

# **Adapting massively parallel graphics processing units for geo-physical flow simulation with smoothed particle hydrodynamics.**

## **Case for support part a) previous track record**

**Dr. M. Bithell, Prof. K. Richards**  
Department of Geography, Cambridge University  
**Dr. D. Liang**  
Engineering Department, Cambridge University

**Dr. J. Brasington, Prof. N. F. Glasser**  
River Basin Dynamics and Hydrology Research  
Group Aberystwyth University  
**Dr. Igor Rychkov**  
PDRA to be based at Cambridge.

This proposal links together three departments with a track record in the modelling of fluid flow, and overlapping interests in the use of computation to understand and predict the effects of rapidly evolving flows both on the natural environment and areas of human habitation. Several members of the team have a past history of working together and regular group meetings will help both to strengthen existing working relationships and extend the base of shared knowledge amongst the project partners.

### **Project team and expertise**

The PI (MB) is currently assistant director of research in computing in the Geography department at the University of Cambridge. Past work has concentrated on numerical modelling of natural systems, including the ozone hole, stratosphere-troposphere exchange and climate modelling. Current research is interdisciplinary and directed toward understanding the interaction of environmental processes with human systems, and the adaptation of social dynamics to climate variability at a range of time-scales, particularly where this involves impacts on eco-systems and their interaction with water distribution.<sup>1-6</sup> Methodologically much of this work involves modelling the interaction of many particles, using computational tools that focus on discrete entities for the representation of social and natural systems. The current proposal builds both on expertise in modelling fluids, and more general computational expertise with high-performance computing and visualisation built up as a result of managing the IT strategy for the whole of the Geography department. The current project will provide an essential component for the extension of current work on the impact of natural hazards on human communities, especially those vulnerable to flooding.

DL is University Lecturer in Civil Engineering Fluid Mechanics at the University of Cambridge, with a joint position between Division A (Energy, Fluid Mechanics and Turbomachinery) and Division D (Civil, Structural, Environmental and Sustainable Development). Early work involved the study of scour around submerged pipelines, including modelling the transport of sediment and bed deformation by the flow. As part of an EPSRC project – ‘Flood Risk Management Research Consortium’ (GR/S76304) he was responsible for the development of computer models to predict shallow water flows<sup>7-13</sup>. A numerical scheme, which was first proposed for capturing shockwaves in supersonic air flows, was applied to predict the sharp water surface gradients near flood-fronts<sup>8-10</sup>. The depth-averaged surface and subsurface flow models were combined together to take into account the storage effects of buildings in a floodplain<sup>11</sup>. The two-dimensional flood routing model was dynamically linked with iSIS (a one-dimensional model owned jointly by HR Wallingford and Halcrow), so that water exchanges between floodplains and rivers could be simulated<sup>12</sup>. He was also a key player in developing GIS-based flood mapping software with a major consulting company in the UK. Current research focuses on the study of complex water and granular flows using the mesh-free Lagrangian approaches, including dam-break flows in which the the 3-D Navier-Stokes equations are solved using a Smoothed Particle Hydrodynamics (SPH) model<sup>14</sup>.

JB is director of the River Basin Dynamics and Hydrology Research Group at Aberystwyth University, which incorporates 9 full-time academic staff and 4 post-doctoral researchers. Interests include hydrological modeling, in particular rainfall-runoff and flood inundation modelling; fluvial sediment transport and gravel bed river processes, including monitoring and modeling sediment transport; environmental monitoring including terrestrial, airborne and satellite remote sensing, altimetry and GPS, and digital elevation modelling. Current research focuses on: the development of novel geomatics and remote sensing methods to study to evolution of river systems; methods for monitoring and modelling bed material fluxes and channel adjustment; and the development of numerical simulation models to study flood inundation and intermediate-scale geomorphological processes. JB has developed an international reputation for his work on fluvial geomatics and parallels this research with complementary interests in numerical modelling, in particular the development of reduced complexity hydrological and geomorphological models<sup>15-20</sup>.

IR's first speciality is in the statistical physics of macromolecules and molecular simulation, which he studied at Moscow State University and further extended at Kyoto University and Griffith University in Brisbane<sup>21-23</sup>. In 2007 IR came to the Institute of Geography and Earth Sciences at the University of Aberystwyth in order to develop physically based models of river flow, sediment transport and landscape evolution. IR has introduced the Smoothed Particle Hydrodynamics methodology to both landscape

evolution modelling and smaller scale geophysical fluid problems. Currently underway is development of a reduced-complexity 2D SPH model to serve as a replacement submodel for the water routing used in empirical cellular-automata models. At the same time, IR is developing a general 3D SPH model of water, sediment, and debris to address dam breaking and glacial lake outburst flooding among other problems. IR has also worked on a sub-project to characterize surface roughness and porosity, in order to correctly parameterize and hide boundary details in an SPH simulation.

