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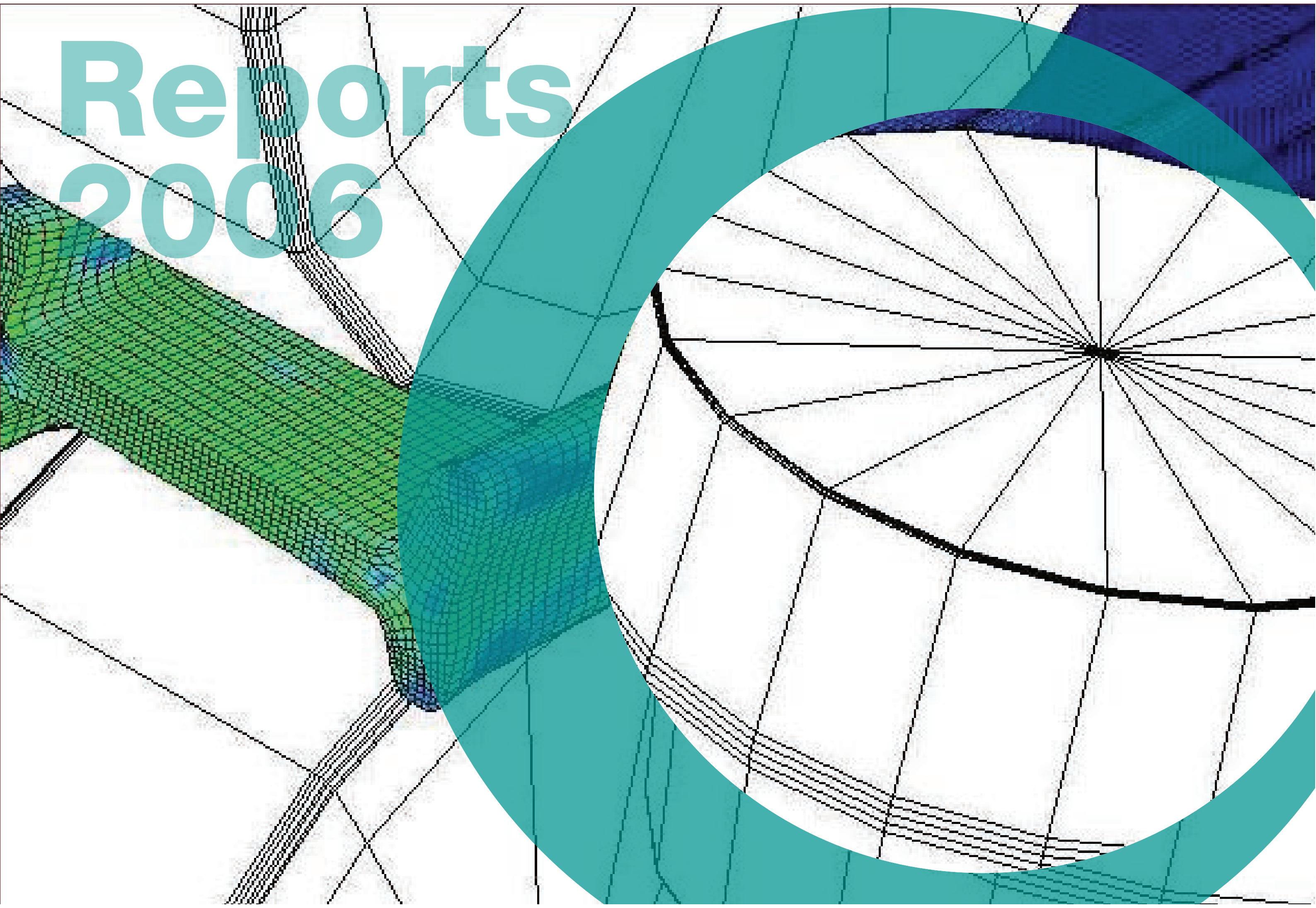

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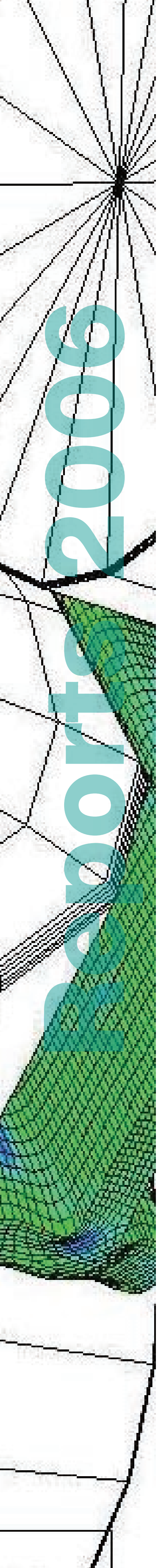
Materials Innovation and Growth Team



