave

For the single sine wave the analytic solution is easily constructed, as only the \( k = 1 \) wavenumber is present in the solution.

\[
\mathbf{u} = \left( \frac{-1}{\lambda - 1} e^{-\lambda \alpha^2 t} + \frac{\lambda}{\lambda - 1} e^{-\alpha^2 t} \right) a_1 e^{i x} \\
= \left( \frac{-1}{\lambda - 1} e^{-\lambda \alpha^2 t} + \frac{\lambda}{\lambda - 1} e^{-\alpha^2 t} \right) \sin (\alpha x) \tag{2.25}
\]
Recalling the exact solution:
\[ u_0 = e^{-\nu \alpha^2 t} \sin(\alpha x) \] (2.26)

The ratio of solution over exact solution now becomes:
\[ r = \frac{u}{u_0} = \frac{-1}{\lambda - 1} e^{(1-\lambda)\nu \alpha^2 t} + \frac{\lambda}{\lambda - 1} \] (2.27)

Or in case of resonance:
\[ u = (1 + \nu \alpha^2 t) a_0 e^{i\omega \tau - \nu \alpha^2 t} \]
\[ = (1 + \nu \alpha^2 t) e^{-\nu \alpha^2 t} \sin(\alpha x) \] (2.28)

The ratio of solution over exact solution now becomes:
\[ r = \frac{u}{u_0} = (1 + \nu \alpha^2 t) \] (2.29)

These results are given in figure 4.10.

It can be clearly seen the lag of the solution becomes larger with smaller coupling parameters. While the amplitude of the solution is decreased.

**Burgers shock**

These results are given in figure 4.11. The results is similar to the sine wave, the lag of the solution becomes larger with smaller coupling parameters. The shock shape changes due to the diffusion; the coupling does not have an significant influence.
3. Discussion

In general overlap coupling is able to reproduce the reference solution relatively accurately. But the coupling parameter should not be chosen too small. In most cases overlap coupling will lead to a solution which lags the reference solution. In the flux-divergence case with correction error and \( \lambda > 1 \), however, the solution will lead the reference solution. In convection cases this means the solution is shifted, while in diffusion cases the amplitude remains larger than the reference solution.

Coupling of the burgers shock can result in shape deformations. This is especially true in the convection cases. This deformation is due to different coupling behavior for each wavenumber, as \( T_\text{par} \) and \( T_\text{hom} \) are functions of \( k \). The different temporal behavior of the particular and homogeneous part of the solution also contributes to the deformation.

Analytically stable methods are obtained as long as the coupling parameter is positive. The flux-divergence case with convection error also allows a negative coupling parameter. However, there seems to be no reason to prefer a negative coupling parameter. Therefore the coupling parameter will be restricted to be positive from now on.

Resonance can occur in specific cases. In these cases the coupling term will be a continuous source. For flux-divergence coupling with convection this results in unbounded growth of the solution. For variable and flux-divergence coupling with diffusion this results in solution which decays much slower than the reference solution. The ratio solution over reference solution grows linearly in time.
Chapter 5
Linear convection-diffusion with overlap coupling

In this chapter, the coupling equation from the previous chapter will be extended to the full 1D convection-diffusion equation with coupling:

$$u_t + F(u)_x = \lambda c(u_0, u)$$  \hspace{1cm} (0.1)

Hence the time rate of change of the solution is governed by the net influx and the difference between the solution $u$ and the reference solution $u_0$. The relative importance of these two contributions is governed by the coupling parameter $\lambda$.

Just like in the previous chapter, a linear equation is considered, which is simple to analyze and inexpensive to compute numerically. The length of the domain, $L$, and the convection velocity, $\alpha$, are both chosen to be unity for simplicity. A periodic boundary condition is used to circumvent problems at the boundary.

The same initial conditions will be used for analysis:

- A single Sine wave
- A Burgers shock

Errors have to be introduced in the formulation, which will be partly corrected by the overlap coupling. Two types of error are considered:

- Convection error
- Diffusion error

The variable-coupling method will be discussed in section 1 while flux-divergence coupling will be discussed in section 2. In both sections the analytic solution will be derived first. After this some limit cases will be discussed to get some basic understanding of both coupling methods.

Finally the discrete system of equations, obtained by using the methods given in chapters 2 and 3, is analyzed. Numerical stability is checked for both coupling methods. This is done for the all-scale coupling and the three different types of VMS-coupling. It will be shown that variable coupling is more applicable than flux-divergence coupling for a number of reasons.
1. Variable coupling
For 1D linear convection-diffusion with convection and diffusion errors and variable coupling, the governing equation is:

\[ u_t + (a + a_c)u_x - (\nu + \nu_c)u_{xx} = \lambda(u_0 - u) \]  
(1.1)

1.1 Analytic solution

1.1.1 Particular solution
The particular solution of equation 1.1 is determined using the solution decompositions given in equations 1.1 and 2. This results in the following relation:

\[ (-aiok - \nu \alpha^2 k^2) + (a + a_c)iok + (\nu + \nu_c)\alpha^2 k^2)b_k = \lambda(a_k - b_k) \quad \forall k \]  
(1.2)

Which can be simplified to:

\[ (a_c iok + \nu_c \alpha^2 k^2)b_k = \lambda(a_k - b_k) \quad \forall k \]  
(1.3)

or:

\[ a_k = T_k^{par} a_k \quad \forall k \]  
(1.4)

with the transfer coefficients:

\[ T_k^{par} = \frac{\lambda}{a_c iok + \nu_c \alpha^2 k^2 + \lambda} \]  
(1.5)

This complex number can be split in a real and imaginary part:

\[ Re(T_k^{par}) = \frac{\lambda(\nu_c \alpha^2 k^2 + \lambda)}{(a_c iok)^2 + (\nu_c \alpha^2 k^2 + \lambda)^2} \]
\[ Im(T_k^{par}) = -\frac{\lambda a_c iok}{(a_c iok)^2 + (\nu_c \alpha^2 k^2 + \lambda)^2} \]  
(1.6)

These transfer coefficients are almost identical to the ones in equations 1.16 and 1.17. Substituting \( a = -a_c \) and \( \nu = -\nu_c \) will yield the exact same expression.

Resonance

Resonance occurs when \( T_k^{par} \) becomes singular. This happens when convection error is absent \( (a_c = 0) \) and the penalty parameter is exactly \( \lambda = -\alpha^2 k^2 \). However in the following section it will be clear this choice of \( \lambda \) will lead to instability right away. Hence this resonance case can be ignored.

1.1.2 Homogeneous solution
The homogeneous part of equation 1.1 is:

\[ u_t + (a + a_c)u_x - (\nu + \nu_c)u_{xx} = -\lambda u \]  
(1.7)

Which has a solution of the form:

\[ u = \sum c_k e^{-(\lambda + (\nu + \nu_c)\alpha^2 k^2)t + iok(x - (a + a_c)t)} \]  
(1.8)

The method is stable if \( \lambda + (\nu + \nu_c)\alpha^2 k^2 \geq 0 \) or:

\[ \lambda \geq -(\nu + \nu_c)\alpha^2 k^2 \leq 0 \]  
(1.9)

Hence \( \lambda \geq 0 \) will always be stable.

The \( c_k \) can be derived using \( a_k \), the coefficients of the exact solution:

\[ c_k = T_k^{hom} a_k \]  
(1.10)
Where $T^\text{hom}_k$ is simply defined as $T^\text{hom}_k = 1 - T^\text{par}_k$, see appendix III:

$$\text{Re}(T^\text{hom}_k) = \frac{(\alpha_0a_a)^2 + \nu_c\alpha_0^2k^2(\nu_c\alpha_0^2k^2 + \lambda)}{(\alpha_0\alpha_k)^2 + (\nu_c\alpha_0^2k^2 + \lambda)^2}$$

$$\text{Im}(T^\text{hom}_k) = \frac{-\nu_c\alpha_0a_a}{(\alpha_0\alpha_k)^2 + (\nu_c\alpha_0^2k^2 + \lambda)^2}$$

(1.11)

### 1.1.3 Total solution

The total solution is the sum of the particular and homogeneous solution:

$$u = \sum T^\text{par}_k a_k e^{-(\lambda + (\nu + \nu_c)\alpha_0^2t)} + \sum T^\text{hom}_k a_k e^{ik(x - at)} - i\alpha_0^2k^2t + \sum T^\text{hom}_k a_k e^{iak(x - at)} - i\alpha_0^2k^2t$$

(1.12)

### 1.2 Limit cases

In this subsection the following limit cases will be discussed:

- Convection error with convection
- Convection error with diffusion
- Diffusion error with convection
- Diffusion error with diffusion

### 1.2.1 Convection error

In the case of convection error the transfer coefficients are identical to the ones in subsection 1.2.1.

