C1. Project Description

PROJECT TITLE

Live coding of complex flood simulations with uncertainty quantification

AIMS AND BACKGROUND

Emergency services responding to environmental disasters (such as floods and bushfires) increasingly use computational simulations to model rapidly developing threats. Such simulations involve elaborate mathematical models overlayed on realistic terrain at scales relevant to local communities. They need to incorporate field data (weather conditions, water levels etc) and they are very demanding computationally, requiring high-performance computing in order to run effectively. In order to be useful for decision makers, simulations need to accommodate rapidly-changing scenarios and field data, and they need to properly quantify and communicate the uncertainty in their predictions. Developing such simulations requires insights from applied mathematics, software engineering, high-performance computing and human-computer interaction.

Aims

This research addresses the need for real-time simulation of environmental disasters through a *live coding* (or 'live programming') approach to rapid scenario modelling including uncertainty. We specialise our concerns to environmental models of inundation with the three main aims of:

1. **Developing new inundation models** (riverine floods, storm surges and tsunamis) that use sparse grids and reduced basis approaches to *quantify uncertainty* to dramatically increase the speed and usefulness of model predictions.

2. **Prototyping and optimising these models using live coding** to interactively search and optimise their parameter and solution spaces in real time. Such an approach will accelerate the development of stand-alone simulations. It will also be explored in the context of live, deployed simulations to, for example, make traditionally "offline" aspects of quantifying uncertaintly into interative and "online" simulations.

3. **Deploying and redeploying these models** on realistic, high-performance-computing (HPC) systems, including local compute clusters and the cloud. Live coding will be used to dynamically redeploy models across changing HPC systems configurations in order to optimise the efficiency of computations and to cope with the compute node failures expected in volatile emergency-management scenarios.

The outcomes of this research will enable decision makers to examine environmental disaster scenarios in real-time, even with computationally-intensive models. Through this, they will develop an intuitive understanding of the uncertainty relationships in the system—from uncertainties in input data through to representations of uncertainty in model outputs.

Background

Uncertainty quantification describes a collection of mathematical techniques that allow the predictions of computational simulations to be bounded probabilistically. The area is important in HPC simulations of scientific and engineering systems where it is desired to know how likely the outcomes of a simulation will be when various assumptions underlying the simulations are open to doubt. When uncertainty is included in a model, the essential dimensionality of the problem is increased markedly and sophisticated mathematical techniques are required to stop the cost of computation exploding (the so-called "curse of dimensionality"). This project will exploit new mathematical techniques that combine reduced order models (such as sparse grids and reduced basis methods) with uncertainty quantification. **Sparse grids** [3] are known to reduce the effects of the curse of dimensionality and recent work in our group has found new ways to incorporate gradient information and multi-fidelity models into sparse grid approximations [6, 9, 5]. **Reduced basis models** normally involve the computation of a large number of bounding 'offline' simulations that are examined together with an 'online' simulation to quantify its

uncertainty. With our live-coding approach, we plan to modify this approach so that the bounding simulations are also 'online' and 'live' in a way that allows them to be extended and interpolated and steered in real time.

Live coding describes software systems that support the direct intervention of the programmer in a program's run-time state so that code changes can be hot-swapped into running programs, allowing for extremely fast exploration and iteration of new ideas and system updates. As the ambition of live-coding has grown, support systems and languages have evolved to, for example, create, modify and interact with cyberphysical systems in real-time. Such an approach has been described as "with-time programming" [20] because it allows for timing constraints on a running system, including human-computer-interaction constraints, to be explicitly modelled and guaranteed. The present project will make use of the **Extempore live-coding software environment**[1] that can **harness and steer scientific simulations** (written in ABI compatible languages such as C, C++ and Fortran) in real time. Such an intervention in the world of HPC simulation radically changes the landscape and ambition of simulation codes; no longer do they need to be considered as hands-off batch processes running on supercomputers, but they can now be interacted with on-the-fly while a simulation is in progress. We envision that there will be several benefits of the application of live-coding to our problem: firstly, it will enable us to **rapidly prototype our simulation software** to deliver robust systems for disaster emergency response; secondly, live coding will allow us to **maintain and tune a set of, traditionally-offline simulations used to quantify uncertainty in real time**; and thirdly, the use of live coding will allow us to **adjust and optimise our systems for better efficiency** and to cope with compute node failure in the volatile HPC systems expected in disaster management situations.

