Chapter 2

Proper Orthogonal Decomposition

2.1 Introduction

Coherent structures play an important role in the turbulence research of the last decades. In many visualizations of turbulent flows one can see coherent structures. They develop, move through the flow, merge with other coherent structures, disappear, and reappear. Some structures have been called names: lambda-vortices, Taylor-vortices, Taylor-Görtler vortices, mono-, di-, and tri-pole vortices (see Fig. 1.2). In general it is hard to give a mathematical definition of a coherent structure.

We define a coherent structure by the proper orthogonal decomposition (POD). POD is an unbiased way to define a coherent structure. The POD has been introduced to the turbulence community by Lumley in 1967 [32]. Before that time it was already known in statistics as the Karhunen-Loève expansion. In the meteorology it is known as principal component analysis or empirical orthogonal functions (EOF). An example of this can be found in the Ph.D. thesis of Selten [49], in which he used EOF's for an efficient description of the large-scale atmospheric dynamics. An extensive treatment of the principal component analysis can be found in [43].

Lumley proposed to define a coherent structure with functions of the spatial variables that have maximum energy content. That is, coherent structures are (linear combinations of) $\boldsymbol{\sigma}(\boldsymbol{x})$'s which maximize the following expression

$$\frac{\langle(\boldsymbol{\sigma}(\boldsymbol{x}), \mathbf{u}(\boldsymbol{x}, t))^2\rangle}{(\boldsymbol{\sigma}(\boldsymbol{x}), \boldsymbol{\sigma}(\boldsymbol{x}))} \tag{2.1}$$

In this expression (f, g) is the L^2 inproduct $\int_\Omega f\overline{g}\mathrm{d}\Omega$ and $\langle\cdot\rangle = \lim_{T\to\infty}\frac{1}{T}\int_0^T \cdot dt$. So, if $\boldsymbol{\sigma}(\boldsymbol{x})$ maximizes (2.1), it means that if the flowfield is 'projected' along $\boldsymbol{\sigma}(\boldsymbol{x})$, the average energy content is larger than if the flowfield is 'projected' along any other structure, e.g. a Fourier mode. In the space orthogonal to this $\boldsymbol{\sigma}(\boldsymbol{x})$ the maximization process can be repeated, and in this way a whole set of orthogonal functions $\boldsymbol{\sigma}_i(\boldsymbol{x})$ can be determined. The power of the POD lies in the fact that the decomposition of the flowfield in the POD eigenfunctions converge optimally fast in L^2-sense.

The POD did not much receive attention the mid 80's due to its computational requirements. Since a lot of flow-data is needed a large computer-memory is required, and to treat this data a fast computer is needed. Early applications of the POD have been reported by Bakewell *et al.* [5] who applied the POD to a turbulent pipe flow, and by Payne *et al.* [40] who applied the POD to a turbulent wake behind a cylinder. Both used experimental data with a coarse resolution and determined only the first POD eigenfunctions.

In the last ten years the POD has been applied to a lot of different flows and geometries, resulting in an extensive list of articles. Here we will mention some of them. For a more extensive list of articles the reader is referred to Berkooz *et al.* [9]

The POD eigenfunctions in the wall region of a turbulent boundary layer have been computed by Herzog [26], who used experimental data. Rempfer [45, 46, 47] also computed the POD eigenfunctions of a turbulent boundary layer, he used numerical data. Rempfer computed the 3D eigenfunctions whereas Herzog used Fourier modes in the homogeneous directions.

A POD of a turbulent shear layer can be found in Hilberg *et al.* [27]. They computed the POD in two dimensions. Manhart *et al.* [34] computed the POD of a turbulent shear layer above a square rib at a Reynolds number of about 50,000. Rajaee *et al.* [44] used experimental data to determine the POD in the first pairing process of a free-shear-flow.

Other flows of which POD's are reported are the mixing layer [16, 21, 22, 55], thermal convection [39, 52, 53], channel flow [51, 6], flow around an airfoil [15], flames [2], and wakes [14].

Most of these POD computations use Fourier modes in the homogeneous directions or consider only one or two space directions. A full 3D POD is mostly expensive and has not been applied often, examples are [34, 39, 45, 53]. For all these full 3D POD's the so-called 'snapshot' method of Sirovich [50] has been used, a method which is considerably cheaper than the direct computation of the POD.

The POD's are often used for a low-dimensional description of the turbulent flow. For example Aubry *et al.* [4] used the POD eigenfunctions of Herzog [26] to derive a low-dimensional dynamical system for the wall region of a turbulent boundary layer and found that the pressure signal of the outer part of the boundary layer triggers the bursting events associated with streamwise vortex pairs. Other low-dimensional dynamical systems with POD eigenfunctions are reported in [14, 15, 21, 44, 45], for example.