MATERIALS MODELLING – GROWTH AND INNOVATION PROSPECTS

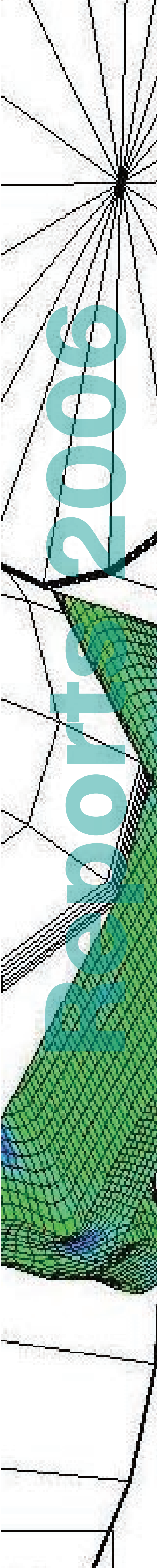
by

members of the EPSRC Materials Modelling Strategic Task Group, chaired by Professor Marshall Stoneham FRS

Foreword

At the inaugural Town Meeting of the IGT in February 2005 the Science and Technology Task Force breakout session suggested that members of the Materials Modelling Strategic Task Group, which advises EPSRC on its current Initiative in materials modelling, should summarise the status and future UK needs in materials modelling research and training. This report has been prepared by members of that group in response.

The report draws upon earlier reports in this field, notably Predictive Modelling of Materials in the UK (DTI, February 2001) by a group chaired by Professor Marshall Stoneham FRS, and also on those elements of the 2000/2001 Foresight exercise which remain relevant today. It also draws on inputs from recent consultative events including regional meetings of the broad materials research community held by EPSRC in 2004, a presentation and breakout group on materials modelling at the IGT Town Meeting on 7 June 2005, and modelling-relevant aspects of the Report on an EPSRC Theme Day on Nanotechnology on 16 June 2005.



PUTTING MATERIALS MODELLING IN CONTEXT

Context (I): Scope and Drivers

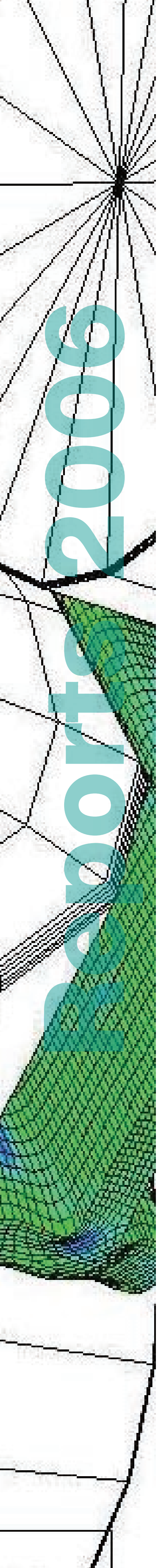
Materials modelling, also described as predictive materials modelling, is a framework of understanding for materials information; a means of scoping new situations to establish priority; a way to predict quantitatively in novel areas; and a route to improving the testing and reliability of existing processes.

The drivers are the reduction of risks and costs, improvement in efficiency and effectiveness, and the opening up of opportunities. Much of the current publicly supported UK activity and policy builds on the 2001 DTI/OST Foresight Report on this topic (A M Stoneham, A Howe, T Chart), and has been also been motivated to some extent by subsequent US and European developments.

The overall concept of materials modelling comprises a very wide diversity of needs and activity. Modelling must capture realistic practical situations and a representative range of problems. There is a very wide range of materials and behaviour and the variety of need, of materials studied and of properties should not be underestimated. This variety includes:

- Metals, ceramics, semiconductors, polymers, layered and composite systems,...;
- Structural and functional properties;
- Equilibrium, metastable and non-equilibrium systems; electronic and excited states ...;
- Possible extreme conditions of pressure, temperature, stress. ..;
- During processing for manufacture and during the operational life of key products (including testing in operation)

An important feature and source of research challenges is that key length and time scales cover many orders of magnitude.



Context (II): Scales

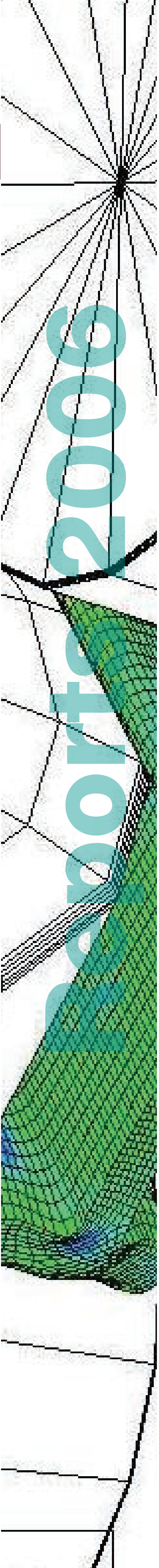
The tools and techniques in use or required at the different length scales can be summarised as:

The Macro (engineering) scale: Good commercial software exists (FE, FD, CFD) for many cases (electromagnetics, elasticity, simple fluids; hosts for flow-or stress-dominated processes and component in-service models). There are some gaps, e.g. for turbulence, or history-independent processes, especially involving fluid-solid transition and interaction, or processes involving the close coupling of a range of phenomena.

