Chapter 1
Computing Surrogates for Gas Network Simulation using Model Order Reduction

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Abstract CPU-intensive engineering problems such as networks of gas pipelines can be modelled as dynamical or quasi-static systems. These dynamical systems represent a map, depending on a set of control parameters, from an input signal to an output signal. In order to reduce the computational cost, surrogates based on linear combinations of translates of radial functions are a popular choice for a wide range of applications. Model order reduction on the other hand is an approach that takes the principle structure of the equations into account to construct low-dimensional approximations to the problem. We give an introductory survey of both methods, discuss their application to gas transport problems and compare both methods by means of a simple test case from industrial practice.

1.1 Introduction

Gas network simulation is a challenging problem that can become large scale, if one considers a realistic network. Being able to simulate these large models accurately and efficiently is however becoming increasingly more important as gas is used more widely as an energy source. In order to optimize processes related to gas pipeline operation or other gas network problems it is important to be able to simulate the flow of gas within complex pipe networks in realtime. This is a challenging problems since the flow within a pipe is a complex physical phenomenon and the network itself can be very large and complex, spanning entire continents with pipelines joined by numerous junctions. Writing the system as a set of equations for discrete values of the pressure and flows or possibly other important states, the system size can increase to an order of tens of thousands. Since the equations are

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highly nonlinear differential algebraic equations this is already a challenging problem. Creating surrogate models in general can often solve the problem. Since we are interested in solutions of equations, the functions to be modelled are only given implicitly. Model order reduction is however a technique that is used to reduce the complexity of dynamical systems or sometimes parameter dependent equations. The reduction of the dimension will typically reduce the computational time. Possibly it allows us to compute a solution, where standard solvers fail due to the complexity of the system. One of the problems for gas networks is for example to compute a stationary solution for a given fixed configuration of supplies and demands within a network. Reduced Order Modelling is particularly powerful when used during an optimization algorithm where one needs to solve the equations several times. If a trust-region method is used, one is even able to give at least heuristic error estimators, or bounds. In certain cases it can be interesting to create a surrogate of the solution vector by interpolation methods. One of these methods is radial basis metamodelling. RBF metamodelling is a very powerful technique since it can be used to interpolate any given smooth data set.

In Sect. 1.2 we give a detailed explanation of the modelling of gas within a pipe. We explain the benchmark equations often used as well as the approximations we will apply for modelling the whole network. We show the effects of this approximation in Sect. 1.5.1. We summarize in Sect. 1.3 the radial basis function interpolation methods. Section 1.4 on model order reduction gives a very brief general introduction into model order reduction and a summary of the model order reduction technique we used, which is called proper orthogonal decomposition. We will show first results in Sect. 1.5 in reducing two different ways of modelling the gas network. One is a dynamic model and one a stationary one. In the stationary case we also compare it to a radial basis surrogate in which we can see the advantage and limitations of this model.

1.2 Gas Network Simulation

Modelling and simulation of a gas network is a challenging problem for many reasons. One of the reasons is that gas pipe network simulation connects combinatorial aspects, through the network topology, with continuous behaviour within individual components. The physics within these components are often complex and one needs to find suitable approximations. The gas flow within one individual pipe is described by nonlinear partial differential equations. Adding valves, for example, the solution of the system is no longer differentiable. Because the problem can be arbitrarily complex, we will have to limit ourselves within this chapter. We cannot address all the challenges of gas networks, but rather mean to describe and discuss certain aspects of a simplified, though still practically relevant version of the problem.

We will mainly follow [Ste07, HMS10, ES] for the mathematical modelling of the gas network. We are going to discuss a dynamical model and a quasi-stationary model to describe the gas flow within a pipe. The topology of a pipe network, after

[Ste07], is modelled as a directed graph $\mathscr{G} = (\mathscr{A}, \mathscr{N})$, where the vertices are supply nodes $\mathscr{N}_+$, demand nodes $\mathscr{N}_-$ and interior nodes $\mathscr{N}_0$ (junctions),

$$\mathscr{N} = \mathscr{N}_+ + \mathscr{N}_- + \mathscr{N}_0.$$

The edges of the graph can constitute pipes, connections, compressors, valves, regulators or other components of a realistic gas network. We will, however, restrict ourselves to a network that consists of pipes only. This is certainly a strong simplification. On the other hand, the main focus of this chapter is to develop a fast surrogate for the problem. One can still explain the techniques of surrogate modelling we use as well as address issues within the simulation of gas networks, namely the problem of finding a stationary solution for a given configuration.

An edge is denoted by $ij \in \mathscr{A}$, where the flow is directed from i to j. Within each pipe we want to model the physics of the gas by thermodynamic conservation laws. This is based on [ES].

We now assume that $x \in [0,L]$ is the independent variable along the length of a pipe segment , where L is the length of the segment (D its diameter). The other independent variable if one considers time varying problems is the time t.

Conservation of mass yields the so-called continuity equation (1.1) and conservation of momentum the pressure loss equation (1.2). These equations form a coupled PDE together with the equations of the state of a real gas (1.3). Together they are called the isothermal Euler equations.

$$\partial_t \rho + \partial_x q = 0 \tag{1.1}$$

$$\partial_t q + \partial_x p + \partial_x(\rho v^2) + g\rho\,\partial_x h = -\frac{\lambda(q)}{2D}\rho v|v| \tag{1.2}$$

$$p = \gamma(T)\, z(p,T)\, \rho \tag{1.3}$$

The dependent state variables are gas density $\rho(x,t)$, gas velocity $v(x,t)$, gas pressure $p(x,t)$ and gas temperature $T(x,t)$. From density and velocity of the gas we can calculate the gas flow $q(x,t) = \rho(x,t)\, v(x,t)$. The network of pipes can have a given geodesic height $h(x)$. The friction coefficient $\lambda(q)$ can be determined by a variety of formulæ. The simplest one is

$$\lambda = 0.067 \left(\frac{158}{\mathrm{Re}} + \frac{2k}{D} \right)^{0.2},$$

where Re is the Reynolds number and $k = 0.03$mm the equivalent roughness of the pipe [LIW04]. If we even consider an approximation of Re, λ will be a constant number independent of q. $z(p,T)$ is a compressibility factor that can also be computed by several formulæ [LIW04]. It denotes the deviation from the behaviour of an ideal gas ($z = 1$) and may even be approximated by this ideal behaviour without the loss of practical utility of the equations. $\gamma = RT$ is a field determined by temperature and a gas constant R [LIW04]. The full term γz is often approximated by the square of the sound velocity $a \approx 300 m/s$ in practice. Making use of the described simplifications yields

$$\begin{aligned} \partial_t \rho + \partial_x q &= 0 \\ \partial_t q + \partial_x p + \partial_x(\rho v^2) + g\rho\,\partial_x h &= -\frac{\lambda}{2D}\rho v|v| \\ p &= a^2\rho. \end{aligned}$$