This chapter consist of 5 sections. Section 2.2 discusses the mathematical formulation of the POD, the properties of the POD eigenfunctions, the snapshot POD, and the space-time symmetry which can be used to reduce the computational requirements. In Section 2.3 the method of Sirovich is described. This method has a close relation with the space-time symmetry of the snapshot POD. Section 2.4 describes the Galerkin projection of the Navier-Stokes to derive the low-dimensional dynamical system. In Section 2.5 closure models are formulated. These closure models are used to compensate for the non-resolved POD eigenfunctions.

2.2 Mathematical formulation of the POD

In this section POD eigenfunctions are shown to be eigenfunctions of the space-correlation tensor. For an accurate approximation of this tensor it is necessary to perform a long and expensive flow-simulation. The computation of the eigenfunctions is even more expensive, if not impossible.

To overcome this problem another time-discrete formulation of the POD is introduced. This formulation has the same interesting properties as the continuous one when applied to the data which is used to compute it. It has a close relation with the so-called "snapshot method" of Sirovich [50], which is introduced in the next section, as a method to compute the POD eigenfunctions.

In the first subsection the original continuous POD as introduced by Lumley [32] is described, in the second the snapshot POD is introduced, and in Section 2.2.3 the space-time symmetry of the snapshot POD is described.

2.2.1 Continuous POD

By calculus of variation (see appendix A) it can be shown that a necessary condition for $\boldsymbol{\sigma}(\boldsymbol{x})$ to maximize expression (2.1) is that it is a solution of the following Fredholm integral equation of the second type (see [36]):

$$\int_{\Omega} \mathbf{R}(\boldsymbol{x}, \boldsymbol{x}')\boldsymbol{\sigma}(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' = \lambda\boldsymbol{\sigma}(\boldsymbol{x}) \tag{2.2}$$

where Ω is the flow domain, and $\mathbf{R}$ is the space-correlation tensor:

$$\mathbf{R}(\boldsymbol{x}, \boldsymbol{x}') = \langle \mathbf{u}(\boldsymbol{x})\mathbf{u}^T(\boldsymbol{x}')\rangle$$

This space-correlation tensor is symmetric and positive definite. Therefore, according to the Hilbert-Schmidt theory, equation (2.2) has a denumerable set of orthogonal solutions $\boldsymbol{\sigma}^i(\boldsymbol{x})$ with corresponding real and positive eigenvalues λ^i. The eigenvalue with the largest magnitude is the maximum which is achieved in the maximization problem (2.1). The second largest eigenvalue is the maximum of the maximization problem restricted to the space orthogonal to the first eigenfunction:

$$\max_{\boldsymbol{\sigma} \in \mathbf{L^2}} \frac{\langle (\boldsymbol{\sigma}, \mathbf{u} - (\mathbf{u}, \boldsymbol{\sigma})\boldsymbol{\sigma})^{\mathbf{2}}\rangle}{(\boldsymbol{\sigma}, \boldsymbol{\sigma})} \tag{2.3}$$

The third largest eigenvalue is the maximum achieved when restricted to the space orthogonal to the first two eigenfunctions, and so on. The eigenfunctions of (2.2) have some interesting mathematical properties.

The eigenfunctions are orthogonal as mentioned, and can be normalized:

$$(\boldsymbol{\sigma}^i, \boldsymbol{\sigma}^j) = \delta_{ij} \tag{2.4}$$

The closure of the span of the POD eigenfunctions is equal to the set of all realizable flowfields. Therefore we can use it as a basis for the flowfield.

$$\mathbf{u}(\boldsymbol{x}, t) = \sum_{i=1}^{\infty} a^i(t)\boldsymbol{\sigma}^i(\boldsymbol{x}) \tag{2.5}$$

The coefficients $a^i(t)$ in equation (2.5) are determined by

$$a^i(t) = (\mathbf{u}(\boldsymbol{x}, t), \boldsymbol{\sigma}^i(\boldsymbol{x})) \tag{2.6}$$

Stated otherwise, $a^i(t)^2$ is the amount of energy of $\mathbf{u}(\boldsymbol{x},t)$ in the 'direction' of $\boldsymbol{\sigma}^i$. The total energy is the sum of the $a^i(t)^2$ in the different 'directions':

$$e(t) = (\mathbf{u}(\boldsymbol{x},t), \mathbf{u}(\boldsymbol{x},t)) = \sum_{i=1}^{\infty} a^i(t)^2 \tag{2.7}$$

The coefficients $a^i(t)$ are uncorrelated and their mean values are the eigenvalues λ^i:

$$\langle a^i(t) a^j(t) \rangle = \delta_{ij} \lambda^i \tag{2.8}$$

The eigenfunctions do not necessarily span the space $L^2(\Omega)$, since the kernel of $\mathbf{R}$ may be not empty. This is also the power of the POD, because the POD selects just those flowfields that we want to select, namely the realizable flowfields. Another consequence is that properties of the realizable flowfield are taken over by the POD eigenfunctions. For instance, the eigenfunctions are divergence-free and satisfy the boundary conditions. If the geometry and boundary conditions have certain symmetries and when flow-realizations remain flow-realizations when transformed under this symmetries the POD eigenfunctions are invariant under these transformations. For example the 3D driven cavity flow (see Chapter 3) has a symmetry-plane at z=0.5, therefore the eigenfunctions will be odd or even with respect to this symmetry-plane.