Atomic and nanoscale (up to 1010 atoms at most, less than grain size): Commercial and academic software is available (for electronic structure, molecular dynamics etc). There remain some significant gaps, and some over-confidence in “first principles”.

Meso scale (microstructural) There are no general methods, and “brute force” methods are often misguided. The meso-scale is often identified as the main rate-limiting step. Top-down and bottom-up methods may work well and there are several successful approaches for defined materials areas. However extremal behaviour (e.g. fracture) remains largely unresolved.

At all scales there is real scope for new ideas. Approaches to the understanding and prediction of irreversible phenomena, non equilibrium and extremal behaviour are largely empirical.



MAIN ISSUES

Issues (I): Modelling needs at the different length scales

Examples of the current issues and needs in predictive materials modelling at the various length scales include:

- **Macro scale:**

Improved modelling of coupling flow- and stress-related phenomena: here, anything but the most rudimentary modelling is very difficult; in modelling turbulence when chemical reactions or supersonic conditions or multiple phases are involved. Algorithms are not themselves the primary limiting factor; rather, there is a need to capture macro-scale representations of the physics. This requirement is itself likely to expose limitations in the analysis software capability, especially where the paradigm which best represents the phenomena changes dynamically (e.g. continuum to particulate).

- **Meso/microstructure:**

Systematic (though not necessarily universal), reliable methods are needed. Ways are needed to model microstructures for extremal behaviour (fracture, electrical breakdown, fatigue), which in many cases cannot be predicted at all, and the easier fallback of averaging is often used. There are unresolved questions about how to include soft solids (e.g. adhesives) and biomaterials.

- **Atomic/Nanoscale:**

There are significant gaps, such as behaviour far from equilibrium; non-adiabatic processes, where quantum matters.

- **Practical and effective coupling strategies**

are needed, so that models involving several length or time scales can be treated effectively by non-specialists.

- **Timescales:**

Whole-lifetime modelling - prediction of lifetime events from initial properties - remains a "valley of death" barrier for many structural applications

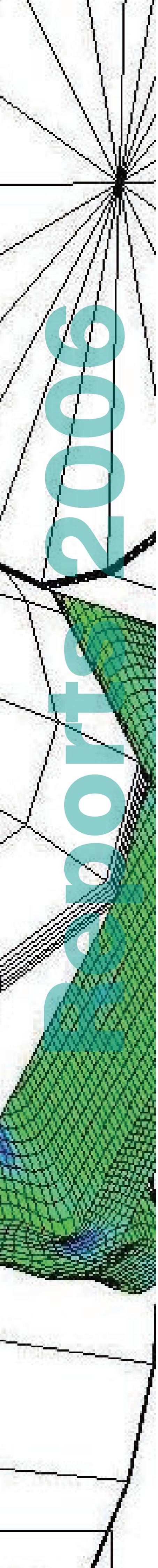
- **Characterisation and its interpretation:**

There are important issues of what measure to pick, what the data means, especially taking 2D to 3D and then to properties- a framework of understanding is what is really needed, which can be helped by modelling but may also be a precondition in terms of the skills and teams needed to make modelling work. For some purposes, eg production control, the precision of sensing/characterisation has been greatly enhanced (eg laser ablation) so considerable practical precision is already available.

- **Inspection**

remains a problematic area which is sometimes neglected, but is essential for incorporation into structural models

It is worth noting that there are many incomplete efforts "hidden in drawers" as well as in the formal literature (some flawed), that have not led to useful tools. Yet knowledge of such experience, including of failure, can be useful.



Issues (II): Education

Education of/ for whom:
Industry is international, hence issues of student grants and citizenship rules are important. It is proper to emphasise industry's future needs over a significant outlook period (5-10 years), rather than past and present needs. There is a need for continuing professional development, not just M.Sc. training.

Education to recover discarded experience:
Different industries are at different phases of their use of modelling so ways should be explored of eliciting and sharing existing knowledge, recouping losses of know-how, records, reports, software & hardware.

Education about what:
"Defining the problem" issues are as important as software application expertise. The need is for capability to operate when major industry changes.