### Steering committee

In addition to the PI and two Co-Is, a steering committee will assist with the management of the project. The additional members of this committee will bring considerable experience in environmental modelling and monitoring to bear on the project, and help to ensure that the software development is kept relevant to the NERC community and that its further adoption and development is likely. The committee will include the PDRA, investigators, KR, professor of Geography at the University of Cambridge, with a long-standing interest in flood hydrology and hydraulics<sup>2,5,6,15,17,18</sup> and NFG, professor of physical geography in the Institute of Geography and Earth Sciences at the University of Aberystwyth, with research expertise in the processes and reconstruction of glacial lake outburst floods<sup>24,25</sup>.

### Contributions to competitiveness and quality of life

The research team has a strong history of focussing research on major challenges related to environmental change, with contributions to NERC strategic science themes in the areas of climate, natural hazards, biodiversity and earth system science. The current proposal also promises to add to the NERC technology theme by increasing the effectiveness with which environmental processes can be modelled.

In addition both JB and DL have collaborations with engineering consultancies (Hannah Reed and Associates, JBA and Halcrow). JB also has a DTI funded partnership with Ambiental Plc to support transfer of new 2D codes for hydraulic modelling. He is also a member of the Aberystwyth University-based river science consultancy firm, Fluvio.

### References

1. Bithell, M., and Brasington, J., (2009), "Coupling agent-based models of subsistence farming with individual-based forest models and dynamic models of water distribution", *Environmental Modelling and Software*, 24, 173-190. doi:10.1016/j.envsoft.2008.06.016
2. Bithell, M., Brasington, J., and Richards, K.S., (2008), "Discrete-element, individual-based and agent-based models: tools for interdisciplinary enquiry in geography?", *Geoforum*, 39, 625-642. doi:10.1016/j.geoforum.2006.10.014
3. Bharwani, S., Bithell, M., Downing, T.E., New, M., Washington, R., and Ziervogel, G., (2005), "Multi-Agent Modelling of Climate Outlooks and Food Security on a community Garden Scheme in Limpopo, South Africa", *Phil Trans. Roy. Soc. Ser. B*, 360, 2183-2194.
4. Ziervogel, G., Bithell, M., Washington, R. and Downing, T., (2005), "Agent-based social simulation: a method for assessing the impact of seasonal climate forecast applications among smallholder farmers", *Agricultural Systems* 83, 1-26
5. Richards, K., Bithell, M., Dove, M and Hodge, R (2004) "Discrete element modelling: methods and applications in the environmental sciences." *Phil. Trans. Roy. Soc. London, Ser A* 362, 1-20
6. Richards, K., Bithell, M., and Bravo, M (2004) "Space, time and science: towards a geographical philosophy." In: *Common Heritage, Shared Future: Perspectives on the Unity of Geography*; eds Matthews, JA and Herbert, D T, London, Routledge
7. Liang D, Falconer RA and Lin B. Improved numerical modelling of estuarine flows. *Proceedings of the Institution of Civil Engineers – Maritime Engineering*, Thomas Telford, 2006, 159 (1): 25-35
8. Liang D, Falconer RA and Lin B. Comparison between TVD-MacCormack and ADI-type solvers of the shallow water equations. *Advances in Water Resources*, ELSEVIER, 2006, 29 (12): 1833-1845
9. Liang D, Lin B and Falconer RA. A boundary-fitted numerical model for flood routing with shock-capturing capability. *Journal of hydrology*, ELSEVIER, 2007, 332: 477-486
10. Liang D, Lin B and Falconer RA. Simulation of rapidly varying flow using an efficient TVD-MacCormack scheme. *International journal for numerical methods in fluids*, John Wiley & Sons, 2007, 53:811-826
11. Liang D, Falconer RA and Lin B. Coupling surface and subsurface flows in a depth averaged flood wave model. *Journal of hydrology*, ELSEVIER, 2007, 337: 147-158
12. Liang D, Falconer RA, Jiang C and Wang X. Numerical simulation of flood flows due to levee breaches. *Proceedings of 32nd IAHR Congress*, 2007, Venice, Italy, Theme A1.d, pp 1-10
13. Liang D, Falconer RA and Lin B. Linking one- and two-dimensional models for free surface flows. *Proceedings of the Institution of Civil Engineers – Water Management*, Thomas Telford, 2007, 160: 145-151
14. Liang D. Examining shallow water assumptions for modeling dam-break floods. *SPHERIC newsletter*, 2008, 5: 4 (<http://wiki.manchester.ac.uk/spheric/>)
15. Richards, K.S., Brasington, J. and Hughes, F.R.M. 2002. Geomorphic dynamics of floodplains: ecological implications. *Fresh. Biol.*, 47, 559-579.
16. McMillan HK, Brasington J. 2008. End-to-end flood risk assessment. *Wat. Resour. Res.*, 44, W03419.
17. Brasington J, Richards K. 2007. Reduced-complexity, physically-based geomorphological modelling. *Geomorph.* 90: 171-177.
18. Hodge R, Richards K, Brasington J. 2007. A physically-based bedload transport model. *Geomorph.* 90: 244-262.
19. McMillan HK, Brasington J. 2007. Reduced complexity strategies for modelling urban floodplain inundation. *Geomorph.*, 90: 226-243.
20. Brasington J, Vericat D, et al. 2008. Reach-scale retrieval of alluvial bed roughness. *EGU Meeting*, 10: EGU2008-A-01295
21. Rychkov, I. 2005. Block copolymers under shear flow. review. *Macromolecular Theory and Simulations*, 14:207 – 242.
22. Rychkov, I. And Yoshikawa, K., 2004. Structural changes in block copolymer solution under shear flow as determined by nonequilibrium molecular dynamics. *Macromolecular Theory and Simulations*, 13:257.
23. Rychkov, I. and Yoshikawa, K., 2004. Nonlinear rheological behavior associated with structural transitions in block copolymer solutions via nonequilibrium molecular dynamics. *Journal of Chemical Physics*, 120:3482.24
24. Quincey DJ, Richardson SD, Luckman A, Lucas RM, Reynolds JM, Hambrey MJ, Glasser NF. 2007. Early recognition of glacial lake hazards in the Himalaya using remote sensing datasets. *Global and Planetary Change*, 56:137-152.
25. Hambrey, M.J., Quincey, D.J., Glasser, N.F., Reynolds, J.M., Richardson, S.J., Clemmens, S. 2008. Sedimentological, geomorphological and dynamic context of debris-mantled glaciers, Mount Everest (Sagarmatha) region, Nepal, *Quaternary Science Reviews* 27, 2361–2389