The differences in signs between equations 1.5, 1.12 and 1.6, 1.11 is eliminated due to the assumption $\nu_c = 0$. The only difference is the definition of the normalized penalty: $\lambda_0 = \frac{\lambda}{\alpha_0}$. 

**Single sine wave**

For the single sine wave the analytic solution is easily constructed. As only the $k = 1$ wavenumber is present in the solution, hence the transfer coefficients become:

$$T^\text{par}_1 = \frac{\lambda_0^2}{1 + \lambda_0^2} + i\frac{\lambda_0}{1 + \lambda_0^2}$$

$$T^\text{hom}_1 = \frac{1}{1 + \lambda_0^2} + i\frac{-\lambda_0}{1 + \lambda_0^2}$$

(1.13)

Resulting in the following solution:

$$u = \left( \left( \frac{1}{1 + \lambda_0^2} + i\frac{-\lambda_0}{1 + \lambda_0^2} \right) e^{-(\lambda + i\alpha_0\alpha_k)t} + \left( \frac{\lambda_0^2}{1 + \lambda_0^2} + i\frac{\lambda_0}{1 + \lambda_0^2} \right) \right) a_k e^{ik(x - at)} - i\alpha_0^2k^2t$$

(1.14)

In the case of pure convection, $\nu = 0$.

$$u = \left( \frac{1}{1 + \lambda_0^2} \sin (\alpha(x - (a + \nu_c)t)) - \frac{\lambda_0}{1 + \lambda_0^2} \cos (\alpha(x - (a + \nu_c)t)) \right) e^{-\lambda \cdot t}$$

$$+ \left( \frac{\lambda_0^2}{1 + \lambda_0^2} \sin (\alpha(x - at)) + \frac{\lambda_0}{1 + \lambda_0^2} \cos (\alpha(x - at)) \right)$$

(1.15)
In the case of pure diffusion, \( a = 0 \).

\[
\begin{align*}
\mathbf{u} &= \left( \frac{1}{1 + \lambda_0^2} \sin (\alpha(x - a_e t)) \right) - \frac{\lambda_0}{1 + \lambda_0^2} \cos (\alpha(x - a_e t)) \right) e^{-(\alpha + \nu \alpha^2 k^2) t} \\
&+ \left( \frac{\lambda_0^2}{1 + \lambda_0^2} \sin (\alpha x) + \frac{\lambda_0}{1 + \lambda_0^2} \cos (\alpha x) \right) e^{-\nu \alpha^2 k^2 t}
\end{align*}
\]

(1.16)

The results of equations 1.15 and 1.16 are given in figures 5.1 and 5.2.

From these equations it can be seen that the particular solution has the correct decay rate. However, as can be seen in the figures there is an amplitude error. This is due to the homogeneous part of the solution which decays too fast. Notice that there is no phase error.

**Burgers shock**

For the burgers shock, the analytic solution is as given in equations 1.12 and 1.15 with the appropriate \( a_e \). The results for pure convection (\( \nu = 0 \)) are given in figure 5.3 and the results for pure diffusion (\( a = 0 \)) are given in figure 5.4. As the amplitude and phase error is a function of wavenumber, the shock shape deforms. This effect is smaller when higher coupling parameters are chosen.
Figure 5.1: The solution for the sine wave with $a = 1.0 \, \nu = 0.0 \, a_c = 0.1 \, \nu_c = 0.0$

$t = 1.0$

$t = 2.0$

$t = 3.0$

$t = 5.0$

Figure 5.2: The solution for the sine wave with $a = 0.0 \, \nu = 0.01 \, a_c = 0.1 \, \nu_c = 0.0$
Figure 5.3: The solution for the shock $a = 1.0 \; \nu = 0.0 \; a_c = 0.1 \; \nu_c = 0.0$

Figure 5.4: The solution for the shock with $a = 0.0 \; \nu = 0.01 \; a_c = 0.1 \; \nu_c = 0.0$
1.2.2 Diffusion error
In the case of diffusion error, hence $a_c = 0$, the real and imaginary parts transfer coefficients of the particular solution become:

$$
Re(T_{k}^{\text{par}}) = \frac{\lambda(\nu_c^2 \alpha^2 k^2 + \lambda)}{\nu_c^2 \alpha^2 k^2 + \lambda} = \frac{\lambda}{1 + (\frac{\lambda}{\nu_c^2 \alpha^2 k^2})}
$$

$$
Im(T_{k}^{\text{par}}) = 0
$$

(1.17)

And the transfer coefficients for the homogeneous solution:

$$
Re(T_{k}^{\text{hom}}) = \frac{\nu_c^2 \alpha^2 k^2(\nu_c^2 \alpha^2 k^2 + \lambda)}{(\nu_c^2 \alpha^2 k^2 + \lambda)^2} = \frac{\nu_c^2 \alpha^2 k^2}{1 + (\frac{\lambda}{\nu_c^2 \alpha^2 k^2})}
$$

$$
Im(T_{k}^{\text{hom}}) = 0
$$

(1.18)

Where the normalized coupling parameter is defined as $\lambda_0 = \frac{\lambda}{\nu_c^2 \alpha^2 k^2}$. The real and imaginary parts of the transfer coefficients as function of the coupling parameter are given in plot a figure 5.5. This can be translated into the magnitude and the argument of the complex transfer coefficients which is directly related to the amplitude and phase error:

$$
||T_{k}^{\text{par}}|| = \sqrt{Re(T_{k}^{\text{par}})^2 + Im(T_{k}^{\text{par}})^2} = \frac{1}{(\frac{\lambda}{\nu_c^2 \alpha^2 k^2}) + 1}
$$

$$
\arg T_{k}^{\text{par}} = \arctan\frac{Im(T_{k}^{\text{par}})}{Re(T_{k}^{\text{par}})} = 0
$$

(1.19)

And:

$$
||T_{k}^{\text{hom}}|| = \frac{1}{|\frac{\lambda}{\nu_c^2 \alpha^2 k^2}| + 1}
$$

$$
\arg T_{k}^{\text{hom}} = 0
$$

(1.20)

The amplitude and phase errors as function of the penalty parameter are given in plot b figure 5.5.

![Figure 5.5: Transfer coefficient for diffusion error with variable coupling](image)

Single sine wave
For the single sine wave the analytic solution is easily constructed. As only the $k = 1$ wavenumber is present in the solution, hence the transfer coefficients become:

$$ T_1^{par} = \frac{\lambda_0}{1 + \lambda_0} $$
$$ T_1^{hom} = \frac{1}{1 + \lambda_0} \tag{1.21} $$

Resulting in the following solution:

$$ u = \left( \left( \frac{1}{1 + \lambda_0} \right) e^{-(\lambda + \nu \alpha^2 k^2) t} + \left( \frac{\lambda_0}{1 + \lambda_0} \right) a_k e^{i\omega k(x-\omega t) - \nu \alpha^2 k^2 t} \right) $$

$$ = \left( \frac{\lambda_0}{1 + \lambda_0} + \frac{1}{1 + \lambda_0} e^{-(\lambda + \nu \alpha^2 k^2) t} \right) e^{-\nu \alpha^2 k^2 t} \sin(\alpha(x - \omega t)) \tag{1.22} $$

In the case of pure convection, hence $\nu = 0$.

$$ u = \left( \frac{\lambda_0}{1 + \lambda_0} + \frac{1}{1 + \lambda_0} e^{-(\lambda + \nu \alpha^2 k^2) t} \right) \sin(\alpha(x - \omega t)) \tag{1.23} $$

In the case of pure diffusion, hence $\omega = 0$.

$$ u = \left( \frac{\lambda_0}{1 + \lambda_0} + \frac{1}{1 + \lambda_0} e^{-(\lambda + \nu \alpha^2 k^2) t} \right) e^{-\nu \alpha^2 k^2 t} \sin(\alpha x) \tag{1.24} $$

The results of equations 1.23 and 1.24 are given in figures 5.6 and 5.7. In the two equations it can be seen both the particular and homogeneous solution have the correct convection speed. However the particular solution has the correct decay rate while the homogeneous solution has a faster decay.

