

NEW AND EMERGING THEMES IN INDUSTRIAL AND APPLIED MATHEMATICS

Final Report of the NEST SUPPORT project NETIAM

edited by Melvin Brown and Robert Leese Smith Institute

This report has been produced with thanks to the coordinators and participants of the NETIAM project.

European Commission Directorate-General for Research Structuring the European Research Area Anticipating Scientific and Technological Needs (NEST activity); Basic Research

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EXECUTIVE SUMMARY

Mathematics and the formulation of unexplored research challenges

The NETIAM project has used mathematics as a tool to integrate the approaches of science from many disciplines. New theoretical and computing techniques, and collaborative formulation of unexplored research challenges, enable mathematics to play a vital part in the research process much earlier than previously. This novel project has linked multidisciplinary teams under four themes covering complex problems of sociology, economics, manufacturing and natural sciences. The project has identified three underpinning mathematical methodologies and eleven diverse application areas for multidisciplinary research, and it has examined the infrastructures that are required to support such activity.

The European integration of expertise that has occurred in NETIAM has increased the potential for dissemination and application of research results by overcoming existing intellectual and administrative fragmentation. In total, 125 researchers of many different disciplines from 15 countries have participated in the workshops, and many hundreds more have been reached as part of the project's dissemination initiatives. Through ongoing vision and well organised collaboration, the NETIAM project has provided a benchmark for the use of mathematics in the formulation of unexplored multidisciplinary research challenges in a wide range of areas.

Four key themes

NETIAM has five participating organisations, from five EU Member States and is coordinated by the Smith Institute (United Kingdom). They have held thematic workshops on the following areas:

- Mathematical modelling of criminality in the urban environment
- New multidisciplinary challenges in modelling the business environment
- Challenges in visualisation, simulation and design for virtual porous materials
- Complexity in modelling proteins and interfaces at the molecular level.

The themes were chosen by the partners for their challenging interdisciplinarity and their emerging opportunities for using novel mathematics. They have demonstrated how, by working at a European level, mathematics can provide a common language with which to approach multidisciplinary research.

A fifth capstone workshop drew on the work of the thematic workshops and proposed an integrated summary of topics, methodologies and consortia for adventurous research activity. New multidisciplinary consortia have since been formed, with mathematics playing a central role, and new proposals have been submitted to the NEST programme¹ to support research in the underpinning themes.

Strategy: Mathematics, industry and society in Europe

Following its five thematically based workshops, the NETIAM Strategy meeting of leading figures from mathematics communities across Europe identified the need for sustained activity to raise awareness and use of mathematics, in industry, government, academic communities and in society generally at all levels. Under the title 'Unleashing Mathematics', the project has established a strategic initiative to help deploy the power and flexibility of mathematics for exploiting opportunities for

¹ NEST: New and Emerging Science and Technology, Framework Six Programme of the European Commission.

innovation across a broad spectrum of industry and society. The use of mathematics will be a crucial element in achieving the European Union's ambition to become the world's most dynamic knowledge-based economy.

The NETIAM Consortium

The NETIAM consortium partners are:

Smith Institute for Industrial Mathematics and System Engineering, UK Ventspils University College, Latvia Fraunhofer Institute für Techno- und Wirtschaftsmathematik, Germany Technische Universiteit Eindhoven, Netherlands Università degli Studi di Firenze, Italy

Together, the five partners represent a critical mass that has allowed the strategic planning of interdisciplinary mathematical research on a scale never before seen in Europe. They have brought to NETIAM a common commitment to working on an interdisciplinary basis and a varied expertise in mathematical modelling, demonstrated by extensive track records. Existing networks such as ECMI and MACSInet had enabled the partners to become familiar with each other's particular strengths and collaborators, and hence to fully realise the potential of the collective strategic approach to new and emerging areas that NETIAM has adopted. Moreover, the NETIAM workplan was constructed so that all five partners contributed to the planning and reporting of all workshops, with representatives of all partners participating in all workshops. These steps minimized any risk that the workshops might become disconnected and maximized the opportunity for highlighting common mathematical frameworks across different workshop themes.

The strategic and management leadership was provided by the NETIAM Management Board which comprised:

- Dr Hilary Ockendon (University of Oxford), Chair
- Dr Melvin Brown (Smith Institute), Project Manager
- Dr Robert Leese (Smith Institute), Partner and Project Coordinator
- Prof Robert Mattheij (Technische Universiteit Eindhoven), Partner
- Prof Mario Primicerio (Università degli Studi di Firenze), Partner
- Dr Andreas Wiegmann (Fraunhofer-Institut f
 ür Techno-

und Wirtschaftsmathematik), Partner

Prof Aivars Zemitis (Ventspils University College), Partner

Project objectives and major achievements

The overall objectives of NETIAM are:

- **Objective**: to raise the role of mathematics by identifying areas of high adventure and opportunity that are prime future topics for NEST, other parts of FP6 and other research programmes, and to provide advice to managers of research programmes on behalf of the mathematical community.
- **Objective**: to assemble teams of researchers that are in a position to generate proposals into NEST, other parts of FP6 and other research programmes.

