NETIAM

New and Emerging Themes in Industrial and Applied Mathematics

Challenges in visualization, simulation and design for virtual porous materials

Report of a workshop held Kaiserslautern, Germany, on 29th & 30th September 2004

Prepared by the Smith Institute on behalf of the NETIAM Project

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The NETIAM project web site can be found at http://www.netiam.net.

Executive Summary

Through a series of five workshops at different venues across Europe, the European FRAMEWORK 6 project NETIAM (New and Emerging Themes in Industrial and Applied Mathematics), aims to use mathematics in the formulation of unexplored multidisciplinary challenges, to increase awareness of this role across academic disciplines and end-users, and to identify strengthening mechanisms for multidisciplinary collaboration.

In its third Thematic Workshop, held in Kaiserslautern, Germany on 29-30 September 2004, 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 non-wovens.

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[1]. 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 concerns the microscale impact mechanics of the particle (which may be minute) with the filter matrix. This 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 ultrafilters, tissue engineering, catalysis and fuel cells to the preservation of our architectural heritage and to the trapping of bacteria and perhaps even viruses.

[1] N. A. Fuchs. The mechanics of aerosols. Pergamon, 1964.

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 all the quality control it can receive 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 which 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 theme 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.

The programme of each of the NETIAM workshops is highly flexible, interactive, and responsive to emergent ideas, so distinguishing them from more traditional conference and seminar events. The Firenze[2] and Ventspils[3] workshops have provided insight into the mechanisms and challenges in stimulating ideas for novel multidisciplinary research topics and collaborations; these aspects will be addressed more fully in the subsequent capstone Plenary Workshop in March 2005.

The proceedings and output from the Kaiserslautern workshop are recorded in this report for dissemination amongst the workshop participants and the wider public and research communities. The report is intended as a resource of ideas for future multidisciplinary research activity on the topic of Challenges in visualisation, simulation and design of virtual porous materials and related areas. It is also the third of four Thematic Workshop reports which will form the basis of the final Plenary Workshop in March 2005, in which the ideas emerging from the Thematic Workshops will be integrated into substantial themes and collaborations for novel and multidisciplinary research.

[2] See http://www.smithinst.ac.uk/Events/Firenze/FirenzeReport

[3] See http://www.smithinst.ac.uk/Events/Ventspils/VentspilsReport

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1 Introduction

On 29th to 30th September, 2004, a workshop on Challenges in visualisation, simulation and design of virtual porous materials was a held in Kaiserslautern, as part of the European FRAMEWORK 6 project: NETIAM (New and Emerging Themes in Industrial and Applied Mathematics), which emphasizes new and emerging applications of mathematics in the real world. (An outline of the NETIAM project and its aims is given in Appendix A.).

The Kaiserslautern workshop is the third of four multidisciplinary Thematic Workshops. Each Thematic workshop uses mathematics to help identify and formulate unexplored multidisciplinary research challenges, and to form new multidisciplinary collaborations for high adventure research. The Thematic Workshops will be capped by a Plenary Workshop to consolidate the emerging opportunities.

This report records the setting, aims, processes and outcomes from this workshop. It has three audiences; the European Commission NEST programme, the participants in the workshop and the wider public and research community, for which it is intended as a resource of ideas for future multidisciplinary research activity on the topic of the visualisation, simulation and design of virtual porous materials and related areas. The report will form the basis of the NETIAM Plenary Workshop discussions on this topic.

This report is organised into three parts: The main body describes the processes of the workshop and summarises the key points arising from the presentations and discussions during the workshop. In a second section copies of the presentations made duing the workshop are given as a point of reference. Finally, appendices provide background information on the NETIAM project, details of the Kaiserslautern workshop participants, and related reference material.

2 Background to the Workshop

2.1 Workshop setting and aims

The aim of the Kaiserslautern workshop is to connect those mathematical methodologies that have greatest potential to predict the properties of complex porous materials, to understand how geometry influences these properties and ultimately how to design materials so that they have improved properties. As a specific example, the visualisation, simulation, analysis and design of filter materials with respect to filtration efficiency, pressure drop, and filter life time will be considered.

New production processes and new materials vastly increase the possibilities of making cheaper and better materials. Large numbers of production parameters and material choices as well as choices for material recombination together with shortened product cycles due to increased global competition as well as lack of experience with new materials and production processes make traditional trial and error approaches for material improvement obsolete. A particular challenge lies in the randomness of materials (for example, Non-woven or foams) on small scales. Thus, many researchers in this field from material science, computer science and mechanical engineering have begun to use simulation and models to predict improvements under material variation.

Whereas there is a vast mathematical literature on individual aspects of virtual porous materials, the use of mathematical models and methods from a unified perspective is still at its dawn, and most works that treat all aspects of real world problems stem from mechanical engineers, computer scientists and material scientists.

a) The issues in the *visualization of virtual porous materials* as well as real materials include, but are not limited to the need for

- very large 3d data sets,
- complex and changing geometries as well as complex properties such as flow fields, displacement fields, electric fields, magnetic fields,
- representative, instructive agglomerate information and
- easily accessible detail information.

b) Regarding the *analysis of materials,* it is necessary to create models of materials that include all the relevant features needed to correctly predict their properties. Issues here include but are not limited to

- extraction of 3d features from 2d images,
- 3d image acquisition and image processing,
- stochastic geometric models for random materials and
- bridging of scales from microns for geometric material features to metres for products assembled from these materials.

c) Regarding the *virtual design of materials* issues include but are not limited to

- computation of material properties,
- finding porous media material models with few parameters
- continuous and discrete optimization methods,
- dealing with constraints on manufacturability and
- dealing with non-modelled side conditions, e.g. production cost.

According to the list above, the mathematical works fall in three main categories:

- Visualization and Image analysis
- Stochastic geometry and Material Description
- Porous material design based on the simulation of material properties

With the broader setting of the NETIAM project, the most desirable outcomes of the workshop and the follow-on discussions were stated to participants as (i) the identification of areas of high adventure and opportunity that are prime future topics for NEST, other parts of EC Framework and other research programmes, and (ii) the formation of multidisciplinary collaborations to generate proposals in those areas.

2.2 Workshop participation

A list of invited workshop participants is given in Appendix B. The participants were invited to provide an outline of their interests in the topic of the workshop and also to provide literature references, which they thought would be relevant to the event. See Appendix C. This material provides an outline of the landscape against which the Kaiserslautern workshop took place, and against which new adventurous research agendas for the topic of the workshop are to be set.

The event was coordinated Dr Andreas Wiegmann of ITWM, Kaiserslautern, Germany, and project coordination and facilitation support were provided by Dr David Allwright and Dr Heather Tewkesbury of the Smith Institute.

2.3 Workshop programme and format

2.3.1 Location and programme

The workshop took place at Seehotel Kaiserslautern. Use was made of one ‘forum’ room and and one other room to enable two separate break-sessions. The format of the workshop was designed to encourage the widest exploration of possible approaches. The initial plan for the use of the available time is outlined below.