INVESTIGATORS

The personnel involved in this project will be CIs Gardner, Strazdins, Roberts and Hegland, two Post-doctoral Research Associates and four PhD students. This project is split equally between the ANU Research School of Computer Science and the ANU Mathematical Sciences Institute. The four CIs are senior academics with many years of experience in running projects and many years of experience working with each other. Although CI Gardner is the lead CI on this grant application, the management structure of the project will be flat and deeply collaborative.

CI Gardner will be responsible for the overall project. He is a senior academic with many years of experience in computational science, high performance computing, virtual reality, Human Computer Interaction and computer music. He was director and head of school of ANU Computer Science from 2008 to 2013 and is presently the Associate Dean of Higher Degree Research in the ANU College of Engineering and Computer Science. In recent years, CI Gardner has been leading a research group that has developed the live coding "Extempore" programming system. This system originated in the creative arts to support live computer music, but has now been shown to be able to harness and interactive with traditional computational science applications in real time with negligible performance overhead. CI Gardner has a 40% research allocation and his term as Associate Dean will expire in 2018 providing him with opportunity to provide the proposed 20% allocation to the present project. **CI Strazdins** will be responsible for the high performance and distributed computing components of the project, based on his expertise in high performance computing, where he has a number of significant and well cited publications [2, 24, 1]. CI Strazdins has a 40% research allocation, leaving sufficient research time to cover the proposed 15% allocation to this project. **CI Roberts** will lead the inundation modelling, and uncertainty quantification components, based on his expertise in computational fluid dynamics and the use of sparse grid based uncertainty quantification [5, 11, 19, 16]. CI Roberts has a 40% research allocation, with no current grant obligations, leaving sufficient research time to cover the proposed 20% allocation to this project. **CI Hegland** will be responsible for the sparse grid and reduced model component of the project, based on his extensive expertise in computational mathematics, in particular his expertise in the analysis of the combination technique for sparse grids [2, 8, 1]. CI Hegland has a 60% research allocation. In 2018 will he contribute 20% of his research time to the DP150102345, and potentially a 20% contribution to LP160100624 leaving sufficient research time to cover the proposed 20% allocation to this project.

Our project is strengthened by a collaboration we are building with Dr Bert Debusschere and Dr John Jakeman both from Sandia National Laboratories, USA. They both have very strong records in uncertainty quantification research. Dr Jakeman has expertise on uncertainty quantification techniques based on his extensive expe-

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[1] http://extempore.moso.com.au

rience in using adaptive sparse grids, having applied such techniques to complex modelling problems [11, 10, 9] and has already collaborated with CI Roberts (his former PhD supervisor) [11]. Dr Debusschere has extensive expertise in uncertainty quantification through to fault tolerant numerical solvers, having already collaborated with CI Strazdins [21].

One post-doctoral fellow, to be situated in the Research School of Computer Science (RSCS), will develop large portions of the live programming tools and software interface which will interact with the scientific models and will conduct experiments on live scenarios where human actors mimic the interactions and information flows involved in the group dynamics of disaster response with simulation support. Due to the large skill set and responsibilities of this position it has been factored into the budget at level B3. One possible candidate for this position is Dr Ben Swift who is currently a post doc in the RSCS and has work extensively in HCI and has collaborated extensively with CI Gardner, on work relevant to this project [14, 15, 25, 26, 27].

A second post-doctoral fellow, to be situated in the Mathematical Sciences Institute (MSI), will need to have a very different skills set to the computer science research fellow. This research fellow will develop the numerical methods for computing sparse grid surrogates and reduced basis models which will be used to efficiently propagate uncertainties in model applications of tsunami and flood surge events. This position is budgeted at level B1 (raising to B2 in year 3). One possible candidate for this position Dr Brendan Harding, who is the former PhD student of CI Hegland and who has collaborated with CIs Hegland, Strazdins and Roberts on work relevant to this project [1, 2, 6, 8, 24].