These over-arching objectives are comprised of several more focused objectives, which have been achieved with input to each from all five of the NETIAM consortium partners.

• **Objective**: to bring together European researchers around four crossdisciplinary themes, so as to identify potential research breakthroughs, with mathematics at their core, that will be prime motivators for interdisciplinary efforts in new science and technology, and hence help to define the next generation of innovation in the European Research Area.

Summary of work and achievement: four thematic workshops have been held as planned and a summary of the final reports from each is given in this report. Success has been demonstrated in both the number of workshop participants (125 in total from 15 different countries) and the quality of their scientific contributions, as demonstrated by the wealth of material in the workshop reports. It is intended that dissemination of the NETIAM reports to all participants and to the wider communities from which they are drawn, will stimulate still further ideas for multidisciplinary research.

Objective: to demonstrate how, through careful modelling and analysis, mathematics provides a common language with which to describe interdisciplinary research challenges in the chosen themes, leading to the necessary cross-disciplinary cohesion.
 Summary of work and achievement: all of the thematic workshops have been successful in demonstrating the use and potential use of mathematics in a multidisciplinary context, and have had a strong multidisciplinary participation. Each workshop report is rich source of ideas and collaborative partners for researchers wishing to embark research programmes relating to

the areas covered by the four thematic workshops.

- **Objective**: to define gaps in the research knowledge base that need to be addressed if innovative thinking is to shed light on the chosen themes. **Summary of work and achievement**: the format of each workshop was designed to allow ample time for facilitated discussion aimed at identifying gaps in current knowledge and research. The gaps identified have been the basis for identifying the 11 application areas, the mathematical methodologies and the potential consortia that have emerged for novel multidisciplinary research. They are presented in detail in the Capstone Workshop report and are summarised in this report.
- Objective: to identify the barriers, in terms of organisation and scientific culture, to the research that will fill these gaps in knowledge.
 Summary of work and achievement: these issues were discussed in the thematic workshops. More particularly, prior to the Capstone Workshop, NETIAM participants were invited to assess the novelty and importance of the research areas highlighted by the thematic workshops. The need to fill the identified gaps was then further explored during the Capstone workshop. For each of the 11 proposed research areas, barriers and specific enablers for the pursuit of the proposed multidisciplinary research were discussed. The conclusions are included in the report of the Capstone Workshop.
- Objective: to recommend process enablers, for the formation of multidisciplinary collaborations, that will enable exciting and potentially high-benefit proposals to be brought forward and to provide generic guidance on how to conduct multidisciplinary research programmes.
 Summary of work and achievement: The process of invited participation, proposed by individual workshop coordinators and overseen by the NETIAM Management Board, has proved highly successful in achieving the required mix of skills and disciplines to explore the workshop themes. Equally important has been the use of dedicated workshop facilitators and rapporteurs (in this case provide by Technology Translators of the Smith Institute). The workshop programme and largely common format is reported in each of the five workshop reports: briefly, each consisted of presentations on the workshop theme(s) followed by plenary and break-out working sessions. The workshops have provided a model for the formation of multidisciplinary collaborations. As

of the publication date of this report, the NETIAM-proposed multidisciplinary research programmes remain to be established, so it is not yet possible to report complete experience and guidance on conducting such activity.

An additional Strategy Meeting was added to the NETIAM plan, after the thematic workshops had been completed; it had the following objective:

 Objective: to give the mathematics community in Europe the opportunity to formulate a strategic 'action plan' in response to the experiences of the NETIAM project.
 Summary of work and achievement: The Strategy Meeting of 20 leading

Summary of work and achievement: The Strategy Meeting of 20 leading representatives of the mathematics community in Europe and from industry has launched a long term initiative, entitled 'Unleashing Mathematics - A Driving Force for Industry and Society in Europe', to construct an Action Plan for Mathematics in Industry and Society to begin in 2007.

Four multidisciplinary themes

The programme of each of the four NETIAM thematic workshops was highly flexible, interactive, and responsive to emergent ideas, so distinguishing them from more traditional conference and seminar events. Each workshop provided insight into the mechanisms and challenges in stimulating ideas for novel multidisciplinary research topics and collaborations; these aspects were also addressed more fully in the subsequent Capstone Workshop. The proceedings of each workshop (see NETIAM Reports section) are summarised below.

Mathematical modelling of criminality in the urban environment

Thematic Workshop, Firenze, Italy, 7-8 June, 2004

In its first Thematic Workshop, the NETIAM project explored opportunities for multidisciplinary research under the title 'Mathematical Modelling of Criminality in the Urban Environment'. The workshop was attended by some 24 researchers from 9 countries, including social scientists, geographers, physicists, and mathematicians.

There were three opening presentations on challenges in crime mapping, the geography of crime and the sociology of crime. In these presentations, the participants sought to identify the key observations that will underpin any realistic model of criminality within a closed urban community.