By construction the POD eigenfunctions are optimal with respect to energy content. That means that any other set of N modes contains less energy on time average than the first N POD eigenfunctions. This property leads to the expectation that when only a relatively small number of POD eigenfunctions are retained in a Galerkin projection we can approximately reproduce the dynamics of the turbulent flow.

For a more mathematical description of the POD, and proofs of some of the stated properties the reader is referred to [9] and [7], e.g.

When applied to the velocity field the first POD eigenfunction is almost the mean flow provided the variations of the fluctuating velocities are not too large in areas with zero mean flow. Therefore the POD is mostly applied to the fluctuating part of the velocity. An advantage of this approach is that the POD eigenfunctions of the fluctuations satisfy homogeneous boundary conditions. Another advantage is that we do not have to solve an equation for the mean flow in the low-dimensional dynamical system.

2.2.2 Snapshot POD

For the snapshot POD we need a set of N snapshots $\mathbf{u}_n(\boldsymbol{x})$ of the fluctuating velocity field. The snapshots are taken at different times from a simulation

$$\mathbf{u}_n(\boldsymbol{x}) = \mathbf{u}(\boldsymbol{x}, t^n) \tag{2.9}$$

The times t^n are usually equally spaced in time but this is not necessary. The only requirement is that the snapshots are linearly independent.

The maximization problem (2.1) can be reformulated for the snapshots

$$\max_{\boldsymbol{\sigma}} \frac{\frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{\sigma}(\boldsymbol{x}), \mathbf{u}_n(\boldsymbol{x}))^2}{(\boldsymbol{\sigma}(\boldsymbol{x}), \boldsymbol{\sigma}(\boldsymbol{x}))} \tag{2.10}$$

Just like in the continuous case, $\boldsymbol{\sigma}$ is defined up to a constant, so we may assume $(\boldsymbol{\sigma}, \boldsymbol{\sigma}) = 1$. It is convenient, also for the next subsection, to formulate (2.10) in terms of a minimization problem instead of a maximization problem. Maximizing the square of the projection of $\mathbf{u}$ in the 'direction' $\boldsymbol{\sigma}$ is equivalent to minimizing the square of $\mathbf{u}$ minus its projection along $\boldsymbol{\sigma}$. Indeed,

$$\begin{aligned} (\mathbf{u}_n - (\mathbf{u}_n, \boldsymbol{\sigma})\boldsymbol{\sigma}, \mathbf{u}_n - (\mathbf{u}_n, \boldsymbol{\sigma})\boldsymbol{\sigma}) &= \\ (\mathbf{u}, \mathbf{u}) - 2(\mathbf{u}, \boldsymbol{\sigma})^2 + (\mathbf{u}, \boldsymbol{\sigma})^2(\boldsymbol{\sigma}, \boldsymbol{\sigma}) &= (\mathbf{u}_n, \mathbf{u}_n) - (\mathbf{u}_n, \boldsymbol{\sigma})^2 \end{aligned}$$

So the maximization problem (2.10) is equivalent to the minimization problem

$$\min_{\boldsymbol{\sigma}} \frac{1}{N} \sum_{n=1}^{N} (\mathbf{u}_n - (\mathbf{u}_n, \boldsymbol{\sigma})\boldsymbol{\sigma}, \mathbf{u}_n - (\mathbf{u}_n, \boldsymbol{\sigma})\boldsymbol{\sigma}) \tag{2.11}$$

The solution(s) of (2.11) $\boldsymbol{\sigma}^1$ is supposed to be an approximation of the $\boldsymbol{\sigma}^1$ of the continuous POD. The second POD eigenfunction $\boldsymbol{\sigma}^2$ is now the minimization of

$$\min_{\boldsymbol{\sigma}^2} \frac{1}{N} \sum_{n=1}^{N} (\mathbf{u}_n - (\mathbf{u}_n, \boldsymbol{\sigma}^1)\boldsymbol{\sigma}^1 - (\mathbf{u}_n, \boldsymbol{\sigma}^2)\boldsymbol{\sigma}^2, \mathbf{u}_n - (\mathbf{u}_n, \boldsymbol{\sigma}^1)\boldsymbol{\sigma}^1 - (\mathbf{u}_n, \boldsymbol{\sigma}^2)\boldsymbol{\sigma}^2) \tag{2.12}$$

We can go on minimizing until we have filled the whole space spanned by the N snapshots $\mathbf{u}_n$. The minimization problem for all N $\boldsymbol{\sigma}^i$'s will be

$$\min_{\boldsymbol{\sigma}} \frac{1}{N} \sum_{n=1}^{N} (\mathbf{u}_n - \sum_{i=1}^{N} (\mathbf{u}_n, \boldsymbol{\sigma}^i)\boldsymbol{\sigma}^i, \mathbf{u}_n - \sum_{i=1}^{N} (\mathbf{u}_n, \boldsymbol{\sigma}^i)\boldsymbol{\sigma}^i) \tag{2.13}$$

with $\boldsymbol{\sigma} = (\boldsymbol{\sigma}^1, .., \boldsymbol{\sigma}^N)$. It may be recalled that loosing the correct ordering of the $\boldsymbol{\sigma}^i$ isn't important, since we can re-order them in any prescribed way.