**Burgers shock**

For the burgers shock the analytic solution is as given in equation 1.12 with the appropriate $a_k$. The results for pure convection ($\nu = 0$) are given in figure 5.8 and the results for pure diffusion ($\omega = 0$) are given in figure 5.9.
Figure 5.6: The solution for the sine wave with $a = 1.0$, $\nu = 0.0$, $a_e = 0.0$, $\nu_e = 0.01$

Figure 5.7: The solution for the sine wave with $a = 0.0$, $\nu = 0.01$, $a_e = 0.0$, $\nu_e = 0.01$
Figure 5.8: The solution for the shock with $\alpha = 1.0$, $\nu = 0.0$, $\alpha_e = 0.0$, $\nu_e = 0.01$

Figure 5.9: The solution for the shock with $\alpha = 0.0$, $\nu = 0.01$, $\alpha_e = 0.0$, $\nu_e = 0.01$
2. Flux divergence coupling
For 1D Linear convection with model errors and with flux divergence coupling the governing equation is:

\[ u_t + (a + a_c)u_x - (\nu + \nu_c)u_{xx} = \lambda((au_{tx} - \nu u_{tx}) - (au_x - \nu u_{xx})) \]  

(2.1)

2.1 Analytic solution
2.1.1 Particular solution
The particular solution of equation 2.1 is determined using the solution decompositions as given in equations 1 and 2. This results in the following relation:

\[ ((-aiok - \nu a^2 k^2) + (a + a_c)iak + (\nu + \nu_c)a^2 k^2) b_k = \lambda(aiok + \nu a^2 k^2)(a_k - b_k) \quad \forall k \]  

(2.2)

Which can be simplified to:

\[ (a + a_c \nu a^2 k^2) b_k = \lambda(aiok + \nu a^2 k^2)(a_k - b_k) \quad \forall k \]  

(2.3)

Or:

\[ b_k = T_k^{par} a_k \quad \forall k \]  

(2.4)

With the transfer coefficients:

\[ T_k^{par} = \frac{\lambda(aiok + \nu a^2 k^2)}{ia_c \nu a + \nu a \nu a^2 k^2 + \lambda(aiok + \nu a^2 k^2)} = \frac{\lambda}{\sigma_k + \lambda} \]  

(2.5)

With:

\[ \sigma_k = \frac{ia_c + \nu a \nu a k}{ia + \nu a k} \]  

(2.6)

Which can be split in a real and imaginary part:

\[ Re(\sigma_k) = \frac{aa_c + \nu a \nu a^2 k^2}{a^2 + \nu a^2 k^2} = \frac{\gamma_a Re^2 + \gamma_k k^2}{Re^2 + k^2} \]  

\[ Im(\sigma_k) = \frac{(a \nu - a \nu a) \nu a k}{a^2 + \nu a^2 k^2} = \frac{(\gamma_a - \gamma_k) Re k}{Re^2 + k^2} \]  

(2.7)

With:

\[ Re = \frac{\nu a}{a} \quad \gamma_a = \frac{a_c}{a} \quad \gamma_k = \frac{\nu a}{\nu} \]  

(2.8)

Now the transfer coefficients from equation 2.5 can be split in a real and imaginary part:

\[ Re(T_k^{par}) = \frac{\lambda(Re(\sigma_k) + \lambda)}{Im(\sigma_k)^2 + (Re(\sigma_k) + \lambda)^2} \]  

\[ Im(T_k^{par}) = \frac{-\lambda Im(\sigma_k)}{Im(\sigma_k)^2 + (Re(\sigma_k) + \lambda)^2} \]  

(2.9)

Resonance

Resonance occurs when \( T_k^{par} \) becomes singular. This happens when \( Im(\sigma_k) = 0 \) and \( \lambda = -Re(\sigma_k) \) or in other terms:

\[ \gamma = \gamma_k = \gamma_a \]  

\[ \lambda = -\frac{\gamma a Re^2 + \gamma_k k^2}{Re^2 + k^2} = \gamma \]  

(2.10)
In this case equation 2.1 becomes:
\[ \mathbf{u}_t + a \mathbf{u}_x - \nu \mathbf{u}_{xx} = -\gamma (a \mathbf{u}_x - \nu \mathbf{u}_{xx}) \]  
(2.11)

Instead of the decomposition given in equation 2 the decomposition given in 3 is used. Substitution in equation 2.11 yields:
\[ (1 + (-aiok - \nu \omega^2 k^2)(1 + t) + (1 + t)aiok + (1 + t)\nu \omega^2 k^2) \mathbf{b}_k = -\gamma (aiok + \nu \omega^2 k^2) \mathbf{a}_k \]  
\[ \forall k \]  
(2.12)

This simplifies to:
\[ \mathbf{b}_k = -\gamma (aiok + \nu \omega^2 k^2) \mathbf{a}_k \]  
\[ \forall k \]  
(2.13)

Hence:
\[ \text{Re}(T_k^{\text{par}}) = -\gamma \nu \omega^2 k^2 \]  
\[ \text{Im}(T_k^{\text{par}}) = -\gamma a ik \]  
(2.14)

2.1.2 Homogeneous solution

The homogeneous part of equation 2.1 is:
\[ \mathbf{u}_t + (a + a_0) \mathbf{u}_x - (\nu + \nu_0) \mathbf{u}_{xx} = -\lambda (a \mathbf{u}_x - \nu \mathbf{u}_{xx}) \]
\[ \mathbf{u}_t + (a + \lambda \alpha + a_0) \mathbf{u}_x - (\nu + \lambda \nu + \nu_0) \mathbf{u}_{xx} = 0 \]  
(2.15)

Which has a solution of the form:
\[ \mathbf{u} = \sum c_k e^{(-\nu + \lambda \nu + \nu_0) x^2 \alpha^2 t + i \omega k (x - (a + \lambda \alpha + a_0) t)} \]  
(2.16)

The method is stable if \( \nu + \lambda \nu + \nu_0 \geq 0 \) or:
\[ \lambda \geq \frac{-\nu + \nu_0}{\nu} = 1 - \frac{\gamma \nu}{\nu} \quad \text{or} \quad \nu = 0 \]  
(2.17)

The \( c_k \) can be derived using \( \mathbf{a}_k \), the coefficients of the exact solution:
\[ c_k = T_k^{\text{hom}} \mathbf{a}_k \]  
(2.18)

Where \( T_k^{\text{hom}} \) is simply defined as \( T_k^{\text{hom}} = 1 - T_k^{\text{par}} \), see appendix III:
\[ \text{Re}(T_k^{\text{hom}}) = \frac{\text{Im}(\sigma_k)^2 + \text{Re}(\sigma_k) (\text{Re}(\sigma_k) + \lambda)}{\text{Im}(\sigma_k)^2 + (\text{Re}(\sigma_k) + \lambda)^2} \]
\[ \text{Im}(T_k^{\text{hom}}) = \frac{\lambda \text{Im}(\sigma_k)}{\text{Im}(\sigma_k)^2 + (\text{Re}(\sigma_k) + \lambda)^2} \]  
(2.19)

Or in case of resonance:
\[ \text{Re}(T_k^{\text{hom}}) = 1 + \gamma \nu \omega^2 k^2 \]
\[ \text{Im}(T_k^{\text{hom}}) = \gamma a ik \]  
(2.20)

2.1.3 Total solution

The total solution is the sum of the particular and homogeneous solution:
\[ \mathbf{u} = \sum T_k^{\text{hom}} \mathbf{a}_k e^{(-\nu + \lambda \nu + \nu_0) x^2 \alpha^2 t + i \omega k (x - (a + \lambda \alpha + a_0) t)} + \sum T_k^{\text{par}} \mathbf{a}_k e^{i \omega k (x - at) - \nu \omega^2 k^2 t} \]
\[ = \sum (T_k^{\text{hom}} e^{(-\lambda \nu + \nu_0) x^2 \alpha^2 t + i \omega k (x - a \alpha + a_0) t} + T_k^{\text{par}}) \mathbf{a}_k e^{i \omega k (x - at) - \nu \omega^2 k^2 t} \]  
(2.21)

Or in case of resonance:
\[ \mathbf{u} = \sum T_k^{\text{hom}} \mathbf{a}_k e^{i \omega k (x - at) - \nu \omega^2 k^2 t} + \sum T_k^{\text{par}} (1 + t) \mathbf{a}_k e^{i \omega k (x - at) - \nu \omega^2 k^2 t} \]
\[ = \sum ((1 + \gamma (aiok + \nu \omega^2 k^2)) - \gamma (aiok + \nu \omega^2 k^2)(1 + t)) \mathbf{a}_k e^{i \omega k (x - at) - \nu \omega^2 k^2 t} \]
\[ = \sum (1 - \gamma (aiok + \nu \omega^2 k^2) t) \mathbf{a}_k e^{i \omega k (x - at) - \nu \omega^2 k^2 t} \]  
(2.22)
2.2 Limit cases
In this subsection the following limit cases will be discussed:

- Convection with convection error
- Diffusion with convection error
- Convection with diffusion error
- Diffusion with diffusion error

2.2.1 Convection with convection error
In this case \( \nu = \nu_c = 0 \) hence:

\[
\begin{align*}
\Re(\sigma_k) &= \frac{\omega \nu_c}{\alpha^2} = \gamma_a \\
\Im(\sigma_k) &= 0
\end{align*}
\]  
(2.23)

Now the transfer coefficients become:

\[
\begin{align*}
\Re(T_{k}^{\text{par}}) &= \frac{\lambda (\Re(\sigma_k) + \lambda)}{(\Re(\sigma_k) + \lambda)^2} = \frac{\lambda}{\gamma_a + \lambda} = \frac{\lambda_0}{1 + \lambda_0} \\
\Im(T_{k}^{\text{par}}) &= 0
\end{align*}
\]  
(2.24)

And the transfer coefficients for the homogeneous solution:

\[
\begin{align*}
\Re(T_{k}^{\text{hom}}) &= \frac{1}{1 + \lambda_0} \\
\Im(T_{k}^{\text{hom}}) &= 0
\end{align*}
\]  
(2.25)

Where the normalized coupling parameter is defined as \( \lambda_0 = \frac{\lambda}{\gamma_a} \). The real and imaginary parts as function of the coupling parameter are given in figure 5.10.