The immediate result was the decision to separate into two breakout sessions charged with identifying the theoretical framework within which each of the following themes could be considered quantitatively:

- 1. Modelling Acts of Crime
- 2. Modelling Criminal Behaviour

The outputs were

1. Acts of crime are perpetrated over relatively *short time and length scales*, as evidenced by phenomena such as repeat victimization, burglary localization, hot spots and crime elasticity (better law enforcement in one area makes neighbouring areas vulnerable). A mathematical model must be able to predict these phenomena in terms of *external forces* such as weather, law enforcement and ease of access. It must be a spatio-temporal model, which may be continuous or discrete and which could draw *analogies with biological predation* under the action of *foraging predators*.

2. Criminal behaviour depends on many *urban indices* such as poverty, education, ethnicity and housing, and criminals must be classified as, say, juvenile, adult, drug-dependent etc. Hence a *population dynamics model* is called for, similar to those that have been successful in describing *homelessness* and *contagion* in mathematical biology. The model could be continuous or agent-based, it must apply over relatively long time scales and it must be capable of being eventually incorporated into a larger social *network model*.

When these two themes were drawn together in the closing session, it became apparent that not only should they be *developed jointly*, because of the close coupling of many of the variables, but also that a *third 'control space'* theme should be constructed; this would model the interactive coupling with the effects of social and law enforcement policy and public opinion.

New multidisciplinary challenges in modelling the business environment

Thematic Workshop, Ventspils, Latvia, 2-3 August, 2004

In its second Thematic Workshop, the NETIAM project explored opportunities for multidisciplinary research under the title 'New Multidisciplinary Challenges in Modelling the Business Environment'. The workshop was attended by some 69 researchers from 9 countries, including social scientists, economists, physicists, and mathematicians.

There were four opening presentations, covering macroeconomic modelling and econometric models with an input/output core, financial engineering, economic consequences of insurance price fluctuation, and the emergence of collective states in economic systems. In these presentations, the participants sought to identify the key challenges and observations that will motivate and underpin any realistic models of the business, socio-economic and political environment.

The immediate result was the decision to separate into four breakout sessions charged with identifying the theoretical frameworks within which each of the following themes could be considered quantitatively:

- The coupling between macro-economic modelling and social networks
- Risk stochastics in economic modelling (time series)
- Modelling the transition economies
- Socio-political environment, labour, accessibility, corruption

The breadth and diversity of feedback from the four sessions reflected the fact that this is the most ambitious of the four NETIAM themes. It is so large and interdisciplinary that it is a difficult challenge even to identify those topics where mathematicians can add significant value to the methodologies used by sociologists, economists, politicians, and managers. Concerning this challenge, the social science factors that were considered to be crucial to the business environment were:

• transport, communications, labour supply, corruption, leisure activities, human resources/education.

The corresponding economic factors were:

• tax policy, pensions policy, currency value, insurance policy.

The mathematical methodologies that emerge as being best suited to handle this wide range of human activity fall into two categories:

1 Data Management and Statistical Modelling

New directions for this burgeoning area of mathematical science abound in the realm of business risk, where the novelty lies in modelling corruption and mismanagement and in assessing the business implications of social risks such as gambling, health and unemployment. The most promising methodologies are time series and stochastic analysis, but both will be plagued by insufficient data compared to more traditional risk analysis in, say, finance or weather forecasting. A desirable outcome of a research programme based on these premises is the development of new kinds of insurance policies.

2 'Ad hoc' prediction models for the evolution of the business environment

It was absolutely clear that, in this wide-open area, the way ahead is via a generalised theory of dynamic network modelling. The basic network structure needs to comprise interlinked nodes, each of which may have a multi-dimensional behaviour involving many socioeconomic variables of which only a few will be coupled to other nodes. The network should be able to nucleate and evolve new nodes, and also to have a learning capability. This is an exciting new direction for the mathematical theory of differential-algebraic systems; but it is not a completely new challenge because two traditional, but very elaborate 'ad hoc' network models are already in use. However, they have never been subject to serious mathematical scrutiny and their nodal parameters need to be prescribed subjectively. There is, nonetheless, one reliable paradigm in which the social modelling is represented by a very simple network and utility functions at the nodes describe the econometrics. The development of this paradigm to make it a quality control for the larger codes is an exciting challenge.

Assuming progress can be made with 1 and/or 2 above, the resulting predictions will only be of practical value providing two other quite different challenges are met. Firstly, many social norms/indices need to be quantified before the models from either 1 or 2 can be used to predict optimal policies. Secondly, the research must be explicable in terms that are transparent to policy makers. Neither of these challenges can be addressed by the mathematical community alone but they must both be overcome if mathematics is to make a genuine contribution to this outcome.

Challenges in visualization, simulation and design for virtual porous materials

Thematic Workshop, Kaiserslautern, Germany, 29-30 September 2004

In its third Thematic Workshop, the NETIAM project explored opportunities for multidisciplinary research under the title 'Challenges in Visualization, Simulation and Design for Virtual Porous Materials'. The workshop was attended by some 27 researchers from 8 countries, including physicists, computer scientists, and mathematicians.

