(Hyper) Reduced Order Models For Moving Meshes

Literature Review & Research Project

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Index Terms

Finite Elements, Galerkin, Reduced Order Models, Moving Piston, Deforming Mesh, ALE, (M)DEIM, POD, Model Truncation

Contents

1 RESEARCH PROJECT

This thesis focuses in the efficient numerical solution of parametrized unsteady PDEs with moving meshes.

Parametrized PDEs can be numerically solved with the finite element method (FEM), which leads to an algebraic system of equations whose solution can be computationally expensive to obtain, especially for complex geometries or elaborate models. One refers to this FEM model as the *Full Order Model* (FOM),

$$\frac{du_h}{dt} + A_h\left(t;\mu\right)u_h = f_h\left(t;\mu\right). \tag{1}$$

When the problem is unsteady, that is, when the differential operators contain terms that change in time, or the mesh moves in time (effectively changing the integrals of the weak form), the algebraic operators need to be reassembled for each timestep.

When this is the case, many-query procedures and access to field values or calculated outputs for different parameter values μ can become cumbersome, or even infeasible due to computational costs, both in time and memory. To circumvent the efficiency issues, one can build a *Reduced Order Model* (ROM), whose solution is fast in time and light in storage. This ROM is based in ad-hoc empirical basis functions to represent the solution, whose support typically spans the whole domain.

However, due to the change in time of the operators, using a standalone reduced basis to represent the solution is not enough to remove all the overheads of the FEM model. The operators still need to be assembled and projected in the reduced space for each timestep. The reduced basis of the solution does shrunk the overall dimension of the system, but it cannot remove the overhead derived from the inevitable change in the operators. We would state to have an *offline-online coupling*, since information from the FOM is required to assemble the ROM. To overcome this issue, a system approximation technique is introduced. We then talk about an *Hyper Reduced Order Model* (HROM).

1.1 Outline of the Reduction Process

The construction of the ROM has mainly two stages:

- Offline stage: construction of the ROM ingredients.
- Online stage: assembly of the ROM to solve the PDE for unseen parametrizations.

During the offline stage, the costly algebraic problem is solved for a subset of the parameter space. Snapshots of the matrices, vectors and solutions are stored and processed via algebraic reduction algorithms, in order to obtain a reduced basis for each of them.

An example of reduction algorithms would be the Discrete Empirical Interpolation Method (DEIM) and its matrix version (MDEIM). These reduction algorithms need to rely on a procedure to construct the basis, in our case we will use the Proper Orthogonal Decomposition (POD).

The offline stage scales with the dimension of the Full Order Model, N_h, which is governed by the number of nodes in the mesh and the polynomial degree for the FEM basis. Once the offline stage is over, a basis for each operator of the algebraic problem has been produced, of representative[1] size $N \ll N_h$. A projection matrix $\mathbb{V}$ is derived from the solution reduced basis,

$$\mathbb{V} \in \mathbb{R}^{N_h \times N}. \tag{2}$$

This matrix will be used to project once and for all the algebraic operator reduced basis elements, our HROM building blocks. The reduced bases for the solution and the algebraic operators are then used during the online stage, where for unseen parameters a small algebraic system is built and solved,

$$\frac{du_N}{dt} + A_N\left(t;\mu\right)u_N = f_N\left(t;\mu\right). \tag{3}$$

At this stage, it is paramount that the assembly of the operators[2] is independent of the original problem size N_h. We state to have a perfect *offline-online decoupling*.

Once the reduced problem has been solved, the solution can be projected back to the original physical mesh,

$$u_h = \mathbb{V}u_N. \tag{4}$$

Following these steps, access to field values or calculated outputs can be obtained lightly, provided the overall procedure is *certified*: to prove in the online stage that the solution is sufficiently close to what it would have been if the actual FOM had been assembled and solved.

All the above is presented graphically in Figure 1.