![Figure 5.10: Transfer coefficients for flux-divergence coupling with convection and convection error](image)

Single sine wave

For the single sine wave the solution is:

\[
    u = T_1^{harm} e^{i\omega(x - (\lambda a + a_c) t)} + T_1^{par} a_1 e^{i\omega(x - at)} = \frac{1}{1 + \lambda_0} \sin (\alpha(x - (\lambda a + a_c) t)) + \frac{\lambda_0}{1 + \lambda_0} \sin (\alpha(x - at))
\]

These results are given in figure 5.11.

Figure 5.11: The sine wave solution for flux-divergence coupling with \( a = 1.0 \), \( \nu = 0.0 \), \( a_c = 0.1 \), \( \nu_c = 0.0 \)

Again the particular part of the solution has the correct evolution in time as can be seen in equation 2.26, however, the homogeneous part of the solution as an erroneous convection speed. Both parts do not decay, hence the solution is a combination of two sine waves traveling at different speeds. These two sine waves have a constant amplitude, but due to the different wave speeds the total solution has a varying amplitude and phase error. At some specific times the waves coincide again and the correct solution is obtained. See for example the solution for \( \lambda_0 = 1.0 \) at \( t = 5.0 \).
Burgers shock

The results for the burgers shock are given in figure 5.12. The same as for the sine wave applies here.

**Figure 5.12:** The shock wave solution for flux-divergence coupling $a = 1.0$, $\nu = 0.0$, $a_c = 0.1$, $\nu_c = 0.0$

The particular part has the correct convection speed and does not decay, while the homogeneous part of the solution as an erroneous convection speed and also does not decay. The solution is a combination of two shock waves traveling at different speeds, so the position of both shocks don’t match and the initial single shock is split in two separate shocks traveling at different speeds. At specific times the shocks coincide and the correct solution is obtained. See for example the solution for $\lambda_0 = 1.0$ at $t = 5.0$.

### 2.2.2 Convection with diffusion error

In this case $\nu = a_c = 0$ hence:

\[
Re(\sigma_k) = 0 \\
Im(\sigma_k) = -\frac{\nu_c \alpha k}{a^2} = -\frac{\nu_c \alpha k}{a}
\]

(2.27)

Now the transfer coefficients become:

\[
Re(T_{km}^{\text{par}}) = \frac{\lambda(Re(\sigma_k) + \lambda)}{Im(\sigma_k)^2 + (Re(\sigma_k) + \lambda)^2} = \frac{\lambda^2}{(\frac{\nu_c \alpha k}{a})^2 + \lambda^2} = \frac{(\frac{\lambda}{\lambda_k})^2}{1 + (\frac{\lambda}{\lambda_k})^2}
\]

\[
Im(T_{km}^{\text{par}}) = \frac{\lambda Im(\sigma_k)}{Im(\sigma_k)^2 + (Re(\sigma_k) + \lambda)^2} = \frac{\lambda \nu_c \alpha k}{(\frac{\nu_c \alpha k}{a})^2 + \lambda^2} = \frac{(\frac{\lambda}{\lambda_k})}{1 + (\frac{\lambda}{\lambda_k})^2}
\]

(2.28)
And the transfer coefficients for the homogeneous solution:

\[
\begin{align*}
Re(T_{k}^{\text{hom}}) &= \frac{Im(\sigma_{k})^2 + Re(\sigma_{k})(Re(\sigma_{k}) + \lambda)}{Im(\sigma_{k})^2 + (Re(\sigma_{k}) + \lambda)^2} = \frac{(\frac{\nu_{\text{dc}} k}{a})^2}{(\frac{\nu_{\text{dc}} k}{\lambda a})^2 + \lambda^2} = \frac{1}{1 + (\frac{k}{\lambda})^2} \\
Im(T_{k}^{\text{hom}}) &= \frac{\lambda Im(\sigma_{k})}{Im(\sigma_{k})^2 + (Re(\sigma_{k}) + \lambda)^2} = \frac{\lambda^2 \nu_{\text{dc}} k}{(\frac{\nu_{\text{dc}} k}{\lambda a})^2 + \lambda^2} = \frac{1}{1 + (\frac{k}{\lambda})^2}
\end{align*}
\] (2.29)

Where the normalized penalty is defined as \( \lambda_0 = \frac{\nu_{\text{dc}}}{\nu_{\text{ct}} a} \). The amplitude and phase errors as function of the penalty parameter are given in the second part of figure 5.13.

This can be translated in the magnitude and the argument of the complex transfer coefficients which is directly related to the amplitude and phase error:

\[
\begin{align*}
||T_{k}^{\text{par}}|| &= \sqrt{Re(T_{k}^{\text{par}})^2 + Im(T_{k}^{\text{par}})^2} = \sqrt{\left(\frac{(\frac{\nu_{\text{dc}}}{\lambda})^2}{1 + (\frac{\nu_{\text{dc}}}{\lambda})^2}\right)^2 + \left(\frac{(\frac{\lambda}{\nu_{\text{dc}}})}{1 + (\frac{\nu_{\text{dc}}}{\lambda})^2}\right)^2} \\
&= \sqrt{\left(\frac{\lambda}{\nu_{\text{dc}}} \frac{\nu_{\text{dc}}}{\lambda}\right)^2 + \left(\frac{\lambda}{\nu_{\text{dc}}} \frac{\nu_{\text{dc}}}{\lambda}\right)^2} \\
\arg(T_{k}^{\text{par}}) &= \arctan\left(\frac{Im(T_{k}^{\text{par}})}{Re(T_{k}^{\text{par}})}\right) = \arctan\left(-\left(\frac{\lambda}{\nu_{\text{dc}}} \frac{\nu_{\text{dc}}}{\lambda}\right)\right) = \arctan\left(-\frac{1}{\frac{\lambda}{\nu_{\text{dc}}} \frac{\nu_{\text{dc}}}{\lambda}}\right) \\
&= \arctan\left(\frac{(\frac{\lambda}{\nu_{\text{dc}}})^2}{1 + (\frac{\nu_{\text{dc}}}{\lambda})^2}\right) (2.30)
\end{align*}
\]

And:

\[
\begin{align*}
||T_{k}^{\text{hom}}|| &= \sqrt{\left(\frac{1}{1 + (\frac{\nu_{\text{dc}}}{\lambda})^2}\right)^2 + \left(\frac{(\frac{\lambda}{\nu_{\text{dc}}})}{1 + (\frac{\nu_{\text{dc}}}{\lambda})^2}\right)^2} = \sqrt{\frac{(\frac{\lambda}{\nu_{\text{dc}}})^2}{(1 + (\frac{\nu_{\text{dc}}}{\lambda})^2)^2} + \frac{(\frac{\lambda}{\nu_{\text{dc}}})^2}{(1 + (\frac{\nu_{\text{dc}}}{\lambda})^2)^2}} = \sqrt{\frac{1}{1 + (\frac{\nu_{\text{dc}}}{\lambda})^2}} \\
\arg(T_{k}^{\text{hom}}) &= \arctan\left(\frac{(\frac{\nu_{\text{dc}}}{\lambda})}{1}\right) = \arctan\left(\frac{\lambda}{\nu_{\text{dc}} \frac{\nu_{\text{dc}}}{\lambda}}\right) (2.31)
\end{align*}
\]

The amplitude and phase errors as function of the penalty parameter are given in the second part of figure 5.13.