A necessary condition for $\boldsymbol{\sigma}^i$ to minimize equation (2.13) is that it has zero first order variation, which leads to

$$\boldsymbol{\sigma}^i = \frac{\frac{1}{N}\sum_{n=1}^{N} (\mathbf{u}_n - \sum_{j=1, j\neq i}^{N} (\mathbf{u}_n, \boldsymbol{\sigma}^j)\boldsymbol{\sigma}^j)(\mathbf{u}_n, \boldsymbol{\sigma}^i)}{\frac{1}{N}\sum_{n=1}^{N} (\mathbf{u}_n, \boldsymbol{\sigma}^i)^2} \tag{2.14}$$

We seek for solutions for which the correlation coefficient of $(\mathbf{u}_n, \boldsymbol{\sigma}^i)$ and $(\mathbf{u}_n, \boldsymbol{\sigma}^j)$ is zero if $i \neq j$. For these solutions (2.14) reduces to

$$\boldsymbol{\sigma}^i = \frac{\sum_{n=1}^{N} \mathbf{u}_n (\mathbf{u}_n, \boldsymbol{\sigma}^i)}{\sum_{n=1}^{N} (\mathbf{u}_n, \boldsymbol{\sigma}^i)^2} \tag{2.15}$$

Both the left- and right-hand of equation (2.15) are functions of space. The denumerator of the right-hand side is constant, we call this denumerator c_i. A necessary condition for $\boldsymbol{\sigma}^i$ to satisfy equation (2.15) is now

$$\boldsymbol{\sigma}^i(\boldsymbol{x}) = \frac{1}{c_i} \sum_{n=1}^{N} \mathbf{u}_n(\boldsymbol{x})(\mathbf{u}_n(\boldsymbol{x}), \boldsymbol{\sigma}^i(\boldsymbol{x})) \tag{2.16}$$

The right-hand side of this equation can be rewritten as

$$\begin{aligned}
\frac{1}{N}\sum_{n=1}^{N}\mathbf{u}_n(\boldsymbol{x})(\mathbf{u}_n(\boldsymbol{x}),\boldsymbol{\sigma}^i(\boldsymbol{x})) &= \frac{1}{N}\sum_{n=1}^{N}\mathbf{u}_n(\boldsymbol{x})\int_\Omega \mathbf{u}_n(\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' = \\
\int_\Omega \frac{1}{N}\sum_{n=1}^{N}\mathbf{u}_n(\boldsymbol{x})\mathbf{u}_n(\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' &= \int_\Omega \mathbf{R}(\boldsymbol{x},\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' \qquad (2.17)
\end{aligned}$$

where $\mathbf{R}(\boldsymbol{x},\boldsymbol{x}')$ is supposed to be an approximation of the space-correlation tensor of the previous section. So $\boldsymbol{\sigma}^i$ has to be an eigenfunction of $\mathbf{R}$ with eigenvalue c_i, and $\boldsymbol{\sigma}^i$ is a solution of (2.15) if

$$\frac{1}{N}\sum_{n=1}^{N}(\mathbf{u}_n,\boldsymbol{\sigma}^i)^2 = c_i \qquad (2.18)$$

This holds, since

$$\begin{aligned}
\frac{1}{N}\sum_{n=1}^{N}(\mathbf{u}_n,\boldsymbol{\sigma}^i)^2 &= \frac{1}{N}\sum_{n=1}^{N}\int_\Omega \mathbf{u}_n(\boldsymbol{x})\boldsymbol{\sigma}^i(\boldsymbol{x})\mathrm{d}\boldsymbol{x}\int_\Omega \mathbf{u}_n(\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' \\
&= \int_\Omega\int_\Omega \frac{1}{N}\sum_{n=1}^{N}\mathbf{u}_n(\boldsymbol{x})\mathbf{u}_n(\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}'\boldsymbol{\sigma}^i(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \\
&= \int_\Omega \mathbf{R}(\boldsymbol{x},\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}'\boldsymbol{\sigma}^i(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \\
&= \int_\Omega \frac{1}{c_i}\boldsymbol{\sigma}^i(\boldsymbol{x})\boldsymbol{\sigma}^i(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = c_i \qquad (2.19)
\end{aligned}$$

Finally we check that the correlation coefficient of $(\mathbf{u}_n,\boldsymbol{\sigma}^i)$ and $(\mathbf{u}_n,\boldsymbol{\sigma}^j)$ is indeed zero.

