

PROJECT	<b>1. SUPERPARAMETERISATION</b>	PROJECT LEADER	<b>Yiannis</b>		
EMAIL LIST	<a href="mailto:mucm-project-super@lists.shef.ac.uk">mucm-project-super@lists.shef.ac.uk</a>	PROJECT TEAM	Peter, Remi, Dan, Henry		
OVERVIEW	<p>Also links to wider issues of model coupling, nesting and aspects of downsizing.</p> <p>Super-parameterisation is a technique in ocean and atmospheric modelling, according to which, models of a fine process are embedded in a coarse model, in an effort to enhance its level of detail in the analysis, while keeping the overall computational complexity low. The present project attempts to super-parameterise an ocean model of deep convection, introducing the novelty of replacing the fine process model with an emulator, which should result in further decrease in the computational effort, compared to traditional superparameterisation.</p> <p>The model we are working with is the MITgcm (global circulation model). This model is very flexible, and can be configured both as the Fine and as the Coarse model in our example. Initially, a volume of water, modelled with a high resolution grid, is cooled down from the top and the evolution of the temperature with time at different depths is observed. This is the Reference run of our problem. In the second stage, the volume of water is modelled with a coarser grid (Coarse model), and in each grid cell, a high resolution model (Fine model) is embedded. The idea is to match the temperature profile of the Reference model with this combination of Coarse and Fine models. In the final step, the Fine models are replaced by emulators, which are much faster, and again we try to match the temperature profile of the reference model, at a fraction of the computational cost.</p>				
ACTIVITIES	<p>a) Build a prototype of a sub-grid-scale emulator within a coarser simulator. To be based on a cut-down ocean model with emulation of a fine-scale mixing model. A deterministic version based on a highly accurate emulator is one approach, but a stochastic version that accounted for uncertainty through a poorer emulator or boundary conditions that are not delivered by the coarser model will also be considered.</p> <p>b) Preliminary exploration of an example in which tropical convection is nested within an atmospheric model</p> <p>After trying a number of configurations, our current setup is as follows,  A 60 x 60 x 10 (x, y, z) Reference model is used for a volume of water equal to (6 x 6 x 2)km.  The Coarse model has a grid of (3 x 3 x 10) and the Fine models (20 x 20 x 10).  A reference run is obtained by cooling for four days a circle of radius ~2km lying on the centre of the surface of the water volume.  We then try to match the resulting temperature profile by combining the Coarse and the Fine models.  An emulator for the Fine model has been built, and replacing the Fine model with it showed negligible differences in the resulting temperature profiles.</p>				
OBJECTIVES	<p>1.1 A paper for the oceanography literature using the cut-down ocean model</p> <p>REVISED OBJECTIVE: a technical report minimum, but preferably a paper to be completed by JULY 2011</p> <p>1.2 A grant application to NERC on superparameterisation, possibly picking up wider issues as above</p>	Target Date	<p><del>Apr 2011</del> Jul 2011</p> <p><del>Apr 2011</del> Sept 2011</p>		
PROGRESS UPDATE	<ul style="list-style-type: none"> <li>Identified Coarse and Fine scale models. The first will be NEMO and second will be MITgcm. The coarse model will track temperature (T), salinity (S) and the three velocity components, u, v, and w in a coarse grid, possibly in a hydrostatic mode. The fine model will resolve small scale processes, like convection, again in terms of T, S, u, v and w, in a non-hydrostatic mode.</li> <li>George Nurser will be the NOC model expert.</li> <li>Due to its high complexity, NEMO will be set up by George.</li> <li>Yiannis has installed and learned how to run the MITgcm model.</li> <li>Current phase: <ul style="list-style-type: none"> <li>Emulate temperature.</li> <li>Doubly periodic mode.</li> <li>Same number of vertical layers.</li> </ul> </li> <li>Need to determine the time stepping interface between the two models. For example, MITgcm needs several time steps to resolve the convective plumes and we need to determine how it will interface with NEMO, without needing to store the state variable of the model for each time step.</li> </ul>			Updated	Jan 2011

	<ul style="list-style-type: none"> <li>• Next phase:             <ul style="list-style-type: none"> <li>• Include S, u, w and v.</li> </ul> </li> <li>• Determine interpolation schemes that will map T, S, u, w, and v between the fine and the coarse grids.</li> <li>• Configurations of the MITgcm are being used for both the fine and the coarse models. The model is configured and run by us, so we can have easy access to data.</li> <li>• The Fine and Coarse models have been coupled successfully. The information being exchanged at the moment is temperature. In the future this should be expanded to velocities, pressure and perhaps salinity.</li> <li>• The results obtained with the combination of the Coarse and Fine models still differ from the reference results. The source of this discrepancy needs to be identified, and minimised to the degree that this is possible. Exchanging more information apart from temperature between the models could be of help, though it's not certain that this is the source of the problem.</li> <li>• An emulator of the Fine model has been built, and the approximation accuracy was deemed satisfactory.</li> <li>• The training points for the emulator however, were obtained by running the combination of the Fine with the Coarse model first. Ideally, we would like to avoid this step, and built an emulator by running the Fine model only. This is work in progress</li> <li>• The inputs and the outputs of the Fine model are highly correlated, as they represent temperatures in successive vertical layers of the water volume. The application of PCA both in the input and output of the model is currently being investigated.</li> </ul>	
		Apr 2011
	<p>Progress has been made on the project and at present we have a Super-parameterised model, which despite the improvements it can admit, is a model with dimensions comparable to those found in the literature, which shows improvements over alternative methods commonly used. The issues that have been addressed specifically are:</p> <ul style="list-style-type: none"> <li>• The results of the superparameterised model (without emulation) are much closer to those of the reference model (see point 3 in April 2011 update). Enlarging the domain helped improving this point.</li> <li>• Point 5 in April 2011 update was tackled, and now the combination of the Coarse + Fine models does not need to be run before an emulator of the Fine model can be built. This was a major step towards transforming this into a practical working system. Lengthening the communication intervals between the Coarse and Fine models helped towards this direction.</li> <li>• Dimension reduction via PCA (point 6 of April's update) has successfully been applied, reducing the number of inputs and outputs from 20 to 5.</li> <li>• Although the results are satisfactory in regions of constant cooling, they tend to deteriorate at the edges of the cooling region. This problem, which was also encountered in alternative approaches, needs to be tackled.</li> </ul> <p>The following dissemination activities are being undertaken:</p> <ul style="list-style-type: none"> <li>• Presentation of a poster in the SMBES Summer School in September 2011.</li> <li>• Technical report due in the end of September.</li> <li>• We believe that the work done so far consists a robust proof of concept, and we are considering writing up a grant application for NERC. We have yet to decide which call for proposals we are going to participate in.</li> </ul>	Sep 2011
<p>ACHIEVEMENTS / OUTPUTS</p>		