Education for careers outside materials modelling: Education in materials modelling is also good preparation for a far wider range of careers.

Issues (III): Industry Needs

Industry aspects 1:
Management of Materials Modelling

Active groups in industry are said to be too small and too transient to be effective. Management expectations from inexperienced individuals are unrealistic. Time pressures mean SMEs can be especially badly placed. The recommendations arising from this are:

Reinforce Knowledge Transfer Partnerships and similar activities. Encourage EIRMA and similar organisations

Longer-term support:
DTI and EPSRC must find ways to support longer-term projects in national labs and especially universities, particularly in collaboration with new industries as well as established ones. The loss of large research laboratories (government and industry) as a national resource has been damaging.

Industry aspects 2:
Recognising opportunities

Too often, **modelling/simulation are perceived as an overhead.** It is minimised unless it clearly determines success. It is often not given credit even when its effects are major, e.g. cancelling doomed projects.

Also, **predictive material modelling is very varied:** many industries may not realise what it can offer (unlike CAD, etc) or identify easily those who could help. The recommendations are:

Case studies and examples of good practice should be given continuing/wider publicity, even before full economic benefits are realised (the world moves fast).

Find ways of recognising the role of Materials Modelling. Finding ways to do so is problematic, but gaining recognition of the whole area is vital if the UK (and Europe) are retain a place on the leading edge of materials technology

Industry aspects 3: The Software Industries
Identified needs in the area of materials modelling software are:

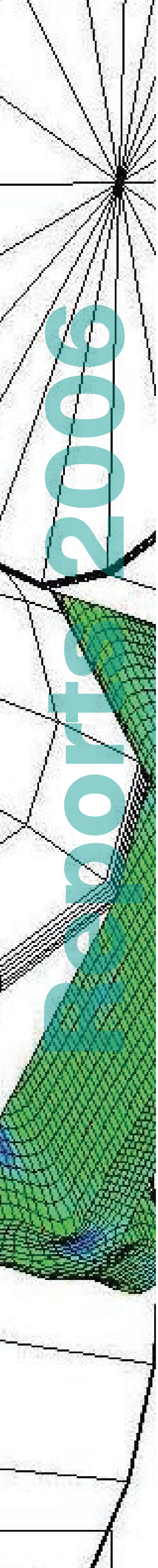
Linking the science base and industrial users to code custodians:
Commercial code is increasingly packaged and has restricted access. Researchers need **open** access.
Materials modellers need to be able to work inter-operably between codes (MPCCI helps), but codes must be able to run on HPC parallel systems (especially clusters). However there may still be problems of code coupling in parallel.

The above are exemplars of modelling infrastructure challenges.

Integrating separate codes for multi-scale simulation is not easy, and is not always the right way to go (e.g. the US national laboratories approach).

Good research code which forms prototypes for commercial product in UK labs and universities. Also, a need often drives industry to create pilot versions of really useful code.
Recommendation: EPSRC should be prepared to encourage academics to develop core analysis technologies, perhaps in conjunction with industry and software houses.

Transformation to a well-packaged PC product for a non-expert modeller is challenging technology development.
Recommendations:
Consider ways of providing support to software houses to aid this step – the production of prototype commercial technology, perhaps analogous to what is done for other new (manufactured) products;
Recognise routes like industry—university—software house as important complements to university—software house—industry.



Issues IV: Hardware needs

The main driving force is international competition. Everyone can use better displays, memory, computer speed, etc, but in the past individual users have not complained much about hardware. **However** there are some challenges which are not being conceived of because the computational demands are so great (as compared with the efforts in the USA)
Also, there is a **gap for some modelling software** – especially coupled macro-level tools which do not naturally scale well on HPC parallel systems.

Recommendation: Research is required on software for coupled macro-level tools which do not naturally scale well on HPC parallel systems.

These challenges aside, the residual computational demands are often satisfied by **cluster technologies with faster interconnects.**

Recommendation: It is important that **no obstacles** are put in the way of effective use of UK computational facilities (e.g., refusing access of industry users to academic facilities under reasonable conditions).

Issues V: **Key/neglected technical areas**

Modelling of joins and welds: The modelling of most aspects of interfaces - joins, welds, adhesives, etc - is still very much at an ad hoc/empirical level, not only in the UK but internationally also (eg Battelle Institute, USA). With no clear leaders, this might represent a niche opportunity for the UK.

Understanding of **grain boundary** issues is a common materials requirement and projects to this effect should be encouraged.
The fundamentals of **crystallisation** are potentially relevant across the natural sciences, including for most materials.

APPLICATIONS

Because modelling is an underpinning activity, "applications" are taken here to include all or any uses to which modelling might be put including research, and not only the end product areas to which modelling contributes.