# Adapting massively parallel graphics processing units for geo-physical flow simulation with smoothed particle hydrodynamics.

## Case for support b) scientific rationale

### 1. Introduction

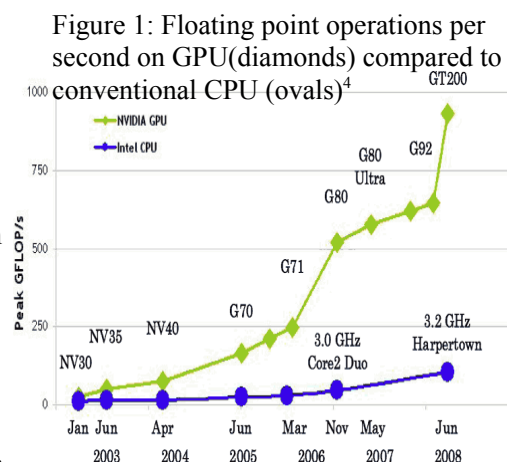
#### 1.1. Project outline

This project will develop a fluid-flow modelling system based on smoothed particle hydrodynamics (SPH) that will run on a new generation of computational hardware based on graphics processing units (GPU). The resulting computational engine is aimed at the simulation of near-surface flows in which the boundaries are often mobile and change rapidly, and which transport significant debris and suspended matter. Examples include glacial outburst floods, lahars, jokulhaups, debris flows and dam-breaks, and at larger scales tsunami, storm surges and flash floods. These represent serious hazards to vulnerable communities, but also present a number of challenges to conventional fluid modelling techniques<sup>1-3</sup>. Many of these hazards may also be of growing significance in the light of climate change. These technologies (SPH and GPU) are currently at the stage where integration is required to bring the new hardware and software together in to applications that have geo-physical relevance, and where development of expertise in the required programming techniques needs to be acquired and made available to the NERC community. As such the level of readiness is at TRL3/4, where prototype applications can be developed and benchmarked against existing solutions that attempt to solve similar problems. The potential benefit is to make highly-parallel, fast, mixed-phase fluid/solid and debris-flow codes at a small fraction of the current cost for conventional parallel hardware.