Figure 5.13: Transfer coefficient for flux-divergence coupling with convection and diffusion error
Single sine wave

For the single sine wave the analytic solution is easily constructed. As only the \( k = 1 \) wavenumber is present in the solution, hence the transfer coefficients become:

\[
T_1^{\text{par}} = \frac{\lambda_0^2}{1 + \lambda_0^2} + i \frac{\lambda_0}{1 + \lambda_0^2} \\
T_1^{\text{hom}} = \frac{1}{1 + \lambda_0^2} - i \frac{\lambda_0}{1 + \lambda_0^2}
\]

Hence the solution is:

\[
u = T_1^{\text{hom}} e^{i\alpha(x - (\lambda a + a)t)} + T_1^{\text{par}} a_1 e^{i\alpha(x - at) - \nu_c a_1^2 t}
\]

\[
= \left( \frac{1}{1 + \lambda_0^2} \sin(\alpha(x - (\lambda + a)t)) - \frac{\lambda_0}{1 + \lambda_0^2} \cos(\alpha(x - (\lambda a + a)t)) \right) e^{-\nu_c a_1^2 t} + \frac{\lambda_0^2}{1 + \lambda_0^2} \sin(\alpha(x - at)) + \frac{\lambda_0}{1 + \lambda_0^2} \cos(\alpha(x - at))
\]

These results are given in figure 5.14. The expected amplitude error due to the diffusion error is

![Graphs showing the solution for different values of \( \lambda_0 \) at various times.](image)

**Figure 5.14:** The sine wave solution for flux-divergence coupling with \( a = 1.0, \nu = 0.0, a_1 = 0.0, \nu_c = 0.01 \) converted into phase error by the coupling term. Both amplitude and phase error become smaller with increased coupling parameters.
Burgers shock

For the burgers shock the analytic solution is as given in equation 2.21 with the appropriate \( a_k \). The results are given in figure 5.15. In this case again the expected amplitude error is converted in
to phase error. These errors become smaller with increasing coupling parameters. As the transfer coefficients \( T_{k}^{\text{par}} \) and \( T_{k}^{\text{hom}} \) depend on the wavenumber the shape of the shock deform if the coupling parameter is not large enough.

2.2.3 Diffusion with convection error
In this case \( a = \nu = 0 \) hence:

\[
\begin{align*}
\text{Re}(\sigma_k) & = 0 \\
\text{Im}(\sigma_k) & = \frac{\omega \nu \alpha k}{\nu^2 \alpha^2 k^2} = \frac{a_c}{\nu \alpha k} 
\end{align*}
\]  

(2.35)

Now the transfer coefficients become:

\[
\begin{align*}
\text{Re}(T_{k}^{\text{par}}) & = \frac{\lambda^2}{\text{Im}(\sigma_k)^2 + \lambda^2} = \frac{\lambda^2}{(\frac{\omega \nu \alpha k}{\nu^2 \alpha^2 k^2})^2 + \lambda^2} = \frac{(\lambda k)^2}{1 + (\lambda k)^2} \\
\text{Im}(T_{k}^{\text{par}}) & = \frac{-\lambda \text{Im}(\sigma_k)}{\text{Im}(\sigma_k)^2 + \lambda^2} = \frac{-\lambda \nu \alpha k}{(\frac{\omega \nu \alpha k}{\nu^2 \alpha^2 k^2})^2 + \lambda^2} = -\frac{(\lambda k)}{1 + (\lambda k)^2}
\end{align*}
\]  

(2.36)
And the transfer coefficients for the homogeneous solution:

\[ Re(T_k^{\text{hom}}) = \frac{1}{1 + (\lambda_0 k)^2} \]
\[ Im(T_k^{\text{hom}}) = \frac{\lambda_0 k}{1 + (\lambda_0 k)^2} \] (2.37)

Where the normalized coupling parameter is defined as \( \lambda_0 = \frac{\lambda_0}{\alpha} \). The real and imaginary parts of the transfer coefficients as function of the coupling parameter are given in plot a of figure 5.16. This can be translated in the magnitude and the argument of the complex transfer coefficients which is directly related to the amplitude and phase error:

\[ ||T_k^{\text{par}}|| = \sqrt{Re(T_k^{\text{par}})^2 + Im(T_k^{\text{par}})^2} = \sqrt{\left(\frac{(\lambda_0 k)^2}{1 + (\lambda_0 k)^2}\right)^2 + \left(\frac{-\lambda_0 k}{1 + (\lambda_0 k)^2}\right)^2} \]
\[ \arg(T_k^{\text{par}}) = \arctan\left(\frac{Im(T_k^{\text{par}})}{Re(T_k^{\text{par}})}\right) = \arctan\left(\frac{-\lambda_0 k}{\lambda_0 k^2}\right) = \arctan\left(-\frac{1}{\lambda_0 k}\right) \] (2.38)

And:

\[ ||T_k^{\text{hom}}|| = \sqrt{\left(\frac{1}{1 + (\lambda_0 k)^2}\right)^2 + \left(\frac{\lambda_0 k}{1 + (\lambda_0 k)^2}\right)^2} = \sqrt{\frac{1 + (\lambda_0 k)^2}{(1 + (\lambda_0 k)^2)^2}} = \sqrt{\frac{1}{1 + (\lambda_0 k)^2}} \]
\[ \arg(T_k^{\text{hom}}) = \arctan\left(\frac{\lambda_0 k}{1}\right) = \arctan(\lambda_0 k) \] (2.39)

The amplitude and phase errors as function of the coupling parameter are given in the plots b and c of figure 5.16.

**Figure 5.16:** Transfer coefficient for flux-divergence coupling with diffusion and convection error
Single sine wave

For the single sine wave the transfer coefficients become:

\[ T^{\text{par}}_1 = \frac{\lambda_0^2}{1 + \lambda_0^2} - i \frac{\lambda_0}{1 + \lambda_0^2} \]
\[ T^{\text{hom}}_1 = \frac{1}{1 + \lambda_0^2} + i \frac{\lambda_0}{1 + \lambda_0^2} \]

Hence the solution is:

\[ u = T^{\text{hom}}_1 a_1 e^{i\alpha(x - a_c t) - (\nu + \omega) \alpha^2 t} + T^{\text{par}}_1 a_1 e^{i\alpha x - \nu \alpha^2 t} \]
\[ = \left( \frac{1}{1 + \lambda_0^2} \sin(\alpha(x - a_c t)) + \frac{\lambda_0}{1 + \lambda_0^2} \cos(\alpha(x - a_c t)) \right) e^{i(\nu + \omega) \alpha^2 t} \]
\[ + \left( \frac{\lambda_0^2}{1 + \lambda_0^2} \sin(\alpha x) - \frac{\lambda_0}{1 + \lambda_0^2} \cos(\alpha x) \right) e^{-i\nu \alpha^2 t} \]

(2.41)

These results are given in figure 5.17.

![Graphs showing the single sine wave solution](image)

**Figure 5.17:** The sine wave solution for flux-divergence coupling with \( a = 0.0 \), \( \nu = 0.01 \), \( a_c = 0.1 \), \( \nu_c = 0.0 \)

As seen in equation (2.41) the homogeneous part of the solution decays faster than the particular part. So eventually only the particular part is remaining. It can be clearly seen the amplitude and phase error of this particular solution becomes smaller with increasing coupling parameter.
Burgers shock

For the burgers shock the analytic solution is as given in equation 2.21 with the appropriate $a_k$.
The results are given in figure 5.18.

\[ \text{Figure 5.18: The burgers shock solution for flux-divergence coupling with } a = 0.0, \nu = 0.01, \alpha_c = 0.1, \nu_c = 0.0. \]

The same applies as in the sine wave. It seems the coupling does not deform the shape of the solution.

2.2.4 Diffusion with diffusion error

In this case $a = \alpha_c = 0$ hence:

\[
\begin{align*}
Re(\sigma_k) &= \frac{\nu\lambda \epsilon^2 k^2}{\nu^2 \alpha^2 k^2} = \gamma \nu \\
Im(\sigma_k) &= 0
\end{align*}
\]

(2.42)

Now the transfer coefficients become:

\[
\begin{align*}
Re(T_{k}^{\text{prw}}) &= \frac{\lambda (Re(\sigma_k) + \lambda)}{Im(\sigma_k)^2 + (Re(\sigma_k) + \lambda)^2} = \frac{\lambda (\gamma \nu + \lambda)}{(\gamma \nu + \lambda)^2} = \frac{\lambda}{\gamma \nu + \lambda} = \frac{\lambda_0}{1 + \lambda_0} \\
Im(T_{k}^{\text{prw}}) &= \frac{-\lambda Im(\sigma_k)}{Im(\sigma_k)^2 + (Re(\sigma_k) + \lambda)^2} = 0
\end{align*}
\]

(2.43)
And the transfer coefficients for the homogeneous solution:

\[
\begin{align*}
\text{Re}(T^{\text{hom}}_k) &= \frac{\text{Im}(\sigma_k)^2 + \text{Re}(\sigma_k)(\text{Re}(\sigma_k) + \lambda)}{\text{Im}(\sigma_k)^2 + (\text{Re}(\sigma_k) + \lambda)^2} = \frac{\gamma_\nu(\gamma_\nu + \lambda)}{(\gamma_\nu + \lambda)^2} = \frac{\gamma_\nu}{\gamma_\nu + \lambda} = \frac{1}{1 + \lambda_0} \\
\text{Im}(T^{\text{hom}}_k) &= \frac{\lambda_0 \text{Im}(\sigma_k)}{\text{Im}(\sigma_k)^2 + (\text{Re}(\sigma_k) + \lambda)^2} = 0
\end{align*}
\]

(2.44)

Where the normalized penalty is defined as \( \lambda_0 = \frac{\lambda}{\gamma_\nu} \). The real and imaginary parts of the transfer coefficients as function of the penalty parameter is given in the second part of figure 5.19.