# PROJECT PLANS

<b>PROJECT</b>	<b>2. BOWEL CANCER</b>	<b>PROJECT LEADER</b>	<b>Ben</b>
<b>EMAIL LIST</b>	<a href="mailto:mucm-project-cancer@lists.shef.ac.uk">mucm-project-cancer@lists.shef.ac.uk</a>	<b>PROJECT TEAM</b>	Jeremy, Dan, Alexis
<b>OVERVIEW</b>	A stochastic health economic model is available in collaboration with Alan Brennan (AP). Alan and collaborators have tried earlier to calibrate this model to observed data, but without any clear idea of what they are doing.		
<b>ACTIVITIES</b>	a) Build an emulator for the stochastic model. Calibrate to observed data, but without incorporating model discrepancy. Use of this model for cost-effectiveness analysis will form a separate project (in the theme of informing decisions) at a later stage. (Grant application could then follow.)		
<b>OBJECTIVES</b>	2.1 Paper (at least a draft) on calibrating this model.	<i>Target Date</i>	<del>Jul 2011</del> Sep 2011
<b>PROGRESS UPDATE</b>	No progress so far. I have not been able to get hold of the model - I am chasing this up. I am also chasing up a second stochastic model and calibration dataset from Richard White and colleagues at the London School of Hygiene and Tropical Medicine.  BY starting 25 <sup>th</sup> April who will take over this project. Extend target date to allow for this.  Received Natural History Model (NHM) and able to run it in Simul8.  Developed foundations for an emulator for the NHM.  Selected procedure for identifying parts of input region from which to build emulator.	<i>Updated</i>	Jan 2011  May 2011  June 2011  August 2011
<b>ACHIEVEMENTS / OUTPUTS</b>	2.1	<i>Achieved</i>	

<b>PROJECT</b>	<b>3. STOCHASTIC FEM</b>	<b>PROJECT LEADER</b>	<b>Noha</b>	
<b>EMAIL LIST</b>	<a href="mailto:mucm-project-sfem@lists.shef.ac.uk">mucm-project-sfem@lists.shef.ac.uk</a>	<b>PROJECT TEAM</b>	Henry, Peter, Yiannis	
<b>OVERVIEW</b>	This will build on work going on with Rolls Royce, who have several SFE models.			
<b>ACTIVITIES</b>	a) Develop methodology for emulating the outputs of SFE models. This will be quite theoretical work, but will include some application using RR models.			
<b>OBJECTIVES</b>	<p>3.1 Draft paper on emulating SFEM outputs (which can be seen as whole distributions). REVISED PLAN: paper will now be on Quadrature/links to design</p> <p>3.2 Funding application to RR to take this work further.</p> <p>3.3 Internal report on emulating SFEM outputs, drawing on ideas from other stochastic emulation projects (projects 4, 5, 10, 11)</p>	<b>Target Date</b>	<p><del>Apr 2011</del> July 2011</p> <p><del>Apr 2011</del> May 2011</p> <p>Sep 2011</p>	
<b>PROGRESS UPDATE</b>	<p>Henry and I are in touch with Ron Bates (Rolls Royce), Giovanni Pistone (Torino) and Eva Riccomagno (Genoa) to start to plan a workshop in March in Genoa. It is to be on "sparse quadrature" which is the preferred method for handling outputs which take the form of Wiener chaos (polynomials of Gaussian Processes). We are at present collecting references, including to an PhD in Italy on the subject. We will give a list of these references, shortly. Henry will be seeing Gianni and Eva at a conference in Spain 12-15 November. Noha will write up a short summary of the work, as soon as I have submitted my PhD.</p> <ul style="list-style-type: none"> <li>Since I have submitted my PhD at last I am working hard to found my knowledge about the Stochastic Finite Elements method. The method is used to solve a system of partial differential equations. A short report on the SFE method and sparse quadrature in engineering uncertainty analysis will be done by April 2011.</li> <li>A workshop in Italy will be attended in the university of Genoa on the 15/03/2011. Henry is giving a short course on Computer Experiments in Diendi workshop on industrial experimentation (joint with Daniele Romano).</li> <li>Rolls Royce Update: A discussion with Dr.Bates and Dr. Avathen at Brunel university with a review to build up a project in the area.</li> </ul> <p><b>Current Updates</b> (by NY)</p> <ul style="list-style-type: none"> <li>I passed my VIVA last month with minor corrections (misprints).</li> <li>Henry and I attended the workshop in Genoa on quadrature. Henry gave a talk on sparse quadrature.</li> <li>Henry gave the short course on computer experiments with my assistance as Daniele Romano cancelled his session. The second session we gave introduced the participants to the MUCM toolkit.</li> </ul> <p><b>Future plans</b></p> <ul style="list-style-type: none"> <li>Now I am working on a poster for using partial entropy sampling design to present in DEMA in Cambridge in August. We are also writing a paper on adaptive designs to be submitted to the ISI the 58th congress in Dublin.</li> <li>I am still working on the SFE and quadrature review to be finished by the end of April.</li> </ul>	<b>Updated</b>	<p>Nov 2010</p> <p>Jan 2011</p> <p>Apr 2011</p>	
<b>ACHIEVEMENTS / OUTPUTS</b>	<p>Noha's PhD VIVA</p> <p>Workshop on Sparse quadrature in Genoa.</p> <p>A short course on Computer Experiments in diendi workshop in Turin on industrial experimentation</p> <p>Collecting references on the Stochastic finite elements</p>	<p>Passed with minor corrections.</p> <p>Sparse quadrature is the preferred method for handling outputs which take the form of Wiener chaos (polynomials of Gaussian Processes).</p> <p>Henry gave the course with my assistance. We also introduced the participants to the MUCM toolkit in the second session.</p> <p>A short report has been written but not finished yet. The method is used to solve a system of partial differential equations. There is a massive literature on this topic especially in engineering applications. The main idea is to</p>	<b>Achieved</b>	<p>Mar 2011</p> <p>Mar 2011</p> <p>Mar 2011</p> <p>Mar 2011 - present</p>