#### 1.2. Hardware considerations

Along with the exponential increase in processor power over the last few decades, a separate strand of development has been taking place in the evolution of computing hardware, namely a rapid increase in the capability of Graphics Processing Units (GPU), in terms of individual core speed, memory access times and parallelization. Indeed, the rate of increase has been larger in recent years than for more general purpose CPU. This has now reached the stage where the typical budget graphics card has 32 cores (often referred to as stream-processors), while high specification cards may contain up to 480 cores yet cost as little as £400. One manufacturer currently quotes computational capability for such devices on the order of 3-4 TFlops, comparable with large-scale compute clusters but at a fraction of the cost. For comparison, the Cambridge HPC computer cluster has 2000 cores and a performance in the range 18-28TFlops (see [www.hpc.cam.ac.uk](http://www.hpc.cam.ac.uk)), but a total installation cost of several million pounds. Rapid increase in memory on these cards (one can currently get up to 4GB per card), is also extending the scale of problem amenable to GPU processing.

In practice the architecture of such devices, in particular the arrangement of internal memory and cache, and the latency with which operations may be carried out, means that direct core-for-core comparison of graphics cards with more traditional parallel CPU arrangements is not meaningful – however, it appears that for some applications a 240 core GPU is capable of delivering much the same performance as a 32 core CPU cluster (see for example [www.ameslab.gov/hoomd/benchmarks.html](http://www.ameslab.gov/hoomd/benchmarks.html)). This tremendous increase in price-performance offers the possibility for massively parallel computing to be delivered at low cost on current desktop computers. Although GPU computing has been possible for a number of years, new software libraries have now significantly simplified the process of developing applications that use GPU for numerical computation. The Nvidia CUDA library, for example, is freely available and specifically aimed at the development of code that exploits the parallelism of GPU for numerical computing. This library in particular includes a development path that, whilst it currently only supports C as a programming language, is planned to incorporate FORTRAN and C++ in the near future. The driving forces behind this technology, namely the computer games and movie industries, are sufficiently well resourced that the rapid advancement of the technology seems likely to continue for the foreseeable future. Other manufacturers are also beginning to develop libraries that likewise are able to exploit the possibilities inherent in stream-processor hardware – examples are Intel's Ct programming model and Apple's OpenCL. However, implementations of these latter frameworks appear to be further from practical application than the CUDA library, for which fully functional code is available ([www.nvidia.com/cuda](http://www.nvidia.com/cuda)).



Although the availability of such libraries eases the process through which this technology can be exploited, the architecture differences from conventional CPU are significant: it is not possible to simply adapt traditional (MPI-based) parallel code and obtain optimal performance. New code needs to be written that uses the architecture efficiently. Expertise currently focussed on developing MPI-based applications (as, for example in the climate modelling community) does not translate to directly to making use of this new technology (although some parametrizations in climate models that are otherwise MPI-based can be ported to GPU hardware<sup>5</sup>). The need therefore exists to develop code directed at geophysical applications that will promote rapid adoption within the NERC the community by making relevant applications freely available.

### 1.3. Smoothed Particle Hydrodynamics (SPH)

SPH is a mesh-free, fully Lagrangian method that simulates fluid flow by tracking the motion of a set of sample particles that represent individual fluid masses. It is one of a family of particle-based methods for granular and fluid flow simulation<sup>6,7</sup>. Pressure forces are calculated by using averages over neighbouring particles and these are used directly to accelerate the particle field. As such it gives direct solution of the advection problem, with very accurate non-diffusive tracer transport, accurate mass conservation, and easy representation of free surfaces, including regions of wetting and drying. In addition it adapts straightforwardly to dynamic and irregularly shaped boundaries, and can be modified to simulate the associated transport of rigid bodies and suspended particulate matter. SPH can also be adapted to simulate flow through porous media and thermodynamic phenomena such as freezing and thawing, and the collapse of semi-solid or composite barriers under internal or external stresses<sup>7</sup>.