There were six opening presentations: 'Visualisation of very large data sets', 'Ventilation, material transport and separation in the human lung', 'Numerical rocks', 'Material geometry: physics and shape of spatially complex matter', 'Parallel algorithms for complex materials', and 'Textiles and nonwovens'.

There were many possible areas within this large area of basic science upon which the breakout groups could have focused. Of the two which emerged, one covered a broad range of applications and the other a broad area of basic mathematical methodology.

Micromechanics of future filtration devices

The classical theory of filters classifies their mechanics according to certain key mechanical chemical and thermodynamic parameters which emerge from paradigm studies of single particle impact on a simple filter element. The applicability of such ideas depends considerably on the ability of scientists to scale up their predictions to practical filters with all their complex geometry.

Modern methodology offers the promise of predicting filter performance far more precisely by using

(i) emerging visualisation techniques (from X-ray or synchrotron data) to represent the filter geometry faithfully,

(ii) modern CFD codes to predict fluid flow through this geometry, even for modern highly irregular filter matrices.

However, there is one basic gap in scientific understanding that needs to be addressed before this strategy can be considered to be reliable. This gap concerns the microscale impact mechanics of the particle (which may be minute) with the filter matrix. It inevitably involves delicate fluid mechanics and surface adhesion mechanics and may also involve electrostatics, coating properties and surface chemistry.

There are also theoretical challenges concerning coupling the particle motion (including coagulation) to the fluid motion, especially when there is a filter cake, or when clogging needs to be predicted.

If these scientific issues can be resolved, there are really exciting applications in prospect ranging from ultra-filters, tissue engineering, catalysis and fuel cells to the preservation of our architectural heritage and to the trapping of bacteria and perhaps even viruses.

From microgeometry of porous media to macro material properties

This is the fundamental multiscale problem of all porous media and it is one where the methodologies cited above pave the way. It is axiomatic (and provable) that fluid flow through a porous medium at the pore scale averages or homogenises itself to Darcy flow in many parameter regimes. It is already possible to explore new regimes by using CFD codes that apply when the Navier-Stokes equations contain inertial terms. However, as flow rates increase, the accuracy of the geometrical representation must be increased, and new codes must be written to compute macroscopic thermodynamic or electromagnetic properties, rather than flow per se. This challenge is waiting to be met because the code predictions can immediately be tested against known homogenised models (Darcy or Biot) and then used to search for new correlations and scaling laws between the microgeometry measures and the macroscale properties. (For Darcy flow the porosity and tortuosity are the principal ones to have been identified.)

This experimental research programme should receive as much quality control as possible from the burgeoning mathematical theories of homogenisation, computational geometry and stochastic partial differential equations, this last being vital in the presence of uncertain tomographic data.

It is even possible that this research could lead to fundamental advances in image processing because it is clear that state-of-the-art voxel visualisations are inadequate to represent porous media with strong inhomogeneities such as fractures. There is a great need for the discretised visualisation to contain geometrical elements that are physically plausible for the porous media under consideration. The problem of making such elements is waiting to be addressed.

It is certain that this research topic will have really strong links with one of the principal NETIAM themes, namely network modelling. At the moment in the oil and filtration industries the passage from microgeometry to macroproperties can only be realised by constructing intermediate scale networks of elements that are believed to provide a reliable stepping-stone between the two scales. The design and reliability of such networks has never been subject to mathematical scrutiny.

Complexity in modelling proteins and interfaces at the molecular level Thematic Workshop, Eindhoven, Netherlands, 2-3 December 2004

This fourth NETIAM thematic workshop identified two important areas of physical and biological science where mathematical innovation could enlighten our understanding of fundamental molecular processes. Despite the apparent disparity between these areas, the emergence of new insights would rely in each case on bringing new *multiscale* analyses to bear.

Understanding interfaces at the molecular level

The more physically based topic is that of the bonding of two disparate materials at an interface, and specifically that of a polymer coating a metal substrate. Despite the importance of such interfaces to the automotive, semiconductor, metal and food industries, there is still no reliable basic understanding of the atomic configurations that are adopted even in the simplest configuration when the interface is nearly flat and the coating and substrate are infinite in extent. Here the new mathematical idea is to systematically use multiscale methodologies to 'match' together

(i) a classical statistical physics theory for the atoms in the relatively wide sublayer where energy and entropy compete in the polymer between its 'long chain' bulk and the nominal interface;

(ii) a density functional theory for the relatively even mixture of atoms in a nanolayer around the interface;

(iii) an atomistic theory for metal atoms deeper into the substrate.