	<p>use the polynomial chaos to represent the stochastic output. This requires choosing a good set of points where the output will be observed at (Design problem). The common technique for choosing such a set of points is the Smolyak grid. Smolyak was initially developed to overcome the dimensionality problem.</p> <p>Three pages were written for the toolkit on the design using the K-L expansion. A long discussion has been going on about the new criterion developed in my PhD<sup>2</sup>. The discussion lead to another criterion or simply to another approximation to the predictive variance.</p> <p>Henry gave a talk about this paper at the conference.</p> <p>The study develops a new criterion based on the maximum entropy sampling criterion. It behaves similarly to the <math>D_s</math> optimality criterion where the interest is just in estimating a subset of the mean parameters. The use of this criterion can be extended to designing for estimating the covariance parameters when the GP model is approximated by the K-L expansion.</p> <p>The paper aims at testing this criterion on different regression models such as Haar regression. The criterion was initially developed for the approximated GP model by the K-L expansion. The paper compares different calculation methods to reach this criterion. I finished coding for the Haar regression and going to try Tony's suggestion to compare between the two approximations. In addition I will do MCMC to find the predictive variance of the required distribution and compare it with the approximated criterion.</p> <p>NY will be leaving MUCM by the end of Sept. and starting a new post at LSE. However she will continue working with Henry and finishing all MUCM work.</p>	<p>Jun 2011 - present</p> <p>Aug 2011</p> <p>Aug 2011</p> <p>Sept 2011</p> <p>Dec 2011</p>
<p>Toolkit pages</p>	<p>A paper titled "A discussion of adaptive design for computer experiments" submitted to the ISI the 58th congress in Dublin.</p> <p>Henry gave a talk at DEMA 2011 about the algebraic method in Statistics: Betti numbers and Alexander duality</p> <p>A poster titled "Partial maximum entropy sampling criterion for computer experiments" was presented at DEMA 2011 conference in Cambridge</p> <p>A paper on the approximated adaptive maximum entropy sampling criterion</p>	

<b>PROJECT</b>	<b>4. SYSTEMS BIOLOGY</b>	<b>PROJECT LEADER</b>	<b>Ian</b>		
<b>EMAIL LIST</b>	<a href="mailto:mucm-project-sysbio@lists.shef.ac.uk">mucm-project-sysbio@lists.shef.ac.uk</a>	<b>PROJECT TEAM</b>	Michael, Alexis, Jeremy		
<b>OVERVIEW</b>	<p>The primary interest in such models is calibration, to estimate transition rate parameters.</p> <p>Systems Biology is a rapidly expanding area which involves the investigation of chemical reaction networks found (usually) within cells. There are a large number of such models available ranging from small (a few rate parameters i.e. inputs, and one or two chemicals) to very large (100's of rate parameters with 80+ chemicals). The vast majority of these networks have been studied using standard coupled differential equations. While these differential equation models are suitable if the numbers of molecules of all chemicals are large, such deterministic models break down for low numbers of molecules which often occur for processes that involve gene translation (as many of these networks do).</p> <p>In these low molecule count cases, stochastic modelling, which describes the number of molecules of each chemical species as a random process, is more appropriate. The stochastic formulation is usually simulated using the Gillespie algorithm, a relatively fast forward simulator, which incorporates various mass action kinetic laws.</p> <p>The primary interest of this Project is to develop emulation techniques for the stochastic systems biology models described above, and to use these to perform history matching and possibly calibration in order to learn about the transition rate parameters, which are of major interest to the Biologists.</p>				
<b>ACTIVITIES</b>	a) Build a case study using an intermediate size regulatory network model. This will include design considerations and discrepancy modelling. Apply history matching (possibly also calibration).				
<b>OBJECTIVES</b>	<p>4.1 Draft paper on history matching a stochastic model.</p> <p>4.2 Grant application to BBSRC (or at least some progress on drafting such an application). REVISED PLAN: Submission within 6 months</p> <p>4.3 NEW OBJECTIVE: Paper from AB's thesis</p>	<b>Target Date</b>	<p><del>Apr 2011</del> June 2011</p> <p><del>Apr 2011</del> Sept 2011</p> <p>Sept 2011</p>		
<b>PROGRESS UPDATE</b>	<p>We have developed a univariate Bayes Linear emulator for stochastic models and applied it to</p> <ol style="list-style-type: none"> <li>a 2-parameter toy model (the Birth-Death process)</li> <li>a 2-parameter simplified version of the Prokaryotic model</li> <li>the full 8-parameter version of the Prokaryotic auto-regulation gene network</li> </ol> <p>In each case we have used the univariate emulator to evaluate implausibility measures and hence to history match the model. In the full Prokaryotic model we have so far performed 3 waves of history matching and found great benefits in accuracy in the second and third waves, allowing for large reductions in the input space. We are now down to less than 0.02% of the original input space, and can now see substantial amounts of structure in the non-implausible volume, especially in wave 3. Provisional tests suggest that a wave 4 would be unnecessary as the wave 3 emulator errors are now substantially smaller than the observational errors, meaning that the non-implausible region cannot be significantly reduced with a more accurate emulator.</p> <p>We have also examined stochastic univariate emulator diagnostics for each of our emulators at each of the three waves, and one can see how the diagnostics improve with each wave due to the increase in emulator accuracy (which is one of the main motivations for such an iterative history matching approach).</p> <p>The above work will form the basis of the paper that is Objective 4.1. This paper should be completed soon, however it has been delayed as we have redone the above example so as to use equivalent simulated data to that of one of Darren Wilkinson's papers that featured inference for this model (essentially we want to use the same xstar).</p> <p>We have also considered the selection of the most informative subset of outputs (in this application these are individual time points on 5 separate time series) to use in the History Match, by a) applying principal variables to the means and the variances of the model outputs b) examining the fraction of input space cut out by each output using a univariate implausibility measure. When determining outputs for use in wave 1 say, criteria b) tends to</p>			<b>Updated</b>	Feb 2011