We now consider a small pipe network and allow for an approximation of $h(x) \equiv h_0$ and $T(x) \equiv T_0$. We will also drop the kinetic energy term, replace $v = \frac{q}{\rho}$, plug the third equation into the second and obtain:

$$\begin{aligned} \partial_t \rho + \partial_x q &= 0 \\ \partial_t q + a^2 \partial_x \rho &= -\frac{\lambda}{2D}\frac{q|q|}{\rho}. \end{aligned} \tag{1.4}$$

We will consider two models for our pipe network, one where the physics within the pipe is modelled by (1.4) and the other were we assume the dependent variables ρ and q are time-invariant as in [HMS10, sec. 2.3] leading to the quasi-static equations

$$\partial_x \rho = -\frac{\lambda}{2Da^2}\frac{q|q|}{\rho}, \quad q = \text{const.} \tag{1.5}$$

Equations (1.4) or (1.5) have to be satisfied for every pipe $ij \in \mathscr{A}$. The pipes are connected at the nodes and for each interior node we have to satisfy Kirchhoff's current law, i. e. the sum of all incoming gas flows equals the sum of all outgoing flows per node. In the following, we will describe how to discretize these two sets of equations inside a given network and see the full set of equations that has to be solved. We start with (1.4) which is the dynamic case and use these to then derive the quasi-static discretized equation in Sect. 1.2.2. This quasi-static case is the stationary solution given a time-independent input. If one considers time dependent inputs, however, one can use these simplified equations to construct time dependent functions for q and ρ. This is a relevant approach in practice and referred to as the quasi-static solution.

1.2.1 Dynamic Equations

Given a network with pipes as edges, experience shows that in practice any rough discretization of $x_i - x_{i-1} \in [1000\text{m}, 5000\text{m}]$ is sufficient. We therefore take discrete points for the pressure only at the nodes and flows q at the beginning and at the end of each pipe. If the pipe is longer than 5km we add artificial interior nodes into the network. We then have a density ρ_i at every node $i \in \mathscr{N}$, and for every pipe segment $ij \in \mathscr{A}$ we have a flow q_{ij}^{out} and a flow q_{ij}^{in}. Here (out) stands for the flow at the end of the pipe, out of the pipe, and (in) for the flow at the beginning of the pipe into the next segment. The dynamic pipe equations are then discretized for a given pipe ij by

$$\partial_t \frac{\rho_i+\rho_j}{2} + \frac{q_{ij}^{\text{out}} - q_{ij}^{\text{in}}}{L_{ij}} = 0$$
$$\partial_t \frac{q_{ij}^{\text{out}} + q_{ij}^{\text{in}}}{2} + a^2 \frac{\rho_j - \rho_i}{L_{ij}} = -\frac{\lambda}{4D_{ij}} \frac{\left(q_{ij}^{\text{out}} + q_{ij}^{\text{in}}\right)\left|q_{ij}^{\text{out}} + q_{ij}^{\text{in}}\right|}{\rho_i+\rho_j}.$$

For every node we have to add an algebraic constraint. Introducing the new variable $y_{ij} = \frac{q_{ij}^{\text{out}}+q_{ij}^{\text{in}}}{\rho_i+\rho_j}$, one can write the full system as:

$$\partial_t \frac{\rho_i+\rho_j}{2} + \frac{q_{ij}^{\text{out}} - q_{ij}^{\text{in}}}{L_{ij}} = 0 \quad \forall e = ij \in \mathscr{A}_{\text{pipe}} \tag{1.6}$$
$$\partial_t \frac{q_{ij}^{\text{out}} + q_{ij}^{\text{in}}}{2} + a^2 \frac{\rho_j - \rho_i}{L_{ij}} + \frac{\lambda}{4D_{ij}} \left|q_{ij}^{\text{out}} + q_{ij}^{\text{in}}\right| y_{ij} = 0 \quad \forall e = ij \in \mathscr{A}_{\text{pipe}} \tag{1.7}$$
$$\sum_{ji\in\mathscr{A}} q_{ji}^{\text{out}} - \sum_{ik\in\mathscr{A}} q_{ik}^{\text{in}} = 0 \quad \forall i \in \mathscr{N}_0 \tag{1.8}$$
$$\sum_{ji\in\mathscr{A}} q_{ji}^{\text{out}} - \sum_{ik\in\mathscr{A}} q_{ik}^{\text{in}} - D_i(t) = 0 \quad \forall i \in \mathscr{N}_- \tag{1.9}$$
$$a^2\rho_i(t) - \hat{p}_i(t) = 0 \quad \forall i \in \mathscr{N}_+ \tag{1.10}$$
$$(\rho_i+\rho_j)\, y_{ij} - (q_{ij}^{\text{out}} + q_{ij}^{\text{in}}) = 0 \quad \forall e = ij \in \mathscr{A}_{\text{pipe}}. \tag{1.11}$$

Equations (1.6) and (1.7) describe the dynamics of the system. Equation (1.8) is Kirchhoff's current law for interior nodes. In (1.9) the sum of flows has to be equal to the demand at the demand node. For the supply node, we have a given pressure $\hat{p}_i(t)$ (1.10). Equation (1.11) is necessary since we introduce the extra variables y_{ij}.

We will consider $\lambda, 1/D_{ij}, 1/L_{ij}, a^2$ as parameters and collect them in a large vector p. The demand flows $D_i(t)$ and the supply pressures $\hat{p}_i(t)$ are considered inputs to the system and are collected in a vector $u(t)$. The states of the system are $\rho_i, q_{ij}^{\text{out}}, q_{ij}^{\text{in}}, y_{ij}$. Collecting all states in a vector x, this system can be written as

$$E\dot{x} = A(p)x + H(p)\,(x \otimes g(x)) + Bu \tag{1.12}$$

where $(g(x))_i = x_i$ or $(g(x))_i = |x_i|$. In a variety of applications one is interested in optimizing a quantity that depends on the states. If one calls that quantity $y = h(x)$ we are in the framework of a dynamical system of the form

$$E\dot{x} = A(p)x + H(p)(x \otimes g(x)) + Bu$$
$$y = h(x).$$

Due to the fact that E is singular this system is a so-called algebraic differential equation (DAE). For general network structures it is an index 1 DAE. Furthermore

it is reasonable to assume $g(x) = x$ for certain networks. Then the dynamical system is purely quadratic. The matrices in (1.12) are sparse and the parameter dependence is linear.

