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Mixed-dimensional models for real-world applications

Jan Martin Nordbotten

We explore mathematical models for physical problems in which it is necessary to simultaneously consider equations in different dimensions; these are called mixed-dimensional models. We first give several examples, and then an overview of recent progress made towards finding a general method of solution of such problems.

1 Mixed-dimensional physical problems

Real-world physical problems often involve processes interacting between different physical "domains" (for instance, water and air), which are naturally considered to be three dimensional. When the interface between the domains itself has properties that must be taken into account, it is often natural to use a model that considers the interface to be two dimensional. So we have a "mixed-dimensional" problem. By a mathematical model, we mean a set of equations that represent a physical system and can be analysed to give numerical solutions that are then interpreted as information about the original system. We are interested here in models that contain equations that are defined on domains of different dimension - subsets of the three-dimensional space $\mathbb{R}^3$, the plane $\mathbb{R}^2$ or the real line $\mathbb{R}$ - and the equations must be solved simultaneously (we say they are *coupled*). Such models are called mixed-dimensional.

In order for a physical problem to be considered as mixed-dimensional, it must contain some features that are naturally either so flat, thin, or small, that they are reasonably represented as surfaces, curves or points, respectively. As we will see, such a categorization depends upon the “scale”, or level of magnification, at which the problem is considered. Nevertheless, we can already give some examples:

- The surface between two liquids, as common language indicates, is often reasonable to model as a surface between two three-dimensional domains.
- The wires of a bridge structure are reasonably modelled as one-dimensional curves connecting three-dimensional structures.
- Since the time of Johannes Kepler (1571–1630), it has been known that even objects as big as planets can sometimes be considered to be points, for example if the problem of interest is to calculate the motion of the solar system.

So, mixed-dimensional models arise in many settings. They have been used in science and engineering literally for hundreds of years; Kepler’s laws of planetary motion are more than 400 years old, and they are not the first such example. On the other hand, mixed-dimensional models have typically been introduced on a case-by-case basis, and their systematic study within a class of mathematical problems, in the sense that they are investigated using recognised tools and techniques that have previously been developed for other similar problems, is a relatively recent development.

Indeed, as an example, the description of the flow of a liquid in a fractured, porous media as a mixed-dimensional problem has recently been given [1]. Analysis of the resulting mathematical models is an active area of research (see for instance [2] and references therein). A second example is the description of blood circulation in the human body, which has to take into account both the flow in vessels (described as networks of 1D segments) and tissue (3D), and leads to problems with coupling across dimensions [5]. This problem is non-trivial to handle, as the most straight-forward mathematical models lead to “singular” solutions, intuitively solutions that are not physically convincing in some way.

1.1 Low dimensional gap: Surfaces

Any interface between two domains can in principle lead to a mixed-dimensional system. However, as mentioned in the introduction, the character of this mixed-dimensional system will depend strongly on the scale we consider. This is most easily understood by looking at something as familiar as the surface between water and air.

Consider first a single drop of water, and imagine that you have a microscope which is powerful enough that you can see individual molecules. If you aim the microscope at a point in the water drop, you would then not see anything resembling what we usually think of as water, you would instead see individual H_2O molecules, moving around essentially randomly with no apparent order. While the majority of molecules are water molecules, you may also once in a while spot an oxygen molecule. If you were now to gradually move the microscope to look closer to the edge of the water drop, you would now see that as you approach the edge, the molecules move less randomly. Indeed, as you get to the edge, the molecules nearly form structured layers, due to the fact that the electromagnetic forces associated with the oxygen molecules outside the drop differ from the forces associated with the water molecules. Finally, when you point the microscope outside the water drop, you see a very sparse amount of O_2 molecules whizzing around, with once in a while a water molecule mixed in. At this finest scale, our description of the world is three-dimensional, and there is no precise concept of a surface between water and oxygen, even though it is easily recognized qualitatively.