1.2 System Approximation

An essential ingredient to achieve a perfect offline-online decoupling is what we call an *affine decomposition* of the algebraic operators. Simply put, it is to say that we can achieve a linear separation in the parameter, time, and spatial domains (the latter represented by the algebraic basis elements),

$$A_h\left(t;\mu\right) = \sum_{q=1}^{Q} \Theta_q(t;\mu)A_{h,q}, \tag{5}$$

where $A_{h,q}$ are constant matrices referred to as the collateral basis, and $\Theta_q(t;\mu) \in \mathbb{R}$ are scalar values.

The easiest example one could come up with of an affine decomposition is the one present in the heat diffusion problem with two different but uniform diffusion parameters k_q across the domain. The affine decomposition would look like

$$A_h\left(t;k_1,k_2\right) = k_1 A_{h,1} + k_2 A_{h,2}, \tag{6}$$

where each matrix $A_{h,q}$ would represent the diffusion operator with support over the subdomain associated with each parameter. For this simple example, the affine decomposition is present naturally within the PDE structure, but this will not always be the case, specially when nonlinearities are present.

However, nowadays it is absolutely possible to obtain an automatic ad-hoc affine decomposition for any operator

1. The reduction of each operator might have required a different number of basis elements, but they should be all of the same order of magnitude $N \ll N_h$ or smaller for the reduction process to be a success.

2. We shall overload notation and refer to *the operator* for both the matrices and the functionals, unless explicit distinction is required.

thanks to grounded algorithms and procedures, like DEIM and MDEIM. This key fact will allows us to achieve a perfect split between the offline and the online stage, as it will allow us to assemble our ROM operators without having to assemble at any point the complete FOM operator.

1.2.1 *Nonlinear Term Reduction*

The reduction of a nonlinear term can be achieved with the same MDEIM technique as the one used for linear operators.

The only difference is that the coefficient functions Θ_q from the affine decomposition depend on the solution values too,

$$A_h\left(t;\mu\ ,u\right) = \sum_{q=1}^{Q} \Theta_q(t;\mu,u) A_{h,q}. \tag{7}$$

Nevertheless, this fact does not necessarily break the convergence and approximation properties derived for MDEIM, so we expect to use it successfully.

1.2.2 *Implicit Nonlinearities*

A nonlinearity can be seen essentially as a characteristic that prevents a linear separation. Despite the apparent linear character of an algebraic equation, from the point of view of the affine decomposition, it could potentially hide a nonlinearity.

The introduction of the time variable t in the shape of the mesh makes it so that the operators change at each time step during the integration loop. Additionally, since the domain geometry will depend on some parameter values too, one cannot explicitly write the affine decomposition of the operators in a closed form. This is implicitly collected by the Jacobian, the transformation that maps integrals over moving meshes to one over a reference fixed mesh.

Another type of nonlinearity would be a term whose integrand contained a nonlinear function applied over the u field, or interactions of the solution with its own derivatives.

1.3 Kick-off Point

The (M)DEIM reduction technique have been successfully used with domains whose boundary is parametrized, but whose mesh remained fixed in time [1].

We aim at extending these results by introducing a moving mesh in time, thus allowing us to obtain an hyper reduced order model which can tackle more complex real-life problems. The additional complexities introduced by the moving mesh are the introduction of the Arbitrary Eulerian Lagrangian formulation (ALE), and the increase in the number of operator snapshots to be collected during the offline stage.

