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Final Report: to EOARD re FA8655-07-1-5049
Workshop: Multiscaled Mathematics in Defense Research and its Spinoffs

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(1) Background /context

International and interdisciplinary researchers of highest quality were drawn together by multi-scaled modelling, analytical and computational challenges, Defense-related mathematics and the numerous spin-off areas. Support was kindly provided by EOARD and EPSRC UK. The workshop held at the Lighthill Institute <<http://www.ucl.ac.uk/lims/>> in May-June 2007 posed new questions to be addressed and discussed non-traditional methodologies. Academia and industry were represented. The growth of interest in biomedical modelling, terrain modelling, impact problems, multi-material predictions and multi-body analyses as well as in social and related issues, homeland security, terrorism and safety was also reflected well in the list of participants.

(2) Key advances and supporting methodology

The major research achievements included much new interaction between participants and their areas along with novelty in terms of methodologies. Advances and methodologies are described under 'DETAILS' below.

(3) Project plan review

The workshop went largely as planned except that the timetable was slightly altered to provide an improved iteration method between active and passive participation, i.e. between talks and discussions. The participants' enthusiasm aided the progress, as did the mixture of their different backgrounds. The rest of the workshop proceeded broadly as proposed.

(4) Research impact and benefits to society

Some of the impact and benefits are covered in detail under (2). The impacts and benefit are multi-faceted from this workshop. Many collaborations were reinforced or began. Close interest from industry included QinetiQ, Dstl [dstl] and Airbus, while Schlumberger came to mind in many areas. Progress towards future potential exploitation is via the collaborations and industrial links just mentioned and via other industry as well as related academia.

(5) Explanation of expenditure

Expenditure went largely as planned.

(6) Further research or dissemination activities

Plans are afoot for much further work, for instance in terms of new research, proposals, visits and presentations some of which have already been instigated. Dissemination includes the detailed summaries which are to be placed on a secure website at LIMS <<http://www.ucl.ac.uk/lims/files.htm>>.

DETAILS

Highlights

Group discussions, summaries, new interactions and recommendations were the highlights of the event. This included publicising certain difficult industrial problems that would benefit from academic involvement in an environment which encouraged such involvement and which would therefore stimulate new research proposals.

Structure of the workshop itself

The structure and methodology relied first on an appropriate mixture of researchers, from the UK and abroad, from academia and industry, from Applied Mathematics and a large number of other disciplines, altogether reflecting the workshop aims as regards industrial, biomedical, environmental and social modelling. This mixture appeared to work. Virtually all the participants (including seven doctoral students) joined in wholeheartedly. The main schedule consisted of alternating sessions of invited short talks (chaired by Paul Dellar, John Ockendon, Stephen Wilson) and breakout group discussions (the leaders of which are mentioned later). In between were suitably lengthy refreshment breaks which also allowed free discussion, while at the end a summary session was held. The detailed pre-workshop schedule is given on the website mentioned earlier in this report and it was followed fairly closely. Yet the event overall was an organic affair with the workshop not being too regimented and with a lot of intellectual leadership coming through the breakout-group activities as it should.

There were at least four breakout groups during each of the three assigned breakout periods of the workshop. The groups were based on the principal planned themes of biomedical /human-risk-interface, terrain /geophysical problems and impact /multi-particle problems, but in addition spinoffs occurred as expected.

The research discussions and actions

- o The talks at the workshop were these:
 - *Long-range forecasting of atmospheric conditions: a mix of weather and climate scales*: Mick Davey, UCL-LIMS
 - *Uncovering physical phenomena with stochastic optimization*: Michele Milano, ASU (Arizona State University USA)
 - *Cerebrovascular modelling for extreme situations*: Nick Ovenden, UCL-LIMS
 - *Interactions of explosives and confinement*: Gary Sharpe, Leeds
 - *Modelling sand movement*: Steve Bishop, UCL-LIMS
 - *Nonlinear multiscale dynamics, nested modeling and HPC simulations of terrain influenced atmospheric flows*: Alex Mahalov, Basil Nicolaenko, Joe Fernando (presented by Alex Mahalov), ASU
 - *Multiscale problems of explosive response, penetration and unrest*: John Curtis, QinetiQ
 - *The runout of the collapse of a granular column*: John Hinch, Cambridge
 - *Simulation models for mesoscale systems: between discrete event simulations and continuum approximations*: Dieter Armbruster, ASU
 - *An environmental stress index and monthly prediction*: Bernd Becker, Meteorological Office
 - *Advanced imaging and web-GIS techniques for terrain and impact crater modelling*: Peter Muller, UCL
 - *Some open icing problems*: Richard Purvis, UEA
 - *Challenges faced by the interventional neuroradiologist*: Fergus Robertson, National Hospital for Neurology & Neurosurgery (NHN) London
 - *A talk on latest HPC developments*: Dan Stanzione, ASU
 - *Computations on environmental modelling*: Nikos Nikiforakis, Cambridge
 - *A talk on recent developments in impact modelling*: Alexander Korobkin, Novosibirsk Russia