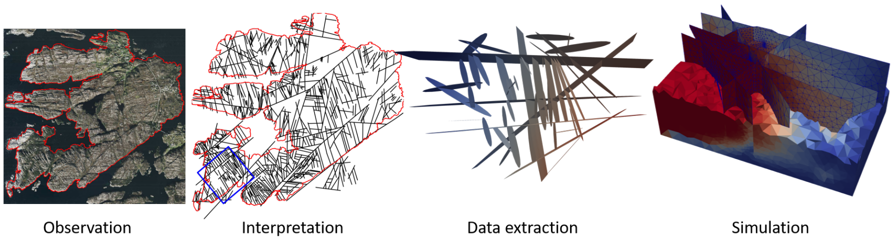

Figure 1: An illustration of a mixed-dimensional geometry with low dimensional gap. Starting on the left of the figure, we see an aerial photograph from the island of Sotra, outside of Bergen, Norway. Then we see a geological interpretation, wherein a 2D planar interpretation of fractures and faults identified at this site has been recorded. The next picture shows the full 3D interpretations of this fracture network, and finally a computer simulation of heat transport is shown. The actual mixed-dimensional domain thereby contains both the rock (3D domains), fractures (2D domains), and their intersections (1D line segments and 0D points).

Without access to such a powerful microscope, your description of a water drop would be very different: Indeed, you may now say that the drop is simply a drop of liquid water with some small oxygen concentration, while air is a gas of oxygen with some small water concentration. Between the liquid and the air is a surface, which in addition to providing a separation between water and air, also induces a pressure difference. This pressure difference, or *surface tension*, is a result of the structuring of molecules near the edge of the water bubble.

In addition to providing a pressure difference, the surface tension also acts to ensure that the surface of the water drop is smooth, that is, if a drop of water is left undisturbed for some time, it will form some nice smooth shape like a sphere. At this intermediate scale, our description of the world is that of two three-dimensional domains, separated by a two-dimensional surface.

You might also be interested in air and water not because you are looking at a water drop, but because you are looking at the surface of the ocean. Now again you observe a region of water and a region of air, and a surface that separates them. But at this scale, you might decide that surface tension is of less importance, and that the world is described sufficiently by considering the surface as simply an interface, and that the important processes to take into account are the currents and winds happening in either the water or the air.

Our example of the surface between water and air reveals a typical characteristic of real systems: Our description depends on the scale we look at, and thus also implicitly on the questions we want to answer. In this example, it is only at the intermediate scale, where interface tension is important, that the system is mixed-dimensional, since at both the finest and coarsest scale the system is described using only three-dimensional equations. A much more complicated example arises in systems of geothermal energy production, wherein heat is distributed in the subsurface rock in part due to flow in complex networks of fractures. An illustration of such a system is given in Figure 1.

Mixed-dimensional systems are often characterized by the span in dimensions, also known as the *dimensional gap*. In the case of surfaces, the difference between the full domain (three dimensions) and the surface (two dimensions) is one, and we therefore refer to problems with domains and surfaces as having low dimensional gap. The concept of low dimensional gap is a bit more general, as we will also consider problems where surfaces intersect in curves or points as having low dimensional gap, as long as the objects of various dimensions are only connected to objects of adjacent dimensionality. That is, we consider three-dimensional domains connected by surfaces (but not curves or points), or two-dimensional domains (surfaces) connected by one-dimensional curves or three-dimensional domains (but not points), and so on.

1.2 High dimensional gap: curves and points

Problems with high dimensional gap are inherently more difficult than those with low dimensional gap. This is because the concept of a surface is usually easy to define, and because the interaction between an object and its surface is well understood in both physical and mathematical terms. In contrast, the interaction between an object and a curve may be less straight-forward.

As an example, consider the setting of a drinking well drilled into a subsurface reservoir of water (called an aquifer). As in the previous section, we can consider this problem at various scales, but it suffices to say that at an intermediate scale, we study the flow in the aquifer with the understanding that the well can be reasonably considered to be a 1D curve (or indeed, often a line segment). Conceptually, we can consider the physical situation wherein there is now flow inside the well, and flow in the aquifer towards the well. The challenge is in determining how these two flows are coupled.

In the case of aquifer flow towards a well, we would like to think of the system as being described by the fluid flow rate and the pressure. In this system, the law of mass conservation is valid, and thus the flow inside the well should equal the (total) flow to the well. On the other hand, it is not so clear how to link the pressure in the well to the pressure outside the well. One would like to think that there should be some relationship between these two, but this runs into the difficulty that pressure is not defined on 1D objects such as a curve.

In physical terms, pressure is defined as force per surface area, (on the molecular scale the concept of pressure is based on the actual collisions between molecules and between molecules and a surface). However, a curve does not have any area, and the probability of a molecule hitting a curve is zero, so any virtual or real measurement of force on a curve would necessarily somehow involve dividing zero by zero. In mathematical terms, pressure is usually understood as a function in a space of functions (technically, a *Hilbert space*[1] often referred to as H_1), which is continuous almost everywhere and for which values on curves or points cannot be guaranteed to exist.