Although fixed- and adaptive mesh methods have been developed to simulate dynamic, free-surface and mobile flow phenomena, SPH permits the generation of complex, 3d flow structures and rigid body interactions naturally, and without the need for persistent, computationally expensive re-gridding. To date, a variety of SPH codes have been developed: however none of these fully exploit GPU technology and those currently emerging are closed-source or directed at non-geophysical applications such as computer graphics, where the target is convincing visualization rather than precision and accuracy. Despite the clear potential gains of developing optimized SPH for geophysical applications, the method remains largely unexploited within the NERC community. The slow adoption of this technology, is, in large part, due to the computationally intensive nature of the method, so that the development of an efficient GPU code is now timely. The slow uptake within the geophysics community is however, in contrast to advances made using SPH in astronomical simulation<sup>9,10</sup>. In this context, MPI-parallel versions of code have specifically been developed to enable large scale models, albeit dependent on expensive supercomputing hardware<sup>11</sup>. While these codes provide a useful template for the development of geophysical SPH, the unconstrained nature of astronomical simulation is unlike typical boundary layer, geophysical flows which are strongly controlled by their topographic boundary conditions. Nonetheless, geophysical applications of SPH are beginning to emerge in a variety of contexts<sup>12-18</sup>, but to date, remain to be fully parallelized and are thus restricted to very narrow spatial and temporal domains.

Developments in discrete computation in other fields have however, indicated the potential of GPU based optimization of particle-based simulation technologies; for example, efficient particle-based GPU code is now freely available for molecular dynamics simulation<sup>19</sup>. This project seeks to adapt these novel parallelization routines for use in geophysical SPH applications. The specific challenge for particle methods is the need for an efficient method of finding the nearest neighbours to any single particle, given that the particles move in an unstructured fashion in three dimensions. This problem has been solved efficiently in molecular dynamics: however, these codes lack the geometric boundary conditions, dynamics of particle interaction and constitutive equation set appropriate for fluid flow simulation. These deficiencies can be remedied using existing SPH algorithms that are available through open-source serial codes<sup>20</sup>, and also in existing SPH code developed by one of the Co-Is (DL). :-

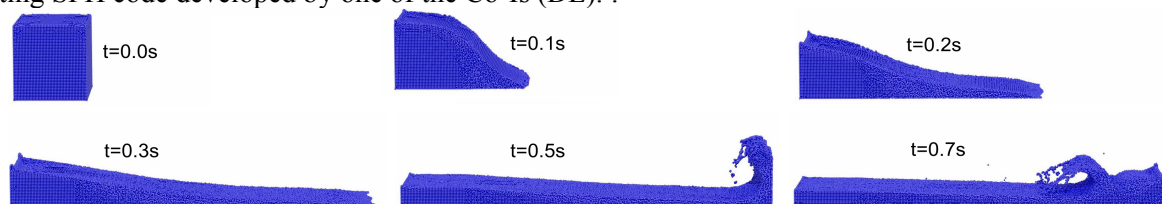


Figure 2: SPH simulation by DL of a  $0.1 \times 0.1 \times 0.1 \text{ m}^3$  water column collapse in a  $0.5 \times 0.1 \times 0.1 \text{ m}^3$  flume

Our primary aims (detailed below) can therefore be met, by integrating pre-existing codes and techniques in order to take advantage of the rapidly advancing GPU technology.

## 2. Aims, Objectives and Wider Relevance

The above introduction suggests that we may be about to witness an order of magnitude change in the availability of highly parallel computing hardware at the small desktop or medium-scale server level. With suitable code, researchers will be able to simulate much larger computational problems (i.e., larger spatial extents, longer duration events, higher resolution dynamics) than previously possible and, moreover, implement this increased computational intensity at low levels of power consumption and with lower a capital outlay. We aim to provide a set of tools for simulation of fluid flow that will allow researchers in the NERC community and in the wider environmental fluid-simulation community to take advantage of this development quickly and easily. For example, we intend that those involved in flood simulation would be able to take advantage of our simulation framework with minimal adaptation, an area which will be of growing importance in future planning for environmental change. Those engaged in modelling of fluid flow for assessing hazard risk in the engineering or town planning fields should also find these models of benefit.

Specifically we aim to:-

O.1. Build a GPU-enabled SPH code suitable for use in geo-physical applications, particularly flows involving water at the Earth's surface. Test the code for stability and internal consistency.

O.2. Test the GPU code against the same set of algorithms running on traditional CPU. Test the GPU enabled code for scalability on different graphics hardware and on GPU clusters.

O.3. Include tests of a variety of boundary models and a variety of different implementations of particle search for their effectiveness in the GPU environment. Include moving boundaries and large suspended solid particles as part of the SPH code.

O.4. Test against code validation datasets. Benchmark the GPU code against traditional fixed-mesh scalar 3D code as currently used for the extreme flow simulation problem associated with outburst floods (dam-break and glacial lake outbursts).