Wednesday, September 29th	**Thursday, September 30th**
08.30 Registration 09.00 Opening, Welcome to Fraunhofer ITWM 09.10 Introduction to NETIAM 09.30 Visualization of very large data sets from porous materials – Christoph Garth 10.00 Ventilation, material transport and separation in the human lung – Wolfgang Koch 10.30 Numerical Rocks – Chris Farmer 11.00 Coffee break 11.30 Material Geometry: physics and shape of spatially complex matter – Klaus Mecke 12.00 Parallel algorithms for complex materials – Adrian Sheppard 12.45 Lunch 14:30 Plenary “Barriers and enablers for multidisciplinary research” 16.00 Parallel Sessions I, II, III 19.30 Dinner	09.00 Parallel Sessions I, II, III 11.15 Reporting Session 12.15 Conclusions – Closing Session 12.45 Lunch

This programme was treated as a flexible framework, in order to respond to emerging lines of discussion. In the event, there was a mix of presentations, forum discussions and parallel break-out discussions. The initial session on Wednesday morning included an introduction to the NETIAM project and the aims of the workshop (see section I), followed by six presentations of some of the important modelling challenges for porous materials. (See sections II-VII). There then followed a mix of forum and break-out discussions, which continued during Thursday morning.

2.3.2 Format and management

Taking the presentations as a starting point, the forum and break-out discussions drew out key issues surrounding visualisation, simulation and design for virtual porous materials. The discussions then progressed to defining challenges requiring attention from multidisciplinary collaborations including mathematicians.

The overall progression of the workshop required careful management to assign agreed tasks to each of the forums and break-out sessions. It is important that the presenters come from domains of the workshop topics and therefore preferably from disciplines other than mathematics. As sub-themes emerged, mathematical skills were subsequently used to help structure and formulate research challenges. A careful balance had to be struck between, on the one hand defining the topic domain challenges in the language of the topic domain, and, on the other, using high-level mathematical modelling approaches to show how progress might be made on those challenges. This approach means that, as intended over one-and-a-half days, rather than forming research pathways, the workshop has provided sign-posts to areas and methods for which new multidisciplinary research is expected to be fruitful. Equally significantly, the workshop has brought together a core body of potential collaborators which has the background and expertise to carry out such research. The stimulation and structuring of groupings of such researchers is one of the aims of the Plenary Workshop.

Two breakout groups were created in comparison to four groups at the Ventpils workshop, mainly due to the number of workshop participants. This enabled the participants to work in different areas whilst maintaining the critical mass required to sustain the groups. Subsequent forum discussions looked at each breakout theme in turn rather than merging the themes back in to one area.

The following sections provide a summary of key points arising in the workshop presentations and discussions

3 Outline of workshop findings

In this section key points from the discussions following each presentation are outlined in note form and broadly in chronological order of their occurrence in the workshop. The original presentation material is given in sections II-VII.

3.1 Visualization of very large data sets from porous materials

Christoph Garth (Computer Science, University of Kaiserslautern).

Refer to section II for more detail.

One discussion to emerge from the talk was about how to visualize data at a “seam” where two different representations, using different non-uniform grids, had to match together. It was pointed out that this is a general problem, and that you have to match the numerics as well as the visualization, and that you want the matching to be numerically efficient. How you do the fitting is problem-dependent: the mathematical model expressed in the PDEs will specify which derivatives are continuous across the interface and which may be discontinuous, and that information must be used to provide a sensible visualization of the seam.

It was also pointed out that there was a strong tendency now to go to smaller unstructured grids in CFD, rather than the larger structured grids that the talk had tended to focus on. This was agreed, but visualization methods are currently better developed for structured grids. It was asked whether a large structured grid could be converted to a much smaller unstructured grid, and then possibly visualized using non-rectangular pixels.

There was discussion of the method of visualizing vector fields by a stream surface (instead of streamlines). In the examples shown, the colour of the surface was used to indicate either time or distance travelled (from a fixed curve) or position round a vortex (in vortex breakdown).

3.2 Ventilation, material transport and separation in the human lung

Wolfgang Koch (Fraunhofer Inst. fur Toxikologie und experimentelle Medizin).
Refer to section III for more detail

In the discussion, it was pointed out that the good mixing achieved in the airflow in the lung does not necessarily need turbulence, but could occur through counter currents.

The question was raised whether the airways form a tree, and it was suggested that although the conducting airways do form a tree, the deep lung may behave more like a porous medium, and there perhaps needs to be a transition between the two models as you go through the generations of the branching system. There was brief discussion of the paper by Owen & Lewis (2001), see page 28.

3.3 Numerical Rocks

Chris Farmer (Schlumberger).
Refer to section IV for more detail

In the discussion, the question was raised how the accuracy of measurement compares with the accuracy of simulation. Chris Farmer inclined to the view that since you do not want numerical error to be dominant you should do quite accurate simulations (even when really the data are uncertain) but also keep track of the way that uncertainty propagates through the workflow.

Work of the IMA at Minnesota with Schlumberger was referred to, in which an initially uniform grid is taken, and then the cells that cross a fault are split.

The question was raised whether upscaling depended on having a separation of length scales between the fine structure and the coarse grid. Really for porous medium flow through rocks you have a continuum of length scales, and you need a homogenization approach that can cope with that.

3.4 Material Geometry: physics and shape of spatially complex matter

Klaus Mecke (Max-Planck-Institut fur Metallforschung, Stuttgart).
Refer to section V for more detail

In discussion, the question of reconstructing permeability based on a measured porosity was raised, and it was said that the Cozeny-Karman formula gives good results.

In discussing the Minkowski functionals $M_n(D)$ for a domain with pore space D, it was pointed out that the standard formula

$$\sum_n \exp(\gamma_n t) \sim \frac{M_0(D)}{4\pi t} - \frac{M_1(D)}{4\sqrt{t/\pi}} + \frac{M_2(D)\pi}{6} \quad as\ t \to 0 \qquad (1)$$

depends on smoothness assumptions about the domain that will not hold for real (e.g. approximately fractal) domains *D*. (Here γ_n are the eigenvalues of the Laplacian on *D* with Dirichlet boundary conditions.)

Other areas mentioned as needing study were
(i) Incorporating physics into the analysis of how physical properties depend on the Minkowski functionals.
(ii) Incorporating time-dependence.
(iii) Dealing with anisotropic properties. (Tensorial Minkowski functionals have been defined but not computed yet.)
(iv) Understanding how the Minkowski functional can capture non-local properties, e.g. whether pores are closed or not. Apparently they can estimate the percolation threshold quite well, but the reason for this is not totally clear.

3.5 Parallel algorithms for complex materials

Adrian Sheppard (Australian National University).
Refer to section VI for more details

No other particular points were raised during discussion, other than the items already covered by AS's presentation.

3.6 Textiles and non-wovens

Martin Dauner (Institute of Textile and Process Engineering, Denkendorf).
Refer to section VII for more details

The question was raised whether the Institute did any simulation of creasing of textiles, or of ropes. It does not, but does simulate things like laying fibres into a structure for forming a helmet. A modified FLUENT code is used, allowing for viscoelasticity.

It was asked whether the Institute worked on surgical materials, and on for instance the question whether a surgical robot using surgical thread has successfully tied a knot. The Institute does work on surgical materials such as threads, but not on simulation of them.

3.7 Forum and break-out session discussions

Two groups were suggested:

(i) Identification of macroscopic material properties from image analysis. This might break down into a first step of image analysis leading to mathematical measures of the structure, geometry and connectivity, followed by a second step taking those measures together with surface and material properties and producing the physical macroscopic material properties (such as permeability).

(ii) Multiscale aspects of filter operation and design, from microgeometry up to macroscopic modelling.