We are requesting ARC funding for **two PhD students**, and we anticipate obtaining funding for **another three PhD students** from Australian Postgraduate Awards. Even though we have designated these PhD students to either computer science or mathematics, the projects will be inter-disciplinary, with all four CIs being on the supervisory panels of each of the students. The total of five PhD students will be split between the two departments—three in RSCS and two in MSI, focusing on specific aspects of the project as described below.

PROJECT QUALITY AND INNOVATION

Computational modelling and simulation is an invaluable support tool for disaster response, allowing emergency services personnel to explore what might happen in the immediate future under various scenarios. But these model simulations can be fraught with uncertainty: some of their *input parameters* may be well known (possibly from reliable sensor data), others may be known only approximately, and others still may only be guessed at. Even with perfect input data, the models themselves entail assumptions and numerical approximations which bound the reliability of their predictions.

The January 2011 Brisbane River floods in south-east Queensland cost 32 lives and caused 2.5 billion dollars worth of damage [29]. In the days leading up to these events, a key issue facing authorities was incorporating their **uncertainty** about the preceding fortnight's rainfall and the forecast rainfall into their modelling. In their report on the causes, impacts and implications of the floods, [29] concluded:

> whilst the dam operators were acting in accordance with the operations manual for the dam, their modelling did not take account of forecast rainfall in determining the predicted dam water level, and this resulted in a sub-optimal water release strategy.

In this one instance, it is speculatively possible that employing tools for decision making under uncertainty would have resulted in a different water release strategy. Our ambition is to build models and support infrastructure that will ensure that all relevant scenarios can be explored properly before such decisions are undertaken.

The overall project described in this application is core to a larger context for our work as shown in Figure 1. We envision a context where real-time and rapidly-varying human demands for simulation results will drive the development of appropriate interfaces and modelling infrastructure including uncertainty. Such simulations will be running on heterogenous HPC compute systems which, themselves, may need to be optimised and redistributed in real-time because of the volatile nature of the deployed environment. Both layers of the simulation environment will be developed and deployed using live-coding infrastructure. The major thrust of this grant application addresses the three main aims described above and is shown as the vertial box on this diagram. Through the research undertaken by the PhD students attached to this proposal, we will also study other important aspects of the entire project context. We now describe these research topics in more detail with a particular emphasis on the overall project's three main aims.
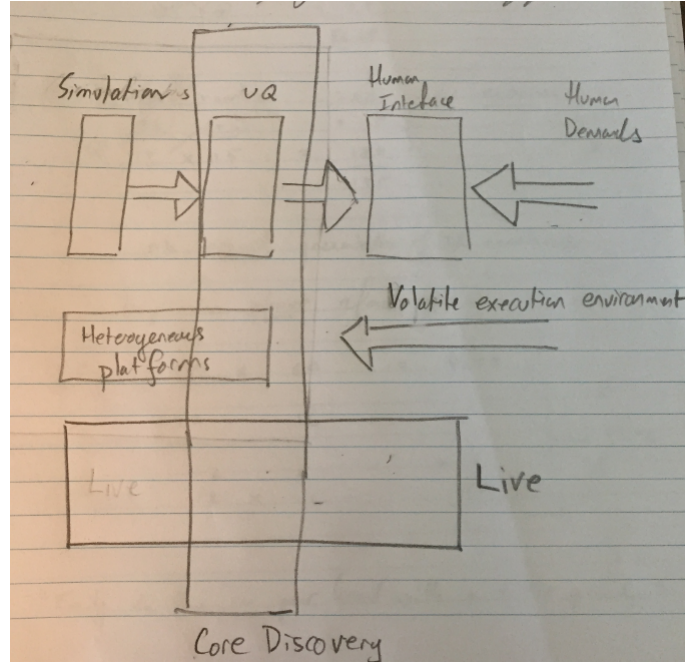
Figure 1: Context of overall project

A storm-surge example

To make matters concrete, we consider the problem of predicting the maximum storm surge water level at a location (or locations) along a coast threatened by a cyclone. We denote the geographical area of interest by Ω (the region threatened by the cyclone) and consider spatial points $(x, y) \in \Omega$. We restrict our interest to times t in an interval of time $T = [t_0, t_1]$ (the duration of the storm). A mathematical model for storm surge is provided by the shallow water wave equations [28]