(The final three talks above were spontaneous offerings at the event. Most talks touched on more than one of the workshop themes, and all or almost all talks fed into the breakout groups below. Copies of the presentations are on the website.)

- o The breakout discussions took place predominantly in the following groups:
 - *Biomedical modelling* led by Alistair Fitt, Nick Ovenden, with Robert Bowles, Sarah Waters, James Oliver, Douglas Cochran, and many others.
 - *Air Vehicles* led by Malcolm Arthur, with Sergei Timoshin, Andrew Lacey, Stephen Wilson, David Allwright, and several others.
 - *Violent Mechanics* led by John Ockendon, Mark Cooker, with Adrian Jones, John Curtis, Gary Sharpe, Mohammed Luheshi, Roman Novokshanov, Andrew Belyavin, Malcolm Cook, and others.
 - *Aspects of impacts* led by Richard Purvis, Guo-Xiong Wu, James Oliver, with Anthony Pollitt, Andrew Ellis, Alexander Korobkin, Peter Hicks, Ian Ford, Fariba Fahroo, Jean-Marc Vanden-Broeck, and others.
 - *Impacts and Craters* led by Peter Muller, with Anthony Pollitt, Frank Smith, Andrew White, and others.
 - *Social modelling* led by Dieter Armbruster, Nick Ovenden, with David Allwright, Robert Bowles, Douglas Cochran, Alistair Fitt, Stephen Glavin, Anthony Hutton, George Klokakis, Andrew Lacey, Alex Smith, Sarah Waters, Alex White, Guo-Xiong Wu and many others.
 - *Terrain and environment modelling* led by Mick Davey, Ian Eames, with Robert Peck, Andrew White, Peter Muller, Joe Fernando, Dan Stanzione, Michele Milano, Alex Mahalov, Basil Nicolaenko, Bernd Becker, Andreas Baas, Andrew Fowler, Paul Dellar, Steve Bishop, Ted Johnson, and many others.

(Copies of the detailed notes on these discussions are available on the website.)

- o Informal discussions also took place at the various breaks and during an evening dinner arranged during a cruise on the Thames.

Outputs

- o Several principal foci emerged by the end of the workshop, leading to 5-7 summaries. These summaries of the group discussions were presented on the final afternoon and are as follows.

Biomedical research (summarised by Alistair Fitt and Nick Ovenden)

The following problem areas arose specifically from concern with cerebral networks and arterio-venous malformations (AVMs), after illuminating discussions with Fergus Robertson of the NHNN, although the application is much wider.

- a) Patient-specific computational modelling of the flow of a tracer through an abnormal vascular structure such as an arteriovenous malformation or an aneurysm. Model should be able to compute the flow in a matter of hours and highlight regions of fast flow, high wall shear stresses and high pressures. The computational platform could be based at UCL using codes developed by Guo Xiong in Mechanical Engineering and colleagues, using lattice-Boltzmann methods (Peter Coveney) or perhaps using a larger platform such as the Centre for Fluid Modelling and Simulation (CFMS), mentioned by Anthony Hutton and currently under development with DTI funding.
- b) A second related problem would be to develop a generic AVM model (consisting of some well-defined multiple branching structures) and resolve the flow in that when coupled to a simplified model of the normal vasculature. The circle of Willis could serve as a focus. This could be used as a benchmark for computational and other methods. Aneurysms and the flow disturbances due to them were mentioned in discussions together with the elasticity of materials, second lobes, and calculation methods. Paul Dellar noted CFD being done currently addressing properties elsewhere in the body, a point also made in the breakout group.
- c) The homogenization of a large network of many branchings into a continuum model appears to be a challenge that could easily form a clear goal of a PhD or other programme in this field. Taking a multiple-branching tree with N generations as N tends to infinity with nonlinear rules at each junction with mild alterations in the structure across the branching downstream was agreed to be an unsolved and useful problem to tackle for research involving very large networks. John Ockendon, Paul Dellar and group members noted possibly relevant work on rivers and estuaries.
- d) The solidification of glue in a fistula. The fistula would be a single flexible tube vessel with varying compliant properties upstream and downstream. The idea would be to examine the gradual setting of a bolus of glue, via its contact reaction with blood and diffusion, as it travels downstream. Extensions include examining how the bolus behaves near a bifurcation or how the addition of a side branch expelling blood affects the shape of the bolus. This task has a clear link to the embolization of an arteriovenous malformation. Two- and three-phase solidification problems in vessels and porous-medium analogies were also noted.
- e) A final paradigm proposed problem is to examine the way an abnormally low resistance connection between arterial and venous systems, such as a fistula or an arteriovenous malformation, *steals* blood supply from normal brain tissue. The idea is to model unsteady flow through a fistula and a branching network consisting of normal vessels and examine how the highly distensible venous system behaves and if the lower perfusion of blood through the normal vasculature is primarily caused by high unsteady venous pressures.