A further topic suggested was the process-based modelling of the structure of materials. For instance, rather than just *measure* the properties of a material, one could have a scientific model of the process that produced the geometry. In a geological context, one would want to model the compaction of grains of sand over long timescales; for an industrial filter one would model the laying down of fibres with friction, bending and non-intersection; for a foam one would model the chemical thermodynamics. This topic was added to the subject area of the first group. There is of course the possibility of combining information from process-based geometric modelling with information from image analysis as a means of (for instance) obtaining better 3D reconstructions from 2D scans.

The second breakout group reached their conclusions after a relatively short period of time and then rejoined the first breakout group.

3.8 Breakout group on identification of macroscopic properties of porous materials

3.8.1 From image to structural measures

In looking at conversion from an image to structural measures, it would be desirable to have a validation of the whole procedure for a structure where the true details of the geometry had been precisely measured or prescribed. In practice a lot of preprocessing of images is done by experience, and verification is done visually, but quantitative validation would be good step forward. Often the imaging process only sees down to a certain scale, and the behaviour on finer scales has to be extrapolated using scaling laws.

In addition to the Minkowski functionals, the geometry and topology of the medial surface of a porous medium was an important structural measure. It was questioned whether the Minkowski functionals could describe permeability, since they are essentially local geometric descriptors, not global: two media might have very similar local structure in terms of pore size, curvature and so on, but the interconnections of the pores may give one medium much higher tortuosity than the other, and so much lower permeability, even though the Minkowski functionals would be essentially identical. The conventional understanding of tortuosity still seemed to capture something vital for flow through porous media that is not captured by the Minkowski functionals.

One point made about imaging processes is that they often do not image exactly the properties that are relevant for an application. For instance X-ray imaging essentially provides electromagnetic information and hence a geometric description of the surfaces. But if an acoustic application is in view then the acoustic parameters cannot necessarily be immediately inferred from the X-ray data: other understanding of the medium has to be used. This then means that the uncertainty in the material model derives partly from the imaging resolution and partly from uncertainty in the physical properties: these two kinds of uncertainty will generally have different effects on the outcomes of simulations.

A recurring theme was that the imaging mechanism should be based on the specific material and properties that you are trying to measure, and that there is a continuing need to improve the quality and resolution of the images acquired.

One aim in imaging would be to reconstruct surfaces directly from Radon projection data. The Centre for Mathematical Morphology at Fontainebleau was referred to in connection with this.

3.8.2 From structural measures to macroscopic parameters

The desired aim in this area is reliable and properly understood correlations between microstructural measures (of geometry, connectivity and so on) and macroscopic engineering properties.

One area that needs further understanding is why the observed correlations work out so surprisingly well. An example is that the percolation threshold correlates well with the Euler characteristic, but this is not understood on the theoretical level. The question was raised how well quantities such as the percolation threshold can be estimated from *local* information. Furthermore, the randomness of the medium needs to be allowed for here, so one is actually asking how a statistical distribution of structural measures is converted into a statistical distribution of macroscopic parameters.

3.8.3 Process-based geometric modelling

The goal here would be to have a mathematical model of the process forming the porous medium, with some unknown parameters in it. Running a simulation of this model would then produce some predicted geometric properties of the material. By comparing those with physical measurements, the actual values of the parameters in the forming process could be inferred. It was pointed out that the porous media we had heard about were formed in many different ways: rocks through geological processes over long timescales – deposition and compaction of sand grains, diagenesis, faulting and fracture; lungs through biological growth and development; filters by laying down mats of fibres, and then blocking and mechanical and chemical degradation during use; and foams by chemical processes. Each of these processes is very complex, and there could easily be elements in any of them that are not captured by a mathematical model, or by its numerical simulation. What will happen when the measurements indicate things that may not support the hypotheses that have been made about the physics?

A further point made was that there is a lot of randomness in any of these processes, and some way must be found of propagating this uncertainty through any model, to provide confidence intervals or regions on the outputs. In some ways, what is needed is not so much a direct numerical simulation of the process that forms the porous medium, but rather an understanding of how the parameters of that process are converted into the parameters governing the statistical distributions of pore size, shape, connectivity etc. The point was also made that the *dynamics* of the formation processes are often complex and if a realistic geometric description of the final state can be obtained in other ways and used in simulation, then in some contexts that is all that is needed. However, in *design* contexts where a given required geometric structure has to be manufactured (e.g. for a filter) then a simulation of the formation process could be more valuable. In the oil industry too, it is necessary to understand how the properties of a porous medium are modified by flow and by chemistry. If CO_2 is sequestered in porous rocks then its weak acidity will over time cause increased erosion, and this is an evolution problem in a porous medium.

3.8.4 The limits of voxel modelling

One of the issues raised here was *What are the limits of voxel modelling?*: if we try to solve a problem with the image cells as the grid cells, without forming any structural measures or any macroscopic model, what are the computational limits on that? It was pointed out that this is not really possible, because you still need a model for what happens in each cell, with parameter values etc: the model may be somewhat simpler, or at least different, at the voxel scale, but you still need one. If you want to compute *directly* on the image in this way, the question was raised whether voxels are the best way to do this or whether you should convert the image to, say, a model of the surface as a set of polygons or a continuum. It was accepted that voxel values are averages, and that even computing on the voxel scale is an approximation. There is always finer scale detail than any image shows, and really you need to extract a multiscale model from the images and all other sources of information available. The area of multiscale inverse modelling needs to be developed. What is the *best* description of a porous medium? Is it a statistical description, as a random field of some kind specified by a relatively small number of parameters, or is it one particular most likely realization with a large number of parameters?

The relationship of this question to the Minkowski functionals was described: the Minkowski functionals are essentially defined for a continuous surface. They can be extended to give a definition on a voxel lattice, but this differs from the continuum definition and the discrete version does not necessarily converge to the continuum version as the mesh size tends to 0 (though in some examples they differ by a factor bounded by π). It is an interesting question whether the discrete version should attempt to mimic continuous curvature, or just look directly at the grid values.

3.8.5 Network models

In many examples of modelling porous media, a network model of some kind is ultimately extracted and used for simulations. The pores of the medium become spheres (nodes) in the network, and the links between pores become tubes (edges) between the nodes. Tortuosity is incorporated by making the length of a tube different from the physical distance between its ends. Such models are valuable not only in prediction but in understanding paths of influence. The physics of what is happening at the pore scale (surface effects, electrochemistry and so on) must be incorporated into the network model parameters. One point raised here is that the rheology of complex fluids, particularly multi-phase or viscoelastic, still poses problems and one may need different models for flow through contractions, elongational flow and so on. Experiments show that in multi-phase flow Darcy's law in the form usually used is not valid, in that, for instance, the flux of oil can show dependence on the pressure gradient in the water. Improvements to the macroscopic models can come from increased understanding of the micro-to-macro transition. Nevertheless, network models are the state of the art in the oil industry, for 3-phase flow, with complex constitutive equations for the phases.

In a network model, it is conventional to think of the fluid flow as taking place along essentially 1-dimensional tubes within a 3-dimensional solid medium. In a filter, the roles are reversed, and it is the solid that is formed from 1-dimensional fibres, and the fluid that flows in the 3-dimensional space around them. Some analogy to a network model could be useful here.

An extension from classical network models would be to use them for acoustics as well as slow flow.

A network model on the microscopic scale would effectively be a voxel model, solving the Navier-Stokes equations on enough pores to simulate macroscopic permeability.

3.8.6 Homogenisation

It was generally considered that there is a need to relate porous media more closely to the standard mathematical theory of homogenization, and of stochastic differential equations.