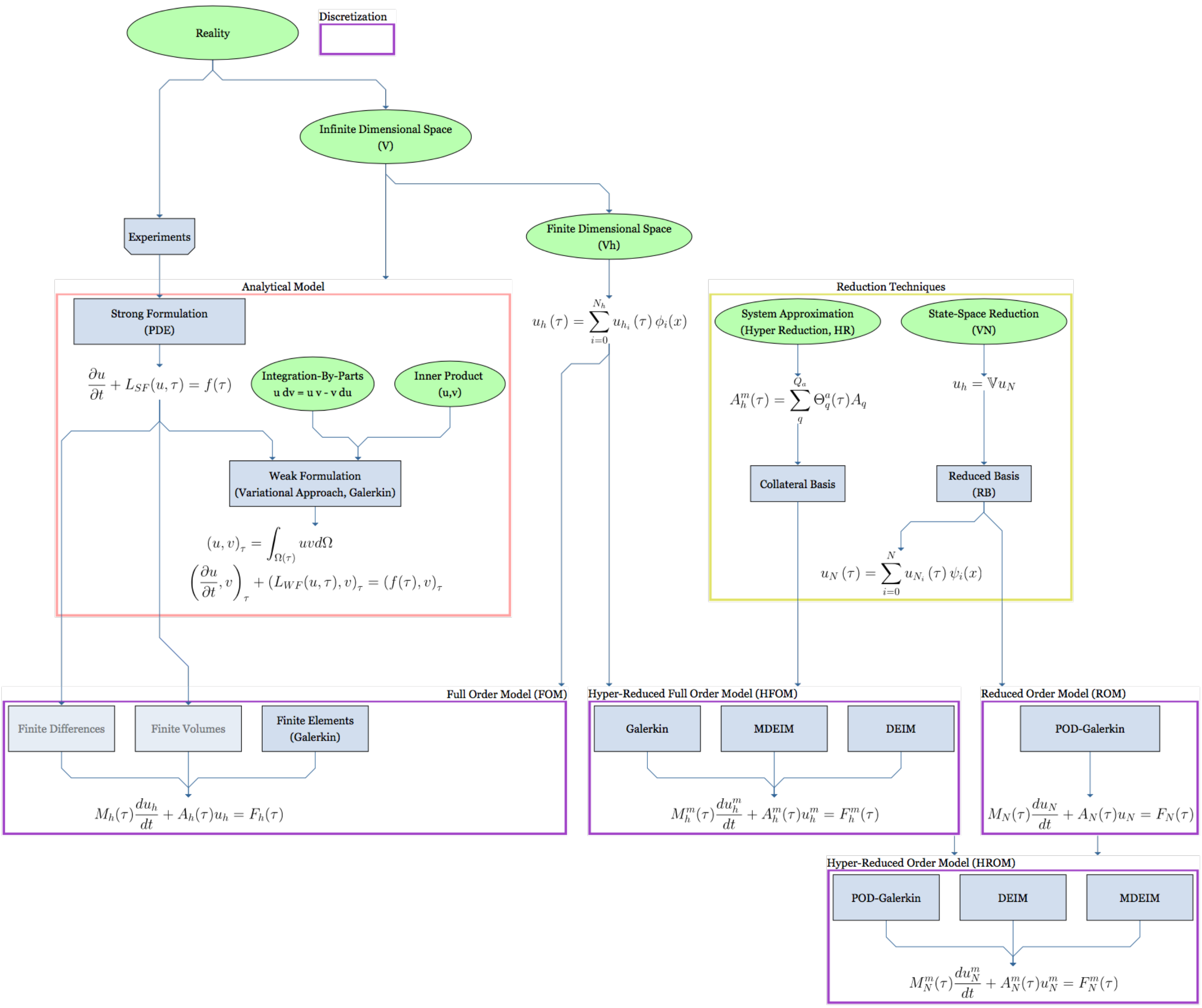

Fig. 1. Building blocks of the transition from reality to discrete reduced order modeling. On the left side we present the traditional finite element course: from the observation of reality a parametrized PDE model is derived (infinite dimensional space, unknown analytical solution). The paremeters allow the model to capture a range of boundary conditions, geometries, and term-domination effects, all of them driven by the same physics. This model can be cast into a weak form and solved numerically via the Galerkin projection (finite dimensional space, Lagrangian piecewise solution). The finite element method is a robust and well-established technique for the solution of parametrized PDEs. However, for three-dimensional domains, or complex modelling terms, the algebraic operators involved (vectors and matrices) can become computationally expensive to assemble and solve, especially for unsteady problems with moving meshes. On the right side, we present two reduction techniques introduced to increase the efficiency of the numerical solution: the construction of a *reduced basis* (RB), also known as state-space reduction; and the determination of a collateral basis for the algebraic finite element operators, known as *system approximation*. The reduced basis is used in substitution of the Lagrangian piecewise functions, the collateral basis is used to skip the assembly of all the entries of each algebraic operator. All in all, the simultaneous use of these two reduction techniques leads to an algebraic hyper-reduced order model, cheaper to assemble and solve than the traditional finite element problem; and for problems with time-dependent matrices, even cheaper than assembling the operators and projecting them unto the reduced basis for each timestep.