**Figure 5.19: Transfer coefficient for flux-divergence coupling diffusion and diffusion error**

*Single sine wave*

For the single sine wave the analytic solution is easily constructed. As only the \( k = 1 \) wavenumber is present in the solution. Hence the solution is:

\[
\begin{align*}
u &= T^{\text{hom}}_1 a_1 e^{i \lambda x - (\nu + \nu_x + \nu_t) \rho t} + T^{\text{par}}_1 a_1 e^{i \alpha x - \nu \rho t} \\
&= \left( \frac{\lambda_0}{1 + \lambda_0} e^{(\nu + \nu_x + \nu_t) \rho t} + \frac{1}{1 + \lambda_0} \right) \sin(\alpha x)
\end{align*}
\]

(2.45)

These results are given in figure 5.20. In this case nothing special happens. The solution has an lower amplitude than the reference solution. This discrepancy decreases when the coupling parameter is increased.
Figure 5.20: The sine wave solution for flux-divergence coupling with $a = 0.0$, $\nu = 0.01$, $a_c = 0.0$, $\nu_c = 0.01$
Burgers shock

For the burgers shock the analytic solution is as given in equation 2.21 with the appropriate $a_k$. The results are given in figure 5.21. Just like with the sine wave the solution has an lower amplitude than the reference solution. This difference decreases when the coupling parameter is increased. The shape of the shock is not severely deformed due to the coupling.

3. Numerical stability
In this section the discrete stability will be analyzed. Upto now, continuous analytic results with coupling on all scales have been considered. Here the VMS variants of the coupling methods will also be considered, using a For both coupling methods this is done for the full-scale as well as the three VMS variants. For normalized penalties three different values are chosen, each representing another fundamentally different situation:

- $\lambda_0 = 0.01$ The original equation dominates the solution, as the coupling term is virtually absent.
- $\lambda_0 = 1.0$ Both coupling and the original equation influence the solution.
- $\lambda_0 = 100.0$ The coupling term dominates the solution.

The numerical stability is tested using shape functions of the order $[2, 2]$. The first number indicates the spatial discretization order and the second number indicates the temporal discretization order. This discretization order is chosen as it is the simplest option which still allows a VMS interpretation: The linear shape functions can be considered as large scales while the quadratic shape functions can be considered as small scales.
3.1 Analysis method

The analysis method is similar to the method used in Fourier analysis of finite-difference methods. But in this case the eigenvectors are not known \textit{a priori} like the eigenvectors for the finite-difference methods which are known to be sampled sine functions. The eigenvectors are part of the solution. Just like a finite difference method the new solution, \(\mathbf{u}^{n+1}\), can be written as a linear combination of the previous solution, \(\mathbf{u}^n\):

\[
LHM\mathbf{u}^{n+1} = RHM\mathbf{u}^n
\]  

(3.1)

Which can be written as:

\[
\mathbf{u}^{n+1} = C\mathbf{u}^n
\]  

(3.2)

Where the amplification matrix, \(C\), is found as follows:

\[
C = LHM^{-1}RHM
\]  

(3.3)

For a stable discretization this matrix should have eigenvalues of a magnitude of unity or smaller.

3.1.1 Time-discontinuous Galerkin

As the shape functions used are designed for a continuous method the eigenvalue problem can be dramatically reduced in size by splitting solution vectors of the current and previous time slab in three parts:

- \(\mathbf{u}_l\) are the lower DOFs (all DOFs with non-zero shape functions on the lower boundary)
- \(\mathbf{u}_h\) are the upper DOFs (all DOFs with non-zero shape functions on the lower boundary)
- \(\mathbf{u}_i\) are the internal DOFs (all remaining DOFs)

Which gives:

\[
\mathbf{u}^{n+1} = \begin{pmatrix}
\mathbf{u}^{n+1}_l \\
\mathbf{u}^{n+1}_h \\
\mathbf{u}^n_i
\end{pmatrix} \quad \mathbf{u}^n = \begin{pmatrix}
\mathbf{u}^n_l \\
\mathbf{u}^n_h \\
\mathbf{u}^n_i
\end{pmatrix}
\]  

(3.4)

As \(RHM\) only has a contribution from the lower time initial condition it is has a structure represented as:

\[
RHM = \begin{pmatrix}
0 & 0 & RHM_{lh} \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]  

(3.5)

This results in an amplification matrix with the structure:

\[
C = \begin{pmatrix}
0 & 0 & C_{lh} \\
0 & 0 & C_{lh} \\
0 & 0 & C_{hh}
\end{pmatrix}
\]  

(3.6)

Combining this with relation 3.2 gives:

\[
\begin{align*}
\mathbf{u}^{n+1}_l &= C_{lh}\mathbf{u}^n_l \\
\mathbf{u}^{n+1}_h &= C_{lh}\mathbf{u}^n_h \\
\mathbf{u}^{n+1}_i &= C_{hh}\mathbf{u}^n_i
\end{align*}
\]  

(3.7)

From this it can be seen the large eigenvalue problem from equation 3.2 is reduced in a smaller eigenvalue problem plus two equations for the secondary DOFs.
3.1.2 Time-continuous Galerkin

Now the lower time solution of the new time slab equals the upper time solution of the previous time slab

\[ u^t_h = u^{t+1}_h \]  

(3.8)

This relation is assured if the matrices \( LHM \) and \( RHM \) are changed to:

\[
LHM = \begin{pmatrix}
I & 0 & 0 \\
LHM_{d} & LHM_{id} & LHM_{idh} \\
LHM_{hd} & LHM_{hd} & LHM_{hh}
\end{pmatrix} \quad RHM = \begin{pmatrix}
0 & 0 & I \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]  

(3.9)

3.2 Analysis results

All analysis are performed on a 32 element mesh and varying CFL-number. The results can be summarized as follows: All-scale coupling is stable in all studied cases, for both variable coupling and flux-divergence coupling. VMS variable coupling is stable in all studied cases. While VMS flux-divergence coupling can be unstable, depending on the presence of physical damping.

4. Discussion

The results of this test case are comparable with the result of the previous test case, the pure overlap coupling case. The reference solution can be reproduced relatively accurately when the coupling parameter is chosen large enough. If not, the solution will differ from the reference solution and the shock shape can be deformed. Analytic stability of the methods is guaranteed as long as the coupling parameter is positive. Introduction of the physical influx term shifts the resonance coupling parameter for variable coupling to the unstable negative range. Hence this does not have to be taken into account. For flux-divergence coupling resonance remains possible for positive coupling parameters. This happens when the introduced errors are exactly canceled by the homogeneous part of the coupling term. In this case the non-homogeneous part of the coupling term acts like a source term which blows up the solution.

The errors introduced in the equations and the coupling term influence in the temporal behavior of homogeneous solution, while for the particular solution the temporal behavior is completely governed by the temporal behavior of the reference solution. As the overlap-coupling method is proposed to minimize physically incorrect behavior, it is desired that the homogeneous part of the solution is as small as possible. Hence it is preferable that the homogeneous part of the solution has a relatively rapid decay. From this perspective the variable coupling has an advantage over flux-divergence coupling, as it always has a decaying homogeneous part. Flux-divergence coupling, in contrast, only has a decaying homogeneous solution when the physical model possesses some diffusion.

The numerical stability analysis showed that all coupling methods are numerically stable, except the VMS implementations of flux-divergence coupling which can be unstable.

Summarizing, there are three reasons for discarding the flux-divergence coupling as a satisfying coupling method:

- Possibility of resonance
- Problematic decay of homogeneous part of the solution
- VMS implementations always unstable

Therefore only variable coupling will be used from now on.
Chapter 6
Burgers equation with overlap coupling

In this chapter the behavior of overlap coupling is investigated for the case where an energy cascade is present. This case illustrates the potential benefits of VMS coupling.