There is a less subtle way to understand why pressure is a difficult variable. If the well is represented as a line segment, it can be thought of as the limiting case of a well with finite radius when the finite radius becomes vanishingly small. A vanishing radius implies a vanishing circumference and this implies that the flow per unit surface area of the well is infinite (as long as the flow does not vanish). But what pressure can drive an infinite flow rate? In some sense the pressure in the well is infinitely high, what mathematicians call a “singularity”.

The solution to this conundrum lies in realizing that the well, despite being considered as essentially a line, still represents something that has a real radius, and that this radius cannot be neglected, even though it is in geometric terms vanishingly small compared to the full size of the aquifer. This is in contrast to the problems with low dimensional gap, where the width of the surface typically plays no explicit role in our understanding of the system.

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[1] A Hilbert space, named after the German mathematician David Hilbert (1862–1943), is a generalisation of the familiar Euclidean spaces. Hilbert spaces can have any number of dimensions, even infinitely many, and their defining characteristic is a geometric one: they admit an “inner product”, which is a generalisation of the scalar product of two vectors in space, which allows the measurement of lengths and angles. Hilbert spaces arise naturally in many areas of mathematics and physics.

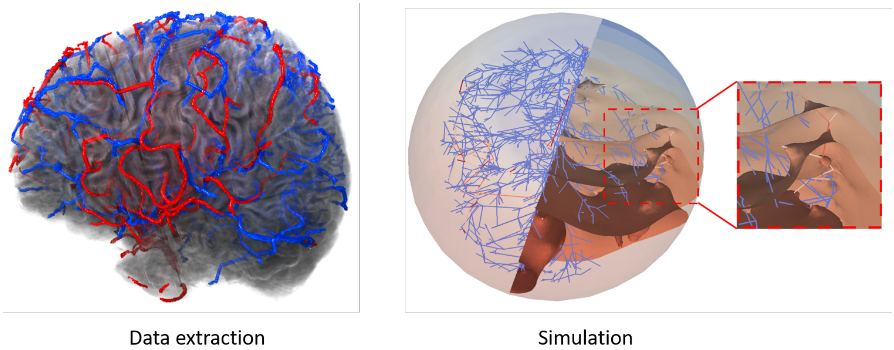

Figure 2: An illustration of a mixed-dimensional geometry with high dimensional gap. Here the arteries and veins (which together make up the vascular system) are rendered by red and blue, respectively. This system is naturally modeled as mixed-dimensional, where the white and gray matter comprise the 3D texture of the brain, while the vascular system is represented as 1D. The interaction between the vascular system and the brain must be understood to be a balance between diffuse leakage from the vascular system (very low in the case of the brain due to the blood-brain barrier), and source terms arising where the arterial and venous trees are terminated due to finite resolution in the images [6, 7].

In Figure 2, we give another, more complex, example of such a geometry, namely, that of the vascular system in the human brain.

2 Mixed-dimensional mathematical models

Once we have identified a mixed-dimensional physical system, we would like to make mathematical models of a similar structure. These models consist of two parts: Equations within each domain and "coupling conditions" between domains. To be precise, let us make an illustration and fix some notation, as in Figure 3. Here we have labeled the two two-dimensional domains Ω_1 and Ω_2, while we have labeled by Ω_3 the one-dimensional curve separating them.

We consider two types of variables. For each domain Ω_i, let χ_i be the vector of what are called *state variables* for that domain. A typical example, as was the case for the aquifer described above, might be $\chi_i = [\rho_i, \mathbf{v}_i]$ if the state variables are density ρ and velocity $\mathbf{v}$. Note that these variables are defined within each domain, so that the velocity would be a two-dimensional velocity in

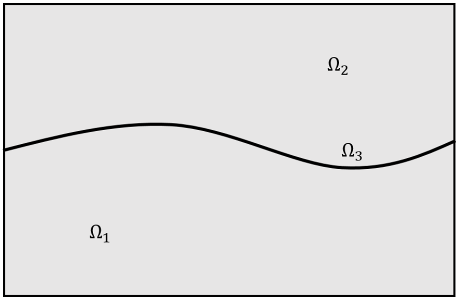

Figure 3: An illustration of a prototypical mixed-dimensional geometry.