From the sources available including the series of EPSRC Materials Challenge workshops held in 2004 across the UK to work up possible future areas for the Materials programme to target EPSRC priorities, from the peer review response to the projects submitted to its Materials Modelling Initiative, and the Nanotechnology Theme Day of June 2005, important applications areas can be identified for materials modelling across the full range of materials, including new and expanding markets as well as new or improved properties and processes for existing materials. In particular several of the "challenge" fields identified by the community for materials as a whole were seen as ripe for the application of materials modelling. The relevant statements/recommendations were:

(I) Nanotechnology:

Materials modelling is vital in predicting the properties of Nanomaterials. The connection between theory of Nanomaterials and the physical properties of the materials is increasingly important and needs research. A number of the existing fundings under the Materials Modelling initiative have begun to tackle important facets at this scale.

At EPSRC's June 2005 theme day it was recognised that at the nanoscale, modelling can analyse and predict properties of systems, processes and other phenomena in ways that complement experiment. For instance, the topic **Nanoparticles, nanoclusters, nanocatalysis,** included the understanding of properties and processes of nanoparticulate catalysts, modelling and catalyst fabrication, and was seen as likely to have major impact in areas such as fuel production, materials production and environmental protection. The issues and opportunities identified for modelling at the nanoscale were, on a 5 and 10-year horizons common to the theme day topics:

Nanotechnology and modelling - 5 year horizon

The nanoscale shows many features that are not evident from scaled-up atomistic calculations, nor from scaled-down macroscopic calculations, though the important links across length and timescales must be recognised. Linking nanoscale phenomena to models of novel manufacturing processes will be important. The dynamic behaviour of complex three-dimensional nanostructures in real time is especially important, and would enable development of better mathematical models of mixed hard/soft structures, like biological systems. Other results from these developments would be the modelling of intentionally-doped or structured nanosystems which would have applications in spintronics, and extensions of the modelling to devices such as displays, solar cells, and radio-frequency tags. It was commented that EPSRC needs to consider the collaboration of computer scientists, physicists, chemists, engineers, in the development of new algorithms, and the availability of next generation computing power for such modelling.

Nanotechnology and modelling - 10 year horizon

Ambitious, imaginative projects need encouragement. Goals might include biomedical systems with realistic modelling of interactions between nanomaterials and biological tissues, the credible modelling of life processes in living cells, and the whole lifecycle modelling of environmental issues including nano-pollution. These imply the integrated models of whole systems. Other developments might include quantum algorithms to model quantum dynamics of nanostructures in dissipative environments. The predictive modelling of highly non-equilibrium systems involving nanoscale components will continue to give challenges, and such challenges will be come even more varied as microelectronics moves to nanoelectronics. These developments will drive collaborations between different scientific communities. It was commented that progress on the 5 year time scale should encourage a culture change within the whole science community, so that many more researchers feel able to span different disciplines.

(II). EPSRC Materials Challenge Workshops (autumn 2004): Comments relevant to modelling;

Advanced materials processing:

Through-process characterisation and through-process modelling were needed to enable the UK to use its considerable capabilities to "leapfrog" in relation to the international competition, for example through multi-scale modelling of materials and processes. Casting and related grain boundary issues were an example.

Structural Integrity:

The UK should strive to maintain its strong position in fields including defect assessment and monitoring (non-destructive evaluation) and experimental/predictive modelling for the design of structures. Modelling applications: Life prediction; mesomechanics; microstructural models, grain boundaries.

Healthcare and Food (considered together, as they have a common interest through soft materials research):

There was scope for novel modelling and analysis of soft solids and interfaces – applicable both to biological environments and to food science and technology; strong potential for modelling to contribute to accelerated high throughput assessment techniques for ever more stringent regulatory approval purposes (drug development analogy); modelling for materials aspects of food processes (colloids, soft solids and interfaces, powders).

Energy and Power:
New models were needed for the materials properties at high temperature, of radiation damage, prediction of long- term service lifetime. Predicting performance and life cycle of materials for high-temperature/high field conventional, nuclear or fusion generation; high structural performance for renewables - light but high strength wind turbine blades or water-borne structures; predicting/producing novel insulation for domestic, public buildings, motors; low-loss transmission of electrical or mass transport of fuels/energy

Transport & Defence- including materials for defence and security: Developing integrated modelling strategies for materials modelling across length scales and phase changes. Modelling of structural - anti-attack and anti-blast properties of novel and improved traditional materials, atmospheric filtering (NBC); horizontal role of novel composites, and the simulation of impact, permeability, flow, and their interactions.