## 3. Methodology

As this is an integration project, we do not expect that all code will need to be generated from scratch. Where possible we will use open-source code that has already solved some of the problems involved in implementing GPU code.

### Particle code and SPH(O1)

As highlighted above, a core component of the SPH method is the need to find neighbouring particles efficiently in order to make the force calculation. This is typically achieved by 'bucketing' the particles into a regular grid, so that nearby particles are easily located in neighbouring (coarse resolution) grid cells. Since SPH requires a local force calculation, this gives an adequate solution to the search problem. However, in order to exploit the hardware efficiently it is necessary to have neighbouring particles in nearby memory locations, and, in general, this means that particles need to be periodically re-ordered in memory as particles change their neighbours during the evolution of the flow. Various techniques exist to manage this problem – notably graph partitioning algorithms, or those based on space-filling curves<sup>11,19</sup>. Experience from within the molecular dynamics community suggests that the space-filling curve approach is more efficient, at least for a slightly older generation of hardware<sup>19</sup>. However, more recent GPU support atomic writes, which allow multiple threads to update global memory independently without conflicts<sup>20</sup>, and this may make a more direct bucketing approach, in which cell occupancy is re-calculated at frequent time-steps equally efficient. For this part of the project, we will review open-source code available from [www.ameslab.gov/hoomd](http://www.ameslab.gov/hoomd) and [nVidia](http://nvidia.com)<sup>20</sup> and adapt these for SPH flow dynamics (c.f. Figure 2 and [21]), incorporating simple static boundary conditions (e.g. flow inside a rigid box). We will then evaluate the speed-up factor of the different algorithms on available hardware versus running the same code on a single conventional CPU.

### Multi-GPU code(O2)

Once we have developed a single GPU-based SPH code, we aim to extend this for direct application on cost-efficient multiple graphics processors. Typically, current top-of-the-range cards are restricted 4GB of memory. This clearly poses a limitation on the size of physical system that can be simulated. However, multiple GPU units can be housed within the same chassis (see for example the Nvidia S1070 which incorporates up to four GPU cards each with 4GB of memory and a total of 960 stream processors). Additionally, depending on the interconnect between GPUs, the scope for further accelerating computation exists by subdividing the computational domain. We will investigate extensions to the single GPU code, by both making use of multi-GPU aspects of the CUDA library, and by using more conventional MPI-based techniques to distribute code over multiple processors<sup>22</sup>. The latter has the advantage that it makes available

a pathway for acceleration of other existing MPI-based code by accelerating those portions that are adaptable to GPUs.<sup>5</sup>

### Boundaries and solid matter(O3)

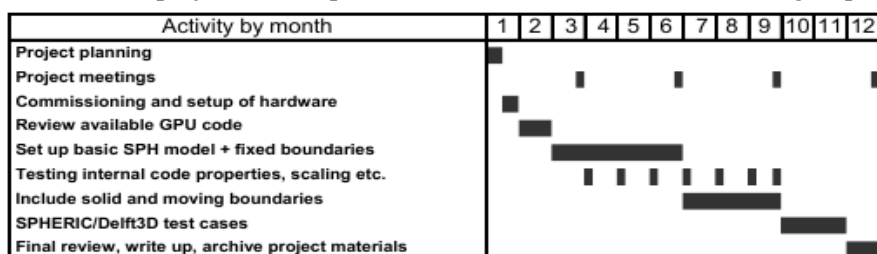
Geometric boundaries in SPH can be treated in a number of different ways. While it may be simpler from the geometric point of view to discretise the boundary using simple primitives, such as sets of bounding planes, this approach oversimplifies the resulting flow dynamics represented by the SPH particles. Alternatives to this simplification include the use of ghost or mirror particles that have the same pressure and density values as an interior fluid particle, but a velocity and position reflected through the boundary surface. This adds computational complexity as it requires extra particles to be dynamically added and removed from the system. In practice it generally proves more useful to represent boundaries using particles with a slightly altered representation of the dynamics – for example boundary particles with prescribed velocities, but which follow the pressure of the neighbouring fluid. Dummy particles can also be used outside solid surfaces in order to match the interior fluid density. The latter approach also gives the option to include large suspended or moving solid objects, binding together the boundary particles so that forces can be transmitted elastically between them<sup>8</sup>, and then allowing the assemblage of bound particles to be moved by the SPH flow. This further allows solid surfaces to be dissolved or melted into the fluid by disaggregating the bound particle clusters, so that we can start to model disintegration and collapse, and thereby study embankment breaches or dam-breaks, including the break-down of the initial barrier confining the fluid, and its advection downstream as large debris. The same sort of mechanisms can also be used to change the shape of bed surfaces dynamically according to the local shear stress. In this case, however, we need to include the possibility of small particulate material being added to the flow. In general the number of SPH particles needed to model a region of interest, such as a river reach below a dam, will not allow for small particles to be directly resolved. These therefore need to be incorporated as a modification to the density and rheology of the flow by passing estimates of the local small-particle density between the SPH particles representing a much larger volume of fluid. The major advantage of SPH here is that the suspended material is accurately advected in the absence of turbulent mixing or settling. In general, however, this is a rather complex problem, as the diffusion of particles through the flow will be mediated by un-resolved turbulent eddies, and the flow rheology is not in general known a-priori, but will depend both on the density and character of the fine suspended material. For this reason in the current work we will initially concentrate on the formulation for incorporating large debris, and use simple parametrizations for any fine suspended material (e.g. modelling this as a Bingham fluid for the rheology<sup>23</sup>, plus the standard diffusion equation for calculating movement of sediment between SPH particles. ).