	<p>be more useful as space reduction is the main goal. If we were deciding on which outputs to instruct the biologists to measure things are a little more complicated and we have not resolved this fully yet.</p> <p>We have been establishing contact with members of the Biology Department at Durham University. Specifically, IV has held several meetings with Dr Junli Liu, a systems biologist here at Durham. Dr Liu has several models that might be of interest to MUCM2 members of various size (we have been discussing two models with 17 inputs and 64 inputs and more recently models with 47 and 100 inputs respectively), but most of the models are currently deterministic. We have been encouraging Dr Liu to explore the stochastic versions of these networks (as the conversion from deterministic to stochastic is quite straightforward). We are also discussing and exploring the possible funding opportunities provided by BBSRC, as relates to Objective 4.2.</p> <p>In terms of funding opportunities we have recently completed a joint bid with three biologists at Durham: Junli Liu (systems biology modeller), Keith Lindsey and Marc Knight (both senior experimentalist in plant biology) for an EPSRC impact award. This is to provide a proof of concept study to explicitly demonstrate MUCM methods at work on two large systems biology models. In this project we would also have the opportunity to direct the biologists to gather experimental data on the most informative parts of the system: a very interesting design question.</p>	
<p><b>ACHIEVEMENTS / OUTPUTS</b></p>	<p>Objective 4.1 Draft paper on history matching a stochastic model: Almost done. Delays due to redoing the example so that we used equivalent simulated data to that used in the literature (we wanted to use exactly the same xstar and input ranges to compare with Darren Wilkinson's mcmc techniques as applied to this model).</p> <p>Objective 4.2 Grant application to BBSRC (or at least some progress on drafting such an application): We have submitted a proposal for an EPSRC impact award to fund a proof of concept study with three biologists at Durham (see above for details). This would form the basis of a future large BBSRC proposal.</p> <p>Issues relevant to this 6 month period:</p> <ul style="list-style-type: none"> <li>• Emulation and history match of 2 simple models: Complete</li> <li>• Set up, emulation and wave 1 history match of full Prokaryotic model: Complete</li> <li>• Wave 2 emulation, history match and physical interpretation of non-implausible volume: Complete</li> <li>• Wave 3 emulation and history match: Complete</li> <li>• Redo above example so the simulated data is consistent with alternative approaches in the literature: Complete</li> <li>• Decision about which univariate combinations of outputs to use for the history match (dimension reduction): Complete</li> <li>• Draft paper on history matching a stochastic model: Almost complete</li> <li>• Discussions regarding BBSRC funding: Ongoing</li> <li>• Application for EPSRC impact funding for joint project with Biologists: Complete</li> </ul> <p>Future Issues of interest:</p> <ul style="list-style-type: none"> <li>• Full multivariate emulation needed (will involve emulation of covariance structures): see the Multi-output Systems Biology topic.</li> <li>• The Design problem (deciding on location, repetition, completion time and proportioning of evaluations between waves). Some thoughts on but nothing concrete as of yet.</li> <li>• Incorporation of Model Discrepancy in the stochastic setting (what are the possible and appropriate MD structures).</li> <li>• Diagnostic measures for stochastic emulators (repetitions vs location: how should we test the emulator?): some progress but more to do.</li> <li>• Incorporation of different data types (e.g. single cell incomplete time-course data): see Multi-output Systems Biology topic.</li> </ul>	<p style="writing-mode: vertical-rl; transform: rotate(180deg);">Achieved</p> <p>Sept 2011</p> <p>Feb 2011</p>

<b>PROJECT</b>	<b>5. AGENT-BASED MODELS</b>	<b>PROJECT LEADER</b>	<b>Alexis</b>
<b>EMAIL LIST</b>	<a href="mailto:mucm-project-agent@lists.shef.ac.uk">mucm-project-agent@lists.shef.ac.uk</a>	<b>PROJECT TEAM</b>	Dan, Jeremy, Ian (if a grant application for an agent-based model project at Durham is successful)
<b>OVERVIEW</b>	Someone at Aston has built an agent model of crowd behaviour. An interesting feature is that agent models often have discrete inputs and/or outputs.		
<b>ACTIVITIES</b>	a) Using the crowd behaviour model develop a simple emulator as a proof of concept.		
<b>OBJECTIVES</b>	5.1 Conference paper on emulating the crowd behaviour model.	<b>Target Date</b>	Apr 2011 Sep 2011
	5.2 NEW OBJECTIVE: obtain and emulate a larger agent based model		Sep 2011
<b>PROGRESS UPDATE</b>	5.1 Brief discussion with local Aston group developing agent based models (28/10/2010). Will get conference paper describing model and later on some java code so we can run the model. The initial model is quite simple with continuous inputs. Number of inputs is 10-12, currently the team has perturbed one-at-a-time 2-3 of them to see effects. Output is percentage of violent people. Time series output is also available. Goal is to build good enough emulator to do sensitivity analysis jointly on entire input set. Implausibility could also be useful to figure out interesting input domain. We will try by end of year to have working emulator (Dec 2010). Goal is to have conference paper in application conference on applying emulation on this type of model. Going through paper describing agent based model. Next step is to obtain code, run simulator and perform exploratory analysis. (22/1/2011) Attended <a href="#">OR Society Simulation Special Interest Group Meeting</a> on the current state of Agent Based Models (ABM). Focus of meeting was on the use of ABM in social science and operational research (24/3/2011). Have obtained code for the crowd control simulator and have started doing exploratory analysis. Elicitation for crowd control simulators. Have obtained <a href="#">initial ranges for all model parameters</a> from domain experts. Have also started discussing which parameters are of interest. Goal is now to start working on sensitivity analysis.	<b>Updated</b>	Jan 2011 Jan 2011 Apr 2011 Aug 2011 Aug 2011
<b>ACHIEVEMENTS / OUTPUTS</b>	5.1		<b>Achieved</b>

PROJECT	<b>6. NONSTATIONARY EMULATION</b>	PROJECT LEADER	<b>Gemma</b>
EMAIL LIST	<a href="mailto:mucm-project-nonstat@lists.shef.ac.uk">mucm-project-nonstat@lists.shef.ac.uk</a>	PROJECT TEAM	Peter, Noha, Yiannis, Jeremy, Michael
OVERVIEW	This will also link to the wider issues of discontinuous outputs.		
ACTIVITIES	a) Review approaches to emulating nonstationary outputs (including treed GPs). Assemble a small collection of suitable models displaying nonstationary and/or discontinuous behaviour.		
OBJECTIVES	<p>6.1 Review (internal report or draft paper)</p> <p>6.2 Two or three suitable models to work with</p> <p>REVISED PLAN: Continue to build a model set, explore 2 or more approaches and begin to write up about work</p>	Target Date	<p><del>Apr 2011</del></p> <p>May 2011</p> <p><del>Apr 2011</del></p> <p>Sep 2011</p>
PROGRESS UPDATE	<p>6.1 Have been looking at use of GMRFs to represent a GP. Specifically, <a href="#">Lindgren et al. (2010)</a> use an approximate solution of stochastic partial differential equations to provide the link between GMRFs and GPs with the matern correlation function. They show how this can be extended to generate GMRFs to represent non-stationary GPs.</p> <p>The Lindgren 2010 approach works quite well in 2 dimensions and although their method is theoretically extendable to more than 2 dimensions, in practice this isn't quite so straightforward. The main problem is with the triangulation of the input space and the subsequent triangulation if further design points are required as a result of the validation process. (Attended RSS read paper 16 Mar 2010). This approach is being put on hold for the time being and am now focusing on more traditional methods of dealing with non stationarity such as Sampson and Guttorp 1992 and Higdon et al 1999.</p> <p>6.2 Have mentioned to members of subgroup (climate and uncertainty) at NOC that I'm looking for such models.</p> <p>We've been looking at using the MIT gcm and although non stationarity is achieved, the output of this model is not ideal for our purposes. A model of the doppler effect is being used as a toy model in 1 dimension and if this is successful some sort of ocean model with an acoustic element where we look at sound speed, current etc might provide a better "real model" example.</p>	Updated	<p>Jan 2011</p> <p>Apr 2011</p> <p>Jan 2011</p> <p>Apr 2011</p>
	Gemma has now left MUCM.	Achieved	