The 1D non-linear convection equation is used. This equation is better known as the Burgers equation. It is the simplest equation with an energy cascade. This cascade transfers energy from large scales to small scales. This cascade is due to a non-linear convection term which is also present in the Euler and Navier-Stokes equations.

First an equivalent of the RANS model is developed for the Burgers equation. This model is accurate but has a low resolution. The solution of this model is coupled to a LES domain with introduced errors.

First all-scale coupling is used to couple the solution. Then the three different VMS-coupling implementations are used and compared with each other. Only variable coupling will be used, as flux-divergence coupling has the risk of unstable VMS implementations and resonance. The only restriction for variable coupling is the choice of coupling parameter. This should be chosen positive to ensure stability, and large to ensure a fast decay of the homogeneous solution.

1. Reynolds-Averaged-Burgers

In this section an equivalent of the RANS (Reynolds-Averaged-Navier-Stokes) model is developed for the Burgers equation. This model will be called RAB (Reynolds-Averaged-Burgers).

Just like the RANS model the RAB model is supposed to be more accurate but should have a low resolution. These demands seem contradicting as a low resolution normally leads to inaccurate results. See the first plot of figure 6.1. This plot present the energy spectrum at $t = 1.0$ for the DNS and RAB method starting from the Burgers shock as given in (appendix B) The order of discretization of the two methods are as follows: DNS $= [5, 2]$ and RAB $= [1, 1]$. While a 100-by-100-element space-time mesh is used (hence $dt = dx = 0.01$). This discretization and initial condition will be used throughout this chapter. It can be clearly seen the RAB solution does not represent the small scales correctly, as these are not present in the low-resolution discretization. However the larger scales, which are present in the discretization, are also not entirely correctly predicted. This is not desirable for the RAB solution.

Instead an appropriate RAB solution is obtained by computing a high-order solution on the same mesh and projecting it into the RAB basis. See figure 6.2. To circumvent spurious wiggles in the
Figure 6.1: Two RAB-results: normal and projection

![Graphs showing comparison between RAB and DNS methods.]

Figure 6.2: RAB-method

RAB-solution it is chosen to have the same mesh for the DNS and RAB. The projection is as follows:

\[ (w, \bar{u} - u_{RAB}) = 0 \]  \hspace{1cm} (1.1)

Where \( \bar{u} \) are the large scales which are in the polynomial space \( P = [1,1] \), or with other words these are the linear shape functions. In this specific case where the RAB and DNS domains have the same mesh, the RAB is exactly the DNS without the higher orders, the energy spectrum of this projection method is given in the second plot of figure 6.1.

The small scales are still incorrect, however, the larger scales now follow the DNS solution exactly until the resolution of the discretization becomes a problem. This is exactly the behavior of the RAB which is desired.

2. All-scale variable coupling

To test the coupling methods artificial errors are introduced. This is similar what has been done for the convection-diffusion equation. However, in this case the errors are only introduced in the large-scale equations. As a result of this the small scales will be governed by an unmodified equation. Now there is no need to couple the small scales as these are governed by the correct equations. Using equation 3.10, the errors are introduced as follows:

\[ B_{TDG}(w_j, U) + E(w_j, u) = 0 \]  \hspace{1cm} (2.1)

Where \( E(w_j, u) \) is the introduced error. Three different error types are chosen:

- Diffusion error: \( E(w, u) = (w_x, u_x \bar{u}) \)
- Convection error: \( E(w, u) = -(w_x, a_i \bar{u}) \)
- Convection-diffusion error: $E(w; u) = -(\partial_w^2 \psi w + \alpha_\psi \nabla \cdot \nabla \psi)$

For these three errors the solution and spectrum at $t = 1.0$ for all-scale variable coupling are given in figures 6.3 to 6.5. In these figure it can be seen that the larger the penalty the better the solution matches the DNS solution. However, the eye-ball norm is deceiving in this case. The figures also show that the energy spectrum of the solution starts to match the RAB spectrum. This could be expected as this solution has been used as reference solution for the coupling.
Due to the low resolution of the RAB solution, the small scales of the LES are less accurate when the coupling parameter is increased. Eventually, when the coupling parameter is chosen large enough the small scales will be completely absent. This is not a desired property of the overlap-coupling method. The whole idea behind the overlap coupling is to have small scales present in these overlapped regions.

3. VMS variable coupling

In the previous section the small scales are badly represented when the coupling parameter is increased. However, these scales need no coupling. The small scales are governed by the correct physical equations, as the errors are only introduced on the large scales equations.

In this case the VMS-coupling is expected to give better results. These methods only give a restriction to the large scales, while the small scales are allowed to develop freely.

The solution and spectrum at $t = 1.0$ for the all three types of VMS variable coupling are given in figures 6.6 to 6.14.

Type-I and type-III VMS give virtually similar results and are able to let the small scales develop freely, even for high coupling parameters.

For type-II VMS these observations are not true as can be observed on the spectrum. The small scales do not develop freely at higher values of coupling parameters and at a coupling parameter $\lambda = 100.0$ the large scale part of the spectrum is above that of the reference solution. While at higher coupling parameters (e.g. $\lambda = 10000.0$) singularity problems arise and a solution can not be obtained. This occurrence of this singularity problem was already anticipated in section 2.2. This VMS type offers no improvement in the behavior of the small scales compared with the all-scale variable coupling.

For Type-I and type-III VMS the solution approaches the DNS solution when the coupling parameter is increased. This effect is slightly less stronger than in the results of the all-scale variable coupling presented in the previous section. But this could be expected as the VMS coupling is less strict. The difference with the results from the previous section are the small scales, which tend to be represented better when the coupling parameter is increased. Especially type-I gives good results in the small scale region of the spectrum. For type-III VMS this is not entirely true; at some point the small scales start to deteriorate.
Figure 6.6: Solution and spectrum of VMS-I variable coupling with diffusion error

Figure 6.7: The solution and spectrum of VMS-I variable coupling with convection error

Figure 6.8: The solution and spectrum of VMS-I variable coupling with convection-diffusion error
Figure 6.9: The solution and spectrum of VMS-II variable coupling with diffusion error

Figure 6.10: The solution and spectrum of VMS-II variable coupling with convection error

Figure 6.11: The solution and spectrum of VMS-II variable coupling with convection-diffusion error
Figure 6.12: The solution and spectrum of VMS-III variable coupling with diffusion error.

Figure 6.13: The solution and spectrum of VMS-III variable coupling with convection error.

Figure 6.14: The solution and spectrum of VMS-III variable coupling with convection-diffusion error.
Chapter 7
Conclusions

This thesis has examined the fundamental properties of a new overlap coupling approach intended for application to combined RANS/LES computations. Two basic methods were considered, one based on variable coupling and one based on flux divergence coupling. Both all-scale and VMS variants of each method were examined.

Analytic solutions for the all-scale case have been derived to predict the basic behavior of the coupling methods. In order to model the discrepancy between LES and DNS at large scales, artificial errors were introduced. The analytic solutions were expressed in terms of particular and homogeneous components. In general the temporal behavior of the homogeneous part of the solution is affected by the errors and the coupling parameter, while the temporal behavior of the particular part of the solution is completely governed by the reference solution. The goal of the overlap coupling method is to minimize physically incorrect behavior; therefore it is desired that the homogeneous part of the solution be as small as possible and has a relatively rapid decay. From this perspective, variable coupling has an advantage over flux divergence coupling, as it always has a decaying homogeneous solution. Flux divergence coupling, in contrast, only has a decaying homogeneous solution when the physical model possesses some diffusion.

Continuous all-scale stability is satisfied for both methods when the coupling parameter is taken positive. If this is not the case the homogeneous part of the solution will grow without bound. Another source of analytic instability is resonance. This can occur when the homogeneous part of the flux divergence coupling is exactly canceled by the artificial errors. This can result in an unbounded growth of the particular solution.

Both all-scale coupling methods are discretely stable (as long as they are also continuously stable) for all cases which were tested. The proposed VMS variants of variable coupling are always discretely stable, but for flux divergence coupling they are unstable when there is not enough physical damping. Eventually flux divergence coupling was discarded as a satisfying coupling method for the following three reasons:

- Problematic decay of homogeneous part of the solution
- Possibility of resonance
- VMS implementations can be unstable

Although useful for understanding the basic properties of overlap coupling, the all-scale variants do not lead to appropriate representations of the small scales for LES regions. Three variants of VMS
coupling were proposed to address this issue. VMS type II does not give an improvement in the small scales, and results in a deterioration of the large scales, accompanied by conditioning problems. Therefore it is discouraged to use type II. In contrast VMS types type I and III give improvements in the small scales part of the solution while matching the desired large-scale behavior. With type I VMS the small scales improve with increasing coupling parameter, while for type III VMS this is only true until a certain coupling parameter value after which the small scales start to deteriorate. Therefore VMS type I is favored over type III.