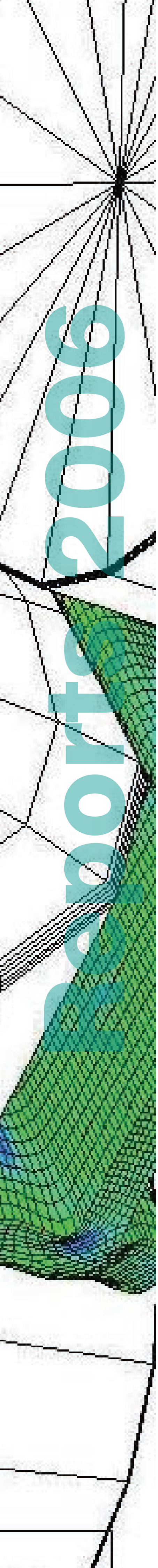
New materials for medical/biological techniques (biocompatible scaffolds tissue engineering, stem cells, medical and NBC textiles and composites).

Sustainability: modelling for predictive materials selection for novel uses and processes for conventional crops and materials (wood, arable crops)

Multifunctional materials: These materials combine a range of possible combinatorial property issues along with novel processing challenges, for example in built-in actuation/sensing in structural materials, or in technical textiles, presenting especially complex challenges when combining disparate properties and processing requirements.

Other applications noted from other EPSRC inputs to programme planning included:

Soft solids and interfaces - understanding interface and texture issues for food, medical, engineering flow purposes.



WHAT THE REST OF THE WORLD IS DOING: COMPETITOR ANALYSIS

Competition (I): International context

The most significant competition appears at first sight to come from the US, where national laboratories - Lawrence Livermore, JPL, Los Alamos, etc, as they devote large sums to computing power, and to software which is networked to universities. Certainly the UK reduction of national labs in the 1980s assumed that knowledge networking substitute would work, but this was not so effective. As mentioned elsewhere in this report, the US funding approach may not gain as much advantage as it appears when the relative ineffectiveness of "brute force" approaches to link across different scales is appreciated, as it is still essential to implement modelling in a "smart", computationally efficient way.

The UK is very strong, along with other world groups, in numerical modelling in metals at the macro-scale- there are no clear world leads elsewhere. However, in predicting structure etc at the meso-scale then although the UK was at the start of this activity, in Europe, Japan and especially the USA, there are now rather more sophisticated efforts.

In some fields, eg metals, leading UK universities are well linked with industry and to the EU (eg Delft) , having benefited from the former Coal & Steel community ongoing research levy which paid for networking/pilot research activity.

Competition (II): UK Funding – an update

The 2001 Foresight Report, the International Review of Materials, and other inputs, led to a new Materials Modelling initiative funded by EPSRC along these lines:

- Proposals should be relatively large (500K-1500K) and encouraged to be collaborative across the UK;
- Problem posing and strategic approaches to capturing multi-scale behaviour should be a key component, with code development and running large codes only secondary aspects;
- The proposals should be ambitious, aiming to take the UK alongside or ahead of the world leaders at the end (say 5 years);
- The proposals should link to industries likely to be significant at the end of the project (say 5 years), not just those currently active.

Modelling

Pending the decisions on a third call expected to be completed in February 2006 the results of the Initiative so far have been that 7 consortia proposals were funded from ~100 outlines submitted, with 17 excellent short-listed proposals. The best proposals clearly encouraged students and post-docs to gain experience in problem posing and strategic approaches to predictive materials modelling. All funded proposals involved multi-institutional teams, and the teams had established viable links to the relevant industries, including external advisory committees. The successful teams also had strong international links and were judged as being seriously likely to make the UK world-leading in their areas. As required, they addressed industries likely to be important in say 2008-2010 (materials for fusion reactors, nucleation and interfaces in biomedical contexts, the role of fluctuations in micro- and nano-electronics).

The topics covered by the proposals were: Biological interfaces with materials; materials mechanical properties for fusion power plants; Nano-CMOS electronics; Non-adiabatic processes; interfaces in ceramic and metallic alloys; Polymer nano-composites; and the engineering of functional (eg photonic) coatings.

Subsequent reflection by the EPSRC Materials Modelling Strategic Task Group on the EPSRC projects funded indicated that exciting science was being funded but also that some gaps remained: They were generally focussed at one (typically nano-) scale; they did not generally move up the T&L scales to have impact in an engineering context; there was little genuine multi-scale work in a tightly coupled sense; and most compute efforts were well contained within cluster or even fully loaded PC systems. The useful comparitor here was with international efforts where major work on coupled multi-physics & multi-scale analyses on HPC systems was well underway, usually with bespoke software to capitalise on the HPC systems.

Overall, in the first two calls there was strong emphasis on the materials science and relatively little on engineering end of the spectrum, and the balance is being addressed in third call to complete the planned funding of £10m over 3 calls. Separately, internationally prominent modelling activity is being undertaken by the 6-institution Microscale Polymers Processing consortium (MUPP2) led by Leeds University, which has attracted £5.5m EPSRC renewal funding for 3D modelling and control of the polymers extrusion process. This group has attracted and retained significant support from multinational polymers processing industry over several years and combines world-class polymer physics with process technology and modelling at the forefront of its field.