1.2.2 Quasi-Static Equation

Starting from Eq. (1.5) we follow [HMS10, Eq. (6)] for an explicit solution, which is a discretization of the pipe with nodes at the beginning and end of the pipe only:

$$\begin{aligned}
\partial_x \rho &= -\frac{\lambda}{2Da^2}\frac{q|q|}{\rho}, \quad q = \text{const},\\
\Rightarrow \partial_x(\rho)\rho &= -\frac{\lambda}{2Da^2} q|q|, \quad q = \text{const},\\
\Rightarrow \frac{1}{2}\partial_x(\rho^2) &= -\frac{\lambda}{2Da^2} q|q|, \quad q = \text{const},\\
\Rightarrow \partial_x(p^2) &= -\frac{a^2\lambda}{D} q|q|, \quad q = \text{const},\\
p_j^2 - p_i^2 &= -\frac{a^2\lambda}{D_{ij}} q_{ij}\left|q_{ij}\right| L_{ij}, \quad q_{ij} = \text{const}.
\end{aligned}$$

Together with Kirchhoff's laws at the nodes the full algebraic system is given by

$$p_j^2 - p_i^2 + \frac{a^2\lambda L_{ij}}{D_{ij}} q_{ij}|q_{ij}|L_{ij} = 0 \text{forall} ij \in \mathscr{A}, \tag{1.13}$$

$$\sum_j q_{ij} - \sum_k q_{ik} = 0 \text{ for all } i \in \mathscr{N}_0, \tag{1.14}$$

$$\sum_j q_{ij} - \sum_k q_{ik} - D_i = 0 \text{ for all } i \in \mathscr{N}_{\text{in}}, \tag{1.15}$$

$$p - \hat{p}_i = 0 \text{ for all } i \in \mathscr{N}_{out}. \tag{1.16}$$

With the parameters $a^2, \lambda, L_{ij}/D_{ij}$ collected in p, the pressures and flows (p_i, q_{ij}) collected in x, and $\hat{p}_i$ as well as D_i collected in u we get

$$A(p)x + H(p)\,(x \otimes g(x)) + Bu = 0, \tag{1.17}$$

where $(g(x))_i = |x_i|$ or x_i again. In some cases one can assume the relevant x to be positive as in the dynamic case. Then $g(x) = x$ and the system is quadratic.

1.2.3 Discussion of non-linearity

The gas flow within the pipe network leads to the moderate non-linearity of the quadratic term and possibly to a discontinuity due to the absolute value. Nevertheless further elements like connections, valves and regulators may introduce stronger non-linearity or can even cause a loss of smoothness within the solution. Connections do not introduce non-linearity, since they can be thought of as simple, very short pipes with a constant relative pressure loss. If valves are seen as either open or closed, they will not introduce any further non-linearity either. An opening or closing procedure of a valve would cause a non-continuity within the state and should therefore be modelled differently, i. e. by a smooth transition. The remaining elements, the regulators or control valves, do introduce strong non-linearity, since they will usually reduce gas pressure, but do not interfere if the gas pressure is too low to be reduced. It is to be made sure that the solution algorithm of the DAE can deal with such non-smoothness, either by appropriate adaptation of the algorithm itself, or by a smoothing procedure. The character of these kinds of non-linearities or discontinuities should be studied further. Within the scope of this chapter and with model order reduction in mind, we will consider the moderately non-linear part only, since regulators will not essentially contribute to the size of the system.

1.3 Radial Kernel Interpolation

Before we give a detailed overview of model order reduction of gas transport problems, we introduce a more general interpolation approach for comparison. Radial basis function (RBF) interpolation is a very intuitive black-box interpolation approach that is easy to implement and makes very general assumptions about the function that is to be approximated. Recall, for example, the quasi-static equations in matrix form (1.17). If we use an RBF approach, we do not consider the state x, but only the implicitely defined function of parameters p onto one (or more) outputs y.

$$f:\ p \in \Omega \subset \mathbb{R}^d \to y \in \mathbb{R}$$

However, if there is no output defined one can consider the whole state vector as output. The assumptions of RBF interpolation about the approximand f are, simply put, continuity and smoothness. Since we are dealing explicitly with an implicitly defined function, we cannot make these assumptions in general. On the other hand, we are dealing with a mildly non-linear setting, where we can in practice expect continuity and smoothness most of the time. The RBF interpolant is then given by the linear combination of M translates of a radial function $\phi(r), r \in \mathbb{R}$,

$$s:\ x \in \Omega \subset \mathbb{R}^d \to \sum_{i=1}^{M} \lambda_i \phi(||x - x_i||), \tag{1.18}$$

for given interpolation points $x_1,\dots,x_M$. Here, we adopt the convention from the RBF literature, where x denotes a parameter from Ω, while in the MOR literature x denotes a state. $||.||$ stands for the 2-norm or Euclidean norm of a d-dimensional vector. Although other norms have been used, many results in the literature are obtained for this specific choice, refer to [Buh03, Fas07, Chap. 10] for a brief discussion of alternatives. The coefficients λ_i are determined by M interpolation conditions

$$s(x_j) = f(x_j) \qquad \forall j \in [1,...,M] \tag{1.19}$$

of a sampling $f(x_j), x_j \in \mathscr{X} \subset \Omega$ of the parameter space Ω. The choice of this sampling strongly determines the quality of the approximation. Since the interpolation is only dependent on Euclidean distances, scattered samplings that do not lie on a regular grid can be considered without any difficulty.

Classical choices of radial basis functions are infinitely differentiable functions such as (inverse) multi-quadrics $\phi(r) = (\varepsilon^2 r^2 + 1)^\beta, \beta \in \mathbb{R}$ or Gaussians $\phi(r) = e^{-\varepsilon^2 r^2/2}$. The so-called shape parameter $\varepsilon > 0$ scales the width of the functions and thus influences the quality of the approximation critically. Other important choices of radial basis functions are finitely-differentiable, such as the Matérn-class of radial functions and the so-called polyharmonics [BRS12] as well as radial functions with compact support. A prominent example among compactly supported radial functions are the Wendland functions [Wen10, Fas07]. Wendland functions speed up the setup and evaluation of the interpolant, thereby trading computational expense against accuracy. Since RBF interpolants can always be set up and evaluated comparably fast within our framework of the gas transport problem, we do not consider radial functions with compact support in the following, nor will we report on any other accelerating approaches.

1.3.1 Convergence rates

In order to be able to derive general properties of RBF interpolation, radial basis functions are seen as symmetric positive definite reproducing kernels $K(x,y)$ that induce certain Hilbert spaces [Sch97]. The main idea is to choose the kernel K as the translate of a radial function

$$K(x,y) = \phi(||x-y||).$$

Then the theory of reproducing kernels can be applied and error estimates as well as convergence rates of RBF interpolation can be concluded. The Hilbert space induced by a kernel is called its "native" Hilbert space, and properties of the kernel such as the radial symmetry and its translation invariance are responsible for the innate structure of this induced space. Not strictly positive definite functions such as the popular multiquadrics can be incorporated into the framework as conditionally positive definite kernels. Polynomial detrending which allows to exactly reproduce

polynomial functions of a low degree plays an important role in industrial practice as well as in the theory of conditionally positive definite reproducing kernels. We will use polynomial detrending and conditionally positive definite kernel interpolation within this chapter without a thorough theoretical treatment, though. The reason is that we are mainly concerned with the basic practical questions of its application to gas network problems. The interested reader is referred to the introduction of the topic in [Sch97] as well as to the very comprehensible and practical treatment in [Fas07] and to the comprehensive account of all the theory involved that is given in [Wen10].