2 Literature Review

In the following, we present the relevant literature used in this work. We have used mainly two types of papers: methodology and applications. The former present a numerical method or formulation which we use, the latter make use of it for specific applications. We were especially interested in the applications to see how previous works dealt with inhomogeneous boundary conditions, on which will be discussed later on in the work and the review.

2.1 Burgers Terms and Piston Models

Regarding the target PDE to work with, we decided upon several constraints: it had to be one-dimensional (to ease implementation), contain non-trivial terms (to make the problem interesting), and be physically sound (to validate the outcome).

The first two constraints are satisfied by an advection equation with a nonlinear Burgers-like convective term. The Burgers equation showed up in the gas dynamics literature several decades ago [2]–[5], for which under controlled conditions a range of implicit analytical solutions exist [6], including for moving domains [7].

Nevertheless, most of the mentioned solutions are either asymptotic, computed in a moving frame of reference[3], or defined for an infinite or fixed domain. Additionally, to obtain results integral formulations have to be solved (the simple solutions are only defined for fixed domains). Hence, it could become cumbersome to attempt to replicate the results found in these papers.

Luckily, removing viscosity and body forces (which are strong assumptions), and making use of the isentropic condition, we can transform the Navier-Stokes equations into a one-dimensional equation [8], [9] in terms of velocity. At the discretization level though, we will add an artificial viscosity term, to make sure the solution remains stable [10].

This result is a simple yet complete PDE to model the movement of a piston, which can be validated with derived computations such as mass conservation, and whose solution makes intuitively sense when plotted.

Compared to modern problems with moving domains, the piston is quite simple in nature; and yet it allowed many aerodynamicists to push forward the barrier of knowledge back in the days, when computational power was not so easy to access [11].

2.2 Deforming Mesh (ALE)

Because the piston problem is a defined in a moving domain, one needs to modify the departing PDE to account for the movement of the mesh nodes, with the introduction of a convective term governed by the mesh velocity vector. In fact, this needs to be done even for domains with fixed boundaries, where the interior mesh nodes move in time (front-tracking or shock-capturing schemes could be an example of such situations). This leads to the Arbitrary Lagrangian Eulerian (ALE) formulation.

3. It is important to make the distinction between a *moving domain* and a *moving coordinate system*. The former is deformed around the same neighborhood in space, whilst the latter is displacing itself across space.

An introduction to the details of the ALE formulation in a simple setting can be found in [12]–[14]. In these works, stability arguments and implementation details for finite elements and simple PDE models are provided. Work [12] contains lengthy and easy-to-read derivations which explain neatly the differences between conservative and non-conservative weak forms. For reasons that will become aparent later on, in this thesis we need to solve the non-conservative weak form, at least to use the current formulation of the system aproximation technique which we intend to use.

For a complete and generic development of the subject, in higher dimensions and for complex problems, we refer the reader to [15], [16].

Regarding the stability of the integration scheme, the concept of *(Discrete) Geometric Conservation Law* (D-GCL) shows up [17]–[20]. Briefly, how the domain deforms and how this deformation is accounted for *in the discretization* of the continuous problem, could lead or not to instabilities in the solution; for the movement of the mesh could introduce artificial fluxes in the discretization. As a general rule of thumb, to guarantee some notion of stability, the scheme should be able to reproduce the constant solution (under the appropriate boundary conditions).

This D-GCL condition can be further explored for simple problems. In [12] they prove how the Implicit Euler integration scheme becomes conditionally stable for a linear advection-diffusion problem if the non-conservative weak formulation is solved. So in a way, the worst case scenario would be that we have to lower the time step.

As a final note, we would like to point out that a problem with a deforming domain could also be tackled with space-time finite elements [21]. In fact, as it is the case for us, if the boundary movement is prescribed, the domain in a space-time context will be a fixed one. However, we disregarded this line of work because it could make the implementation much more complicated.

This ends the literature review regarding the FOM model. We now present the literature oriented towards the construction of the ROM.