Air vehicle research (summarised by Malcolm Arthur)

Issues arising from the breakout group were summarised as follows.

- a) Significant questions concerned aero-elastic effects for endurance UAVs (which have unusual shapes and flexibility), aerodynamics with control systems and control effectors, and icing on rotorcraft (the formation, subsequent break-off and trajectories) as well as on fixed wing vehicles (formation, removal and engine intake difficulties) and in terms of self-adapting control in response to ice.
- b) Rotorcraft also suffer from sand or snow recirculation and from erosion of blades by sand, hail or ice fragments.
- c) Problems arise in assembling tools from component parts such as boundary-layer models with aero-elasticity, suitable sufficient resolution of physical processes, grids and algorithms self-adapting to the flow regime (e.g. turbulent motions), black-box modelling. Computer hardware exploitation, prediction of vortex breakdown positions and laminar flow control through distributed roughness are also crucial but problematic.
- d) Modelling to utilise the full flight envelope (UCAVs), to reduce noise in the cabin of or radiated from a rotorcraft, and to help decision-making on which vehicles were also mentioned.
- e) Highlighted modelling opportunities are in boundary layers with aero-elasticity, in the $2/3$ law for laminar flow control, in control of ice break-off, in sand and hail blasting, and in exploiting adaptive grids. Frank Smith mentioned work on boundary layers with flexible walls, forming a biomedical connection, and interacting boundary layer studies which may be relevant.

Violent mechanics (summarised by Mark Cooker)

The main points to emerge from this group are as follows.

- a) Short time scales and high strain rates are typical features. The applications and motivations concern shaped charges, detonation and blasting. Theory and analysis on fluids, solids and thermo-mechanics are key here.
- b) Research is required on detonation mechanics: casing deformation, fluid modelling, casing fracture, Gurney's law, and shaped charge geometries are all very open to questioning and improvement.

- c) Rock blasting involves many time scales and physical processes; there is detonation with expansion of gas into rock and fractures; movement of the rock; movement of the debris. Comparison exists with shrapnel modelling and there are connections with so-called behind armour damage.
 - d) In penetration of a shaped charge jet fundamental questions surround the penetration speed, the depth, the mechanics, in addition to the possible plasticity of the target material. Similar problems occur with rod penetration especially with regard to the break-up of the rod after penetration.
 - e) Sand penetration was also mentioned, including the model treatment of sand as a fluid and issues associated with wet sand.
- Work by Ian Eames possibly relevant to e) was mentioned by a participant. The multi-scale nature of the area is clear.

Aspects of impacts (summarised by Richard Purvis)

Quite specific points were made.

- a) Inkjet printing, icing on blades and elsewhere, and slamming-type impacts are of concern.
- b) Research is needed on: comparisons between asymptotics (e.g. for small or large times) and relatively direct numerical work; and effects which are usually neglected such as in air cushioning, bubbly liquid entrapment, elastic bases, three spatial dimensions, liquid-liquid impacts and planing.
- c) Drying of inkjet ink after impactation, and droplet impact on less than ideal surfaces, are also in need of study. The surfaces here are for instance bumpy or covered in ice.
- d) Spallation depth and shape as functions of the impact speed and impactor size are unknowns worthy of fundamental investigation.

Impact craters: mathematical modelling (summarised by Peter Muller)

Again specific points were made.