Our main assumptions of continuity and smoothness, we mentioned earlier, can be seen in terms of properties of the native space. If the approximand f lives in the native space of a radial basis function, the literature provides upper bounds for error estimates depending on the fill distance $h = \sup_{x\in\Omega} \min_{x_j\in\mathscr{X}} ||x - x_j||$ of a sampling $\mathscr{X}$. Here h is a quantity that measures how well a sampling $\mathscr{X}$ covers the parameter space Ω. These error bounds typically are given such that they have a factor which depends on h and a second factor which depends on $|f|_{\mathscr{N}_K(\Omega)}$, where $|.|_{\mathscr{N}_K(\Omega)}$ is the norm of the native space of the kernel K. In other words, the given error bounds try to separate the influence of the sampling from that of the approximand f. Both factors do depend on the kernel K, though – a fact which assigns an important role to our choice of the radial function ϕ. A general rule of thumb is that we can obtain better convergence rates with respect to h, if the approximand is infinitely smooth and thus can be approximated by an infinitely smooth RBF interpolation. Gaussians and multiquadrics allow for exponential convergence orders in the best case if we keep ε constant [Fas07, Chap. 15], while the known best bounds for finitely smooth radial functions such as the Matérn class of functions and thin plate splines are polynomial. The Matérn functions

$$\phi(r) = \frac{K_{\beta-d/2}(r)r^{\beta-d/2}}{2^{\beta-1}\Gamma(\beta)}, \qquad \beta > d/2$$

have Sobolev spaces $W_2^\beta(\mathbb{R}^d)$ as their native spaces $N_\phi(\mathbb{R}^d)$ [Fas07, Chap. 13] with

$$W_2^\beta(\mathbb{R}^d) = \left\{ g \in L_2(\Omega) \cap C(\Omega) : \quad D^\alpha g \in L_2(\Omega)\ \forall |\alpha| \le \beta, \alpha \in \mathbb{N}^d \right\},$$

where Ω is bounded and D^α denotes the distributional derivative with multi-index α. The native spaces of Gaussians and multiquadrics are smaller. If we try to approximate a function f which lives in $W_2^\beta(\mathbb{R}^d)$ but outside the native space of a multiquadric or Gaussian, the expected convergence rate becomes polynomial again, even if we apply a multiquadric or Gaussian kernel, and is therefore comparable to the convergence of finitely smooth RBF interpolation [Sch96]. Although their native space is rather small, we will therefore mainly use multiquadrics in our experiments.

1.3.2 Shape parameter selection

Apart from the important choice of the type of radial basis, there are several other parameters to consider that influence the approximation quality. The most obvious of them is the scaling parameter ε, which is also called shape parameter or "width" in the literature and which determines if the translate of a basis function has a more local or global influence. The discussion about the choice of ε is very similar to that of the basis function itself. Some researchers therefore argue that very flat and thus smooth and global functions yield the most accurate approximations [FW04, FZ06].

Unfortunately, flat basis functions cause numerical ill-conditioning, so that the high-accuracy results cannot be obtained with the described standard method. The solution of the system of interpolation conditions (1.19) leads to large coefficients λ_i introducing numerical cancellation errors within the interpolant, recall (1.18). If this ill-conditioning grows too strong, the theoretically favourable convergence rates are lost [Fas07, Chap. 17].

Several remedies have been suggested in the literature, such as a computationally more expensive expansion of the interpolant s by a rational polynomial of finite order [FW04, FLF11]. Other authors use numerical preconditioning of the system or certain basis transformations [PS11, Fas07, Chap. 34]. In practice, the problem of ill-conditioning becomes important if the approximand f exhibits strong local non-linearity, while most of the function is rather smooth. If this is the case, the simplest solution is to locally adapt the shape parameter so that it takes a different value for each basis function. The goal is to use smoother basis functions in smoother areas of the approximand and less smooth basis functions in more non-linear regions. Such an adaption of ε was originally proposed by [KC92], is easy to implement and potentially even enlarges the native space of infinitely smooth radial basis functions (it does not for the finitely smooth Matérn class functions and thin plate splines [BRS12]). Unfortunately, it cannot be made sure that the system is still non-degenerate when varying ε, although this method has often been used in practice with good results [FZ06]. If degeneration of the system is an issue, we like to point out some very similar approaches like non-stationary multilevel iteration [Fas07, Corr. 32.1] and adaptive univariate interpolation by scaled multiquadrics [BLS02]. The details of the selection of ε in these methods are beyond the scope of this chapter. The simplest rule of thumb is that the variable shape parameter should decrease in a "stationary" way, i. e. according to the decrease in the fill distance h. The simple gas transport problems considered in this chapter do not make it necessary to apply any of these measures at all. Also the example on p. 289 of [Fas07, table 32.6] shows that a simple uniform choice of ε can still give good approximation results compared to a multilevel approach. However, if a problem exhibits strong local non-linearities, we recommend to try one of the adaptive or multilevel approaches.

1.3.3 Sampling and refinement

A different, though related question is how to select the samples in $\mathscr{X}$. Since the error bounds are given in terms of the fill distance h, it is intuitive to select $\mathscr{X}$ such that h is minimized. Random or quasi-random samplings (Halton points) are most common. Other empirical choices of $\mathscr{X}$ consider numerical stability or local non-linearity of the approximand f. Since all these topics have already been discussed in the contect of the choice of ε, we omit most of the discussion here for brevity and refer to [Fas07] for more details. The most important result is that non-uniform samplings may be necessary to approximate locally non-linear functions f, but may cause ill-conditioning. The remedies are essentially again preconditioning, basis transformations, iterative refinement of the sampling and local adaption of the shape parameter such as in multilevel iteration.

Among the black-box surrogate methods, radial basis function interpolation can be compared to Kriging. Reference [SSS$^+$11] draws the comparison between intrinsic Kiging and general conditionally positive definitite kernel interpolation. As to [SSS$^+$11] radial kernels correspond to Kriging with covariance functions of a weakly stationary and isotropic random field.

1.4 Model Order Reduction (a special form of surrogate)

Model order reduction can be seen as a form of surrogate modelling which was originally developed in systems and control theory for dynamical systems. It is neither a black-box approach nor a physical surrogate. MOR can be understood as an interpolatory method that takes the general form of the function that should be approximated into account. It is today a wide area of research with many applications. For a first introduction into the topic of MOR consult [SvJ08, Ant05, BMS05].

The main idea behind model order reduction is that there is a redundancy within the system. The dynamical system for example has a large state space, but most of the solution trajectories lie on a lower dimensional subspace. The idea is to solve a system only on that lower dimensional subspace, therefore reducing the size of the state space.

We will introduce the concept of projection-based MOR as a surrogate for dynamical systems of the following problem type:

$$\begin{aligned} E\dot{x} &= Ax + f(x) + Bu \\ y &= Cx + h(x) \end{aligned} \tag{1.20}$$

where $u(t)$ is an input function, $x(t)$ the state vector and $y(t)$ the output function. The idea of the projection-based MOR is to find projection matrices $V, W \in \mathbb{R}^{n\times r}$ with $W^T V = I$ and $r < n$ such that $x \approx V\hat{x}$ where $\hat{x} \in \mathbb{R}^r$ solves the reduced equations

$$\begin{aligned} \hat{E}\dot{\hat{x}} &= \hat{A}\hat{x} + \hat{f}(\hat{x}) + \hat{B}u \\ \hat{y} &= \hat{C}\hat{x} + \hat{h}(\hat{x}) \end{aligned} \tag{1.21}$$

where $\hat{E} = W^T EV, \hat{A} = W^T AV, \hat{B} = W^T B, \hat{C} = CV, \hat{f}(\hat{x}) = W^T f(V\hat{x}), \hat{h}(\hat{x}) = h(V\hat{x})$. With this step we have reduced the number of states in the system (the unknowns) as well as the number of equations. The projection we described above is called a Petrov-Galerkin projection if $V \neq W$ and a Galerkin projection if $V = W$.