These three theories have a completely different mathematical character but they all highlight the role played by the Gibbs free energy, and this will be of vital importance when matching the theories together. The resulting composite theory will not only allow cohesive forces to be predicted with confidence, but stage (ii) will reveal defect structure in the interface itself. This is the all-important stage at which quantum mechanical effects cannot be avoided and the only way this can be done for any realistic number of atoms is by exploiting the dramatic reduction in the dimensionality of the governing differential equations that density functional theory offers.

If this methodology can be perfected on this paradigm class of problems, it should be relatively easy to generalise it to study cases of imperfect contrast (so called 'loops' and 'trains' in the polymer), steps and/or ledges at the metal interface, the effect of impurity atoms such as oxygen and perhaps even to areas like quantum dot fabrication.

Understanding protein molecules in the cellular environment

There is an urgent need to gain a better quantitative understanding of the behaviour of protein molecules in a cell. From a physico-chemical viewpoint the principal challenge is to predict the evolution of both large and small protein molecules as they move through the complicated pathways between each other and the deformable cell skeleton and its microtubules and lipid bilayers. This is not just a problem in mechanics because of the numerous reactions that can occur between all the kinds of molecules in the cell and because of the important effects of electrical, thermal and chemical gradients. However it is clear that the *geometry* of the protein molecule is its most important mathematical characteristic as far as its reactivity is concerned (the geometry being most conveniently defined by its van der Waals surface). Moreover, user-friendly three-dimensional visualisations of this geometry are now becoming readily available, and there is much current interest in the apparently close relation between geometry and biological functionality.

In this highly complex situation, it was proposed that the first requisite was to understand how the classical theory of immiscible multiphase flow in a porous medium could be generalised to highlight the roles played by both the geometry of the dispersed phase in the pores and by the highly deformable nature of the porous 'matrix'. This multiscale approach will be similar in spirit to the well-developed Buckley-Leverett theory as used so successfully in the oil recovery industry.

Such a paradigm will ignore reactions in the first instance but it is anticipated that these reactions will ultimately be incorporated as a body force distributed through the disperse phase in a way that is crucially dependent on the protein molecule geometry. It is also hoped that the model will provide a basis for understanding transport across the 'bridges' between the cytoplasm and the nucleus.

Opportunities for mathematics in multidisciplinary research

Capstone Workshop, Oxford, UK, 14-15 March 2005

In the Capstone Workshop of the series, the NETIAM project summarised and further examined the opportunities for multidisciplinary research identified by the preceding four thematic workshops. The workshop was attended by 20 researchers from 6 countries including mathematicians and physical, economic and social scientists. The proceedings of this workshop are available in a report which may be downloaded from the NETIAM website at <u>www.netiam.net</u>.

Topics for multidisciplinary research activity

Presentations were made by the local organisers of the earlier thematic workshops to summarise the findings in each of the workshop themes:

- Mathematical modelling of criminality in the urban environment
- New multidisciplinary challenges in modelling the business environment
- Challenges in visualisation, simulation and design for virtual porous materials
- Complexity in modelling proteins and interfaces at the molecular level.

Three underpinning themes of importance to all these diverse areas emerged

- 1. Modelling phenomena over disparate time and length scales
- 2. Dynamic network modelling
- 3. Visualisation and computational geometry.

Each of these underpinning themes was discussed in relation to the topics arising in the preceding thematic workshops. Common areas of challenge and important distinctions between the areas were highlighted in the discussions.

The following eleven application areas, covering one or more of the themes, have been proposed for further research activity as a result of the workshop.

> Bonding forces between organic and inorganic materials Filter (porous) media design Self-organized crime space analysis Opportunity networks in crime Time-evolution of criminality in urban areas Coordination between businesses Characterisation of protein geometry Dynamic social and economic networks Pricing insurance policies in high risk environments Quantifying economic freedom Institutional governance and corruption.

In the workshop report, the corresponding mathematical methodologies and other disciplines required have been highlighted for each application, and multidisciplinary European consortia with the skills to undertake work in each area have been identified. Taking each application area in turn, the structure of the relevant science base has been analysed and, where possible, opportunities have been sought for influencing science policy to facilitate progress.

Infrastructure and mechanism

The Capstone meeting also addressed the issues of mechanism and structure in order to re-visit the last of the NETIAM objectives. A number of points emerged:

The NETIAM approach is very application-oriented, not mathematics-driven, and for good reason. It is difficult to bring people together in a multidisciplinary environment unless there is a *common* point on the horizon to aim for: this is the underlying philosophy of the NETIAM approach, and is one of the reasons why identifying and focusing the problem is half the work. NETIAM has laid the groundwork in identifying and outlining areas for adventurous multidisciplinary research.

The listed applications and methodologies do not imply that the methodologies are adequate — rather it means that they are the *starting points* for the applications. New mathematics and new developments may be required: there is no telling what **new mathematics** may be stimulated by the problems arising in any of these application areas. Developments in mathematics can either be stimulated by problems arising from *outside* mathematics itself, or from within, and NETIAM has been concerned with the first kind of developments. It is also important to realise that NETIAM is not representative of mathematics as a whole; rather, it is at the interface of mathematics with industrial and multidisciplinary applications.