$$\begin{aligned}
\frac{1}{N}\sum_{n=1}^{N}(\mathbf{u}_n,\boldsymbol{\sigma}^i)(\mathbf{u}_n,\boldsymbol{\sigma}^j) &= \frac{1}{N}\sum_{n=1}^{N}\int_\Omega \mathbf{u}_n(\boldsymbol{x})\boldsymbol{\sigma}^i(\boldsymbol{x})\mathrm{d}\boldsymbol{x}\int_\Omega \mathbf{u}_n(\boldsymbol{x}')\boldsymbol{\sigma}^j(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' \\
&= \int_\Omega\int_\Omega \frac{1}{N}\sum_{n=1}^{N}\mathbf{u}_n(\boldsymbol{x})\mathbf{u}_n(\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}'\boldsymbol{\sigma}^j(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \\
&= \int_\Omega \mathbf{R}(\boldsymbol{x},\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}'\boldsymbol{\sigma}^j(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \\
&= \int_\Omega c_i\boldsymbol{\sigma}^i(\boldsymbol{x})\boldsymbol{\sigma}^j(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = 0 \qquad (2.20)
\end{aligned}$$

So, in conclusion, we have found a set of solutions $\{\boldsymbol{\sigma}^i, i = 1, N\}$ for the minimization problem (2.11), that are also solutions of the following degenerate integral eigenvalue problem

$$\int_\Omega \mathbf{R}(\boldsymbol{x},\boldsymbol{x}')\boldsymbol{\sigma}^i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' = \lambda^i\boldsymbol{\sigma}^i(\boldsymbol{x}) \qquad (2.21)$$

with $\mathbf{R}(\boldsymbol{x},\boldsymbol{x}') = \frac{1}{N}\sum_{n=1}^{N}\mathbf{u}_n(\boldsymbol{x})\mathbf{u}_n(\boldsymbol{x}')$. The eigenvalue λ^i $(= c_i)$ is also the maximum in equation (2.10). It is known (see [36]) that the solutions of such an integral equation are linear combinations of the snapshots $\mathbf{u}_n$ with coefficients q_n^i

$$\boldsymbol{\sigma}^i = \sum_{n=1}^{N} q_n^i \mathbf{u}_n \tag{2.22}$$

Now we can re-order them such that the larger the index the larger the minimum achieved in equation (2.11). The solution of the minimization problem is unique if all the minima are different, and we have found the solution. If two or more minima are equal the corresponding eigenfunctions are not unique, but have to be orthogonal and have to span the two or more dimensional space in which orthogonal projections are minimal. In the latter case we have found such a solution, which is not unique. In practical computations the minima will almost always be different, so then we have found the unique solution.

Now it is easy to verify that the POD eigenfunction of the snapshot POD have the same properties if applied to the snapshots which are used to compute them, as the POD eigenfunctions in the continuous POD. The maximum energy content follows from the construction. The POD eigenfunctions span exactly the space spanned by the snapshots, i.e. the space of the realizable flowfields. Because the POD eigenfunctions are linear combinations of the snapshots, the eigenfunctions satisfy a linear combination of the boundary conditions of the snapshots. In our case these are homogeneous boundary conditions, so the POD eigenfunctions satisfy homogeneous boundary conditions. For the same reason the eigenfunctions are divergence-free. The POD eigenfunctions are orthogonal by construction.

If we subtract the mean of the snapshots from the snapshots, the sum of the new snapshots is zero. So, they are not linearly independent anymore. The new snapshots span a space of dimension $N-1$, so we get one POD eigenfunction with a zero maximum. In practice this will not be much of a problem because we only want to retain a small number of POD eigenfunctions with the largest maxima.

2.2.3 Space-time symmetry

The POD can be seen as a bi-orthogonal decomposition (see for example [3]). Also the time-dependent part in equation (2.5) forms orthogonal (see equation (2.8)) modes.

For the snapshot POD from the previous subsection we can reformulate the minimization problem (2.13) as

$$\min_{a_n^i, \boldsymbol{\sigma}^i} \frac{1}{N} \sum_{n=1}^{N} (\mathbf{u}_n - \sum_{i=1}^{N} a_n^i \boldsymbol{\sigma}^i, \mathbf{u}_n - \sum_{i=1}^{N} a_n^i \boldsymbol{\sigma}^i) \tag{2.23}$$

A necessary condition for a_n^i and $\boldsymbol{\sigma}^i$ to minimize equation (2.23) is that the first order variations δa_n^i and $\delta \boldsymbol{\sigma}^i$ are zero. This leads to the following equations for $\boldsymbol{\sigma}^i$ and a_n^i

$$\begin{aligned} \boldsymbol{\sigma}^i &= \frac{\frac{1}{N}\sum_{n=1}^{N}(\mathbf{u}_n - \sum_{j=1, j\neq i}^{N} a_n^j \boldsymbol{\sigma}^j) a_n^i}{\sum_{n=1}^{N} {a_n^i}^2} \\ a_n^i &= \frac{(\mathbf{u}_n - \sum_{j=1, j\neq i}^{N} a_n^j \boldsymbol{\sigma}^j, \boldsymbol{\sigma}^i)}{(\boldsymbol{\sigma}^i, \boldsymbol{\sigma}^i)} \end{aligned} \tag{2.24}$$