In order to measure the quality of the reduced system we need a measure for the error. One can measure the error by $\|x - V\hat{x}\|$ for an appropriate norm. This is the focus of proper orthogonal decomposition (POD), which we will explain in more detail in Sect. 1.4.1. One can also measure the error in the output. When measuring the error in the states we are focusing on the input to state map, where in the second case in which we measure the error in the output we are interested in the input to output map. Other widely used model order reduction methods are Krylov subspace methods, moment-matching, balanced truncation or the reduced basis method.

A problem in projection methods for general nonlinear systems is that even if one can reduce the number of states and equations considerably it could be still very expensive to evaluate $\hat{f}(\hat{x}) = W^T f(V\hat{x})$ since in the evaluation of this process one has to create the full large state vector $V\hat{x}$ and evaluate the large vector valued function f to then project it back down. For linear, quadratic or other more simple systems this additional evaluation of the full system can be avoided as certain matrices can be precomputed. For general nonlinear functions on the other hand one has to use EIM or DEIM [BMNP04, CS10] which we will not explain here, since the considered gas network problems show only mild non-linearity.

Different model order reduction methods have different guarantees on the error created by replacing the original model with the reduced model. Some methods have strict error bounds and others only heuristic error estimators. However not so much is known for nonlinear systems and especially for nonlinear differential algebraic systems. Another big challenge of nonlinear DAEs is that reducing the system can lead to a system that has no solution. Therefore, there are still many issues to be solved that need further theoretical investigations.

1.4.1 Proper Orthogonal Decomposition (POD)

We are interested in reducing the system (1.20). Since POD tries to find a good approximation in the state we are not interested in the output behaviour. POD finds a projection matrix W to minimize $\|x - W\hat{x}\|$ for a given norm $\|\cdot\|$ at least approximately. POD is a Galerkin projection method, which means we only have to find one matrix W. The method we describe is sometimes referred to as the method of snapshots [Sir87]. The general underlying concept of POD is within some communities also called Principal Component Analysis (PCA) or Karhuenen-Loeve decomposition. Given samples $x_1, \ldots, x_N$ of any kind (could be solutions or outcomes of a process in general) the method extracts a basis $u_1, \ldots, u_\ell$ that solves the following

minimization problem

$$\min_{u_1,\ldots,u_\ell} \sum_{k=1}^{N} \left\| x_k - \sum_{i=1}^{\ell} \langle x_k, u_i \rangle u_i \right\| \quad \text{s.t.} \quad \langle u_i, u_j \rangle = \delta_{ij}. \tag{1.22}$$

The solution to this problem is directly connected to the singular value decomposition of the matrix $Y = [x_1, ..., x_N]$. Given the SVD of $Y = U\Sigma V^T$ the solution to (1.22) for the standard Euclidean inner product and Euclidean norm is obtained by the first ℓ left singular vectors which are the first ℓ columns of U. Here we assume that the singular values in Σ are ordered. Per definition of the SVD U and V are orthogonal matrices and Σ is a diagonal matrix.

For a dynamical system as given above, what we would really like to do is solve the following optimization problem

$$\min \int_0^T \left\| x(t) - \sum \langle x(t), u_i \rangle u_i \right\|^2 \mathrm{d}t \quad \text{s.t.} \quad \langle u_i, u_j \rangle - \delta_{ij}. \tag{1.23}$$

Since this is difficult and we do not always know the solution $x(t)$ everywhere in time we solve the approximated version of this. Here we pick times $t_1, \ldots, t_N$ and look at solutions at these discrete time steps $x(t_1), \ldots, x(t_N)$, the so-called snapshots. We typically consider a fixed input function $u(t)$. The optimization problem (1.23) reduces to (1.22).

Given the singular vectors u_i of the snapshot matrix $Y = [x(t_1), \ldots, x(t_N)]$ we have that

$$x(t_k) \approx \sum_{i=1}^{\ell} \langle x(t_k), u_i \rangle u_i = \sum_{i=1}^{\ell} \hat{x}_i(t_k) u_i = W\hat{x}(t_k)$$

where W is given by the matrix $W = [u_1, \ldots, u_N]$. Since this is true for all discrete time steps t_k it can be considered as evidence that it is true at arbitrary times giving us that

$$x(t) \approx W\hat{x}(t)$$

We are not able to compute $\|x(t) - W\hat{x}(t)\|$ at every t but we minimize

$$\sum_k \|x(t_k) - W\hat{x}(t_k)\|.$$

If the system is furthermore dependent on a parameter this is typically extended by creating snapshots for several parameter values and times. All the snapshots will be put into one large matrix Y and the rest can be done as described above.

1.5 Surrogates for Gas Network Modelling

In this section we will discuss approaches to verify the discussed simplifications for the pipe equations as well as the different surrogate models constructed by model order reduction methods as well as radial basis function surrogates.

We will start with a gas network consisting of one pipe only in which we compare the quasi-static approximation with the dynamic approximation and the simulation of the full isothermal Euler equations. We will see the advantages and limitations of our two approaches. Furthermore we discuss in detail solving a larger example network using the quasi-static equations in the pipe. We construct a surrogate with POD model order reduction as well as with a radial basis function metamodel. The third test is a simulation of the dynamic model on that given network and its surrogate, computed by POD.

1.5.1 Pipe Equation Comparison

As a first verification of the pipe equations we are considering one long pipe ($L =$ 100km) with a given pressures at the inlet and outlet. This example was studied in [HMS10]. For comparability we use the same constants $a = 377.9683\text{m/s}, \lambda = 0.011$, $D = 0.5\text{m}$. The pressure at the inlet will always be given by constant 45bar and the pressure at the outlet varies smoothly from $p_O(0) = 40\text{bar}$ to $p_O(T) = 45\text{bar}$. We have different test cases with fast and slow changing inlet pressure profiles as well as one oscillating profile.

1. $p_O(t) = p_O(0) + \frac{p_O(T)-p_O(0)}{2}(1-\cos(\pi\frac{t}{T}))$ for $T = 1,3$ and 6h
2. $p_O(t) = p_O(0) + \frac{p_O(T)-p_O(0)}{2}(1-\cos(4\pi\frac{t}{T}))$ for $T = 12\text{h}$

We compute the flow at the inlet and outlet by three different sets of equations. First we solve the benchmark model, the isothermal Euler equations given by (1.1)–(1.3). These equations are discretized using a second-order relaxed method with adaptive characteristics speeds, see [HMS10] and the references therein. In [HMS10] the underlying grid has 2001 spatial points and uses a CFL-condition of 0.49. We do not adhere to this choice of discretization and construct a graph out of the pipe by adding 19 nodes such that the pipe segments all have a length of 5km. This as discussed above is the maximal length we allow for our network. Apart from the full isothermal equations we also solve the DAE given by (1.6)–(1.11). And the third solution is the quasi-static solution given by solving Eqs. (1.13)–(1.16). One can solve them on the network as above with the 19 added nodes or directly on the whole pipe. The solution will be the same since the flow in the beginning and end of the pipe (or pipe segment) is always the same.

