C1. Project Description

PROJECT TITLE

Live coding of environmental 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 can be very demanding computationally, requiring high-performance computing in order to run effectively.

Until now, environmental simulations for disaster management have lacked a systematic treatment of the effects of uncertainties in their predictions. The inclusion of properly quantified uncertainty would allow decision makers to better estimate the risks of taking particular decisions. In a well-known example, discussed below, a report into the 2011 Brisbane floods found that water released from a dam adopted a sub-optimal strategy because modelling did not properly account for uncertainties in the forecast rainfall.

Developing enhanced environmental simulations that properly quantify uncertainty and that provide information to decision makers in real time requires insights from applied mathematics, software engineering, high-performance computing and human-computer interaction. In this project, we tackle this challenge in a unique way by employing a software engineering approach known as "live coding".

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. Although our ultimate ambition is to investigate a wide range of environmental simulations, in the present project we specialise our concerns to **models of inundation** with the three main aims of:

1. **Developing inundation models that quantify uncertainty**. Our case studies will include riverine floods, storm surges and tsunamis and we will use sparse grids and reduced basis approaches to quantify uncertainty.

2. **Prototyping and optimising these models using live coding**. We will use live coding to search and optimise the very large parameter and solution spaces of our models in real time with human experts. In this way, live coding will accelerate the development of stand-alone simulations. It will also be explored in the context of live, deployed simulations to make traditionally "offline" aspects of quantifying uncertainty into iterative and "online" simulations.

3. **Dynamically optimising computer systems support for these models in real time.** Here, live coding will be used to dynamically redeploy models across changing high-performance-computing (HPC) systems in order to optimise the efficiency of computations and to cope with the networking and compute-node failures expected in volatile emergency-management scenarios.

The outcomes of this research will be to demonstrate that effective environmental simulations can be developed to enable decision makers to examine disaster scenarios in real time with quantified uncertainty. By considering uncertainty, decision makers 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 obtain results in human-relevant timescales. 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 increased effective dimensionality, and recent work in our group has found new ways to incorporate gradient information and multi-fidelity models into sparse grid approximations [6, 8, 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 make the bounding simulations also 'online' and 'live' in a way that allows them to be extended, 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 allow users to modify cyberphysical systems in real-time. Such an approach has been described by CI Gardner as "with-time programming" [18] 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). 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 use of live-coding in our project: firstly, it will enable us to rapidly prototype our simulation software with human participants to deliver robust, stand-alone systems for emergency response; secondly, the use of live coding in a deployed system will allow us to enliven and tune a set of traditionally-offline simulations to potentially optimise the quantification of uncertainty in real time; thirdly, the use of live coding will allow us to adjust and optimise our compute systems for better efficiency and to cope with network and compute-node failures 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 five 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. Even though CI Gardner is the lead CI on this application, the management structure of the project will be flat and deeply collaborative.

CI Gardner will be responsible for the overall project and for leading Aim 2. 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 and it has recently been shown to effectively harness and "enliven" HPC computational science applications in real time with negligible performance overhead. CI Gardner has a 40% research allocation, his term as Associate Dean will expire before 2018, and he has no other grant commitments at the present time, 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 (Aim 3), based on his expertise in high performance computing, where he has a number of significant and well cited publications [2, 20, 1]. CI Strazdins has a 40% research allocation and has no present grant commitments in 2018, leaving sufficient research time to cover the proposed 20% allocation to this project. **CI Roberts** will lead the inundation simulation model development and will collaborate with CI Hegland to provide leadership of the uncertainty quantification part of the project (Aim 1). CI Roberts has extensive expertise in computational fluid dynamics and uncertainty quantification [5, 10, 17, 14]. CI Roberts has a 40% research allocation, with no

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

current grant obligations, leaving sufficient research time to cover the proposed 20% allocation to this project. As mentioned, **CI Hegland** will collaborate with CI Roberts in the leadership of the mathematical aspects of this project. He will also lead the reduced-basis aspects of uncertainty quantification. CI Hegland has extensive expertise in computational mathematics and is well-known for his expertise in the analysis of the combination technique for sparse grids [2, 7, 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 with Dr Bert Debusschere and Dr John Jakeman both from Sandia National Laboratories, USA. Dr Debusschere has extensive expertise in uncertainty quantification and fault tolerant numerical solvers and has already collaborated with CI Strazdins [19]. Dr Jakeman has expertise on uncertainty quantification techniques based on his extensive experience in using adaptive sparse grids, having applied such techniques to complex modelling problems [10, 9, 8] and has already collaborated with CI Roberts (his former PhD supervisor) [10]. Both of these experts have agreed to visit ANU and to host project participants at Sandia, however administrative issues prevent them becoming formal PIs on this application.