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}(uh) + \frac{\partial}{\partial y}(vh) - R = 0, \tag{1a}$$

$$\frac{\partial uh}{\partial t} + \frac{\partial}{\partial x}\left(u^2 h + \frac{1}{2}gh^2\right) + \frac{\partial}{\partial y}(vuh) + gh\frac{\partial b}{\partial x} - \frac{h}{\rho}\frac{\partial P}{\partial x} - S_{fx} - S_{wx} = 0, \tag{1b}$$

$$\frac{\partial vh}{\partial t} + \frac{\partial}{\partial x}(uvh) + \frac{\partial}{\partial y}\left(v^2 h + \frac{1}{2}gh^2\right) + gh\frac{\partial b}{\partial y} - \frac{h}{\rho}\frac{\partial P}{\partial y} - S_{fy} - S_{wy} = 0, \tag{1c}$$

Here $h(x, y, t)$ is the depth of water and $u(x, y, t)$ and $v(x, y, t)$ are the x and y horizontal components of water velocity. The functions h, u and v are defined on the space $\Omega \times T = \mathcal{D}$. The equations include the constants g (the gravitational constant) and ρ (the density of water). Other terms constitute input data to the model: the bathymetry $b(x, y)$, is the elevation of the ocean bed; the rate of rainfall on the region over time is R; the atmospheric pressure is given by P; the x and y components of the frictional force generated by the flow of the surge over the ocean bed are given by S_{fx} and S_{fy} and the x and y components of the surface stress force (generated by wind) are given by S_{wx} and S_{wy}.

Our previous work [19, 16] has shown that these equations, and their approximation using the AnuGA package, provide a reliable model of general flows associated with inundation due storm-surge as well as riverine flooding and tsunamis. As is evident, there are many opportunities for uncertainty in the input data defining this model. If we denote by $\mathcal{P}$ the space representing the possible variation in both the **input parameters** (R, b, P, S_f, S_w) and the **design parameters** (emergency response actions such as raising or lowering flood barriers and releasing or diverting flow from upstream rivers or flood basins) then the aim of uncertainty quantification is to obtain useful relationships between the parameter vector $\mathbf{p}$ ($\mathbf{p} \in \mathcal{P}$) and output quantities such as the maximum storm surge height as a function of location. A completely general parameter space $\mathcal{P}$ may lead to an intractable problem and it is sensible to look for a lower dimensional manifold $\mathcal{C} \subset \mathcal{P}$. This can be done algorithmically or by using a specific reduced model, however, even such lower-dimensional approaches still necessitate numerous simulations of our model problem to quantify the uncertainty in our quantity of interest. **In addressing Aim 1**

of this project, we will study the shallow water wave equations in realistic flood innundation contexts in order to understand the relationship between their inputs and uncertainty. This research will be facilitated by new developments combining sparse grids [3], reduced basis methods [13, 18, 4, 17] and uncertainty quantification. In particular, by using sparse grids and reduced basis models we will be able to compute *surrogates of the full problem* which have significantly fewer unknowns and are thus cheaper to compute whilst maintaining a high order of accuracy. A sparse grid surrogate of the model can also be computed in an offline phase, so that in an online phase model solutions can be efficiently estimated using the surrogate model. For many problems sparse grids can also be used over $\mathcal{D}$ when computing solutions to the full model to speed up the construction of a reduced basis. We will compute sparse grid solutions via the 'combination technique' [7].

Live Coding for Uncertainty Quantification

This project will make use of the *Extempore* live-coding software environment.Extempore has already been used for the live modification and real-time visualisation of particle-in-cell plasma-physics simulation codes with negligible performance overhead compared to batch-mode execution in C [25].

Such a live deployment of a traditional, batch-oriented HPC simulation allows a user to modify the domain size and shape, the initial and boundary conditions, and various other parameters of a simulation while that simulation is running. It is of use for optimising software for later, stand-alone, deployment as well as for harnessing and steering simulation codes after deployment.