Figures 1.1 and 1.2 show a comparison of the isothermal equations, our slightly simplified dynamic discretized equation solved in time by an implicit Euler as well as the quasi-static solution for the pressure profiles (1). One can see of course that

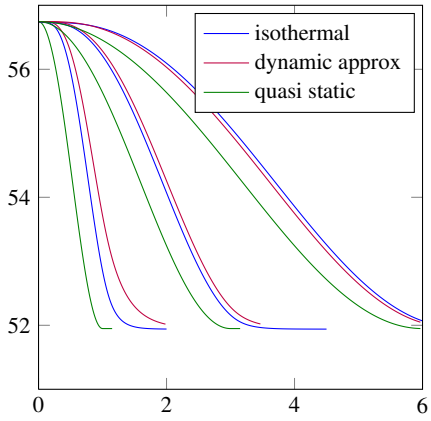


Fig. 1.1 Case (1.) Flux at the inlet

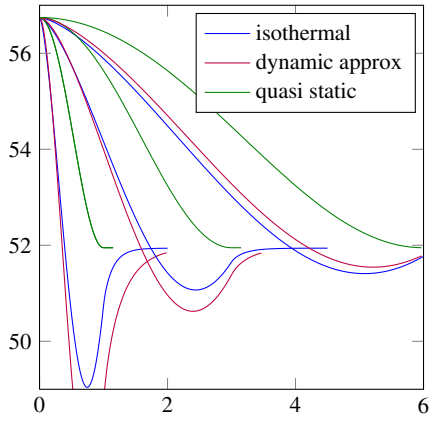


Fig. 1.2 Case (1.) Flux at the outlet

the quasi-static solution is the same at the inlet and the outlet and is nonsmooth at the final time. The dynamic approximated solution shown in red is closer to the isothermal benchmark solution the slower we change the pressure at the inlet. However it is significantly better than the quasi-static solution which is used often in practical applications. Figures 1.3 and 1.4 compare the two different models for oscillating

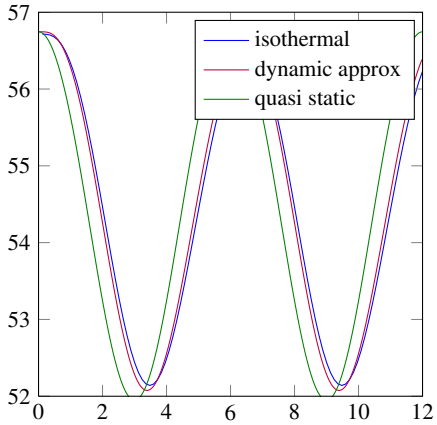


Fig. 1.3 Case (2.) Flux at the inlet

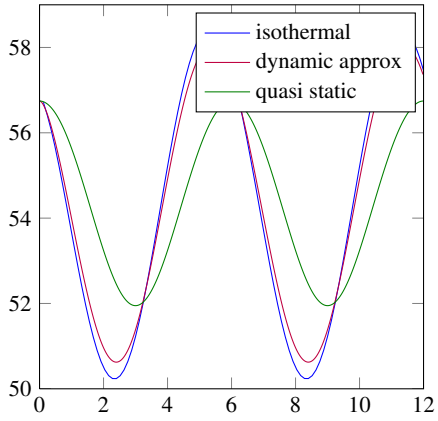


Fig. 1.4 Case (2.) Flux at the outlet

boundary pressure.

In general one can see that at the inlet the quasi-static solution is a decent approximation, where at the outlet it is not. For slowly varying pressure profiles the dynamic approximation is a very good approximation. This simplification produces a system that is quadratic (if set up accordingly to ensure $g(x) = x$) and can there-

fore be approximated more efficiently by model order reduction methods than the full isothermal equations, which justifies its use.

1.5.2 Test Example

We will compute the surrogate in the two following sections based on a model that is a modified version of a part of a true gas network. It consists of 17 nodes, 16 pipes, 1 supply node and 8 demand nodes. Its graph structure can be seen in Fig. 1.5. The lengths of the pipes are given by

$$\begin{aligned} L_{1,2} = 46\text{m}, L_{2,3} = 7\text{m}, L_{3,4} = 3080\text{m}, L_{4,5} = 4318\text{m}, L_{5,6} = 323\text{m}, L_{5,7} = 790\text{m}, \\ L_{7,8} = 1820\text{m}, L_{7,9} = 1460\text{m}, L_{9,10} = 2368\text{m}, L_{10,11} = 1410\text{m}, L_{11,12} = 296\text{m}, \\ L_{11,13} = 3979\text{m}, L_{13,14} = 119\text{m}, L_{13,15} = 3881\text{m}, L_{15,17} = 687\text{m}, L_{15,16} = 6114\text{m} \end{aligned}$$

and the diameters of the pipes are constant 0.206m. We will also assume $\lambda = 0.0003328$ and $a = 430.5\text{m/s}$ in the following if not specified otherwise. Furthermore the supply pressure is 44.5bar and the demands are given by

$$\begin{aligned} D_4 = 0.21\text{kg/s}, D_8 = 34.86\text{kg/s}, D_9 = 0.22\text{kg/s}, D_10 = 2.83\text{kg/s}, \\ D_{12} = 1.81\text{kg/s}, D_{14} = 1.04\text{kg/s}, D_{16} = 2.85\text{kg/s}, D_{17} = 1.45\text{kg/s}. \end{aligned}$$

However, we will also consider a trivial input vector where all demands are zero and the supply (or generally all supplies) are constant p_0. Then setting all pressures to p_0 and all flows to 0 is always a trivial solution of the equations. Since even computing stationary solutions for arbitrary demand and supply distributions can be difficult one has to use such a trivial solution as starting configuration sometimes.