One post-doctoral fellow will be situated in the Research School of Computer Science (RSCS) and 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, a former PhD student of CI Gardner, and someone who has deep expertise relevant to this project [12, 13, 22, 23, 24]. Another possible candidate is Mr Andrew Sorensen who is a software developer, a published researcher, and a world recognised live-coding exponent of many years experience. Mr Sorensen is about to complete his PhD, studying with CI Gardner, based on his work with the Extempore system of which he is the lead author.

A second post-doctoral fellow will be situated in the Mathematical Sciences Institute (MSI) and 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 inundation, tsunami and flood surge events. This position is budgeted at level B1. 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, 7, 20].

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 be for specific projects in computer science or mathematics, all of their projects will be interdisciplinary, with all four CIs being on the supervisory panels of each of the students.

PROJECT QUALITY AND INNOVATION

Significance and Practical Research Challenge: 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 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 [26]. 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, Honert and McAneney [26] concluded:

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

Our ambition is to build models and support infrastructure that will ensure that an appropriate range of relevant scenarios can be explored properly before such decisions are undertaken.

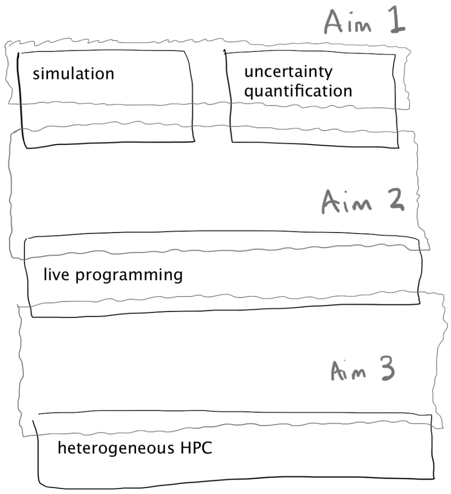

Figure 1: Aims and topic areas for the project. (Note: We represent this figure in a sketch-like fashion to represent the conceptual and high-level nature of these topics and their interactions. In reality there will be additional overlappings between them that is not shown here.)

The aims and topic areas for this project are 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.

The environmental focus of this project fits into the Science and Research Priority of "Environmental Change". Our approach is directed towards the Practical Research Challenge of improving the precision of the environmental modelling of systems undergoing rapid and dramatic change. The dynamic disaster scenarios that we target are thought by many to be increasing in frequency and severity due to climate change.

Framework/Advancing Knowledge – AIM 1: We illustrate our approach to Aim 1 with a concrete example. Consider the problem of predicting the maximum storm surge water level at a location (or locations) along a coast threatened by a cyclone. If 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 [25]

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

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

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

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/time domain $\mathcal{D} = \Omega \times T$. The equations include the graviational constant g and the density of water ρ. Other terms constitute input data to the model: the bathymetry (elevation of the ocean bed) $b(x, y)$; the rate of rainfall on the region over time R; the atmospheric pressure P; S_{fx} and S_{fy} the x and y components of the frictional force generated by the flow over the ocean bed and S_{wx} and S_{wy} the x and y components of the surface stress force generated by the wind.

Our previous work [17, 14] 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, we will study the shallow water wave equations in realistic flood inundation contexts in order to understand the relationship between their inputs and uncertainty and we will take advantage of new developments combining sparse grids [3], reduced basis methods [11, 16, 4, 15] and uncertainty quantification. 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 and 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.

Framework/Advancing Knowledge – AIM 2: 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 [22].

The ability to steer HPC simulations in real time has the potential to improve simulations including the quantification of uncertainty – both for software *development* and for software *deployment*. 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 decision maker 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 simulation models will help us to *rapidly scope and deliver robust software*. The "liveness" that this approach brings can also be deployed into the uncertainty quantification models in very novel ways. 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 enliven the traditionally-offline simulations so that they can be restarted, modified, spawned and explored at the same time that the online simulation is running. The potential advantage of this approach will be to optimise the quantification of uncertainty in real time.

Such a research agenda in live coding is one that includes human-computer interaction (HCI) as well as software engineering. HCI research questions include understanding the realistic time-scales of human-in-the-loop interaction with environmental simulations, both for software development and for decision making in real time. For our human-in-the-loop live coding experiments, we will be soliciting participation from emergency services personnel, environmental scientists and other experts (see Feasibility). Interaction protocol analysis will include both logged events at the interface and video protocols. 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 [24].