Mathematics *is* **the common denominator** of the NETIAM projects, but there is an urgent need for it to be more generally appreciated as the common denominator in science, industry and society. It is necessary to communicate the NETIAM methodology, so that others can see how they can apply the same methods. NETIAM has demonstrated how mathematics can be used in novel areas; that message must be communicated at a high level, by and through the mathematics networks around Europe. This issue was addressed in the subsequent NETIAM Strategy Meeting.

Strategy: Mathematics, Industry and Society in Europe

Strategy Meeting, Oxford, UK, 4-5 July, 2005

In the NETIAM Strategy Meeting, partner coordinators of the NETIAM project and 15 other leading figures from the mathematics community in Europe and from industry explored the interface between mathematics, industry and society, to determine how Europe can best reap the practical benefits of the ideas and opportunities created by its mathematical community.

The group aimed to address a wide range of issues including: the organisation of interdisciplinary mathematics, the mix of private and public investment, measuring the value of interdisciplinary mathematics, creating awareness of the value mathematics, and accommodating different national/regional cultures.

An almost immediate and sustained focus of the discussions was the urgent **need to increase awareness of the role and value of mathematics in society**, **in industry and as an aspect of our culture**. A wide range of challenges and mechanisms to address this issue were discussed, and it was agreed that a sustained period of action by the mathematics community, perhaps over 10-20 years, would be required to enable society to reap the full benefits of mathematics. In the short term of 1-2 years, it was proposed that a comprehensive marketing and publicity campaign would be directed towards the public, industry, the mathematics community and other disciplines. To carry forward this programme, the meeting proposed that an alliance of representatives from mathematics communities in Europe be formed, and that its strategy be implemented through an executive sub-group to be drawn from its membership. The meeting approved the preparation of an action plan for wide dissemination across Europe.

Following the Strategy Meeting, this initiative has been outlined by the participants under the title **Unleashing Mathematics - A Driving Force for Industry and Society in Europe,** and it is being widely disseminated in a brochure, through the NETIAM website <u>www.netiam.net/Unleashing</u>, and through other channels. Drawing on the cumulative experience spread across Europe, the 'Unleashing Mathematics' initiative aims to set up a team of committed researchers and policymakers from academia, industry and government agencies. Its mission will be to identify the best way of coordinating interdisciplinary mathematics in Europe and to construct an Action Plan for Mathematics in Industry and Society to begin in 2007.

The Strategy Meeting report, and further details of the 'Unleashing Mathematics' initiative may be requested from the NETIAM coordinator, whose contact details are provided at the end of this report.

Plan for using and disseminating knowledge

Knowledge dissemination

A NETIAM website at <u>www.netiam.net</u> is maintained by the Smith Institute to disseminate workshop reports and information on the project's activities. The site also provides links and information to support those wishing to participate in the NEST programme.

Through its multidisciplinary participation, each workshop has acted as a vehicle for the engagement with and dissemination of information about activities in NEST. Each workshop participant has been provided in advance with briefing material describing the objectives and expected outcomes of the workshop, together with explanation of the opportunities and mechanisms by which they can contribute to the workshop. Each participant has also been given details of the NEST activity and encouraged to disseminate their knowledge of NEST to colleagues in their home institutions.

A workshop report has been produced for each Thematic Workshop and for the Capstone Workshop. These reports record the proceedings, participation and ideas emerging from each workshop. Each report has been disseminated to the workshop participants, published on the NETIAM website and delivered to the NEST Project Officer at the European Commission. The web links for the reports have also been disseminated more widely to research and press organisations across Europe.

The NETIAM Strategy Meeting, which was added to the project plan at the end of Period 1, was recorded in note form for the participants, and for dissemination by them individually. As a first step in the initiative formulated by the Strategy Meeting, a four-page brochure entitled 'Unleashing Mathematics' has been produced and is being widely disseminated. It aims to garner the active support of committed researchers and policymakers from academia, industry and government agencies to help develop and implement an Action Plan for Mathematics in Industry and Society.

Organisations to which there has been dissemination include:

Engineering and Physical Sciences Research Council La Repubblica Latvian press Nature FP6UK UK Department of Trade and Industry European Consortium for Mathematics in Industry (ECMI) European Research Consortium for Informatics and Mathematics (ERCIM News) Mathematics, Computing and Simulation for Industry (MACSInet) Numerical Analysis Digest (US based e-digest) Institute of Mathematics and its Applications (UK) CORDIS News (web article) CORDIS Wire (web article)

Raising public participation and awareness

The Smith Institute, on behalf of the consortium, has prepared a brief NETIAM project summary, in the style of a press release, in English, of two pages. The summary is accessible to the nonspecialist at school level, university or in the general public, and also provides a useful overview for researchers in all disciplines. The document highlights the key role that mathematics can play in multidisciplinary research and summarises mechanisms for enabling the identification and conduct of such research. The document can be found at http://europa.eu.int/comm/research/fp6/nest/pdf/nest_project_factsheets2003a.pdf

and has been disseminated to all NETIAM partners for distribution.