The example of the Biot model for acoustics in a saturated poroelastic medium was discussed. This requires certain measurements (of porosity, flow resistivity etc) from which the macroscopic model parameters are found. Some of the participants had used this but found that in certain circumstances many of the parameters did not matter. This provides a nice short cut, when it happens, but one needs to know in each set of circumstances why such short cuts work: sometimes it is satisfactory to needs to know in each set of circumstances why such short cuts work: sometimes it is satisfactory to treat the solid as rigid, whereas in a filter the fibres cannot transmit elastic waves so a different simplification occurs.

This example was considered as a possible paradigm of what we have to do more generally: find a minimum number of microscopic measures that suffice to provide a model for the particular macroscopic behaviour under consideration. The correlations between the microscopic and macroscopic parameters will need to be established through cross-validating combinations of mathematical analysis, numerical computations, and experimental work.

3.8.7 Application areas

Many of the applications dealt with fluid flow through a porous medium, often of a multi-phase fluid, or a fluid containing solid particles. Nevertheless, there are other macroscopic properties that can be of interest, such as the acoustic and thermal properties, and elastic or electromagnetic properties (both static and harmonic). It was considered that doing computational electromagnetics on a porous structure was a considerable challenge.

Fuel cells and tissue engineering are other application areas.

3.8.8 Summary

We need a Mathematical Macro- and Nano-Morphology for porous materials.
The ingredients of this need to include:
(i) Appropriate measures of microstructure (porosity, tortuosity, Minkowski functionals, scaling laws) and of the uncertainty and inhomogeneity of microstructure.
(ii) Appropriate correlations from microstructure measures to macroscopic parameters (permeability, relative permeability, thermal, elastic, electromagnetic)
(iii) Validation and verification of these measures and correlations, to be obtained by the mathematical theory of homogenization and stochastic differential equations, numerical computation, and experimental work.
(iv) Process-based geometric modelling, predicting the microstructural parameters from the physics of the formation process.
(v) Direct generation of non-voxel geometric models from images

3.9 Breakout group on multiscale (microgeometrical) aspects of filter design

Aspects covered here included not only conventional filters, but also other situations where a fluid carrying particles flows through a porous medium and the trapping of particles is of importance. A significant amount of work has already been done on filter design (see additional material in Appendix D) but there are several interesting challenges ahead which include:

(i) Modelling filters for risk assessment purposes (filter lifetime, modelling the accumulated damage due to cracking and chemical deterioration)
(ii) Models for filtering agglomerate particles, (e.g. diesel soot) both in man-made filters and in the lungs.
(iii) Models for the restructuring of particles on filters due to environmental factors (e.g. temperature and humidity).

(iv) Designing both the geometry and materials of filters with specific reference to the particle characteristics and the fluid in the required application.
(v) Modelling filter action including the microscale surface chemistry, electrostatics, particle impacts on fibres, coatings, fibre cross-section and surface roughness.
(vi) Modelling the cleaning of filters – the reverse problem.

Potential applications included:
(i) Preservation of cultural heritage (degradation of stone buildings and statues by rain, pollution, soot etc).
(ii) Tissue engineering (trapping of cells in a tissue scaffold, growth of cells in the scaffold, degradation of scaffold, flow of nutrients and waste products to and from the cells).
(iii) Other medical devices involving filtering (artificial kidney, liver).
(iv) Filters for bacteria (and possibly viruses) for medical and anti-terrorism applications.
(v) Filters for environmental remediation.
(vi) Catalytic converters.
(vii) Fuel cells (involving surface chemistry, catalyst particles etc).

The filter modelling code developed by ITWM could be a useful starting point to address such challenges, and transfer of knowledge from other disciplines would enable Europe to be world leading in this field.

4 Barriers and Enablers for Multidisciplinary Research

4.1 Barriers

The potential barriers identified were:

(i) Any multidisciplinary research programme must be carefully designed and managed to create one common vision for the group of researchers, otherwise fragmentation of the project can occur.
(ii) Goals for each party are both scientific and output-oriented. For example, some researchers may be able to produce publications while others may need to transfer their technology for the benefit of others. In this case, the academic career of an individual researcher can be jeopardised, even though working with different disciplines may widen their experience. Project reviewers and others will need convincing of the added value created by the project.
(iii) Universities are under increasing pressure to exploit intellectual property. It is necessary to sign a collaboration agreement before the start of any EC project. This can be messy, and may have to go to a vote, which is not necessarily conducive to a scientist's way of thinking.
(iv) Multidisciplinarity means changing the research goals for each party. The global optimum is not necessarily the local optimum – indeed it is unlikely to be for all project partners.
(v) Refereeing procedures at National and European levels often do not include multidisciplinary researchers.

4.2 Enablers

Potential enabling steps would include:

(i) Better communication of the mathematics in products, processes and services would reflect the relevance of mathematics to society, and make it more visible to the general public.

(ii) Industrial and Governmental uptake of mathematics would be increased if a coherent marketing strategy quantifying the added value of mathematics could be developed.
(iii) There should be a common language or glossary, which can be used to present the work to non-specialists.
(iv) Mathematics is unique in its underpinning nature, and as such it needs special treatment. Industrial mathematicians are driven by intellectual curiosity about problems; they have an interest in the whole world. Mathematicians working with physicists and engineers could add value to all multidisciplinary technical projects.
(v) More multidisciplinary meetings (as offered by ECMI and ESGI) would stimulate new collaborations including mathematicians. The UK's Faraday Partnership for Industrial Mathematics operates a team of Technology Translators to identify and facilitate multidisciplinary collaborations. A similar European network would increase rate of innovation and relevance of multidisciplinary research in Europe.

5 Objective Review and Prospect

The Thematic workshops are guided by the five underpinning NETIAM objectives listed in section A.2.2 of Appendix A. The outcomes and prospect from the Kaiserslautern workshop may be evaluated against these objectives as follows:

Objective: *to bring together European researchers 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.* ***Measure:*** *quantity and quality of participation in the four Thematic Workshops and the level of wider dissemination.*

The Kaiserslautern workshop brought together a body of some 27 researchers from 8 countries, including computer scientists, physicists, and mathematicians. The materials provided by participants prior to the workshop, and the presentations and discussions during the workshop provided a firm and common basis for the participants to identify multidisciplinary research challenges within or related to visualisation, simulation and design of virtual porous materials. It is intended that dissemination of this report to all participants and to the wider communities from which they are drawn, will stimulate still further ideas for collaborative research in this area.

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.* ***Measure:*** *clarification of the mathematical content in each theme, and its presentation in the reports from each Thematic Workshop.*

The workshop has successfully demonstrated how the methods and language of mathematics can help to draw out key issues and challenges. The first steps were in understanding current research in areas relevant to modelling the business environment. The process of cross-disciplinary collaboration and elucidation over the short period of 1.5 days with 27 participants was demanding, but it was made highly productive by the adapatability and willingness of all disciplines to participate actively and with openness to different approaches and outlooks. Here is evidence that mathematics can help to bring cross-disciplinary cohesion.

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.* ***Measure:*** *explicitly reported identification at each Thematic Workshop of lacunae in quantitative understanding.*

Many gaps in understanding and in the data required to support better models of the business environment emerged during the course of the workshop. Such gaps have been identified as questions and needs throughout section 3, although they have not been assembled in a single list. Prior to the Plenary Workhop, the workshop participants will be invited more systematically to assess whether these gaps are, in some cases, also gaps in the wider research knowledge base. Experience at Firenze, Ventspils and Kaiserslautern, suggests that such activity is not possible during a Thematic Workshop.