Framework/Advancing Knowledge – AIM 3: 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 [20, 21] and other results that demonstrate that such computations can be made robust [7, 2, 1]. We will then 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 [19]. 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 on the current phase of the simulation. Of live-coding systems, only *Extempore* has the flexibility and agility to facilitate such 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).

International collaboration: We have already mentioned the active collaboration that we have with researchers at Sandia laboratories in the USA. Uncertainty Quantification is a topic of very great interest in the computational science community. Our very novel approach to this problem involving live coding is bound to generate huge interest and further opportunities for international collaboration as this project progresses. Already we have delivered one invited workshop on the Extempore system at the major SC conference in Austin, TX in 2015.

Dissemination: We describe plans for publication below. As discussed in the project description and under feasibility, we plan to establish contact with disaster management agencies to scope the human interface needs of users and to engage emergency services personnel as human participants in live-coding experiments. This industry engagement will disseminate our work to these stakeholders and will hopefully lead to downstream collaborations over time. Even though we will be concentrating the bulk of our efforts on studying reduced mathematical models, as time permits we plan to make our simulations as close to the real-world as possible, including the use of realistic topographic data for flood simulations. This greater realism is bound to generate much interest in the media and the community. Arising from this interest, we envision that many future projects may involve active collaboration with emergency services and industry across Australia and overseas.

FEASIBILITY

Project design: This research has been 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 3.5 year timeframe. The expertise of the CIs is unique and well aligned with this project. All of the CIs know each other well and all have sufficient research capacity to deliver their fractional engagement with the project.

Apart from the CI's, there will be two postdoctoral research associates and five PhD students (two funded from this project and three funded from competitive scholarships): one postdoctoral fellow and two PhD students in Mathematics will study the simulation (inundation) equations in realistic topographies together with the calculation of uncertainty (with one student focussing primarily on the simulations and the other primarily on the associated quantification of uncertainty). In Computer Science, one postdoctoral fellow and three PhD students will study the application of live coding to uncertainty quantification of the inundation simulations, with one PhD student focusing on human-in-the-loop optimisation with expert participants, one PhD student focussing on HPC systems optimisation, and the third PhD student studying the wider human-computer-interaction context of real-time disaster management. Expert participants in our studies will be solicited from local emergency authorities (ACT Emergency Services, the Australian Maritime and Safety Authority and the Australian Federal Police) and from local environmental scientists (ANU Fenner School, ANU Research School of Earth Sciences, Geosciences Australia and the CSIRO).

The anticipated duration of PhD study in computer science and mathematics is slightly over 3.5 years and this grant application has planned and budgeted for 3.5 years for the two ARC-funded PhD scholarships. In the fourth year of the project, the two research associates will have finished their terms, but the CIs will continue to supervise all of the PhD students through to completion.

We anticipate a number of Honours and other student projects concerned with the overall context of our research as there are many fascinating mathematical and computing problems involved in developing robust simulations of environmental disasters.

Environment: 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 and a new building is presently being constructed at ANU to locate these two schools together. This co-location of academics in these two areas will be particularly fruitful for the present project.

Facilities: The ANU is well-endowed with suitable facilities to carry out this project. Of particular note is the new building mentioned above and the HPC facilities, and associated support, located on campus. Since the early 1980s, ANU has housed the largest supercomputers in Australia. The cloud computing facilities at the NCI national facility, located at ANU, will provide one of the testbeds for this project.

BENEFIT

Solutions to the core scientific problems identified with the three main aims of our project will be of high impact and will lead to the future development of software infrastructure for environmental disaster modelling including the quantifying of uncertainty, and for the software engineering use of live-coding in general. As noted above, we anticipate being able to win scholarship funding to add an additional three PhD students to the project team, and we will also supervise several undergraduate projects. We assess in our budgeting that an ARC investment of about $1Million will be accompanied by about $590K of cash and in-kind contribution from the ANU. The larger team of APA PhD students and undergraduate project students would increase this in-kind contribution to a nominal level of $850K.

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 addresses the mathematical challenges (through new approaches to uncertainty quantification) and the software engineering challenges (through live coding for rapid prototyping) and the systems support challenges (coping with volatile and rapidly changing systems environments) of this very important area.

In addition to the academic benefits of the research program described here, there are potential follow-on projects in close collaboration with industry and possibly even the seeding of spin-off 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 [17, 14] 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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