<b>PROJECT</b>	<b>7. DECISIONS THAT EXPAND MODELS</b>	<b>PROJECT LEADER</b>	<b>Jonathan</b>
<b>EMAIL LIST</b>	<a href="mailto:mucm-project-decision@lists.shef.ac.uk">mucm-project-decision@lists.shef.ac.uk</a>	<b>PROJECT TEAM</b>	Ian, Michael, Henry
<b>OVERVIEW</b>	<p>We have found a more interesting application to study for this project. The focus has shifted to decision making within well test analysis and deconvolution. As the deconvolution project is the focus of JAC's co-funding, this allows for a strong synergy across both projects.</p> <p>In well test analysis, time series of pressure and rate observations are recorded. These measurements are then "deconvolved" to generate a reservoir response function which characterises the features and properties of the reservoir and is the primary object of study and inference. Accurately learning about the response function is therefore crucial to the analysis of the well test, and identifying which test regimes are best for achieving this goal is of interest. The deconvolution problem has a number of aspects of a decision problem:</p> <ol style="list-style-type: none"> <li>1. Determining the optimal well test regime for learning about the reservoir response function</li> <li>2. Extending the above problem to learning about the reservoir itself, rather than the response function (making the link to reality)</li> <li>3. Using all of this information to perform a classification of the reservoir</li> </ol> <p>Performing a single deconvolution is a relatively inexpensive operation computationally. However, the problem is complicated by the presence of substantial uncertainty on the input data which then propagates into sizeable uncertainty on the deconvolution output. We can capture this uncertainty on the outputs by performing many simulations using possible rates and pressures which are consistent with the original data and our error specification. Each of these simulated deconvolutions will have differing levels of accuracy which will vary depending on our choice of well test regime. Given a utility for the accuracy of the deconvolution, we can produce an expected (average) utility using this (now-expensive) simulation method. To identify optimal decisions would require an exhaustive exploration of the utility surface over the decision space. However, due to the computational expense of the operation that will not be possible - instead expected utility will be emulated. Maximisation of the emulated expected utility (via history matching techniques) will then identify the good regions of decision space.</p>		
<b>ACTIVITIES</b>	<ol style="list-style-type: none"> <li>a) Simple emulator-based decision making for deconvolution</li> <li>b) Linking the decision-making to reality</li> <li>c) The classification problem in deconvolution</li> </ol>		
<b>OBJECTIVES</b>	<ol style="list-style-type: none"> <li>7.1 Clear plan of work for a further 6 months to complete this project.</li> <li>7.2 Documentation of uncertainty analysis for Droshky model</li> <li>7.3 Exploration of the deconvolution problem, statistical formulation</li> <li>7.4 Identification of "optimal" well test regimes for learning about the response function in a well test given a known reservoir</li> <li>7.5 Identification of "optimal" well test regimes for learning about the response function in a well test given an unknown reservoir with unknown properties</li> <li>7.6 Extension to inference about the reservoir (link to reality)</li> </ol>	<b>Target Date</b>	<p>Apr 2011 Sep 2011</p> <p>May 2011</p> <p>August 2011</p> <p>October 2011</p> <p>December 2011</p> <p>2012</p>
<b>PROGRESS UPDATE</b>	<ol style="list-style-type: none"> <li>1. Decisions in Deconvolution             <ol style="list-style-type: none"> <li>a. Statistical formulation of the problem</li> <li>b. Outline method for decision-making</li> </ol> </li> <li>2. Marathon Reservoir Simulation             <ol style="list-style-type: none"> <li>a. Durham have submitted a proposal for a substantial decision support project with BG</li> <li>b. Identified initial goals for analysis of the Marathon model.</li> <li>c. Initial analysis principally complete.</li> <li>d. Analysis of Marathon model documented; sent to Bob Parish.</li> </ol> </li> <li>3. BG Decisions Support             <ol style="list-style-type: none"> <li>a. Durham are pursuing a decision support project with BG involving decisions related to the placement of appraisal wells.</li> </ol> </li> </ol>		<b>Updated</b>
<b>ACHIEVEMENTS / OUTPUTS</b>	<ol style="list-style-type: none"> <li>7.1 "<i>Uncertainty analysis for cumulative oil production from the Droshky Reservoir Model</i>," J A Cumming, Internal Report, June 2011</li> </ol> <p>"<i>Decisions in Deconvolution</i>," J A Cumming, Internal Report, In progress.</p>	<b>Achieved</b>	

<b>PROJECT</b>	<b>8. BUILDING THE COMMUNITY</b>	<b>PROJECT LEADER</b>	<b>Tony</b>
<b>EMAIL LIST</b>	<a href="mailto:mucm-project-community@lists.shef.ac.uk">mucm-project-community@lists.shef.ac.uk</a>	<b>PROJECT TEAM</b>	Jo, Dan, Jeremy, Henry, Michael, Peter, Yiannis
<b>OVERVIEW</b>	Reaching out to new user groups via email lists, open days, short courses and continuing development of the Toolkit and website.		
<b>ACTIVITIES</b>	<ul style="list-style-type: none"> <li>a) Set up and management of our own server to host mucm.ac.uk at Sheffield as well as the Toolkit and associated software.</li> <li>b) On-going development of the Toolkit</li> <li>c) Build wider community contact lists of people working in this field</li> <li>d) Identify conferences at which to give short courses</li> </ul>		
<b>OBJECTIVES</b>	<ul style="list-style-type: none"> <li>8.1 MUCM Server: installation and transfer/update of website/toolkit</li> <li>8.2 Toolkit: release 8 – REVISED DATE OF JULY 2011</li> <li>8.3 Set up wider community MUCM mailing list and continue to build</li> <li>8.4 Confirm at least one conference at which to give a short course</li> <li>8.5 Complete and polish a set of basic short course modules</li> <li>8.6 Confirm additional short courses for 2011</li> <li>8.7 Fix venue and dates for UCM 2012 and set up programme committee</li> <li>8.8 Complete new-look website</li> </ul>	<b>Target Date</b>	<ul style="list-style-type: none"> <li><del>Apr 2011</del> July 2011</li> <li><del>Feb 2011</del> <del>Apr 2011</del> July 2011</li> <li>Nov 2010</li> <li>Apr 2011</li> <li>Sep 2011</li> <li>Aug 2011</li> <li>Sep 2011</li> <li>Aug 2011</li> </ul>
<b>PROGRESS UPDATE</b>	<ul style="list-style-type: none"> <li>8.1 I have been enquiring at Sheffield about the best way to provide all the UCM community services at Sheffield. After initial contacts this has been shelved while I concentrate on the toolkit release 7. I will get back to this in the New Year.  We will have our own virtual server at Sheffield. The Computer Centre will help to set this up and run it, but we are currently exploring how that would work and what services it will be realistic to provide.  Progress with the web server has been slow. The computing centre at Sheffield were approached to set up a MUCM server to cover the regular website, the wiki and the toolkit website, as well as possible future services like a preprint repository and a networking forum. It seems that even though we have some money for this they are not really very keen on doing it. So the topic will be referred to the forthcoming team meeting for discussion.  Progress on the web server continues to be rather slow, but we are still hopeful of having the initial system installed by the end of September. This will include a preprint management system. However, initial assessment of this suggests that it might require rather a lot of work (probably by Jo) to load all of our existing papers and presentations into the system. Tony will invite discussion at the team meeting in Durham about how to proceed on this.</li> <li>8.2 Release 7 (the final release officially under MUCM1) is delayed until the last minute - 31 December 2010. At that point, it has to include the final two case studies, since that will be claimed in our final report to EPSRC. In connection with this, we realised that release 6 still did not include any material on calibration, which is essential for CS2 to link to (and probably</li> </ul>	<b>Updated</b>	<ul style="list-style-type: none"> <li>Dec 2010</li> <li>Jan 2010</li> <li>Mar 2010</li> <li>Dec 2010</li> </ul>