DTI's Technology Programme has recognised the importance of materials modelling in its planning and featured Design, Modelling and Simulation in its 3rd call (assessed in November 2004), attracting large demand at the outline stage and resulting in ?7 being funded in the materials modelling field, of which ?1 has academic involvement.

Competition (III) USA: NSF joint activity
A joint all-materials call by EPSRC with NSF under its multinational Materials World Networks calls has not produced any major emphasis on modelling over 3 years to date of operation; one project has been funded broadly relevant to metals modelling.

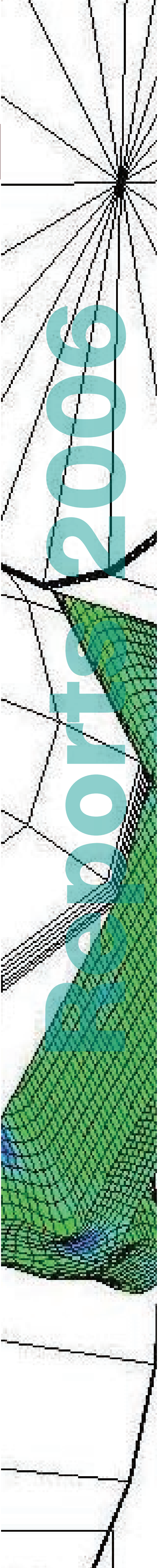
Competition (IV): Joint European efforts
Insufficient evidence has been presented to consider strength of joint European modelling projects or networking efforts that may be funded by the EU or ESF (eg Framework programmes, ESF EuroCORES and networks, COST, though it is highly likely that the UK would be a key participant in many.

Competition (V) Far East
No international comparison has been attempted with the Far East.

Competition (VI) Canada: The NRC has expressed an interest in the UK's Materials Modelling Programme and EPSRC has providing some pump-priming funds to initiate the necessary contacts. It is too early to establish the respective strengths and mutual benefits for the UK consortia funded to do so

Competition (VII) Eastern Europe/accession states:- as in many fields of physical sciences, there has been an influx of or access to many well-skilled modellers, theorists and mathematicians from the former east bloc, but no evidence of direct competition in major areas of modelling.

VIII – Nanotechnology: The EPSRC Nanotechnology theme day held on 6 June 2005, which considered the outcomes of recently completed EPSRC grant activity, observed that the UK as a whole had some real strengths in modelling at the nanoscale but that the grants seen at the theme day did not reflect this (note that this considered only completed grants, and so did not include those funded under the Materials Modelling Initiative, which does include work at the nanoscale).



RECOMMENDATIONS, WITH PRIORITIES

1. How to identify and define the problem

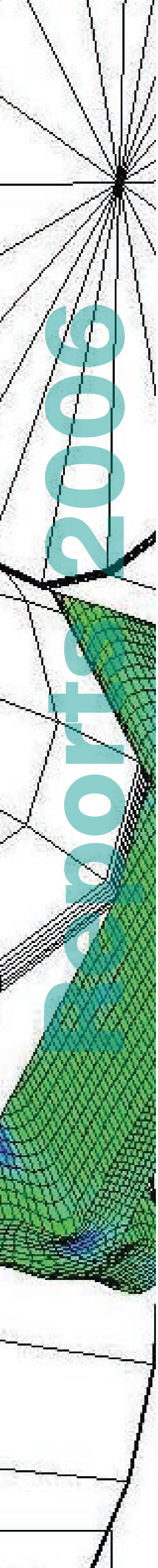
There is no shortage of technology-related materials areas for which modelling could make a major contribution. Some need long-term developments; others may need only the well-chosen, informed application of standard methods; still others will be a consequence of change in a rapidly-evolving new technology. In many cases, the need will start in an ill-posed way, and will involve aspects outside the direct experience of the modeller. Perhaps the **major need is training in how to decide what needs doing and how to implement it on a time scale determined by the technology.** This is far more important than training in any specific modelling method or code.
Related to this need is **gaining experience in the likely accuracy and effectiveness of standard codes.** Thus it is just as important to avoid over-confidence in the words “first principles” as it is to realise the limitations of turbulence models.

2. Microstructures and Mesoscopics

For very many (probably most) materials problems, there is a natural length scale for the key calculations. This may be the atomic scale, or the engineering scale. What happens at the intermediate mesoscale is still important. For instance, one would like a good treatment of turbulence, or history-independent processes (especially involving the fluid-solid transition) that can be used within engineering-scale calculations. One would like to be able to tackle coupling flow- and stress-related phenomena (eg modelling turbulence when chemical reactions or supersonic conditions or multiple phases are involved), capturing macroscale representations of the physics. The fundamentals of crystallisation are potentially relevant across the natural sciences, including for most materials.

