Hierarchical Model Adaptivity

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Overall goal: The goal of this project is to develop a model adaptive approximation strategy that in real time is able to choose the appropriate PDE model to approximate over portions of the domain. Thus the scheme is able to couple hierarchical models for use in, for example, atmospheric approximation.

Motivation, theme fit, methods and description: Hierarchical modelling is a common feature in many application areas. Indeed, most large scale geophysical simulations are built upon the basis of modelling phenomena with systems of PDEs. Depending on the application and the scale of the features needing to be simulated various levels of approximation are conducted, based on some underlying physical reasoning, resulting in a hierarchy of PDE models. At the top level of this hierarchy sits a PDE system that contains all information currently known about the process. For example, climate models contain a huge amount of information, including atmospheric composition, hydrology, impacts of ice sheets, human influence, vegetation, oceanographic aspects, solar inputs and so on. These extremely complicated mathematical models are far too complex to construct any analytical solution method for the resultant system, so, practically, reductions are made, with information being ignored so that the system has a lower complexity. Naturally, this reduction gives rise to hierarchies of models.

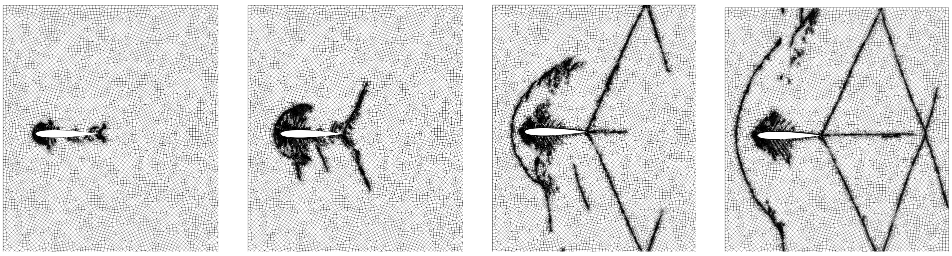

Figure 1: A sequence of adaptive meshes for a supersonic flow around an aerofoil. Notice the mesh is refined as shocks develop and coarsening as the bow shock becomes prominent.

The use of dynamic mesh adaptivity to increase efficiency in computations is well studied. In evolution problems this is particularly important as discontinuities and small scale features propagate in time (Figure 1). This begs the question, how does one decide when and where to add and remove degrees of freedom? Often in practical situations, this is done through gradient indicators. Here, one refines the mesh in regions where the gradient of the solution is large and coarsens when the gradient is small. These can work remarkably well in most situations; however, cases can be constructed where this indictor fails to be a reliable criterion for refinement [Lakkis, Pryer (2011)]. This motivates the a posteriori analysis of these problems. The main goal of an a posteriori analysis is to construct computable bounds for the error that are efficient, reliable and localisable. These are called *a posteriori estimators*. Although in principle an upper bound is sufficient to obtain an approximation guaranteed to be below some tolerance, local lower bounds are also necessary to ensure the approximation is close to being optimal, in the sense of using an almost minimal number of degrees of freedom.

Mesh refinement is not the only mechanism for numerical adaptivity, however. A new area currently being investigated is 'model adaptivity'. This is where an a posteriori estimator is suitably decoupled to enable local selection of the correct model in the hierarchy. This means areas of the computational domain will solve one model and other areas potentially a different one.

This goal does raise further practical questions though, for example, how can different models be coupled together in a smooth fashion without creating artefacts? When different models are coupled together, errors can appear at the interface and propagate into the domain, polluting the simulation of both models. This could result in the numerical method itself becoming unstable. It is known that linking models together in an ad-hoc fashion can give rise to numerous artefacts. Ghost forces, for example, become apparent when coupling atomistic models of crack propagation with continuum models, they represent a localised inconsistency in the steady state of the atomistic region. This is well documented in the engineering literature although never really satisfactorily treated until [Makridakis, Mitsoudis, & Rosakis (2013)], where an *energy compatible* method of coupling the atomistic description with a discretisation of the continuum region was proposed. In essence this approach involved additional terms arising on the interface. It is expected that coupling numerical models, possibly over different scales, will also lead to such numerical artefacts. One possibility of treating this could be the introduction of additional terms on the interface ensuring compatibility or coupling in a multigrid fashion over a hierarchy of mesh levels.

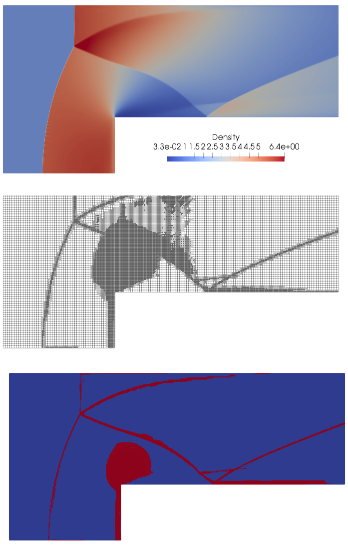

Figure 2 – A model adaptive approximation of the forward facing step problem at Mach 5. Notice the shocks in the density (top) are resolved through mesh refinement (middle). The model is coupled and is the NSF in the red region (bottom) and Euler's

As already mentioned different models will each have different levels of complexity and levels of accuracy in the description of the underlying physics over different scales. An illustrative example is the compressible Euler equations which are the limit of the Navier-Stokes-Fourier equations when heat conduction and viscosity go to zero. Arguably the Navier-Stokes-Fourier system provides a more accurate description of reality since viscous effects, which are neglected in Euler's equation, play a dominant role in certain flow regimes, for example in Prandtls' boundary layers. These effects, however, are negligible in large parts of the computational domain where convective effects dominate. Computationally, the viscous terms force a more restrictive Courant-Friedrichs-Lewy condition and, for stability purposes, it is often desirable to avoid the effort of handling these terms in certain regions, that is, to only solve the Navier-Stokes-Fourier system where it is absolutely necessary and make use of simpler models on the rest of the domain. The mathematical quantification of when and where to do this is, in general, an open problem, however progress has been made in this direction in [Giesselmann & Pryer (2017)].

The aim of this project is to a posteriori quantify the errors committed both through model reductions and numerical discretisation. This allows for adaptive coupling of different models in the already developed hierarchies based on localised error estimates in real time duration simulation (Figure 2).

MRes project: The MRes project focuses on a linear flow governed by Stokes problem. It's reduction to the vectorial Laplacian will be examined through an a posteriori error analysis. The resulting model coupling will be implemented and tested for robustness. Note there is significant novelty here, in that the model reduction is achieved through local elimination of one of the variables rather than sending a specific parameter to zero. This is anticipated to lead to a good quality publication.

Extension to PhD: The direction of the PhD depends on the directions preferred by the student. Some examples of possible extensions include:

- The efficient solution of the model coupled algebraic systems.
- The extension to more physically relevant atmospheric models.

References:
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