### Testing (O4)

Initially we will need to test the code for stability, convergence, robustness and internal consistency. Tests at this level will be built into the code as it is developed in a module-by-module basis so that any code-modifications can be run through a standard test suite as soon as they are implemented. This will also facilitate later code development by others. The model output will then need to be validated to ensure fidelity to fluid flow and maintenance of accuracy with changes of resolution. For this purpose we will use the datasets that can be found at the Smoothed Particle Hydrodynamics European Research Interest Community (SPHERIC) website ([wiki.manchester.ac.uk/spheric](http://wiki.manchester.ac.uk/spheric)). These data provide information on initial conditions, velocity profiles and surface wave-forms for a variety of experimental set-ups. Finally we will test the code against a typical grid-based serial code that has been used for outburst flood modelling, such as Delft3D<sup>25</sup>.

#### 4. Programme and plan of research

The research will take place in five sections:- 1)Project planning and initial commissioning and set-up of the hardware, ensuring that the correct libraries are in place and running smoothly (1 month). 2) Review of pre-existing GPU codes (1 month) 3)Major code development to get the SPH algorithms set-up and running (4 Months ) 4) Include large solid matter and moving boundaries (3 months). Internal consistency testing of serial code and test of code running on conventional CPU against GPU code, including test of boundary algorithms, test of scaling of parallel code over different classes of GPU and on multi-GPU clusters will take place alongside the code development. 5)Testing and validation of output using datasets from the SPHERIC website and test against serial code such as Delft3D in one case of geo-physical relevance (2 months). One month will be set aside for project write-up, dissemination of results and archiving of project materials.



## 5. Project Management

The project will be managed by MB, who will take on the day-to-day supervision of the PDRA and the general tasks of keeping the project on track. Expertise and guidance will be provided by the Co-Is who will also be involved in code development (DL) and testing (JB) and ensuring that the project produces useful and meaningful geo-physical outcomes. A steering committee comprising the PI, Co-Is, PDRA and KR + NFG will also be established to help ensure that the project goals are being met and to advise on dissemination, distribution and archiving of the project material. Quarterly meetings of the project team will be held, including the steering committee, in order to ensure adequate communication between team members.

## 6. Deliverables and stewardship

The primary output will be fully documented open-source SPH code that will run on widely available hardware and is designed for use with highly dynamic surface flows. This will make particle-based geo-physical fluid code a practicable tool for running on desktop machines at scales that are of interest to hydrologists, geomorphologists, sedimentologists, planners and engineers. Additionally it will deliver the ability to include dynamic surfaces, large particulate matter, and to model collapse of solid structures in much decreased model-run times compared with current serial code. Documentation will be made using a standard source-code annotation system such as Doxygen that produces output in both html and pdf, suitable for wide dissemination. Since the developments will be based on open-source code, the products of the project will also be open source and freely available for modification by others.

Datasets and software will be made available initially on a project website. At the end of the project these will be copied to a long term archive with public access such as the Cambridge DSpace system and suitable NERC datacentres. Publications will be submitted to international journals and conferences as appropriate during the lifetime of the project.