2.3 Reduced Basis

We do not aim here at providing a comprehensive review of the whole field (for that could be a complete work by itself), but rather to present a good starting point from which the interested reader could start, and of course, the framing of this thesis.

A problem's complexity and its computational cost are typically something that scale together. Hence, the idea of finding a smaller subspace to represent the solution and reduce calculation times is justified.

This idea of using a problem-dependent basis with global support to solve numerically discretized PDEs is well known. The first references in this line date back to the 80s, with pioneering works in structural analysis [22]. Since then, this idea has become increasingly popular, with many papers and books explaining methods and applications for steady and unsteady problems [23]–[29], including the Navier-Stokes equations [30]. In fact, Burgers' model has been already tackled for a fixed domain [31].

In the following, we present a narrative for Reduced Basis methods in the finite element context, to frame our use of it. We understand and admit that there might be other narratives that suit the field, but the following has proven helpful to understand the ingredients of the ROM.

Our narrative takes the perspective of: where does the basis come from? Or in other words, how many mathematical tools are necessary to obtain it? The construction of the reduced basis needs to take into account the following facts: there must a sampling strategy in the parameter space, the reduced basis must converge to the span of the solutions, and it must be computationally efficient.

The most plain vanilla version of reduced basis is a collection of solutions for several parametrizations. However, the elements of this basis are likely to be almost linearly dependent[4], and no approximation arguments have been used to obtain it.

So, the first step one can take is to use a greedy procedure [32], [33]. That is, the elements of the basis are still solutions of the PDE, but they are combined iteratively, by choosing the next element which minizimes the error made by the current basis within a randomly selected parameter space (hence the name greedy, in terms of approximation accuracy). This procedure only requires the finite element discretization, and one can prove it will converge to the whole span. The difficulty in this procedure is the efficient estimation of the error of the basis at each iteration. However, it has become the established method to approach steady models [34].

The next step one can take is to rely on an external methodology to construct the basis from a collection of solution snapshots. We add an additional item to our mathematical toolbox, the Singular Value Decomposition (SVD) [35], which allows us to compress the span of the solution space efficiently with optimal convergence properties. This is known as the Proper Orthogonal Decomposition (POD) method [36]. It has been widely used in many contexts to obtain a basis from a collection of solutions automatically, or to analyze the underlying dynamics of a flow field [37].

It has a wider application than the greedy method, since we could use experimental data too, to obtain a reduced basis which we then use to solve a numerical model efficiently. Of particular interest is the application made in [38], where they used the POD over an analytical solution with and without a deforming grid to split effects and analyze convergence rates.

Finally, for unsteady problems one may have the combination of both, the POD-Greedy method [34], [39]. This method uses the automatic compression feature provided by the POD in the time dimension, and the greedy approach to parameter selection in the parameter space.

For our work, we will use a physics-driven approach for the sampling strategy in the parameter space, and a nested POD strategy for the time and parameter spaces [1].

Finally, some words need to be said about the handling of the inhomogeneous boundary conditions that we will encounter. It was difficult to find specific literature about this aspect, for most papers and books deal with either homogeneous boundary conditions, scalar-multiplicative shapes [40], [41], or do not dedicate many lines to this implementation detail.

Neumann boundary conditions do not pose a problem, since they are naturally encoded in the weak form. So a suitable approach is to transfer the essential boundary conditions to the weak form too, via a lifting technique [42]. Hence, the target model problem that we reduce becomes one with homogeneous boundary conditions, for which the results from most references apply.

2.4 System Approximation

We reach now the final block of the literature review. In this section we review the methodology used to efficiently approximate the algebraic operators that arise from the discretization. Using an algebraic approach in the reduction scheme is of great advantage, since then most results can generalize to other discretization schemes.

We start by reviewing the approximation methodology for functions and functionals (vectors). The one for matrices is its natural extension.

The seeds of the methodology lie in what is called the Empirical Interpolation Method (EIM) [43]–[45]. It generates an ad-hoc affine decomposition of a parametrized function, by splitting the dependency into some real-valued parameter-dependent functions and a parameter-independent collateral basis. The values of the functions are obtained by enforcing that certain entries of the vector are exactly matched by the ad-hoc decomposition (hence the name interpolation). The entries at which the interpolation should be enforced are computed during the basis creation, and they represent those locations where the approximation behaves worse. The collection of the entries is referred to as the *reduced mesh*. The collateral basis is generated with function valuations following a greedy procedure [46].