It is intended that this report will be a source of ideas and collaborative partners for researchers wishing to embark research programmes relating to the visualisation, simulation and design of virtual porous materials.

Objective: *to identify the barriers, in terms of organisation and scientific culture, to the research that will fill these gaps in knowledge.* ***Measure:*** *specific discussion of these issues in Thematic Workshops, with conclusions presented in the NETIAM final report.*

Barriers were discussed in the dedicated "Barriers and Enablers" session of the Kaiserslautern workshop, as a result of the difficulty in addressing these issues during previous workshops. See section 4.1 of this report.

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.* ***Measure:*** *recommendations in the NETIAM final report.*

Enablers were discussed in the dedicated "Barriers and Enablers" session of the Kaiserslautern workshop, as a result of the difficulty in addressing these issues during previous workshops. See section 4.2 of this report.

6 Concluding observations

6. 1 Science

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.

6.1.1 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[4]. 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.

[4] N. A. Fuchs. The mechanics of aerosols. Pergamon, 1964.

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 concerns the microscale impact mechanics of the particle (which may be minute) with the filter matrix. This 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 ultrafilters, tissue engineering, catalysis and fuel cells to the preservation of our architectural heritage and to the trapping of bacteria and perhaps even viruses.

6.1.2 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 all the quality control it can receive 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 which 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 theme 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.

6.2 Mechanism

In distinction to more traditional conference and seminar events, a large part of the programme of each of the NETIAM workshops is highly flexible, interactive, and responsive to emergent ideas. Ventspils workshop has provided insight into the mechanisms and challenges in stimulating ideas for novel multidisciplinary research topics and collaborations. The fourth and fifth NETIAM objectives regarding barriers and enablers for multidisciplinary research (section A.2.2 of Appendix A) were explicitly addressed within the Kaiserslautern workshop and a summary of these discussions is recorded in section 4. NETIAM participants will be asked to address the third, fourth and fifth objectives, in preparation for the Plenary Workshop in March 2005, where they will be discussed in more detail.

Workshop Presentations

I Introduction
II Visualisation of very large data sets from porous materials
III Ventilation, material transport and separation in the human lung
IV Numerical Rocks
V Material Geometry: physics and shape of spatially complex matter
VI Parallel algorithms for complex materials
VII Textiles and non-wovens

Appendix A: The NETIAM Project – Overview and Aims

A.1 Overview

NETIAM is supported under the NEST (New and Emerging Science and Technology) programme of Framework 6. It aims to demonstrate how mathematics can be used in the formulation of unexplored multidisciplinary research challenges, to increase awareness of this role across a wide range of research disciplines, end-users in industry, business and government, and to develop mechanisms for strengthening and developing multidisciplinary collaborations.

NETIAM is based on four Thematic Workshops on the following themes:

Modelling criminality in the social environment
Challenges in modelling the business environment
Challenges in visualisation and simulation for virtual materials analysis and design
Complexity at the molecular level,

which will be capped by a Plenary Workshop to consolidate the emerging opportunities. The Thematic Workshops will encourage the brainstorming capabilities of the participants in a facilitated 'think-tank' environment. NETIAM will bring together mathematicians and researchers from other sciences, including social science, with end-users in industry, business and government. The results of each NETIAM workshop will be written up in a publicly available report. Drawing on the uniquely cross-cutting position of mathematics for fostering multidisciplinary interactions amongst the sciences, NETIAM will report on new and unconventional opportunities for research. Throughout, emphasis will be placed on ideas that have high potential to yield ground-breaking practical and theoretical insights.

NETIAM is coordinated by the Smith Institute, and the other project partners are Università degli Studi di Firenze, Ventspils University College, Fraunhofer-ITWM and Technische Universiteit Eindhoven. The NETIAM Management Board members are Melvin Brown, Robert Leese, Bob Mattheij, Hilary Ockendon (Chair), Mario Primicerio, Andreas Wiegmann and Aivars Zemitis, all of whom will be participating in the workshop.

The NETIAM project web site can be found at http://www.netiam.net, where output from the NETIAM workshops will be posted.

A.2 NETIAM Objectives

The following objectives are taken from Annex 1 of the NETIAM contract. They form the basis and an essential point of reference for the aims and activities of each NETIAM workshop.

A.2.1 Strategy

The strategic objectives addressed by NETIAM are:

Promotion of interaction with the research community and the identification of opportunities for research under NEST[5]:

- Engagement of the research community in the process of identifying future research opportunities;
- Building awareness of NEST, its aims and modalities.

More specifically, NETIAM aims to demonstrate how mathematics can be used in the formulation of unexplored multidisciplinary research challenges. It aims not only to increase awareness of this role across a wide range of research disciplines, end-users in industry, business and government, but also to develop mechanisms for strengthening and developing multidisciplinary collaborations involving the mathematics community in the European Research Area.

A.2.2 Objectives

In order to fulfil its strategic objectives, NETIAM has the following objectives, associated measures, and internal assessment mechanisms:

- **Objective:** to bring together European researchers around four cross-disciplinary 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. **Measure:** quantity and quality of participation in the four Thematic Workshops and the level of wider dissemination. **Internal Assessment:** by review of reports from Thematic Workshops.

- **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. **Measure:** clarification of the mathematical content in each theme, and its presentation in the reports from each Thematic Workshop. **Internal Assessment:** by review of reports from Thematic and Plenary 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. **Measure:** explicitly reported identification at each Thematic Workshop of lacunae in quantitative understanding. **Internal Assessment:** by review of reports from Thematic Workshops.

- **Objective:** to identify the barriers, in terms of organisation and scientific culture, to the research that will fill these gaps in knowledge. **Measure:** specific discussion of these issues in Thematic Workshops, with conclusions presented in the NETIAM final report. **Internal Assessment:** by review of the final report from the Plenary 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

[5] http://www.cordis.lu/nest/home.html

programmes. **Measure:** recommendations in the NETIAM final report. **Internal Assessment:** by review of the final report from the Plenary Workshop.

Successful outcomes to these first five objectives will provide the foundation from which to achieve the over-arching goals of NETIAM, namely:

- **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. **Measure:** specific suggestions in the NETIAM final report.

- **Objective:** to assemble teams of researchers that are in a position to generate proposals into NEST, other parts of FP6 and other research programmes. **Measure:** emergence of new consortia among NETIAM participants and those to whom the output of NETIAM is disseminated.

The major milestones associated with these objectives are the staging of the five workshops and the issuing of their associated reports two months after each one.