## 7. References not included in part A above

- [1] Liang, D., Lin, B. and Flaconer, R.A. (2007) A boundary-fitted numerical model for flood routing with shock-capturing capability. *Journal of Hydrology* 332, 477-486.
- [2] Kruger, S., Rutschmann, P., Causon, D., Mingham, C. and Ingram, D. (2001). Discussion. Advances in calculation methods for supercritical flow in spillway channels, *Journal of Hydraulic Engineering* 127, 328-330
- [3] Lackey TC and Sotiropoulos F. (2005). Role of artificial dissipation scaling and multigrid acceleration in numerical solutions of the depth-averaged free-surface flow equations. *Journal of hydraulic engineering*, 131, 476-487.
- [4] NVIDIA CUDA Programming Guide 2.1, <http://developer.nvidia.com/object/cuda.html>.
- [5] Michalakes, J. and M. Vachharajani: GPU Acceleration of Numerical Weather Prediction. *Parallel Processing Letters* Vol. 18 No. 4. World Scientific. Dec. 2008. pp. 531--548.
- [6] J. J. Monaghan, (2005). Smoothed particle hydrodynamics, *Rep. Prog. Phys.* 68, 1703–1759.
- [7] Koumoutsakos, P., (2005). "Multiscale flow simulations using particles". *Ann. Rev. Fluid Mech.* 37:457-487
- [8] Keiser, R., Adams, B., Gasser, D., Bazzi, P., Dutre, P., Gross, M., (2005). A unified Lagrangian approach to solid-fluid animation, *Point-Based Graphics*, 2005. Eurographics/IEEE VGTC Symposium Proceedings, 125-148
- [9] Lucy, L.B. (1977). A numerical approach to the testing of the fission Hypothesis. *Astron. J.* 82, 1013-1024.
- [10] Gingold, R.A. and Monaghan, J.J., (1977). Smoothed Particle Hydrodynamics: theory and application to non-spherical stars. *Mon. Not. R. Ast. Soc.* 181, 375-389.
- [11] Springel, V. (2005). The cosmological simulation code Gadget-2.0. *Mon. Not. R. Ast. Soc.*, 364, 1105-1134.
- [12] Cleary, P.W. and Prakash, M., (2004) Discrete-element modelling and smoothed particle hydrodynamics: potential in the environmental sciences. *Phil. Trans. Roy. Soc.*, 362, 2003-2030
- [13] Monaghan J.J. (1994). Simulating free surface flows with SPH. *Journal of computational physics*, 110: 399-406.
- [14] Shao S and Lo EYM. (2003). Incompressible SPH method for simulating Newtonian and non-Newtonian flows with a free surface. *Advances in water resources*, 26: 787-800.
- [15] Dalrymple RA and Rogers BD. (2006). Numerical modeling of water waves with the SPH method. *Coastal engineering*, 53: 141-147.
- [16] Morris JP, Fox PJ and Zhu Y. (1997). Modeling low Reynolds number incompressible flows using SPH. *Journal of computational physics*, 136: 214-226.
- [17] Monaghan JJ, Kos A and Issa N. (2003). Fluid motion generated by impact. *Journal of waterway, port, coastal and ocean engineering*, 129(6): 250-259.
- [18] Antoci C, Gallati M and Sibilla S. (2007). Numerical simulation of fluid-structure interaction by SPH. *Computers and structures*, 85: 879-890.
- [19] Anderson, J.A., Lorenz, C.D. and Travesset, A. (2008). General purpose molecular dynamics simulations fully implemented on graphics processing units. *Journal of Computational Physics* 227 (2008) 5342–5359
- [20] [www.nvidia.com/content/cudazone/cuda\\_sdk/samples.html#particles](http://www.nvidia.com/content/cudazone/cuda_sdk/samples.html#particles)
- [21] SPHysics - open-source smoothed particle hydrodynamics code <http://wiki.manchester.ac.uk/sphysics/>.
- [22] John E. Stone, J.C.P., 2007. Accelerating molecular modeling applications with graphics processors. *Journal of Computational Chemistry*, 28(16), 2618-2640.
- [23] Rodriguez-Paz, M.X., and Bonet, J. (2003) A corrected smooth particle hydrodynamics method for the simulation of debris flows, *Numerical methods for partial differential equations*, 20, 140-163.
- [24] John Biddiscombe, David Graham, Pierre Maruzewski Interactive Visualization and Exploration of SPH Data SPHERIC second international workshop, 51-54.
- [25] Carrivick, J.L., Manville, V. and Cronin, S.J., (2007). A fluid dynamics approach to modelling the 18th March 2007 lahar at Mt. Ruapehu, New Zealand. *Bull. Volcanol.* DOI 10.1007/s00445-008-0213-2