The present report, which captures the integration of outputs and ideas from the NETIAM workshops and from the NETIAM Strategy Meeting, is published for public dissemination to a wide range of organisations across Europe, including industry, government and education.

NETIAM Reports

[1] Mathematical modelling of criminality in the urban environment, Report of the Thematic Workshop held in Firenze, Italy, 7-8 June, 2004.

[2] New multidisciplinary challenges in modelling the business environment, Report of the Thematic Workshop held in Ventspils, Latvia, 2-3 August, 2004.

[3] Challenges in visualization, simulation and design for virtual porous materials, Report of the Thematic Workshop held in Kaiserslautern, Germany, 29-30 September 2004.

[4] Complexity in modelling proteins and interfaces at the molecular level, Report of the Thematic Workshop held in Eindhoven, The Netherlands, 2-3 December 2004.

[5] Opportunities for mathematics in multidisciplinary research, Report of the Capstone Workshop held in Oxford, UK, 14-15 March 2005.

[6] Mathematics, Industry and Society in Europe, Notes of the NETIAM Strategy Meeting held in Oxford, UK, 4-5 July, 2005. Available on request from <u>office@smithinst.co.uk</u>.

References [1-5] may be downloaded from the NETIAM website: <u>www.netiam.net</u>.

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Firenze workshop participants:

(Mathematical modelling of criminality in the urban environment)

Giacomo Aletti	Università degli Studi di Milano, Italy
Daniele Amati	Scuola Internazionale Superiore di Studi Avanzati,
	Trieste, Italy
Francesco Battisti	Università degli Studi di Cassino, Italy
Henri Berestycki	L'École des Hautes Études en Sciences Sociales, France
Melvin Brown	Smith Institute, UK
Jon Chapman	University of Oxford, UK
Claire Cunty	CNRS-UMR Géographie-cités, France
Olof Dahlbäck	Stockholm University, Sweden
Mirta Gordon	Laboratoire Leibniz-Imag, Grenoble, France
Mats Gyllenberg	University of Turku, Finland
Miguel Herrero	Universidad Complutense de Madrid, Spain
Neil Johnson	University of Oxford, UK
Shane Johnson	University College London, UK
Andrew Lacey	Heriot-Watt University, UK
Robert Leese	Smith Institute, UK
Robert Mattheij	Technische Universiteit Eindhoven, The Netherlands
Andro Mikelic	Université Claude Bernard Lyon 1, France
Juan Carlos Nuño	Universidad Politécnica de Madrid, Spain
Hilary Ockendon	University of Oxford, UK
John Ockendon	University of Oxford, UK
Mario Primicerio	Università degli Studi di Firenze, Italy
Beatriz Rumbos	Instituo Tecnológico Autónomo de México
Miguel Virasoro	Università di Roma1 `La Sapienza'
Andreas Wiegmann	Fraunhofer-ITWM, Germany
Aivars Zemitis	Ventspils University College, Latvia

Ventspils workshop participants:

(New multidisciplinary challenges in modelling the business environment)

Giuliano Basso Mārtiņš Bērziņš Uģis Bērziņš Melvin Brown Alistair Fitt Mirta Gordon Gunārs Grizāns Sergejs Hilkevičs Andrejs Jaunzems Per Richard Johansen Juris Roberts Kalniņš Valentinas Kiauleikis Ulrich Nögel John Ockendon Tiiu Paas Mario Primicerio

Energy Solutions, UK Daugavas Vanagi, Germany SLD Consulting, Sweden Smith Institute, UK University of Southampton, UK Laboratoire Leibniz-Imag, Grenoble, France Ventspils University College, Latvia Ventspils University College, Latvia Ventspils University College, Latvia Norwegian Central Bureau of Statistics, Norway Social technology Institute, Latvia Kaunas University of Technology, Lithuania Fraunhofer-ITWM, Germany University of Oxford, UK University of Tartu, Estonia Università degli Studi di Firenze, Italy

Fabio Rossi Jānis Stirna	Università degli Studi di Trieste, Italy KTH, Sweden
Wilma Teness	CC Consulting, Sweden
Heather Tewkesbury	Smith Institute, UK
Vincenzo Vespri	University of Firenze, Italy
Jānis Vucāns	Ventspils University College, Latvia
Andreas Wiegmann	Fraunhofer-ITWM, Germany
Matthias Winkel	University of Oxford, UK
Aivars Zemītis	Ventspils University College, Latvia

A further 44 Latvian participants from government, financial and research institutions attended this workshop on its first day.