We seek for orthogonal solutions with $(\boldsymbol{\sigma}^i, \boldsymbol{\sigma}^j) = 0$ for $i \neq j$, and for uncorrelated a_n^i with $\frac{1}{N}\sum_{n=1}^{N} a_n^i a_n^j = 0$ for $i \neq j$. It then follows that $\boldsymbol{\sigma}^i$ is a linear combination of the snapshots

$$\boldsymbol{\sigma}^i = \frac{\frac{1}{N}\sum_{n=1}^{N} a_n^i \mathbf{u}_n}{\sum_{n=1}^{N} {a_n^i}^2} \tag{2.25}$$

and that a_n^i satisfies the following equation

$$a_n^i = \frac{(\mathbf{u}_n, \boldsymbol{\sigma}^i)}{(\boldsymbol{\sigma}^i, \boldsymbol{\sigma}^i)} \tag{2.26}$$

We can choose a scaling. As before we choose $(\boldsymbol{\sigma}^i, \boldsymbol{\sigma}^i) = 1$. Substituting (2.26) in (2.25) gives the same integral equation (2.21) as in the previous subsection, substituting (2.25) in (2.26) yields the following eigenvalue problem

$$a_n^i = c_i' \frac{1}{N} \sum_{n=1}^{N} A_{n,m} a_m^i \tag{2.27}$$

where $A_{n,m} = (\mathbf{u}_n, \mathbf{u}_m)$. The a_n^i are uncorrelated, as can be checked.

In conclusion we can choose to solve the integral equation of the previous subsection to compute $\boldsymbol{\sigma}^i$, or we can use equation (2.27) and then (2.25). The first option is expensive because it requires the solution of an eigenvalue problem with a dimension of the order of the number of grid cells used to discretize the integral equation. The second option is cheaper, since it requires to solve an eigenvalue problem of dimension equal to the number of snapshots, which is in our case much less than the number of grid cells.

2.3 Method of Sirovich

To determine the POD eigenfunctions we have to solve the Fredholm integral equation (2.2). The dimension of the kernel $\mathbf{R}(\boldsymbol{x}, \boldsymbol{x}')$ is for the 2D case $4n_x n_y$ and in the 3D case $9n_x n_y n_z$ (n_x, n_y and n_z are the number of grid points in the x, y and z direction). Since $\mathbf{R}(\boldsymbol{x}, \boldsymbol{x}')$ is a full symmetric matrix, solving the integral equation directly would exceed today's computer power.

Sirovich introduced the 'snapshot' method [50] to meet this problem. The method is closely related to the space-time symmetry of the snapshot POD. The method of Sirovich uses the ergodicity hypothesis to write

$$\mathbf{R}(\boldsymbol{x}, \boldsymbol{x}') = \lim_{n\to\infty} \sum_{n=1}^{N} \mathbf{u}_n(\boldsymbol{x}) \mathbf{u}_n^T(\boldsymbol{x}') \tag{2.28}$$

In this equation the time dt between the snapshots $\mathbf{u}_n(\boldsymbol{x}) = \mathbf{u}(\boldsymbol{x}, ndt)$ has to be large enough for the snapshots to be uncorrelated. The idea is now to take a finite N large enough for a reasonable approximation of $\mathbf{R}(\boldsymbol{x}, \boldsymbol{x}')$. Substituting (2.28) into the Fredholm integral equation (2.2) results into a degenerate integral equation. Therefore (see also [36]) the solutions are linear combinations of the snapshots:

$$\boldsymbol{\sigma}^i(\boldsymbol{x}) = \sum_{n=1}^{N} q_n^i \mathbf{u}_n(\boldsymbol{x}), \tag{2.29}$$

provided that the snapshots are linearly independent. This condition is likely to be fulfilled since the number of snapshots is much lower than the number of grid cells.

Thus the problem is reduced to finding the coefficients q_n^i of the linear combination. If we substitute (2.29) into the degenerated integral equation we obtain the following eigenvalue problem for the coefficients q_n^i

$$\mathbf{Q}\mathbf{q}^i = \lambda \mathbf{Q}^i \quad \text{with} \quad \mathbf{Q}_{ij} = \frac{1}{N}(\mathbf{u}_i(\boldsymbol{x}), \mathbf{u}_j(\boldsymbol{x})) \tag{2.30}$$

The dimension of this eigenvalue problem is equal to the number of snapshots, which is much lower than the dimension of the eigenvalue problem (2.2).