- a) The broad background is: craters come in various shapes and sizes, with different degrees of erosion and spallation; some are primary, some are secondary effects; major new questions concern improving on the models that have been employed to date, the need for mathematics, and the way forward.
- b) Craters have been classified on their geomorphic properties. What determines their shape, their size (influence of impact speed and the type of materials present) and their representative aspect ratio? Also erosion affects the shape of the sides and the whole crater, spallation affects young craters, while secondary impacts yield linear rays of craters.
- c) Models applied to date are either analogues for laboratory experiments or semi-empirical models. More sophisticated mathematical models have hardly if ever been attempted. There is a need for computational and analytical models to explain basic crater shapes, distribution and shape of secondary products, influence of erosion on the crater rim, influence of water beneath the surface and influence of water within the impacting body.
- d) Possible modelling approaches include ping-pong classical models, PDEs, viscous and inviscid models, hail models, and increased understanding of rock-impacting-rock physics, requiring applied mathematics. A way forward is suggested based on connections with other applications (of what is a huge research area) such as in the impact of small bodies on air vehicle nose cones, and droplet bouncing or displacing, as well as through joint research proposals and meetings.

Social modelling (summarised by Dieter Armbruster)

The following points were drawn from the break-out session and subsequent discussions.

- a) A future workshop was proposed on social science modelling inviting participants from statistics and the social sciences. John Ockendon mentioned that workshops on criminality have already taken place but a follow-up would be a very good idea.
- b) Participants interested in modelling criminality should consider making contact with members of UCL's Jill Dando Institute.
- c) James Moffat from Dstl noted that any models examining how agents make decisions and interact in self-organising ways would be very useful from a Defence perspective. A classic problem is how a self-organising environment consisting of soldiers, civilians and NGOs would evolve over time. Information availability is another factor.
- d) The area is an important one potentially, incorporating analytical and computational social sciences. There is a significant need however for error analysis (or validation) of reduced models as they become increasingly used.
- e) Expertise and skills from Mathematics, Psychology, Probability and Statistics, Data Mining needs to be brought together. 'Big problems' can then be tackled such as pandemics and their public health implications. A workshop would help this.

Environments /terrain (summarised by Mick Davey)

The wrap-up presentation here concentrated on the following.

a) There was a wide range of interests: e.g. in sand movement, virus/malaria spread, large and mesoscale ocean/atmosphere flows, high performance computing, reduced order models, sound propagation, urban models, measurements from space, multiphase flows. Scales ranged from particles to humans to urban areas to weather systems to global climate; activities included observation, modelling and experimentation.

b) A common theme with potential Defence application (among others) that embraced many of these activities was identified as 'the surface environment' (primarily the land surface, but recognising that the sea bed was a related region of interest.) Topics covered by this theme were:

visibility (optical, thermal and radio) and 'obscurance' – relevant to communications;

dispersion (chemical, biological, radiological);

climatic conditions – e.g. heat stress, extreme weather events;

ground conditions – e.g. 'trafficability', mine burial/exposure.

Extreme events were also mentioned.

c) There exist separate complex specialised models for some of these aspects: e.g. the atmospheric boundary layer, urban flow (city, building and personal scale), sand [as well as dust and possibly snow] movement (from particle to dune scale), weather (from mesoscale to global scale), geographic information systems. There exist new computational techniques of embedding models within each other to obtain high resolution and/or resolve particular processes at locations of particular interest; so potentially there are opportunities to link together some of these specialised models beneficially.

d) Discussions on identifying a particular topic that would attract financial support for research or a further specific workshop were brief (time limitations). Potential funders might be NATO, NSF, UK research councils and so on: the point was made that a funder needed to be identified first in order to produce a targeted proposal.

e) Concerning a major challenge, which certainly involves multiple scales, the suggestion was made to investigate sand storms and their typical life cycle: how they arise at the particle level, how they develop and evolve on the weather scale, how they impact the surface operating environment on the human scale, and how that impact might be predicted.

o Outputs from the workshop are also of several other kinds.

Subsequent proposals. Locally, i.e. involving UCL participants, a proposal has been submitted for UK RC support on crater impact prediction using mathematical modelling while two other proposals each with an industrial and a biomedical motivation, one on multi-phase transport and the other on seepage and duct flow, are under construction. Also AFOSR are being approached about an initial study of sand penetration. Two proposals between Nottingham, Southampton and UCL for PhD support in biomedical modelling are being discussed. More broadly see also 'links' and other items below. Other Research Council funding for crater impacts for example may be sought from an EPSRC consortium, a STFC /PPARC-NERC thematic programme, an ESTEC-NASA programme or an NSF-EPSRC-STFC programme.