	<p>also CS3). So Tony has undertaken to write a calibration thread by Christmas!</p> <p>Release 7 finally went live in January. Release 8 is not now likely to happen until April.</p> <p>Other projects have encountered problems in getting going and developing momentum, and Tony thought it best not to load more toolkit development on people right now. Particularly given the uncertainty over the web server. This will also be discussed at the team meeting, but we really need to aim for a new toolkit release no later than June.</p> <p>Release 8 finally went live in early September. Jeremy has done some nice work on revising the home page and several introductory pages. Noha has a couple of pages on adaptive sequential design (with some more work needed on an example) and Tony has extended the basic uncertainty analysis page.</p>	<p>Jan 2010</p>
	<p>8.3 Requested &amp; received names for UCM mailing list. List members have been emailed with opening message and unsubscribe option.</p> <p>Due to high number of list members taken from the SAMO list unsubscribing (and many of these doing so by replying to all) initial list was deleted and then everyone emailed again asking them to subscribe if interested. Membership is now circa 250 and still steadily increasing.</p> <p>This seems to have settled down and a couple of general messages have been sent out. Once the new Sheffield platform for UCM is sorted out, we'll ask list members about adding services and functionality.</p>	<p>Mar 2010</p> <p>Nov 2010</p> <p>Dec 2010</p>
	<p>8.4 Tony will be giving a course in connection with the workshop "Mathematical Science of Understanding and Predicting Regional Climate: A School and Workshop" to be held at the Institute for Mathematical Sciences, University of Singapore. The workshop part runs from 7 to 11 March 2011. It is preceded by a week-long "school", and the MUCM course will form one day of this, 4 March. However, this is a somewhat opportunistic running of the course. Tony was invited to join the workshop and is running the course (on his own) while there. The organisers are paying something for the course to reduce the cost to MUCM of Tony's attendance at this meeting. It is probably not important enough to constitute one of the courses we planned to give at conferences to bring MUCM to the attention of new communities. Possible additional courses will be discussed at the theme day in January.</p> <p>Tony gave the one-day course mentioned above. These slides are now being worked on by Dan and Peter to improve the presentations. They will be giving two 90-minute sessions at the EGU (European Geosciences Union) General Assembly 2011 in Vienna on April 6th. Dan and Peter have set up a DropBox folder to share the presentations and development with others in the team. This includes new Powerpoint templates. Henry has also been involved in a short course based in part on Tony's presentations.</p>	<p>Dec 2010</p> <p>Mar 2011</p>
	<p>8.5 The various presentations made by Tony in March were adapted and polished by Peter and Dan for a short course to the EGU meeting in April. Tony is doing some more work on these for a course he is giving in Austin, Texas, in October</p>	<p>Sep 2011</p>
	<p>8.7 Kenwood Hall, Sheffield has been confirmed as the venue for the next UCM conference and the dates have been set as 2nd - 4th July 2012. The next stage is to form the programme committee.</p> <p>Tony has invited the following people to form the Scientific Programme Committee for UCM 2012 (with him as chair): Derek Bingham, Peter Challenor, Steve Chick, Jon Helton, David Nott, Olivier Roustant, Tom Santner.</p>	<p>Aug 2011</p> <p>Sep 2011</p>
<b>ACHIEVEMENTS / OUTPUTS</b>	<p>8.1</p> <p>8.2 Release 8 of the toolkit went live in early September, 2011</p> <p>8.3 UCM mailing list set up and is being used by members to share information but this will be developed further in terms of adding services and functionality</p> <p>8.4 Tony gave the one-day course mentioned above.</p> <p>8.5 These slides were worked on by Dan and Peter to improve the presentations. They were</p>	<p>Achieved</p> <p>Sep 2011</p> <p>Dec 2010</p> <p>Mar 2011</p> <p>Apr 2011</p>



# PROJECT PLANS

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	<p>given as two 90-minute sessions at the EGU (European Geosciences Union) General Assembly 2011 in Vienna on April 6th. Dan and Peter have set up a DropBox folder to share the presentations and development with others in the team. This includes new Powerpoint templates. Henry has also been involved in a short course based in part on Tony's presentations.</p>	
8.7	Venue & Dates fixed for UCM 2012. Programme Committee invited	Aug 2011 Sep 2011
8.8	New look MUCM website launched	Aug 2011

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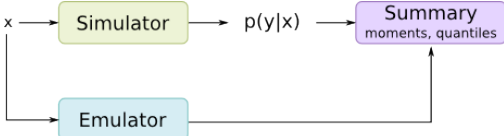


# PROJECT PLANS

<b>PROJECT</b>	<b>9. COUPLED MODELS</b>	<b>PROJECT LEADER</b>	<b>Yiannis</b>
<b>EMAIL LIST</b>	<a href="mailto:mucm-project-coupled@lists.shef.ac.uk">mucm-project-coupled@lists.shef.ac.uk</a>	<b>PROJECT TEAM</b>	Peter, Remi, Dan
<b>OVERVIEW</b>	TBC		
<b>ACTIVITIES</b>	a) TBC b) TBC		
<b>OBJECTIVES</b>	9.1 Find a suitable model	<b>Target Date</b>	Sep 2011
	9.2 Carry out initial investigation		Sep 2011
<b>PROGRESS UPDATE</b>	9.1	<b>Updated</b>	
	9.2		
<b>ACHIEVEMENTS / OUTPUTS</b>	9.1	<b>Achieved</b>	
	9.2		