The main difference with the snapshot POD of the previous section is the approximation of the space-correlation tensor $\mathbf{R}$. The snapshot POD requires only linear independence of the snapshots, which is of course no guaranty that we approximate $\mathbf{R}$. The method of Sirovich, however, uses the ergodicity hypothesis to approximate $\mathbf{R}$, so we can expect the POD eigenfunction to converge to the POD eigenfunctions of the continuous formulation. On the other hand, we can manipulate the snapshot POD by taking those snapshots which we want to see in the POD eigenfunction.

Finally it may be noted that, in one dimension, directly solving the integral equation (2.2) is feasible. Also an iterative method is possible (see [33]).

2.4 Galerkin projection

In this section the POD eigenfunctions are used as a basis for a Galerkin projection of the incompressible Navier-Stokes equations. In this way a system of ordinary differential equations for the coefficients a^i in the expansion of $\mathbf{u}$ in the POD eigenfunctions is derived.

Since the POD eigenfunctions satisfy the continuity equation, we can restrict ourselves to the momentum equation:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \triangle \mathbf{u} \tag{2.31}$$

We write the velocity field as the (time) mean flow $\overline{\mathbf{u}} = \langle \mathbf{u} \rangle$ and fluctuations $\mathbf{u}'$

$$\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}' \tag{2.32}$$

where $\mathbf{u}'$ is expanded in POD eigenfunctions:

$$\mathbf{u}' = \sum_{i=1}^{\infty} a^i \boldsymbol{\sigma}^i \tag{2.33}$$

Substituting equation (2.32) into (2.31) gives

$$\frac{\partial \mathbf{u}'}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \mathbf{u}' + \mathbf{u}' \cdot \nabla \overline{\mathbf{u}} + \mathbf{u}' \cdot \nabla \mathbf{u}' + \overline{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}} = -\nabla p + \frac{1}{Re} \triangle \mathbf{u}' + \frac{1}{Re} \triangle \overline{\mathbf{u}} \tag{2.34}$$

If we substitute (2.33) into this equation we obtain

$$\sum_{i=1}^{n}\frac{\mathrm{d}a^i}{\mathrm{d}t}\boldsymbol{\sigma}^i+\sum_{i=1}^{n}a^i\overline{\mathbf{u}}\cdot\nabla\boldsymbol{\sigma}^i+\sum_{i=1}^{n}a^i\boldsymbol{\sigma}^i\cdot\nabla\overline{\mathbf{u}}+\overline{\mathbf{u}}\cdot\nabla\overline{\mathbf{u}}+\sum_{i,j=1}^{n}a^ia^j\boldsymbol{\sigma}^i\cdot\nabla\boldsymbol{\sigma}^j$$
$$=-\nabla p+\frac{1}{Re}\sum_{i=1}^{n}a^i\triangle\boldsymbol{\sigma}^i+\frac{1}{Re}\triangle\overline{\mathbf{u}} \tag{2.35}$$

Projecting this equation along $\boldsymbol{\sigma}^k$ gives

$$\frac{\mathrm{d}a^k}{\mathrm{d}t}+\sum_{i=1}^{n}a^i(\boldsymbol{\sigma}^k,\overline{\mathbf{u}}\cdot\nabla\boldsymbol{\sigma}^i)+\sum_{i=1}^{n}a^i(\boldsymbol{\sigma}^k,\boldsymbol{\sigma}^i\cdot\nabla\overline{\mathbf{u}})+\sum_{i,j=1}^{n}a^ia^j(\boldsymbol{\sigma}^k,\boldsymbol{\sigma}^i\cdot\nabla\boldsymbol{\sigma}^j)+$$
$$(\boldsymbol{\sigma}^k,\overline{\mathbf{u}}\cdot\nabla\overline{\mathbf{u}})=-(\boldsymbol{\sigma}^k,\nabla p)+\tfrac{1}{Re}\sum_{i=1}^{n}a^i(\boldsymbol{\sigma}^k,\triangle\boldsymbol{\sigma}^i)+\tfrac{1}{Re}(\boldsymbol{\sigma}^k,\triangle\overline{\mathbf{u}}) \tag{2.36}$$

The term $(\boldsymbol{\sigma}^k,\nabla p)$ is zero. Indeed, Gauss theorem states that

$$(\boldsymbol{\sigma}^k,\nabla p)=-(\mathrm{div}\boldsymbol{\sigma}^k,p)+\int_{\Omega}\boldsymbol{\sigma}^k\cdot\boldsymbol{n}p \tag{2.37}$$

both terms on the right-hand side are zero since the POD eigenfunctions are divergence-free and satisfy the (homogeneous) boundary conditions.