In the introduction overlap coupling was proposed for overcoming the lack of small-scale excitation in the zonal approach. The results of chapter 6 show that overlap coupling is indeed capable of overcoming this problem. Therefore it is anticipated that the overlap-coupling method will outperform zonal coupling for RANS/LES applications. In future work this method should be extended to multi-variable and multi-dimensional problems like channel flows and other wall-bounded flows, allowing the overlap and zonal approaches to be compared in the context of turbulent flows.
Appendix I

Exact solution of the convection diffusion equation

The 1D linear convection-diffusion equation is defined as:

\[ u_t + au_x - \nu u_{xx} = 0 \]  \hspace{1cm} (1)

Choosing the solution of the form:

\[ u = \sum a_k e^{\gamma_k t} e^{i\alpha kx} \]  \hspace{1cm} (2)

With:

\[ \alpha = \frac{2\pi}{L} \]  \hspace{1cm} (3)

The derivatives are:

\[ u_t = \sum a_k \gamma_k e^{\gamma_k t} e^{i\alpha kx} \]
\[ u_x = \sum a_k i\alpha k e^{\gamma_k t} e^{i\alpha kx} \]
\[ u_{xx} = -\sum a_k \alpha^2 k^2 e^{\gamma_k t} e^{i\alpha kx} \]  \hspace{1cm} (4)

Substitution in equation (1) yields:

\[ (\gamma_k + ai\alpha k + \nu \alpha^2 k^2) a_k = 0 \quad \forall k \]  \hspace{1cm} (5)

Hence:

\[ \gamma_k = -ai\alpha k - \nu \alpha^2 k^2 \]  \hspace{1cm} (6)

The solution now becomes:

\[ u = \sum a_k e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \]

With \( a_k \) prescribed by the initial condition,

\[ a_0 = \frac{1}{L} \int_0^L u|_{t=0} dx \]
\[ a_k = \frac{2}{L} \int_0^L u|_{t=0} e^{i\alpha kx} dx \quad \forall k \neq 0 \]  \hspace{1cm} (8)
A. The sine wave

The initial condition is:

\[ u(x, 0) = \sin(\alpha x) \quad (A.1) \]

Which has a trivial Fourier decomposition:

\[ b_1 = -i \quad b_k = 0 \quad \forall k \neq 1 \quad (A.2) \]

Hence the solution is:

\[ u = -ie^{i(\omega_0 x - at)} = e^{-i\omega_0^2 t} \sin(\alpha(x - at)) \quad (A.3) \]

A.1 Pure convection

In the case of pure convection:

\[ a = 1 \quad \nu = 0 \quad (A.4) \]

The exact solution is:

\[ u = \sin(\alpha(x - at)) \quad (A.5) \]

Which is plotted in figure L1.

\[ \text{Figure L1: The initial condition and the exact solution for the Sine wave with pure convection} \]

A.2 Pure diffusion

In the case of pure convection:

\[ a = 0 \quad \nu = 0.01 \quad (A.6) \]

The exact solution is:

\[ u = e^{-\nu t} \sin(\alpha x) \quad (A.7) \]

Which is plotted in figure L2.

\[ \text{Figure L2: The initial condition and the exact solution for the Sine wave with pure diffusion} \]
B. The Burgers shock
The initial condition is:
\[ u |_{t=0} = 2x - 1 - \tanh \left( \frac{x - 0.5}{0.01} \right) \]  \hspace{1cm} (B.1)

B.1 Pure convection
In the case of pure convection:
\[ a = 1 \]
\[ \nu = 0 \]  \hspace{1cm} (B.2)

Which is plotted in figure I.3.

**Figure I.3:** The initial condition and the exact solution for the Burgers shock with pure convection

B.2 Pure diffusion
In the case of pure convection:
\[ a = 0 \]
\[ \nu = 0.01 \]  \hspace{1cm} (B.3)

Which is plotted in figure I.4.

**Figure I.4:** The initial condition and the exact solution for the Burgers shock with pure diffusion
Appendix II
Solution decomposition for the convection diffusion equation

Using \( \alpha \) as defined in equation 3 the reference solution and its derivatives are decomposed as:

\[
\begin{align*}
  u_0 & = \sum a_k e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_t & = \sum a_k (-\alpha i k - \nu \alpha^2 k) e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_x & = \sum a_k i \alpha k e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_{xx} & = -\sum a_k \alpha^2 k^2 e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t
\end{align*}
\tag{1}
\]

Normally, the solution and its derivatives are decomposed as:

\[
\begin{align*}
  u & = \sum b_k e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_t & = \sum b_k (-\alpha i k - \nu \alpha^2 k^2) e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_x & = \sum b_k i \alpha k e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_{xx} & = -\sum b_k \alpha^2 k^2 e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t
\end{align*}
\tag{2}
\]

However, in case of resonance the solution and its derivatives are decomposed as:

\[
\begin{align*}
  u & = \sum b_k (1 + t) e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_t & = \sum b_k (1 + t) (-\alpha i k - \nu \alpha^2 k) + 1 e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_x & = \sum b_k (1 + t) i \alpha k e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t \\
  u_{xx} & = -\sum b_k (1 + t) \alpha^2 k^2 e^{i\alpha k(x-\nu t)} - \nu \alpha^2 k^2 t
\end{align*}
\tag{3}
\]
Or if only one specific wavelength \( \omega_r \) gives rise to resonance:

\[
\begin{align*}
\mathbf{u} &= b_{0r}(1 + t)e^{i\omega_r t}e^{i\alpha k_r (x - at) - \nu \alpha^2 k_r^2 t} + \sum_{k \neq k_r} b_k e^{i\omega k(x - at) - \nu \alpha^2 k^2 t} \\
\mathbf{u}_t &= b_{0r}((1 + t)(-i\alpha k_r - \nu \alpha^2 k_r^2) + 1)e^{i\omega_r t}e^{i\omega r (x - at) - \nu \alpha^2 k_r^2 t} \\
&\quad + \sum_{k \neq k_r} b_k (-i\alpha k - \nu \alpha^2 k^2)e^{i\omega k(x - at) - \nu \alpha^2 k^2 t} \\
\mathbf{u}_x &= b_{0r}(1 + t)i\alpha k_r e^{i\omega r (x - at) - \nu \alpha^2 k_r^2 t} + \sum_{k \neq k_r} b_k i\alpha k e^{i\omega k(x - at) - \nu \alpha^2 k^2 t} \\
\mathbf{u}_{xx} &= -b_{0r}(1 + t)i\alpha^2 k_r^2 e^{i\omega r (x - at) - \nu \alpha^2 k_r^2 t} - \sum_{k \neq k_r} b_k i\alpha^2 k^2 e^{i\omega k(x - at) - \nu \alpha^2 k^2 t}
\end{align*}
\]
Appendix III
Determining the coefficients of the homogeneous solution

The complete solution is the sum of the homogeneous and particular part.

\[ u = u_{\text{hom}} + u_{\text{par}} \]  \hspace{1cm} (1)

Where both particular and homogeneous solution are decomposed in Fourier modes:

\[ u_{\text{hom}} = \sum c_k e^{i akx} f_{\text{hom}}(t) \]
\[ u_{\text{par}} = \sum b_k e^{i akx} f_{\text{par}}(t) \]  \hspace{1cm} (2)

Where \( f_{\text{par}}(t) \) and \( f_{\text{hom}}(t) \) are complex functions which evaluate to 1 at \( t = 0 \). The coefficients \( b_k \) are determined using \( b_k = T_k^{\text{par}} a_k \). Now only the coefficients \( c_k \) of the homogeneous solution have to be determined. This can be achieved using the solution at \( t = 0 \) which satisfies \( u_{t=0} = u_{t=0} \). Hence:

\[ u_{t=0} = u_{\text{hom}t=0} + u_{\text{par}t=0} \]
\[ \sum a_k e^{i akx} = \sum c_k e^{i akx} + \sum b_k e^{i akx} \]
\[ = \sum (c_k + b_k)e^{i akx} \]  \hspace{1cm} (3)

Hence using \( b_k = T_k^{\text{par}} a_k \):

\[ c_k = a_k - b_k = a_k - T_k^{\text{par}} a_k \] \hspace{1cm} \forall k
\[ c_k = T_k^{\text{hom}} a_k \] \hspace{1cm} \forall k  \hspace{1cm} (4)

Where \( T_k^{\text{hom}} \) is defined as:

\[ T_k^{\text{hom}} = (1 - T_k^{\text{par}}) \]  \hspace{1cm} (5)
References