PROJECT	<b>10. MULTI-OUTPUT STOCHASTIC MODELS</b>		PROJECT LEADER	Ian
EMAIL LIST	<a href="mailto:mucm-project-multioutput@lists.shef.ac.uk">mucm-project-multioutput@lists.shef.ac.uk</a>		PROJECT TEAM	Michael, Alexis
OVERVIEW	<p>This Project concerns the analysis of multi-output stochastic models. We concentrate on the area of Systems Biology as it has a rich set of models of varying complexity, many of which are ideal for our purposes. This Project therefore has much in common with Project 4: Systems Biology.</p> <p>Systems Biology is a rapidly expanding area which involves the investigation of chemical reaction networks found (usually) within cells. There are a large number of such models available ranging from small (a few rate parameters i.e. inputs, and one or two chemicals (each chemical gives a time series output)) to very large (100's of rate parameters with 80+ chemicals). The vast majority of these networks have been studied using standard coupled differential equations. While these differential equation models are suitable if the numbers of molecules of all chemicals are large, such deterministic models break down for low numbers of molecules which often occur for processes that involve gene translation (as many of these networks do).</p> <p>In these low molecule count cases, stochastic modelling, which describes the number of molecules of each chemical species as a random process, is more appropriate. The stochastic formulation is usually simulated using the Gillespie algorithm, a relatively fast forward simulator, which incorporates various mass action kinetic laws.</p> <p>The primary interest of this Project is to develop emulation techniques for the <b>multi-output</b> stochastic systems biology models described above, and to use these to perform history matching and possibly calibration in order to learn about the transition rate parameters, which are of major interest to the Biologists.</p>			
ACTIVITIES	<p>This topic follows on from Project 4: Systems Biology so please refer to that for more details. In Project 4 we have successfully created a univariate emulator for stochastic models and used it to History Match a variety of models including the Prokaryotic Auto-regulatory gene network (8 inputs, 5 chemical time series outputs).</p> <p>This Project is concerned with emulating and history matching using <b>multiple outputs</b> of a stochastic model. To this end, so far, we have considered the selection of the most informative subset of outputs (in this application these are individual time points on 5 separate time series) to use in the History Match, by</p> <ol style="list-style-type: none"> <li>applying principal variables to the means and the variances of the model outputs</li> <li>examining the fraction of input space cut out by each output using a univariate implausibility measure</li> </ol> <p>When determining outputs for use in wave 1 say, criteria b) tends to be more useful as space reduction is the main goal. If we were deciding on which outputs to instruct the biologists to measure, things are a little more complicated and we have not resolved this fully yet. Identifying the set of outputs to consider (i.e. dimensional reduction) is the first step in a successful multi-output analysis. A full multivariate emulator (which we are in the process of developing) would be based on this subset.</p> <p>We have been establishing contact with members of the Biology Department at Durham University. Specifically, IV has held several meetings with Dr Junli Liu, a systems biologist here at Durham. Dr Liu has several models that might be of interest to MUCM2 members of various size (we have been discussing two models with 47 inputs and 100 inputs), but most of the models are currently deterministic. We have been encouraging Dr Liu to explore the stochastic versions of these networks (as the conversion from deterministic to stochastic is quite straightforward). These models would make excellent large examples to try out a multi-output emulator. We are also discussing and exploring the possible funding opportunities provided by BBSRC.</p> <p>In terms of funding opportunities we (IV and MG) have recently completed a joint bid with three biologists at Durham: Dr Junli Liu (systems biology modeller), Prof Keith Lindsey and Prof Marc Knight (both senior experimentalists in plant biology) for an EPSRC impact award. This is to provide a proof of concept study to explicitly demonstrate MUCM methods at work on two large systems biology models. In this project we would also have the opportunity to direct the biologists to gather experimental data on the most informative parts of the system: a very interesting design question. This work would form the basis of a large proposal to BBSRC.</p>			
OBJECTIVES	<ol style="list-style-type: none"> <li>Identify a case study to work on</li> <li>Report at end of 5/6 months on progress</li> </ol>	Target Date	<p>Sep 2011</p> <p>Sep 2011</p>	
PROGRESS UPDATE	<ol style="list-style-type: none"> <li>We have found three. The Prokaryotic Auto-regulatory gene network as studied in the univariate case will form a suitable case study for this topic, and we have two other more complex models from Junli Liu, one with 47 input parameters and one with approximately 100 input parameters.</li> <li>Some progress made in terms of output subset selection, but delays in the univariate project have had knock-on effects here.</li> </ol>	Updated	<p>Sep 2011</p> <p>Sep 2011</p>	

	<p>Issues relevant to this 6 month period:</p> <ul style="list-style-type: none"> <li>• Decision about which univariate combinations of outputs to use for the history match (dimension reduction): Complete</li> <li>• Consideration of multi-output approaches: Ongoing</li> <li>• Full multivariate emulation needed (will involve emulation of covariance structures): Ongoing.</li> <li>• Discussions regarding BBSRC funding: Ongoing</li> <li>• Application for EPSRC impact funding for joint project with Biologists: Complete</li> </ul> <p>Future Issues of interest:</p> <ul style="list-style-type: none"> <li>• The Design problem (deciding on location, repetition, completion time and proportioning of evaluations between waves). Some thoughts on but nothing concrete as of yet.</li> <li>• Incorporation of Model Discrepancy in the stochastic multi-output setting (what are the possible and appropriate multi-output MD structures?).</li> <li>• Diagnostic measures for stochastic multi-output emulators (repetitions vs location: how should we test the emulator?): some progress but more to do.</li> <li>• Incorporation of different data types (e.g. single cell incomplete time-course data): the main motivation for this topic is to incorporate such data sets.</li> </ul>	
<p><b>ACHIEVEMENTS / OUTPUTS</b></p>	<p>10.1</p> <p>10.2</p>	<p><i>Achieved</i></p>