The ability to stop, modify, or restart computations 'in flight' has the potential to significantly improve the efficiency of an uncertainty analysis. There exist many algorithms, for example adaptive Markov chain Monte Carlo methods [30], which attempt to choose the best samples based on the sampling history. For complex problems however, a domain expert may often have a better idea about the region of the parameter domain where function evaluations should be concentrated. Through live programming within a tight feedback loop a domain expert can incrementally guide the current sampling strategy being used for uncertainty quantification, and in turn be guided by real time information derived from the reduced order model (such as surpluses provided by sparse grid approximation to identify important parameter dimensions and regions of interest), to improve the end result. The resulting strategies are expected to be more aggressive in nature as they are better targeted to the specific problem at hand. The result of this should be more efficient quantification of uncertainty.

In this project, using live coding to accelerate the feedback loop between the vector of input parameters, $\mathbf{p}$, and quantities of interest will give a scientist the ability to interactively *explore* the connection (and the associated uncertainty) between the different dimensions of $\mathbf{p}$ and the overall response of the system. Such a prototyping and optimising of these models (**Aim 2 of our project**) will help us rapidly scope and deliver robust models. The "liveness" that this approach brings will also be deployed into the uncertainty quantification models. For example, reduced-basis methods for uncertainty quantification typically employ a number of "offline" simulations that are used together with an "online" simulation of a system of interest to provide uncertainty estimates for that online simulation; we will apply novel live-coding approaches to such methods where the offline as well as the online simulations are all harnessed and live. The potential advantage of such an approach is that the offline simulations can be restarted, modified, reduced and explored at the same time that the online simulation is running. Such a research agenda in live coding is one that will include human-computer interaction as well as software engineering and we will be looking to identify states of interaction of expert users with our live-coding systems as well as transitions between them – much as we have already done so in the context of computer music [27].

HPC Systems Support

A reliance on high performance computing for the evaluation of scientific models provides additional challenges to the technical side of the project. Specifically, our algorithms must be highly scalable and robust to errors and faults in the computer system layer. We will take advantage of recent developments in both highly-scalable algorithms for the sparse grid combination technique [23, 22] and other results that demonstrate that such computations can be made robust [8, 2, 1].

The *Extempore* system that we have developed has been shown to be able to harness and steer scientific simulation in real time. In this part of the project, **addressing Aim 3**, we will apply live-coding to the real-time steering of the computer systems layer itself. This will involve developing code libraries to assist the

developer in real-time performance-evaluation and tuning of these complex and highly parallel simulations. For example, groups of processes will be allocated to different parts of the simulation. If some parts are delayed relative to others, processes can be 'stolen' from the faster group to improve load balance [21]. Communication bottlenecks can be identified and alternate communication algorithms can be employed to rectify this. Different computational kernels can be selected depending on the current memory system and floating point performance. It should be noted that this fine-tuning is not only application-dependent, but within an application, it depends on the workload selected, and even within that, may depend on the current phase of the simulation. Only Live Programming by *Extempore* has the flexibility and agility to facilitate such a degree of performance tuning.

Live coding of the systems layer of our project will allow rapid prototyping and performance-tuning of our software so that it can be run on realistic (cluster and cloud) HPC computer support. Most importantly, live-coding will allow a computer support expert to optimise the execution of running simulations under conditions where the computer systems may be unreliable or subject to rapid change (as might happen in some disaster-management scenarios).

Project organisation

The two postdoctoral fellows and four of the five PhD students will be concerned with the main aims of this grant application: One postdoctoral fellow and two PhD students in Mathematics will study storm surge equations in realistic topographies together with the calculation of uncertainty. They will work closely with the other post-doctoral fellow and one PhD student in Computer Science to study the application of live coding to uncertainty quantification of these equations. The fourth PhD student will work with the postdoctoral fellow in Computer Science to study live coding of the HPC infrastructure for these systems.

The remaining PhD student will study the human-computer-interaction context of real-time disaster management. Similar to the impact of visually presented geodata on decision making [12], the particular visualisations of uncertainty in our environmental models will need to be systematically evaluated with human participants. Here we will adopt traditional human-factors trials with non-expert participants together with qualitative feedback from emergency services experts. We will solicit qualitative feedback from expert participants from emergency authorities in our local area including ACT Emergency Services, Geosciences Australia, the Australian Maritime and Safety Authority and the Australian Federal Police. Perspectives offered by this participant pool will be important in extrapolating our study results to real world disaster-management.