Ω_1 and Ω_2, but a one-dimensional velocity (along the curve) in Ω_3. In addition to the variables within each domain, we need to keep track of a set of variables which reside on the boundary between domains of different dimension, which we will call $\lambda_{i,j}$ for any pair of domains Ω_i and Ω_j. For the density and velocity example just given, we could select as boundary variables the flows across the boundary, that is, $\lambda_{2,3} = [p_2, u_{n,2}]$, in the sense that the boundary values consist of the pressure at the boundary, p_2, as well as the "normal component" of the velocity on the boundary u_n, where this means the portion of the flow that crosses the boundary.

Then for these three domains and corresponding sets of variables, we would generally obtain a model consisting of five equations, of three different types. We would have two standard, full-dimensional equations representing Ω_1 and Ω_2, and these would be functions of only the variables χ_1 and χ_2 respectively. Then we would have an equation on the lower-dimensional object Ω_3 which is impacted by both of its higher-dimensional neighbors, so it would be an equation in all three of the variables $\chi_3, \lambda_{1,3}$ and $\lambda_{2,3}$. Finally, we would have two equations, one a function of the variables χ_3 and $\lambda_{1,3}$ and the other of the variables χ_3 and $\lambda_{2,3}$, representing the relations between the boundaries of a higher-dimensional domain and its lower-dimensional neighbor.

Equation sets having this form are quite ubiquitous in science. Examples are found in structural engineering (plate reinforced concrete, or the junction between an H-beam and a wall) [3], geophysical engineering (oil, gas and water wells [12], but also structural features such as flow in fractured rock [1]), biomedical applications [5], and even the design of antennas [4].

An important class of examples is when we have what are called *differential equations*, most commonly for the equations that represent the domains (in our example above, Ω_1, Ω_2 and Ω_3). A differential equation is one which relates a given function with its derivatives. In a two- or three-dimensional domain, the derivatives are *partial*, which means they are taken with respect to each of the variables individually. The resulting problem is then called a *mixed-dimensional partial differential equation*. This case is encountered whenever the variables arise from a model where materials are modelled as a continuous mass rather than as a system of particles[2], such as those of fluid dynamics (for instance, the Navier-Stokes' equations), or electromagnetism (the Maxwell equations).

3 Recent developments, and future outlook

Recent work on mixed-dimensional equations is divided along the same lines as the models. Firstly, for problems with low dimensional gap, recent research has sought to unify the variables and equations presented in the previous section. The idea is to explicitly consider a set of mixed-dimensional variables, that is to say, to avoid dividing the variables explicitly by domains. If one imagines such a concept as leading to a mixed-dimensional vector of variables X, representing all the χ_i discussed previously, one might similarly allow for the possibility that our given set of equations could be simplified to a single equation.

The building blocks of such approaches have recently been developed [9, 10], and these results have led to the development of accurate and robust numerical methods [2, 11].

Let us discuss this further for the example of fluid flows, as in [11], with two three-dimensional flows coupled to a two-dimensional flow between them (think of a flow between two parallel plates with a very small distance between them). Under certain conditions, the equations on each of the domains are "elliptic" partial differential equations, which roughly means that they have no discontinuities and are well suited for modelling equilibrium situations. These flows have the property that the rate of volume flow across a unit area (the "flux") is considered to be proportional to the pressure gradient (the direction and rate of change of pressure). The variables χ_i in this case are all understood to be the corresponding pressure. Then for this system, the coupling variables $\lambda_{i,j}$ are recognized as the flow from domain i into the domain j, and the coupling terms can therefore be modeled as proportional to the pressure difference between those domains.

So we have our five equations, as before, three differential equations and two involving the pressure difference between a higher- and lower-dimensional domain. A mixed-dimensional representation of this system is obtained by defining a new mixed-dimensional differential operator that combines the differential operators on each domain with suitably defined "jump" operators involving the neighboring domains. It can be shown that such a definition is sensible,

[2] In order for a function to be differentiable, it must necessarily be continuous.

and moreover, that in this way our five equations can be combined into one, as desired.

Problems with high dimensional gap are less amenable to a unified treatment, and indeed are understood in a case-by-case manner by analyzing the full coupled system (for instance, in [5]). A reasonably accurate understanding of the mathematical structure of these equations has led to recent developments of numerical methods for such problems (see for example [8, 6]).

Image credits

Fig. 1 Courtesy of the Anigma project at the University of Bergen.

Fig. 2 Reproduced with permission from [6, 7].

Fig. 3 Produced by the author.

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Jan Martin Nordbotten *is a professor of mathematics at the University of Bergen*

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Mathematisches Forschungsinstitut
Oberwolfach gGmbH
Schwarzwaldstr. 9 – 11
77709 Oberwolfach
Germany

Director
Gerhard Huisken