Kaiserslautern workshop participants:

(Challenges in visualization, simulation and design for virtual porous materials)

David Allwright	Smith Institute, UK
Martijn Anthonissen	Technische Universiteit Eindhoven, The Netherlands
Iacopo Borsi	University of Florence, Italy
Boris Breidenbach	Max-Planck-Insitut für Metallforschung, Germany
Martin Dauner	Institute of Textile Technology and Process Engineering,
	Denkendorf, Germany
Chris Farmer	Schlumberger Evaluation and Production Services, UK
Christoph Garth	University of Kaiserslautern, Germany
Oleg Iliev	Fraunhofer-ITWM, Germany
Wolfgang Koch	Fraunhofer Inst. für Toxikologie und Experimentelle
	Medizin, Germany
Arnulf Latz	Fraunhofer-ITWM, Kaiserslautern, Germany
Bas van der Linden	Technische Universiteit Eindhoven, The Netherlands
Robert Mattheij	Technische Universiteit Eindhoven, The Netherlands
Klaus Mecke	Max-Planck-Institut für Metallforschung, Germany
Martine Meireles	CNRS and Univ. P. Sabatier, Toulouse, France
John Ockendon	University of Oxford, UK
Julia Orlik	Fraunhofer-ITWM, Kaiserslautern, Germany
George Perera	Perera Software Engineering, Stuttgart, Germany
Mario Primicerio	Università degli Studi di Firenze, Italy
Ewald Quak	SINTEF ICT, Oslo, Norway
Katja Schladitz	Fraunhofer-ITWM, Kaiserslautern, Germany
Adrian Sheppard	Australian National University
Mark Spivack	University of Cambridge, UK
Konrad Steiner	Fraunhofer-ITWM, Kaiserslautern, Germany
Heather Tewkesbury	Smith Institute, UK
Andreas Wiegmann	Fraunhofer ITWM, Kaiserslautern, Germany
Ainars Zemitis	University of Hamburg, Germany
Aivars Zemitis	Ventspils University College, Latvia

Eindhoven workshop participants:

(Complexity in modelling proteins and interfaces at the molecular level)

David Allwright	Smith Institute, UK
Martijn Anthonissen	Technische Universiteit Eindhoven, Netherlands
Alberto Bersani	Università di Roma `La Sapienza', Italy
Enrico Bersani	DataLink Informatica s.r.l, Italy
Tim Boxer	Smith Institute, UK
Monica Bulacu	Rijksuniversiteit Groningen, Netherlands
Christopher Cox	Clemson University, USA
Gero Friesecke	University of Warwick, UK

Christina Giannopapa	Technische Universiteit Eindhoven, Netherlands
Bob Mattheij	Technische Universiteit Eindhoven, Netherlands
John Ockendon	University of Oxford, UK
Miguel Patricio	Technische Universiteit Eindhoven, Netherlands
Mark Peletier	Technische Universiteit Eindhoven, Netherlands
Mario Primicerio	Università degli Studi di Firenze, Italy
Jackie Schooleman	Virtual Protiens B. V., Netherlands
Paul van der Varst	Technische Universiteit Eindhoven, Netherlands
Willem-Pier Vellinga	Rijksuniversiteit Groningen, Netherlands
Andreas Wiegman	Fraunhofer-ITWM, Germany
Bert de With	Technische Universiteit Eindhoven, Netherlands
Aivars Zemitis	Ventspils University College, Latvia

Capstone workshop participants:

(Opportunities for mathematics in multidisciplinary research)

Smith Institute, UK Università degli Studi di Cassino, Italy Smith Institute, UK Smith Institute, UK Technische Universiteit Eindhoven, Netherlands Laboratoire Leibniz-Imag, Grenoble, France Ventspils University College, Latvia University College London, UK Social Technology Institute, Latvia Smith Institute, UK Technische Universiteit Eindhoven, Netherlands University of Oxford, UK University of Oxford, UK Università degli Studi di Firenze, Italy Smith Institute, UK European Commission Ventspils University College, Latvia Fraunhofer-ITWM, Germany Technische Universiteit Eindhoven, Netherlands Ventspils University College, Latvia

Strategy meeting participants: (Mathematics, Industry and Society in Europe)

Jean-Pierre Bourguignon Melvin Brown	Institut des Hautes Études Scientifiques, France Smith Institute UK
Heinz Engl	Johann Radon Institute, Austrian Academy of Sciences
Peter Grindrod	Lawson Software
Helge Holden	European Consortium for Mathematics in Industry
Julian Hunt	University College London, UK
Rolf Jeltsch	ETH Zürich, Switzerland
Philippe Lacour-Gayet	Chief Scientist, Schlumberger
Robert Leese	Smith Institute, UK
Robert Mattheij	Technische Universiteit Eindhoven, The Netherlands
Helmut Neunzert	Fraunhofer-ITWM, Kaiserslautern, Germany
Hilary Ockendon	University of Oxford, UK
John Ockendon	University of Oxford, UK
Mario Primicerio	Università degli Studi di Firenze, Italy
Ewald Quak	Tallinn University of Technology, Estonia
Mike Sheppard	Schlumberger
Bruce Smith	Smith Institute, UK
Martin Taylor	Physical Secretary, Royal Society of London
Bernardus Tubbing	DG Research, European Commission
Aivars Zemitis	Ventspils University College, Latvia

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