APPENDIX B: LIST OF PARTICIPANTS

Dr. David Allwright, Smith Institute (UK)
Dr.ir. Martijn Anthonissen, Dept.of Maths and CS, Eindhoven University of Technology (NL)
Dr. Iacopo Borsi Dept. of Mathematics, University of Florence (ITA)
Boris Breidenbach, Max-Planck-Insitut für Metallforschung, Stuttgart (DE)
Dr. Martin Dauner, Institute of Textile Technology and process Engineering, Denkendorf, (DE)
Dr. C. L. Farmer, Schlumberger Evaluation and Production Services (UK)
Dipl. Math. Christoph Garth, Computer Science, University of Kaiserslautern (DE)
Dr. Oleg Iliev, Fraunhofer ITWM, Kaiserslautern (DE)
Prof. Dr. Wolfgang Koch, Fraunhofer Inst. für Toxikologie und experimentelle Medizin. (DE)
Priv. Doz. Dr. Arnulf Latz, Fraunhofer ITWM, Kaiserslautern (DE)
Dr.ir. Bas van der Linden Dept.of Maths and CS, Eindhoven University of Technology (NL)
Prof. Dr. Robert Mattheij, Dept. of Maths and CS, Eindhoven University of Technology (NL)
Dr. Klaus Mecke, Max Planck Institut für Metallforschung, Stuttgart (DE)
Dr. Martine MEIRELES, Lab. de Génie Chimique, CNRS/Univ. P.Sabatier, Toulouse (FRA)
Prof. Dr. John Ockendon, Oxford Centre for Industrial and Applied Mathematics (UK)
Dr. Julia Orlik, Fraunhofer ITWM, Kaiserslautern (DE)
Dr George Perera, Perera Software Engineering, Stuttgart (DE)
Prof. Dr. Mario Primicerio, Rational Mechanics, Faculty of Sciences, Univ. of Florence (ITA)
Dr. Ewald Quak, SINTEF ICT, OSLO, member of NoE aim@shape (NOR)
Dr. Katja Schladitz, Fraunhofer ITWM, Kaiserslautern (DE)
Dr. Adrian Sheppard, Applied Maths, Australian National University (AUSTRALIA)
Dr. Mark Spivak, Centre for Mathematical Sciences, Cambridge University (UK)
Dr. Konrad Steiner, Fraunhofer ITWM, Kaiserslautern (DE)
Dr. Heather Tewkesbury, Smith Institute (UK)
Dr. Andreas Wiegmann, Fraunhofer ITWM, Kaiserslautern (DE)
Dipl. Math. Ainars Zemitis, University of Hamburg (DE)
Dr.math. Aivars Zemitis, Ventspils University College, Ventspils (LV)

APPENDIX C: PARTICIPANT INTERESTS AND RELEVANT REFERENCES

Dr David Allwright
Technology Translator, Smith Institute
The Smith Institute is a not for profit company working at the interface of industry and academia in the area of industrial mathematics. The Smith Institute manages the Faraday Partnership for Industrial Mathematics in the UK and is coordinating the NETIAM project. David will be facilitating the workshop.

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Examples of partial differential equations with solutions that are rapidly varying functions of the spatial or temporal coordinates appear e.g. in combustion, shock hydrodynamics or transport in porous media. For boundary value problems with solutions that have one or a few small regions with high activity, a fine grid is needed in regions with high activity, whereas a coarser grid would suffice in the rest of the domain. Rather than using a truly nonuniform grid, we study a method called local defect correction (LDC) that is based on local uniform grid refinement.

Advantages of LDC include the usage of simple data structures and simple accurate discretisation stencils. In the LDC method, the discretisation on the composite grid is based on a combination of standard discretisations on several uniform grids with different grid sizes that cover different parts of the domain. Application areas I have been working on include glass modelling, combustion and laser surface hardening.

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M.J.H. Anthonissen, R.M.M. Mattheij, and J.H.M. ten Thije Boonkkamp. Convergence analysis of the local defect correction method for diffusion equations. Numerische Mathematik, 95(3):401-425, 2003.

M.J.H. Anthonissen. Local defect correction techniques: analysis and application to combustion. PhD thesis, Eindhoven University of Technology, Eindhoven, 2001.
M.J.H. Anthonissen, B. van 't Hof, and A.A. Reusken. A finite volume scheme for solving elliptic boundary value problems on composite grids. Computing, 61:285-305, 1998.
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M.J.H. Anthonissen. Plane stokes flow with a free boundary driven solely by surface tension. Technical Report RANA 99-08, Eindhoven University of Technology, Eindhoven, February 1999.

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I am research assistant at Department of Mathematics, University of Florence. I have got my MSc in Industrial Mathematics studying the modelling of groundwater pollution, but I am interested in all research involving porous media flow from both analytical and numerical point of view.
I am collaborating also with the research association I2T3 (Industrial Innovation Through Technological Transfer, Florence), working on projects of applied research. In particular, I am involved in programs studying water/vapour infiltration in textiles and filtration of industrial waste waters.

Boris Breidenbach
Max-Planck-Insitut für Metallforschung, Stuttgart
Doing a PhD at the Max-Planck-Insitut für Metallforschung, I am particularly interested in the characterization of complex materials. As a first step, I am processing experimental data, e.g. tomograms of foams and wet granular materials obtained at the European Synchrotron Radiation Facility (ESRF) in Grenoble, and data from stochastic models like the Boolean grain model, to be able to extract relevant morphological parameters. Our approach focuses on the Minkowski valuations, i.e. the Minkowski functionals and their tensorial generalization. The second step is to explore these valuations and their relation to material properties. There are examples of homogeneous and isotropic materials for which such connections have been established, e.g. with thermodynamic potentials and conductivities. We hope, we will succeed to do something similar for anisotropic materials and tensorial properties like elasticities.

Dr. C. L. Farmer
Schlumberger Evaluation and Production Services (U.K.)
I am interested in the general problem of modelling the geometry and texture of natural systems, in particular the rocks that are found in oil reservoirs. I am also interested in the numerical solution of PDEs, stochastic PDEs, effective medium modelling all with a focus on fluid flow in porous media.

Dipl. Math. Christoph Garth
Computer Science at the University of Kaiserslautern (DE)

Dr. Oleg Iliev,
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I am interested in simulation and design for virtual and real porous materials and media, in particular:
- upscaling effective properties of the porous media;
- development of efficient solvers for solving micro- and macro- scale problems;
- accurate discretizations in the case of highly hereogeneous media;
- solving coupled problems for flow in and around porous medium;
- non-Newtonian flow in porous media, etc.

Some relevant papers are listed below.
O. Iliev and D.Stoyanov, On a flexible tool for upscaling porous media flow problems, Journal on Theoretical and Applied Mechanics, vol.31, No.1, pp.18-30, 2001.
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W.Doerfler, O.Iliev, D.Stoyanov and D.Vassileva,
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* 1998 "Diplom" in Mathematics at the Swiss Federal Technical Institute of Technology/Zuerich with Prof. Ch. Schwab, Diploma-Thesis on p-FEM for hydrodynamic instability problems
* 1998-2001 PhD-Student at the Institute of Mechanics at Darmstadt University of Technology / Sonderforschungsbereich 298 "Deformation and Failure in metallic and granular continua",

* 04/2001 Dissertation (sipervisors Prof. K. Hutter, PhD, Prof. H.D.Alber) "Thermodynamics of structured granular materials"
* 2001-2002 Post-Doc at the Institute of Mechanics at Darmstadt University of Technology / Sonderforschungsbereich 298 "Deformation and Failure in metallic and granular continua",
* since Oct 2002 Post-Doc within Graduiertenkolleg "Engineering materials on different scales: experiment, modellierung and simualtion" at the Institute of Applied Mechanics, University of Kaiserslautern

Research areas:

- continuum mechanics for extendend continua/continua with inherent microstructure on different scales (theory and numerical applications)
- thermodynamics
- granular and porous materials
- segregation in multiphase mixtures

Current research is focused on:

- development of theoretical and numerical formulations for so-called micromorphic materials (to be used for instance to describe the response of metallic foams to various loading/deformation processes)

Prof. Dr. Wolfgang Koch
Fraunhofer Institute für Toxikologie und experimentelle Medizin. (DE)
At Fraunhofer ITEM, models are developed for complex aerosol dynamics, including phenomena of particle growth and particle coagulation in humid and warm environments. Such models are needed both for the simulation of aerosol dynamics both in human lungs as well as in industrial filters. With respect to the human lung, it is particularly important to correctly model and simulate the transient nature of inhalation and exhalation. In a joint project with ITWM, controlled dusting experiments will be performed in industrial filters to test ITEM's models in relation with the flow solver software developed at Fraunhofer ITWM.