In the solid state, there are two broad ways to handle microstructure. Which approach is used depends on the property. For, say, elastic constants, an averaging (perhaps effective medium) approach will be suitable. For, say, fracture, which depends on statistically rare features, it is necessary to look at the properties of many realisations of the microstructure. It is not difficult to create a microstructure that looks reasonable, but it is still an unsolved problem as to how to build a mesostructure that has the right extremal properties. This is inhibiting studies of fracture, electrical breakdown, and fatigue.
Recommendation: **New, non-empirical approaches to the understanding and prediction of irreversible phenomena, non equilibrium and extremal behaviour should be encouraged.**

Systems involving soft solids (e.g. adhesives) and biomaterials should be included in these concerns. There is a **broad need for taking the modelling of joints, welds and adhesives from the empirical level,** and this is a potential niche opportunity for the UK. **Effective and practical understanding of grain boundary issues** is a common materials requirement.



3. Context issues

3.1. Safety issues and regulation for the whole practical lifetime of materials and for their subsequent disposal mean that one cannot simply concentrate on operational performance.
Recommendation: **We encourage whole-lifetime predictive modelling, eg for structural applications, and also the incorporation of inspection elements into structural models.**

3.2. In practice, methods (whether computer-based or analytical) will be used by non-specialists. There is a responsibility on those developing methods to make the assumptions and restrictions very clear. This is especially true of coupling strategies for models involving several length or time scales, where a modest change at one scale may have dramatic consequences at another.

3.3 There is a key role for modelling related to characterisation and metrology: what measure should be picked, what the data means, and especially taking 2D images to 3D and thence to properties. **It is essential to have an appropriate framework of understanding.**

4. Education and training

4.1. Students trained in materials modelling have skills that are valued in many fields. There is no reason to restrict numbers to those necessary for today's materials modelling teams. After allowing moves outside materials modelling, there should be sufficient students trained for industry's future needs over a significant outlook period (5-10 years), i.e., not just past and present needs. **Training must include continuing professional development, not just M.Sc. students.**

4.2. It is in the UK's interest to obtain the best international students. This means that **student grants and citizenship rules should not be restrictive.**

4.3. **Education is needed to recover discarded experience,** by exploring ways of eliciting, recouping and sharing existing knowledge and tools.

5. Industry Needs

5.1 Knowledge Transfer Partnerships and similar activities should be reinforced. Encourage EIRMA (European Industrial Research Managers Association) and similar organisations sharing best practice ideas.

5.2 Longer-term support is crucial: **DTI and EPSRC must find ways to support longer-term collaborative projects in national labs and especially universities,** particularly in collaboration with new industries as well as established ones.

5.3 Industry: There must be **ways to encourage industry (and especially managers) to recognise opportunities for modelling to add value.** One useful way is through **case studies and examples of good practice. These should be given wider, continuing publicity,** even before full economic benefits are realised, as part of a campaign to find ways of recognising the role of Materials Modelling.

6. The Software Industries

6.1 Linking the science base and industrial users to code custodians:
There is much to be gained by finding ways to enable researchers **open** access to code - commercial code is increasingly packaged and has **restricted** access.
There is a need for good research code which forms the prototype for commercial product in UK labs and universities.
Recommendation: EPSRC should be prepared to encourage academics to develop core analysis technologies, perhaps in conjunction with industry and software houses. It is proper to consider ways of providing support to software houses to aid transformation of prototype industrial/academic solutions to a well-packaged PC product for a non-expert modeller.
Recommendation: Recognise routes like industry—university—software house as important complements to university—software house—industry.

6.2 Materials modellers need to be able to work inter-operably between codes (MPCCI helps), but codes must be able to run on HPC parallel systems (especially clusters). However there may still be problems of code coupling in parallel.

Recommendation: Simply enabling inter-operability between codes for modelling at different scales is not the complete answer – **important work needs to be done at the meso-scale to enable 'key' relevant information to be exchanged between the codes with appropriate time and length filters.**

7. Hardware needs

7.1 There will always be some challenges not being tackled in the UK genuinely because the computational demands are so great (cf the USA). Cluster technologies with faster interconnects are a possible way forward for such challenges; grid-based approaches can be effective, but usually it seems necessary to find novel ways to avoid brute-force applications.
Recommendation: Research is required on software for coupled macro-level tools which do not naturally scale well on HPC parallel systems.

7.2 **Recommendation:** There is a need to obviate obstacles in the way of effective use of UK computational facilities (e.g., refusing access of industry users to academic facilities under reasonable conditions)