As with the RB scenario, the generation of the basis can be delegated to a POD procedure, leading to the Discrete Empirical Interpolation Method (DEIM) [47], [48]. Finally, if the columns of a matrix are stacked vertically to *vectorize* it, a matrix-DEIM method can be used (MDEIM) [49]–[52].

These approximation methods are convenient in the finite element context. The calculation of the reduced mesh entries is the sum of evaluations of the weak form for a restricted subset of mesh cells. This operation can be done efficiently in parallel and is much cheaper than assembling the whole operator [1]. Additionally, the collateral basis can be projected in the reduced space, so that the reduced operator is approximated right away.

In all of the above, time can be easily included by treating it as an additional parameter, although the implementation is not so straightforward.

This concludes our literature review.

4. A strong assumption underlying reduced basis methods in this context is that the solutions of the parametrized PDE change smoothly when the parametrization varies.

3 Plan and Scope

The research objective is to build a certified Reduced Order Model (ROM) for a nonlinear Burgers-like parametrized unsteady PDE, within a one-dimensional moving boundary. The main body of the PDE, the geometrical definition of the moving boundary, and the boundary conditions will be parametrized.

The main task at hand is to be able to create a reduced order model not only efficiently, but skipping the Jacobian transformation. Such transformation is usually required in the context of moving meshes, and sometimes it may not even be explicitly available.

Additionally, this could potentially allow us to use our reduction scheme with existing codebases, provided that we can access the operators and some of their entries.

3.1 Research Questions

Of particular interest will be the reduction of the nonlinear term. We will discuss how the approximation error of this term interacts with the approximation error of the remaining operators and the reduced basis itself. Two techniques to reduce the nonlinear will be compared and discussed. One approach is to collect the nonlinear operator snapshots as the FOM is integrated; the other one is to collect the snapshots from evaluations of the nonlinear operator using the reduced basis elements (after all, the solution is a linear combinations of the latter). These two methods could potentially produce different bases, with different approximation errors.

Regarding the movement of the mesh, two types of movements will be analyzed. First, the natural oscillation of the moving piston. This movement spreads out evenly the stretching among the cells, removing the spatial dependency from the Jacobian. Then, a nonlinear mesh movement will be introduced, with the concentration of nodes around specific regions as time changes. These regions will be user-defined, not solution dependent. Our aim is to mimick the effects of shock tracking or mesh refinement techniques, without explicitly using them, to prove the good working of the reduction method, in isolation from specific applications.

The certification of the HROM will be done with a model truncation technique. This is a standard approach, useful due to its generality.

All in all, we intend to exercise in a one-dimensional domain the different techniques we will be using; knowing that since our approach is purely algebraic, it would translate naturally to higher dimensions, albeit more involved codebase implementations details and costs.

3.2 Scope

The project is mainly practice-oriented, in that we shall design, build and evaluate the procedure to construct the HROM. We will use known theoretical results to guide our assessment of the reduction technique, but we do not expect to formulate new ones.

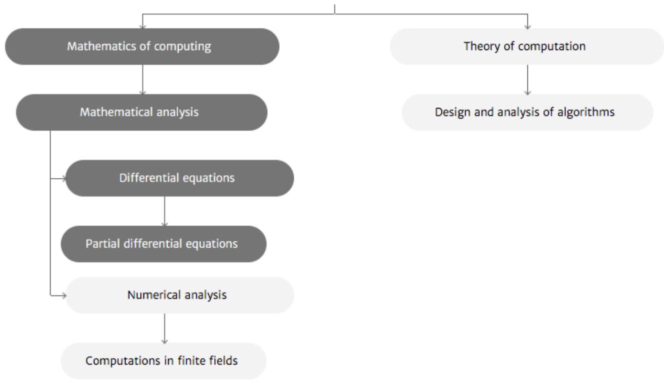

Fig. 2. Conceptual location of the M. Sc. Thesis project.

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