PROJECT	<b>11. EMULATING DISTRIBUTIONS</b>	PROJECT LEADER	Remi	
EMAIL LIST	<a href="mailto:mucm-project-distributions@lists.shef.ac.uk">mucm-project-distributions@lists.shef.ac.uk</a>	PROJECT TEAM	Alexis, Ian, Noha, Peter, Dan	
OVERVIEW	<p>We consider stochastic simulators for which the response to a given input <math>x</math> is a random variable <math>\mathcal{Y}</math>. We are interested in quantifying the uncertainty about <math>y</math>, namely <math>P(y x)</math>. Estimating the full <math>P(y x)</math> can be difficult or even infeasible. An alternative is to estimate some summary measure (such as the mean, variance, quantiles...) which provides "sufficient" (or at least relevant) information about the uncertainty in <math>\mathcal{Y}</math> for the problem at hand.</p> <p>This work package is concerned with emulating the conditional distribution <math>P(y x)</math> (or, as might often be the case in practice, some summary statistics).</p> 			
ACTIVITIES	<ol style="list-style-type: none"> <li>1. Definition of the problem, motivation, when do we want/need to emulate quantiles</li> <li>2. Literature review on existing methods (quantile regression, mixture density networks...)</li> <li>3. Integrate in the emulation framework</li> <li>4. Application to a simple toy model</li> <li>5. Application to a real model (rabies? systems biology? agent-based model?)</li> <li>6. Think about possible applications to/challenges in a dynamic setting (data assimilation)</li> </ol>			
OBJECTIVES	<p>11.1a Literature review on existing methods</p> <p>11.1b Identify problems where one might benefit from emulating quantiles / distributions</p> <p>11.2 Work on methods for emulating quantiles</p> <p>11.3 Application to a simple toy model</p> <p>11.4 Develop case study, e.g. in the rabies model</p> <p>11.5 Draft paper</p>	Target Date	<p>July 2011</p> <p>Sep 2011</p> <p>Sep 2011</p> <p>Oct 2011</p> <p>Nov 2011</p> <p>Dec 2011</p>	
PROGRESS UPDATE	<p>11.1 Literature review (in progress)</p> <p><i>Density estimation methods</i></p> <ul style="list-style-type: none"> <li>• sample-based methods (Monte-Carlo, ensemble methods, unscented methods)</li> <li>• moments (mean, variance, higher moments)</li> <li>• histogram estimation</li> <li>• quantile estimation (linked to CDF, histogram)</li> <li>• PDF-fitting methods (kernel methods - Gaussian, FFT..., neural networks (Mixture Density Networks), splines)</li> </ul> <p><i>Least square regression</i></p> <p>Given a set of observed inputs and outputs <math>(x_i, y_i)</math>, and a fitted model <math>f(x, \theta)</math>, least square regression looks for the value of model parameters <math>\hat{\theta}</math> which minimises the loss function <math>\sum_i (y_i - f(x_i, \theta))^2</math>. In particular, if <math>f(x, \theta) = \theta</math>, minimising the loss function yields the sample mean. This is equivalent to maximising a Gaussian likelihood (the negative log of which is proportional to the square loss function).</p> <p><i>Quantile regression</i></p> <p>If instead of the squared error loss function one uses the absolute error, i.e. <math>\sum_i  y_i - \theta </math>, the optimal estimator <math>\hat{\theta}</math> is the median of the sample [Bishop, 2006, ex. 1.27]. According to [Koenker and Hallock, 2001; Yu et al, 2003], sample quantiles can be obtained similarly by using a "tilted" absolute loss function, <math>\rho_q(x) = q \times I_+(x) - (1 - q) \times I_-(x)</math>, where <math>q</math> is the quantile of interest (e.g. 0.95) and <math>I_+</math> and <math>I_-</math> are the identity function truncated to <math>[0, \infty]</math> and <math>[-\infty, 0]</math> respectively. In particular, for <math>q = 0.5</math>, we get the absolute error loss function which yields the median (0.5 quantile).</p> <p>Here is a proof of the loss function <math>\rho_q(x)</math> yielding the quantile as optimal estimator, adapted from the proof for the squared error loss function found in [Bishop, 2006].</p> <p>We consider the loss function <math>L = \rho_q(x)</math> and look for the values of our fitted model <math>f(x)</math> which minimises the expected loss (under the predictive density function).</p>			Updated

$$E[L] = \int \int [q I_+(f(x) - y) - (1 - q) I_-(f(x) - y)] p(y|x) dx dy \quad (1)$$

$$= q \int \int_{f(x) > y} (f(x) - y) p(y|x) dx dy -$$

$$(1 - q) \int \int_{f(x) < y} (f(x) - y) p(y|x) dx dy \quad (2)$$

We can write its derivative using functional derivation:

$$\frac{\partial E[L]}{\partial f(x)} = q \int_{f(x) > y} p(y|x) dy - (1 - q) \int_{y(x) < t} p(y|x) dy$$

Setting  $\frac{\partial E[L]}{\partial f(x)} = 0$  gives:

$$q \int_{f(x) > y} p(y|x) dy = (1 - q) \int_{f(x) < y} p(y|x) dy$$

and identifying  $\int_{f(x) > y} p(y|x) dy$  as  $1 - \int_{f(x) < y} p(y|x) dy$  leads to:

$$\int_{f(x) < y} p(y|x) dy = q$$

which is the definition of the  $q$ -th quantile.

Like the squared error loss function is linked to a Gaussian likelihood, the quantile ("tilted") error loss function can be linked to an asymmetric Laplacian likelihood [Yu et al, 2003]:

$$p_q(x) = q(1 - q) \exp(-\rho_q(x)).$$

This might be used to fit an emulator to a specific quantile.

References [+](#)

Discussion points

*When should we be using quantiles?*

- when we are interested in predicting rare events (as opposed to extreme events which are really in the tail) or "abnormal" events (e.g. overweight or underweight children as a function of age)
- when  $p(y|x)$  isn't well approximated by a Gaussian (asymmetric, multimodal...) and is too difficult to describe parametrically, then associating our uncertainty with a variance measure can be misleading. Quantiles may be useful in such contexts.

*Applications*

[Yu et al, 2003] review some applications of quantile regression in the literature. These include:

- Medical diagnostics: percentiles can be used to identify unusual health conditions, especially when the reference range depends strongly on the patient's age
- Survival analysis: to quantify the chance of survival after medical operation (e.g. heart transplant), again as a function of patient age
- Finance: risk assessment (lower and upper quantiles)
- Economics: study of income distribution, electricity consumption (lower quantiles indicating background use, higher quantiles indicating peaks in demand linked to air conditioning, etc.)
- Environmental modelling: distribution of rainfall (with lower quantiles linked to drought and higher quantiles to flooding), pollution...
- Detecting heteroscedasticity: in the homoscedastic case, quantiles should be parallel (uniform variance). Non-parallel quantiles can help identify the heteroscedastic nature of a dataset or model output

*Important considerations*

When doing quantile estimation, we need to consider the following:

- Experimental design (more replicate observations might be required to identify higher quantiles)
- Validation (proper scoring rule for quantiles: CRPS?)

11.2 Methods for emulating quantiles TODO

11.3 Application to a simple toy model TODO



# PROJECT PLANS

	11.4	Case study: application to a real model (to be determined)	TODO	
	11.5	Report/Paper	TODO	
ACHIEVEMENTS / OUTPUTS	11.1			Achieved
	11.2			