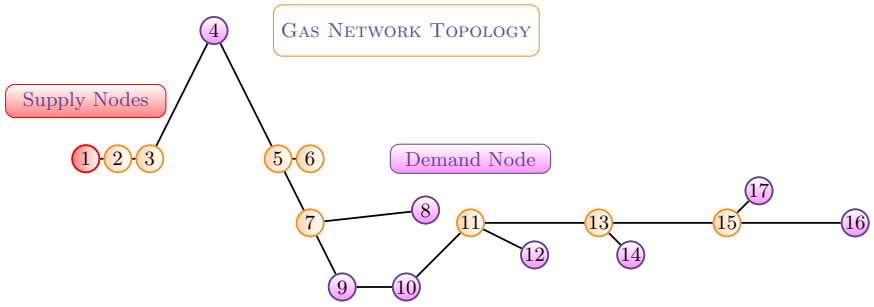


Fig. 1.5 Gas network graph

1.5.3 Quasi-Static Case with POD

The equation is given by (1.17), which we recall here for convenience

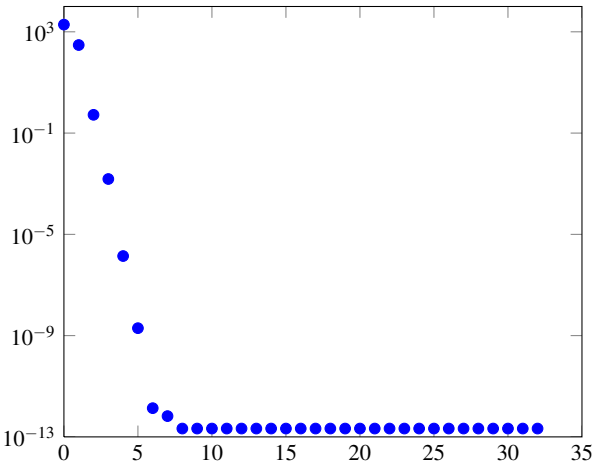
$$A(p)x + H(p)\,(x \otimes g(x)) + Bu = 0. \tag{1.24}$$

The parameter p consists of $\lambda, a^2, D_{ij}, L_{ij}$ and the input u of the pressure at the supply node and the outflows at the demand nodes. Since we are mainly interested in computing stationary solutions with this equation the question is, can one create a good surrogate to find the solution x for a given u? In general applications one typically knows the parameters to be in some range or with some uncertainty. Given the example network described above we compute solutions $x_0, ..., x_N$ for different inputs $u_0, ..., u_N$ with

$$u_i = u_0 + \frac{i}{N}(u_N - u_0).$$

Here u_0 is a trivial solution as described above with $p_0 \equiv 45$bar. This means we are solving the equation for a path of input distributions that move from the trivial solution u_0 to the desired one for u_N, which is the desired input as described in Sect. 1.5.2. We are using the equation solver `fsolve` from [JOP+] to solve the system above. The singular values of the snapshots matrix $Y = [x_0, \ldots, x_N]$ are given by Fig. 1.6.

Fig. 1.6 Singular values



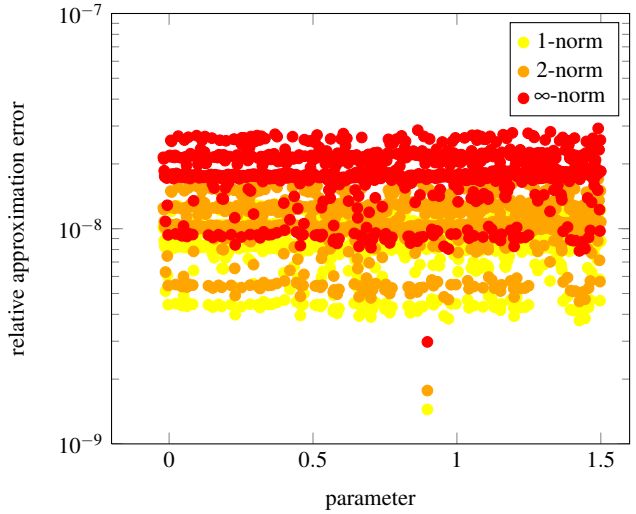
This shows that there is a low-dimensional linear space in which the solutions lie approximately. We create the reduced model by the projection described in Sect. 1.4.1. This is a special case since we do only have to consider algebraic equations, but no differential equations. We however consider a time-varying input system and compute the stationary solution of the system for discrete time steps. Interpreting this sequence of stationary solutions as a time-dependent state we talk about

the quasi-static solution, which can be a reasonable solution as we have seen above if the inputs vary slowly enough. Concretely, given the projection matrix W from the snapshot matrix Y by POD the reduced equation looks like

$$W^T A W \hat{x} + W^T H(p)\,(W \otimes I)\,(\hat{x} \otimes g(W\hat{x})) + W^T B u = 0.$$

Given a tolerance of 10^{-8} we create a reduced model of order 5. Having obtained that reduced model we compute solutions for u_{TEST} which has the same demands as u_N, but the supply is given by 50bar. Furthermore we vary the parameter λ slightly around its given value. The error $\|x - W\hat{x}\|$ is given in Fig. 1.7 for the 1000 different test values of $\lambda \in [0.0002, 0.0006]$.

Fig. 1.7 Different error norms



This shows that, for a given path of input vectors, starting from a trivial configuration, the system is reducible without producing a significant error. Given a configuration u for which the original system is hard to solve one can create a path $u_0, \ldots, u_N = u$ and solve the system starting with u_0 for each u_i, where `fsolve` is started with the solution of the previous problem. It is known that one can still run into a point where the Newton method no longer converges. One can then use the information from before to reduce the system, solve the reduced system and get a more accurate starting value for the quasi-Newton solver. If one is interested in parameter studies for a given input, the above example already shows that the reduced model is a good model for many parameters. One can however also reduce the model based on snapshot solutions for different parameters. We computed a snapshot matrix for values of λ varying from 0.0002 to 0.0006 chosing 40 equally spaced points in between. The reduced model is then of order 4, using the same tolerance of 10^{-8} in the singular values. Given 1000 values of λ between 0 and 1.5

$\lambda \times a^2$	# of samples	order reduced model	error RBF	error POD
$[1.5\times10^{-4}, 4.5\times10^{-4}]\times[150,450]$	33	4	10^{-7}	10^{-6}
$[0, 6\times10^{-4}]\times[0,600]$	100	5	2×10^{-6}	1.6×10^{-7}
$[0, 6\times10^{-4}]\times[0,600]$	100	4	3.5^{-7}	10^{-6}

Table 1.1 Comparing RBF surrogates and POD reduced models

the maximum error of the solution in the reduced system with the solution of the true system is then found to be 10^{-6}.

We also created several RBF metamodels for the solution to this algebraic equation. In order to do that we understand the solution x as an implicitly given function of the parameters and/or the inputs. Multiquadrics, Gaussians and Matérn-class functions have been implemented within a simple interpolation setting. We have not made use of polynomial detrending. Polynomial interpolation is expected to be very efficient and accurate in our example problems, since these problems show a certain polynomial behaviour. On the other hand, such an assumption can probably not be generalized, which is the reason why we refrain from this choice. The shape parameter ε has been selected manually as $\varepsilon = 0.1$. In order to allow for a comparison with POD, the same uniform sampling was used for both methods.

In Table 1.1 we compare creating a surrogate model for the function from the parameters $\lambda \times a^2$ to the state vector x containing the pressures and the flows. In each test we pick a certain parameter range and compute the solution for a number of grid-like distributed points. With that we create an RBF metamodel as well as a reduced order model via POD as above, where the order is again picked by the tolerance of 10^{-8}. We show the maximum error between the approximated and the true solution sampled on $10,000$ grid points.

One can see that if one chooses enough samples within a small enough region one can get almost arbitrarily small errors in the RBF model. This model is however only accurate for the exact region in which we have interpolation points. We again stress the fact that we have assumed the function x of p specified by an implicite function is smooth, which cannot be guaranteed in general. The advantage of the reduced model is that it takes this implicite definition into account and gives good solutions even outside the range which was used to create the model. One can furthermore change other parameters and still get reasonable approximations. One can consider it a disadvantage, on the other hand, that in order to obtain x there is still a system to solve, although of reduced order.