New collaborations. See also 'links' below.

Stimuli to open problems. This output is reinforced by the contributions on the website.

Links. The institutional or personal links appearing are either reinforced or new. The biomedical research and related interests fan out to Nottingham, to Southampton, and to Physio.net as well as locally to the UCL Medical Modelling Group, to Fergus Robertson and colleagues at NHNN, and to many other interested groups nationwide and worldwide. The environmental and terrain modelling connects with research at ASU, at UCL and at the Meteorological Office. The varied studies of impacts link to many widespread concerns including academic researchers at Cranfield, Oxford, UEA, UCL, Nottingham, Novosibirsk, industrial researchers at two branches of QinetiQ (Farnborough and Fort Halstead), and to much other industry including food production. Distortion and shattering of droplets is a shared interest of UCL, UEA and Cranfield (Richard Purvis, David Hammond and the PI). Oil production studies associated with penetration analysis for instance link to Schlumberger, to QinetiQ, to Oxford and to UCL through newly realised networks. Links are being explored involving Dstl, the Meteorological Office and interactive mapping and data (Andrew White, Bernd Becker, Peter Muller). Social-modelling mathematics is suggesting interactions between the Jill Dando Institute and ASU, UCL, Oxford, Heriot Watt, QinetiQ and Dstl (through researchers Johnson, Armbruster, Bishop, Ockendon, Lacey, Curtis, Moffat with the PI and co-I). These links could promote networks with the above people or institutions as hubs.

Unrest. This particular topic arose from talks and discussions on weather forecasting as it affects human performance (Becker, Davey) as well as from pre- and post-workshop discussions on propaganda between John Curtis, the PI and others; both avenues are being pursued. Post-workshop discussion has also taken place on blast, protection, shielding dynamics as an avenue of research.

Complex geometries. Anthony Hutton of QinetiQ (seconded to Airbus) has invited Nick Ovenden to talk to the developers of the CFMS about using their platform to model behaviour through complex geometries. The same approach can be used possibly to simulate embolization. In another development Dan Stanzione of ASU has offered to put the Medical Modelling Group at UCL in touch with Intel to discuss designing chip architectures to run fast lattice-Boltzmann calculations to model flow through complex structures such as arteriovenous malformations.

Icing, sand effects and erosion. Open issues surrounding these influences were common to a least three of the focus areas of the groups.

Crater impacts. A joint study group on the modelling issues here is suggested for Edinburgh in 2008.

Other networks and hubs. There are several possibilities here as hinted at above in ‘links’ onwards; one could form around topics of penetration /fragmentation based on Oxford, UCL, UEA, Leeds (John Ockendon, the PI, Mark Cooker, Gary Sharpe) in academia and two branches of QinetiQ involving John Curtis, John Brown and Malcolm Cook on the industry side.

Additional research interest and possible support. Interest and support additional or alternative to that of EPSRC was suggested several times at the workshop. For AFOSR /EOARD, Fariba Fahroo emphasized a concern with penetration through sand (following Steve Bishop’s talk) while Surya Surampudi mentioned support existing within a computational mathematics programme.

Recommendations and other points

Concerning other points, the website created for the workshop activities and corresponding dissemination is to show particulars of the invited talks (presentations), summaries, listing of the participants, and further handouts and information. Feedback received via forms and emails from the participants was all positive and constructive. The workshop was an exciting event, highlighting the many-faceted role of mathematics in conjunction with engineering, physics, biomedicine and so on as well as in industry; and the location in central London appeared to very suitable. Increased interest in the forthcoming ECMI conference of June-July 2008 in central London was also expressed.

On recommendations covering a wider front, multi-scale analysis and associated new techniques hand in hand with computation were found to be a common feature among the many connections that became apparent. Also a common need is for more mathematical research personnel to be supported in environmental, medical and industrial interdisciplinary fields of research in both established areas and (more especially) emerging areas. Corresponding proposals are implied. There were calls for increased societal modelling, for more medical modellers, for more interdisciplinary workshops, and for more development of new techniques required in new or emerging areas.

Particular recommendations from the workshop concerning the specific focus areas that arose are contained in the summaries described under the heading ‘Outputs’ above. Corresponding proposals are implied.