Koch, W., Friedlander, S.K. “The Effect of Particle Coalescence on the Surface Area of a Coagulating Aerosol”, J. Colloid Interface Sci., 140, p. 419, 1990
Friedlander S.K., Koch, W., Main, H.H. Scavenging of a Coagulating Fine Aerosol by a Coarse Particle Mode, J. Aerosol Sci., 22, p. 1, 1990, 12
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Koch, W., Stöber, W. “A Simple Pulmonary Retention Model for Inhaled Particles Accounting for Dissolution and Macrophage-mediated Removal”, Inhalation Toxicology, 13, p. 129, 2001.
Owen, M.R., Lewis, M.A., The mechanics of lung tissue under high frequency ventilation. SIAM J. Appl. Math., Vol. 61, No. 5, pp1731-1761, 2001.

Priv. Doz. Dr. Arnulf Latz,
Fraunhofer ITWM, Kaiserslautern (DE)
My main research interests are the dynamics of complex fluids as polymers, colloidal suspensions, gels etc. and the mathematical description of the filtration process on microscopic particle scale in complex microstructures and its transfer to medical applications. In recent years I was involved in the development and implementation of a filtration model based on the motion of particles in microstructures under the influence of thermal fluctuations in the fluid (Brownian motion), friction forces between fluid and particle, inertia forces and complex interactions with the microstructure (fibrous media and membranes). One big challenge in this context is the adequate modeling of the adhesion forces between complex shaped particles and structures, whose dimensions are of the same order as the particles itself.

More information on the activities in filtration modeling can be found in :
A. Latz and A. Wiegmann, Simulation of fluid particle separation in realistic three dimensional fiber structures, Proceedings Filtech Europa, I-353 (2003).

Prof. Dr. Robert Mattheij
Department of Mathematics and Computer Science
Eindhoven University of Technology
R Mattheij is full professor of scientific computing at TU Eindhoven. He is past president of ECMI (European Consortium of Mathematics for Industry). He is co-ordinator of MACSI-net (European network on Mathematics, Computing and Simulation for Industry), RTN network on Glass MAGICAL, and Marie-Curie Training Site MASTER. He serves on the editorial boards of Surveys on Mathematics in Industry, SIAM News Electronic Journal for Boundary Elements, International Journal of Nonlinear Modelling in Science and Engineering and Springer Series on Mathematics in Industry. He is chairman of the organising committee of ECMI2004 Eindhoven. He is director of the Master programme Computational Science & Engineering

His present research interests are: numerical analysis of (partial) differential equations, in particular boundary element methods, differential algebraic equations, local defect correction, applications in materials (like glass), chemistry and mechanics.

Dr. Klaus Mecke
Max Planck Institut für Metallforschung (DE)
Material Geometry: physics and shape of spatially complex matter
Spatially complex disordered matter such as foams, gels and porous media are of increasing technological importance due to their shape-dependent material properties. But the shape of disordered structures is a remarkably incoherent concept and cannot be captured by correlation functions alone which were almost a synonym for structural analysis in physics since the very first X-ray scattering experiments. However, in the last 20 years numerous methods such as AFM and computer tomography have been developed which allow quantitative measurements of complex structures directly in real space. Integral geometry furnishes a suitable family of morphological descriptors, known as Minkowski functionals, which are related to curvature integrals and do not only characterize connectivity (topology) but also size and shape of disordered structures. Such functionals can be used to characterize and reconstruct stochastic geometries and to compare real experimental data with stochastic models such as Gaussian random fields or Boolean grain models. Furthermore, Minkowski functionals are related to the spectrum of the Laplace operator, so that structure property relations can be derived for complex materials. Percolation thresholds and fluid flow in porous

media, for instance, can be predicted by measuring the Minkowski functionals of the pore space alone. Also, evidence was found in hard sphere fluids that the shape dependence of thermodynamic potentials of fluids in confining pores can be expressed solely in terms of Minkowski functionals. Finally, a density functional theory can be constructed on the basis of Minkowski functionals which allows an accurate calculation of correlation functions and phase behavior of mesoscopic complex fluids such as microemulsions and colloidal dispersion.

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Research Activity:
Development of membrane and separation processes for particles and colloids ;
Main areas of research include: solid - liquid separation technologies, membrane technology, strategies for wastewater reuse, fine particle separations

Current research focuses around

- Development of methods for characterising structural and transport properties of porous media (light and neutron scattering , microtomography)
- Analysis and description of fouling mechanisms (concentrated colloidal media, fine particulate, aggregates)
- Modelling of transport and hydrodynamics in filtration elements including physicochemical effects

Papers:
F.PIGNON, A. MAGNIN, J.M. PIAU, B.CABANE, M.MEIRELES, P. AIMAR, P.

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Dr. John Ockendon
Oxford Centre for Industrial and Applied Mathematics (UK)
My expertise is differential equations applied to industry in the broadest sense. Over the past 30 years, I have worked on porous materials modelling in the oil, glass, food textile and metal industries, and also in environmental studies. I am also increasingly involved with porous materials modelling in medicine.

Dr. Julia Orlik
Fraunhofer ITWM, Kaiserslautern (DE)
Dr. Orlik is mainly working on three subjects of the multi-scale solid mechanics. The first one refers to the modeling and simulation of the microscopic stress-strain behavior and effective material properties of composite or porous materials. She applies homogenization methods which allow for the computation of average (effective) elastic, viscoelastic, and plastic material properties, accounting for the microstructure and the different constitutive laws. The computation of effective free temperature deformation, swelling, and shrinkage is also possible. The second subject deals with contact problems with micro-rough surfaces, which can also be solved by homogenization methods. Finally, within the third problem complex she considers time-dependent processes for composite bodies, whose macro strength and durability are examined with respect to fatigue, creep strain, impact load, and wear.
More information can be found in the attached flier regarding the topic and a journal paper.

Prof. Dr. Mario Primicerio
Dr. Primicerio is Full Professor in Rational Mechanics at the Faculty of Sciences of the University of Florence (since 1975). He is
Reviewer of Mathematical Reviews
Reviewer of Zentralblatt fur Mathematik
Referee for evaluation of research projects (National Science Foundation-USA; Conseil National Recherche Scientifique- France; CODEST - European Community; Third World Academy od Sciences)
Member of Commitees for Ph.D. examinations in Paris, Delft, Augsburg
Member of the Evaluation Committee I.M.A. Minneapolis - I.A.C. Rome
NATO Senior Fellow at Austin, Texas, USA
Christensen Fellow of St. Catherine's College, Oxford, U.K.
Vice President of the Italian Commission for UNESCO
Socio Corrispondente of the Accademia Nazionale dei Lincei
Socio Corrispondente of the Accademia della Colombaria
President of I2T3 (Industrial Innovation Through Technological Transfer)

and has been Mayor of Firenze (1995-1999)

His current research interest lie in
Tumour growth: the a-vascular case
Models for tumour growth are being discussed incorporating the possible transition of cells through different stages of activity.
Chemotaxis
The concept of "maximum packing" has been introduced and the corresponding free boundary problem has been discussed. Cases of two populations interacting have been also considered, studying the bifurcation of nontrivial stationary solutions.
Blow-up of solutions and their possible continuation are currently studied
Homogenization problems with non - local conditions
Nonlinear diffusion of oxygen and interaction with an array of capillaries has been studied as a model problem in this class. A more general situation incorporating storage of oxygen in hemoglobine has been considered as well.