Thus the coefficients $a^k(t)$ have to satisfy the following ordinary differential equation.

$$\frac{\mathrm{d}a^k}{\mathrm{d}t}+A_{kij}a^ia^j+B_{ki}a^i+C_k=0 \tag{2.38}$$

where

$$\begin{aligned}A_{kij}&=(\boldsymbol{\sigma}^k,\boldsymbol{\sigma}^i\cdot\nabla\boldsymbol{\sigma}^j)\\B_{ki}&=(\boldsymbol{\sigma}^k,\overline{\mathbf{u}}\cdot\nabla\boldsymbol{\sigma}^i)+(\boldsymbol{\sigma}^k,\boldsymbol{\sigma}^i\cdot\nabla\overline{\mathbf{u}})+\frac{1}{Re}(\boldsymbol{\sigma}^k,\triangle\boldsymbol{\sigma}^i)\\C_k&=\frac{1}{Re}(\boldsymbol{\sigma}^k,\triangle\overline{\mathbf{u}})+(\boldsymbol{\sigma}^k,\overline{\mathbf{u}}\cdot\nabla\overline{\mathbf{u}})\end{aligned}$$

We refer to this set as the low-dimensional dynamical system.

2.5 Closure model

We want to use a small number of POD eigenfunctions in the dynamical system (2.38), because it is cheap. The most expensive term in the dynamical system is the term with A_{ijk}. The amount work for this term is proportional to the number of eigenfunctions to the power 3.

The dynamical system (2.38) does not include interaction with the non-resolved modes, therefore the dynamical system will not be able to dissipate enough energy. This is because energy dissipation takes place at small scales and the most energy containing scales, which are the POD eigenfunctions, are the large scales. Therefore we have to model the energy transport to the non-resolved POD eigenfunctions.

The most commonly used assumption in turbulence modeling is that of an eddy-viscosity. It assumes that the influence of small scales on large scales can be modeled by an additional viscosity: an eddy-viscosity. Another way of preventing the high-energy POD eigenfunctions from getting too much energy is the use of a linear damping term. We will use both approaches.

In an eddy-viscosity model for the dynamical system (2.38) the "viscosity" $\frac{1}{Re}$ is multiplied by a factor $1+\nu_{e.v.}$. This kind of model is also used in the Ph.D. thesis of Rempfer (see [45]). He computed the actual eddy-viscosity of his simulation, and found that $\nu_{e.v.}$ is approximately zero for the first eigenfunction, approximately one for the fortieth, and is almost a linear function of the index of the eigenfunction. We also use a linear model, i.e.

$$\nu^i_{e.v.} = i * Constant \tag{2.39}$$

where i is the index of the POD eigenfunction, and the constant is chosen such that for the eigenfunction which maximizes (2.10) $\nu_{e.v.}$ is of the order of one. We have determined the value of the constant by trial and error.

The model with linear damping is based on the average energy exchange between the POD eigenfunctions. Suppose we have a dynamical system in which we retain M POD eigenfunctions. The energy content of a flow realization in the direction of POD eigenfunction $\boldsymbol{\sigma}^i$ is $a^i(t)^2$. The exchange of energy with other POD eigenfunctions in time reads

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}a^i(t)^2 &= 2\cdot a^i(t)\frac{\mathrm{d}}{\mathrm{d}t}a^i(t) = \\
&\quad 2\cdot a^i(t)(-\sum_{j,k=1}^{M} A_{ijk}a^j(t)a^k(t) - \sum_{j=1}^{M} B_{ij}a^j(t) - C_i) = \\
&\quad 2\cdot(-\sum_{j,k=1}^{M} A_{ijk}a^i(t)a^j(t)a^k(t) - \sum_{j=1}^{M} B_{ij}a^i(t)a^j(t) - C_i a^i(t))
\end{aligned} \tag{2.40}$$

On average the energy $a^i(t)^2$ has to be conserved, so the average of $\frac{\mathrm{d}}{\mathrm{d}t}a^i(t)^2$ will be zero. This leads to

$$\begin{aligned}
&\sum_{j,k=1}^{M} A_{ijk}\langle a^i(t)a^j(t)a^k(t)\rangle + \sum_{j=1}^{M} B_{ij}\langle a^i(t)a^j(t)\rangle + C_i\langle a^i(t)\rangle = \\
&\qquad\qquad \sum_{j,k=1}^{M} A_{ijk}\langle a^i(t)a^j(t)a^k(t)\rangle + B_{ii}\lambda^i = 0
\end{aligned} \tag{2.41}$$

We add a linear damping $D_i a_i$ to the dynamical system to enforce (2.41), i.e. the damping factor has to satisfy

$$\sum_{j,k=1}^{M} A_{ijk}\langle a^i(t)a^j(t)a^k(t)\rangle + \lambda^i B_{ii} + \lambda^i D_i = 0 \tag{2.42}$$

Finally we approximate the term $\langle a^i(t)a^j(t)a^k(t)\rangle$ by an average over the coefficients of snapshots used to compute the POD eigenfunctions

$$D_i = -\frac{1}{\lambda^i}[\sum_{j,k=1}^{M} A_{ijk}\{\frac{1}{N}\sum_{n=1}^{N} a_n^i a_n^j a_n^k\} + \lambda^i B_{ii}] \tag{2.43}$$

It may be observed that this model can be extended to a model with linear damping of the form $\sum_{i,j=1}^{M} D_{ij}a_j$ where the coefficients D_{ij} can be solved with the orthogonality constraint on the coefficients a^i.