1.5.4 Dynamic Case

We are now considering the set of equations given by (1.6)–(1.11). Since the flow is no longer constant within the pipe and we add another set of variables we have for the example problem a state space dimension of $65 = 16\times3+17$. Since this is a differential algebraic equation we use POD exactly as described above, where we

consider the solution $x(t)$ given by solving the system for the input $u(t)$ which has constant demands and a varying supply pressure $\hat{p}_1(t)$ given by

$$\hat{p}_1(t) = 44.5 + 2.5 \times \left(1 - \cos\left(\frac{\pi t}{1\text{h}}\right)\right), \quad t \in (0, 1.5\text{h}).$$

We take 100 snapshots of the solution trajecotry $x(t)$ at equidistant time steps for $t \in [0, 1.5\text{h}]$. The singular values of the snapshot matrix are given by Fig. 1.8. Cutting

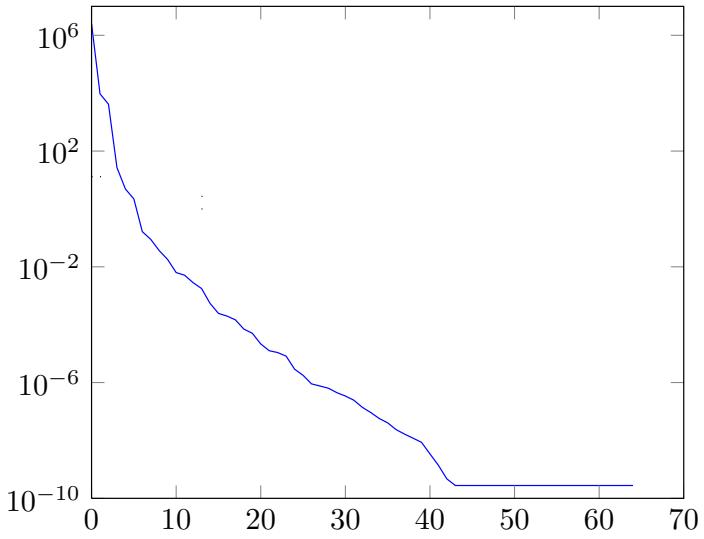


Fig. 1.8 Singular Value Decomposition of Snapshot Matrix

off at 10^{-8}, we create a reduced order model of size 39. To compare we compute the solution at $3,000$ timesteps between 0 and 1.5h. The maximal relative error between the reduced solution and the true solution is then found to be 10^{-8}. This small relative error is not surprising since cutting off the singular values at 10^{-8} is cutting them off at a relative error of $10^{-8}/10^{6} = 10^{-14}$, where 10^{6} is the value of the largest singular value. And since we reduce the model only for a given input function and fixed parameters the solution trajectory lies in that subspace and we can reduce the system to that subspace without creating an error. We can see the flux of the original model and the flux of the reduced model at node number 5 in Fig. 1.9. It shows that there is no difference.

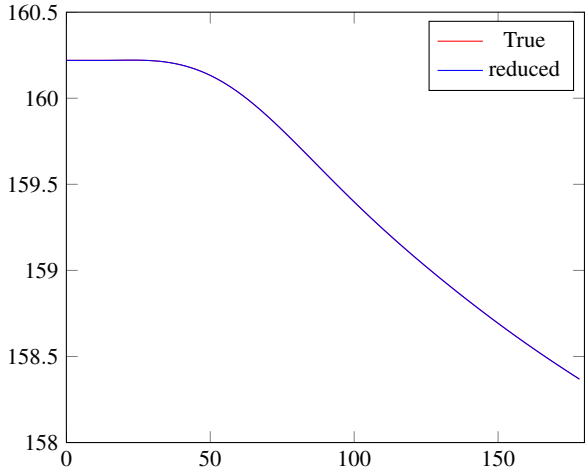


Fig. 1.9 Flux at node 5

1.6 Discussion and Conclusions

We have compared a dynamic approximation to the isothermal Euler equations for a network consisting of one long pipe. We used different outlet pressures and can see that the dynamic approximation is very close to the true isothermal Euler equations, especially if the pressure at the outlet is varying slowly enough. The often used quasi-static approximation is shown to not exhibit the right behaviour, but for very slowly varying inputs could still be a valuable option. We furthermore investigated a part of a realistic gas network with 17 nodes and 16 pipes. We created a reduced model for the quasi-static set of equations by POD. We were able to reduce the model for varying inputs to just 4 unknowns with a relative error of only 10^{-7}. This shows clearly that gas networks are reducible and model reduction is a valued surrogate. We also created RBF surrogates for this problem. Given good sampling points in the whole range one can create very accurate and efficient RBF interpolants. However the reduced model gives good results even outside the sampled parameter values. As discussed in Sect. 1.4 there are many methods for reduced order modelling, however very little is known for nonlinear differential algebraic systems. We tested the POD approach since it is an easy to use method and it works for arbitrary systems. The selected RBF approach works well due to the simple relation between x and p in our example, but might not be applicable to more involved settings.

With respect to the dynamic problem, proper orthogonal decomposition is probably not the most efficient model order reduction scheme. $\mathscr{H}_2$-optimal methods for linear systems that allow for a best-approximation in the $\mathscr{H}_2$ norm of the system can be computed efficiently by an iterative Krylov-subspace algorithm without solving the full system of equations. They have recently been extended to differential algebraic equations and to quadratic problems. However, there are still some issues. It is

not yet fully clarified, how optimality can be achieved with these methods. Neither is it understood in detail, how and when the iterative procedure converges and how the approach is implemented efficiently. Network systems have already been studied as nonlinear DAEs and there exist some tractability and stability results. However, we believe that there are still a lot of possible research topics, in order to arrive at tractable and stable reduced order systems of nonlinear gas transport network problems. One of the main questions is if the reduced order system does still adhere to the algebraic equations. Another question is how quadratic terms and switch state systems can be incorporated into some of the DAE-specific linear MOR approaches.

As to RBF interpolation, too, the dynamic case is more involved. There are very general RBF interpolation methods for PDEs that may have the potential to be adapted for gas networks. One might consider time as a parameter or a set of solutions for discrete time steps as a vector-valued output. In the computer graphics literature there are also RBF methods for the interpolation of implicit functions, which might have the potential to be extended to a multi-dimensional setting and thus to gas network simulation. Of course, the techniques for local strong nonlinearities mentioned in Sect. 1.3 may be of use if the problem setting becomes more demanding.

As has been mentioned earlier, the gas transport network problem can become much more difficult to solve if nonlinear compressors, regulators or other elements are considered. Therefore, the model order reduction problem can become very ambitious, too. Radial basis function interpolation might deal well with smooth nonlinearities but is expected to have difficulties with piecewise continuous functions or switch state systems. Therefore, one of the challenges in this application area is to combine the different approaches in such a way as to benefit from the advantages of each without suffering their disadvantages.

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