Dr. Ewald Quak
SINTEF ICT, OSLO, member of NoE aim@shape (NOR)
SINTEF is a multidisciplinary organisation that finds intelligent, profitable solutions for the public and private sectors' needs based on research and development in technology, the natural sciences, medicine and the social sciences. Technology for a better society is SINTEF's vision. SINTEF is Scandinavia's largest independent research organisation with about 1160 employees of whom around 85% are R&D personnel. There are research activities in visualization within the institute SINTEF Information and Communication Technolgy (ICT) and in materials within the institute SINTEF Materials and Chemistry, which can contribute to future research projects.

Ewald Quak, a senior scientist in the Department of Applied Mathematics of SINTEF ICT, is the technical manager of the EU's IST Network of Excellence AIM@SHAPE (see www.aimatshape.net and also the attached flyers) within shape modelling. The expertise of the network partners in 3D modelling and visualization should be very interesting for the materials community, which in turn provides a challenging application area. Ewald Quak is therefore very much interested in identifying and pursuing some new interdisciplinary out-of-the-box approaches combining these subject areas.

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Dr Sheppard received his PhD from the ANU in 1996, looking at the dynamics of optical solitons and related dynamical systems. He continued this work as a Postdoctoral Fellow at the ULB in Brussels, Belgium before taking up an appointment at the UNSW School of Petroleum Engineering in Sydney, Australia to work on the numerical simulation of multiphase fluid flow through porous media. Since 2001 he has worked at the Department of Applied Mathematics at ANU, developing

parallel algorithms for the analysis of tomographic images, the morphological characterisation of porous materials and the simulation of multiphase transport properties.

Selected Publications

A. P. Sheppard, R. Sok, and H. Averdunk, "Techniques for image enhancement and segmentation of tomographic images of porous materials," Physica A, vol. 339, pp 145-151, 2004
A. P. Sheppard, J. Y. Lee, M. A. Knackstedt, and W. V. Pinczewski, "Volume conservation of the intermediate phase in three-phase pore-network models," Transp. Porous Media, in press, 2004.
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Dr. Mark Spivak
Centre for Mathematical Sciences, Cambridge University (UK)

Our work is largely in wave (especially electromagnetic and acoustic) scattering from surfaces and propagation in random media. Within this we have long-standing collaborations with industry to study radar scattering by electrically large or rough surfaces; materials may be perfectly conducting or more complex absorbent materials. The computational task scales very badly with object size and complexity, and requires novel mathematical and computational methods. The mathematical basis for this is the solution of boundary integrals, and stochastic differential equations.

Visualisation is increasingly central to the project for several reasons including high dimensional data, and the sensitivity to parameters of the material or medium. One aim is relate far-fields to surface /material properties, and ultimately to build this information back into the design process.

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http://www.escience.cam.ac.uk/projects/emgrid and http://www.rcuk.ac.uk/escience/) and
in collaboration with scientists from BAE Systems.

Dr. Katja Schladitz
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Research interests: geometric analysis of volume images of microstructures, geometric modelling of microstructures of materials. Scientific background: integral geometry, stochastic geometry, spatial statistics.
Microstructures of macroscopically homogeneous and microscopically heterogeneous materials are interpreted as realisations of stationary random closed sets (racs). Geometric analysis includes various approaches: estimation of particle features, estimation of features of the racs, model based analysis, spectral analysis. The interest in geometric modelling is threefold - good models allow a more detailed analysis (e.g. for foams), simulated image data is a tool for verifying image analytic procedures, models fitted to real data are needed as input e.g. for simulation of macroscopic material properties.

Dr. Konrad Steiner
Dr. Steiner is head of the department “Flows and complex structures” at Fraunhofer ITWM. He has studied mathematics at the University of Kaiserslautern. Since his work at ITWM, he is interested in numerical methods for computational fluid dynamics, especially Lattice Boltzmann Methods. Microstructure simulation and virtual material design especially concerning porous media is main field in the department and therefore he is quite interested concerning the topics of the workshop.

Dr Heather Tewkesbury
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The Smith Institute is a not for profit company working at the interface of industry and academia in the area of industrial mathematics. The Smith Institute manages the Faraday Partnership for Industrial Mathematics in the UK and is coordinating the NETIAM project. Heather will be facilitating the workshop.

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Dr. Wiegmann is one of the organizers of the NETIAM workshop series and responsible for the organization of this particular one. He received his PhD on numerical methods for elliptic partial differential equations from the University of Washington, Seattle, WA, before joining UC Berkeley and Lawrence Berkeley National Lab for two years as a PostDoc in Alexandre Chorin and James A. Sethian’s group. For almost 5 years he is now a staff scientist at Fraunhofer ITWM and coordinator for the fields of micro structure simulation and virtual material design. In this position, Dr. Wiegmann is responsible for the GeoDict material generator and property simulator, accessible at http://www.geodict.com.

In this field his interests lay in the generation of micro structures, in particular nonwovens, and in the design of materials based on the simulation of their properties. Properties of interest are transport phenomena, strength phenomena, acoustic absorption and most recently, particle filtration capability. In order to perform the material modelling, simulation and design, many aspects of physics and scientific computing have become interesting, including adhesion forces between chemical substances, filtration by electric fields, 3d imaging via synchrotron tomography, numerical methods for very large data sets and parallel computing, to name a few.

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A fuel cell is an electrochemical cell which can continuously convert the chemical energy of a fuel and an oxidant to electrical energy by a process involving an essentially invariant electrodeelectrolyte system. In general hydrogen is considered to be the fuel and oxygen the oxidant.

Although, there are different types of fuel cells like SOFC (Solid Oxide Fuel Cell), PEMFC (Proton Exchange Membrane Fuel Cell), PAFC (Phosphoric Acid Fuel Cell) and others, they have common aspects. A fuel cell consists of an electrolyte layer in between two porous electrodes. Electrodes are in general porous electron conducting layers containing catalyst particles like Pt, Pd, Ni etc. Reactions can only take place in the contact zone where reactant, electrolyte and catalyst meet. Reactions are influenced by the temperature, concentrations of the species and potential differences.

One attempt to model mass transfer, reaction rates and potentials within a fuel cell is macroscopic modelling describing porous media as a homogeneous material and using macroscopic experimental parameters to describe it. It has been shown, that using this approach it is possible to fit numerical results to the experimental values and receive acceptable qualitative behaviour. But this approach fails to describe some crucial problems inside the fuel cell like catalyst poisoning through carbon monoxide or other impurities and also potential dynamics remain unclear.

On the other hand different microscopic attempts have been made to describe various aspects of involved materials including pore geometry, catalyst positions, microscopic flows, but no general solution has been presented till this day. In particular it is often not quite understood how complex the reaction chains are, which are the intermediate reactions, how much does the geometry influence the dynamics.

Lot of work has been invested in this area in the last few decades, but still lot of open questions need to be answered.

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