We also anticipate a number of Honours and other student projects concerned with the overall context of our research.

FEASIBILITY

This research will be framed around problems that address the three main aims of the project. The core scientific objectives of each aim will be able to be achieved with reduced models, making them clearly realisable within the three year timeframe. However we stress that our objective is to make our simulations as close to the real-world as possible, including the use of realistic topographic data for flood simulations.

The Australian National University is a research-intensive university of high international standing where the quality of research in the ERA categories of Information and Computing Sciences (08) and Mathematical Sciences (01) have been assessed as being at the highest level of 5. At ANU, the Research School of Computer Science and the Mathematical Sciences Institute have a long and deep collaboration in numerical and applied mathematics, notably linked to the supercomputing facilities on campus. Indeed, since the early 1980s, ANU has housed the largest supercomputers in Australia and the cloud computing facilities at the NCI National facilities, located at ANU, will provide one of the testbeds for this project.

A new building is presently being constructed at ANU to locate the Mathematical Sciences Institute with the Research School of Computer Science. This co-location of academics in these two areas will be particularly fruitful for the present project.

BENEFIT

Solutions to the core scientific problems of the three main aims of our project will be of high impact and will lead to the future development of software infrastructure for disaster modelling including the quantifying of

uncertainty. As noted above, we anticipate being able to use other funding to add several PhD students, and other project students, to the project team and this larger team will take the entire project in the direction of building actual deliverable software. This larger team will also provide very good value to the ARC in terms of funds invested. Together with the in-kind contributions to the project, we assess in our budgeting that an ARC investment of $x will buy $y worth of research effort. As also discussed, we plan to establish contact with disaster management agencies to scope the visualisation and human interface needs of users.

In a world that is prey to a large number of environmental risks, the societal benefit of improved computational modelling for disaster management is huge. This project addressess the mathematical challenges (through new approaches to uncertainty quantification) and the software development challenges (through live coding for rapid prototyping) and the systems support challenges (coping with volatile and rapidly changing systems environments) of one aspect (flood inundation) of this very important area.

In addition to the academic benefits of the research program described here, there are potential industrial benefits through the seeding of enterprises that develop and deliver guaranteed modelling infrastructure to disaster management agencies.

COMMUNICATION OF RESULTS

We will publish the mathematical results of this project in important venues such as the "SIAM Journal of Scientific Computing","Parallel Computing", and the "Journal of Computational Science" and at the International SIAM conferences in Computational Science and Engineering and Uncertainty Quantification. In computer science, refereed publications associated with major conferences are more prestigious than journals. Our publication targets will be Supercomputing (SC), OOPSLA, ICSE, VL/HCC, IEEE International Parallel and Distributed Processing Symposium (IPDPS), CHI and IEEE Information Visualisation. In both disciplines, we also value the community and high quality of Australian conferences, and we will be submitting work to OzCHI, ASWEC, Computational Techniques and Applications Conference (CTAC) and the International Congress on Modelling and Simulation (MODSIM).

The source code contributions of this project will be released to the public. Both the Extempore live programming system (`https://github.com/digego/extempore`) and the AnuGA [19, 16] shallow water simulation package (`https://github.com/GeoscienceAustralia/anuga_core`) are available on GitHub under MIT and GPLv2 licences respectively. Parallel Sparse Grid Combination codes (ParSGCT) are available from CI Strazdins' website. We are committed to accessible and reproducible computational science, and support these goals by using free software licences and developing our code in the open on GitHub.

MANAGEMENT OF DATA

All research output will be stored on the ANU Data Commons and ANU Digital Collections. Data Commons is a central data repository for ANU research data which has been designed to securely store data and ensure that data are immune to format and media changes. This repository enables data to be accessed and reused with full open-access functionality to the public. Digital Collections accepts journal articles, conference papers, book chapters, working or technical papers and other forms of scholarly communication. It is also a repository for digital images of manuscripts and photographs in other university research collections.

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