Provisional Descriptions of NPSC Projects

Abstract

This document contains descriptions of projects for the submitted Smart Mix research programme of NPSC, the proposed Netherlands Platform for Scientific Computing. This document is not meant for review, nor for referencing, because as yet the descriptions are provisional and need to be further elaborated on plans and deliverables and need further polishing and editing. However, the provisional descriptions do give a sufficiently clear indication of the chosen subjects, the posed challenges, the proposed research and the planned co-operations.

Contents

1 Science

1.1 Grid computing as an enabling tool for scientific computing

1.1.1 Project leader

dr. R. H. Bisseling (Utrecht University)

1.1.2 Project group

Senior researchers:
dr. R.H. Bisseling (Utrecht University, 0.2 fte)
dr.ir. M.B. van Gijzen (TU Delft, 0.2 fte)
prof.dr.ir. B. Koren (CWI, TU Delft, 0.2 fte)
Mrs. drs. M. Nool (CWI, 0.2 fte)
Junior researchers:
2 PhD students (Utrecht University, TU Delft)

1.1.3 Project description and relevance

Generic computational methods will be developed that enable the use of computer grids for a wide range of scientific computing applications. Among the methods are load balancers that take into account different computation rates for computers in a heterogeneous grid, dynamically changing rates, and different bandwidths across the grid. The methods will be based on the Mondriaan method for data partitioning developed in Utrecht in the context of sparse matrices. A solid quantitative basis for modelling grids will be provided by the Bulk Synchronous Parallel (BSP) model, which will be adapted to the case of heterogeneous, dynamically changing grids.

The methods are developed hand in hand with several applications. The prime application is from the area of information retrieval on the Internet, the computation of the Google PageRank of web pages based on the power method for eigenvalue solution. Use of the Grid-Mondriaan package to be developed will give a better storage scheme for storing the web links and for updating the storage over time. A second application, totally different, but which also can benefit greatly from grid computing is the simulation of unsteady, viscous fluid flows in and around complex, moving geometries, such as the simulation of swimming fish. Other applications will be —in principle— all other computational problems from the Scientific Computing Smartmix that may profit from grid computing.

1.1.4 Research questions and challenges

One goal of the project is the development of a data partitioner for a local computer grid or the global Grid that balances computation loads, minimises communication, balances communication loads as well, and all this in a dynamically changing environment. A main research question is how to partition the data well without the partitioning itself becoming the bottleneck. Answers to this question will be based on simplifying assumptions from the BSP model and on approximations of the original data set, using a multi-level approach.

A challenging research question within the context of information retrieval is caused by the huge amount of data involved: how to pre-process the data such that partitioning is feasible at all, and how to do the partitioning itself on a grid computer.

1.1.5 Project plan and deliverables

The project takes a two-pronged approach: *(i)* the sequential Mondriaan program will be made more flexible by developing and implementing algorithms for heterogenous target architectures and dynamically changing ones; *(ii)* scientific computing applications will be used in an early phase to guide the design of Grid-Mondriaan, and to guarantee interoperability between this partitioner, the application, and standard grid middleware.

The methods will be developed and tested for realistic problems on cluster and grid computers. The project brings together the parallel and distributed computing expertise of three institutes. Partitioning algorithms and software (Mondriaan) and the information retrieval application will be largely supplied by Utrecht University, the swimming fish simulation by TU Delft and CWI, and the interfacing to grid middleware and testing on actual grid computers by the CWI. This combined expertise allows to address specific issues that cannot be addressed by each of the partners separately. The outcomes will be:

- new numerical algorithms of general interest for parallel and distributed computing, i.e., contributions to the state-of-the-art in cluster and grid computing;
- new algorithms for Internet computations, such as identification of web spam, personalised PageRanking, and web searching by Latent Semantic Indexing;
- improved capabilities for computing large-scale fluid-flow problems in and around complex, moving geometries.

The total duration of the project is four years.

1.1.6 Track record

Together, Bisseling, Van Gijzen, Koren, and Nool have a strong expertise in parallel computation for a wide range of applications. Each of them has his/her own specialty: parallel and distributed computing algorithms and data partitioning (Bisseling), numerical linear algebra and parallel computing (Van Gijzen), computational fluid dynamics (Koren), and parallel programming (Nool). Together they perfectly supplement each other.

1.1.7 Publications

- R.H. Bisseling. *Parallel Scientific Computation: A Structured Approach using BSP and MPI.* Oxford University Press, Oxford (2004).
- C.T.H. Everaars and B. Koren. Using coordination to parallelize sparse-grid methods for 3D CFD problems. *Parallel Computing*, **24**, 1081–1106 (1998).
- M.B. van Gijzen. Two level parallelism in a stream-function model for global ocean circulation. Proceedings of EURO-PAR 2003, *Lecture Notes in Computer Science*, **2790**, 820–829 (2003).
- M. Nool and M.M.J. Proot. A parallel least-squares spectral element solver for incompressible flow problems on unstructured grids. *Parallel Computing*, **31**, 414–438 (2005).
- B. Vastenhouw and R.H. Bisseling, A two-dimensional data distribution method for parallel sparse matrix-vector multiplication, *SIAM Review*, **47**, 67–95 (2005).

2 Engineering and Design

2.1 Simulation tools for moving-boundary problems in materials science

2.1.1 Projectleader

Prof.dr.ir. P. Wesseling (TUD)

2.1.2 Projectgroup

Senior researchers:
Dr.ir. C. Vuik (TUD, 0.3 fte)
Dr.ir. F. Vermolen (TUD, 0.3 fte)
Ir. P. Koenis (Boal, 0.3 fte)
Junior researchers:
2 PhD students (TUD/Boal)

2.1.3 Project description and relevance

The main goal of the proposal is to develop simulation tools for moving boundary type problems. Problems of this kind are encountered in materials science, self healing materials, optical recording etc. It appears that a good understanding of the particle distribution in alloys is crucial for the required properties. Measurements and modeling are two important tools to enhance this understanding and to observe, which parameters are important to change this particle distribution. The problems originate from (previous) collaborations with industry, Corus, Boal and Alcoa.

2.1.4 Research questions and challenges

Previously, most of the modeling was done by using 1-dimensional geometries and/or a binary alloy. Recently, the applicants have generalized these methods to real 3-dimensional problems. Dissolution of multi-component particles is also possible with this state of the art numerical method. However, a number of challenging problems remains to be solved in order to make the algorithms robust and easy to use in industry. Below the various problems, which should be tackled in the near future are described:

- **Growth**: in the formation of precipitates most models consist of two parts: nucleation and growth. Nucleation is considered in a related NIMR proposal. Thereafter, diffusion controlled growth sets in. It appears from previous experiments that the current implementation is unable to model this phenomenon, inclusion of the Gibbs Thomson effect is necessary to prevent the fingering of the interface of a growing particle, such that the growth of spherical particles can be modeled.
- **Vector Stefan problem**: We are able to solve 3D vector Stefan problems, which are used to simulate dissolution of multicomponent particles. However, it appears that the solution of a crucial non-linear problem, which is part of the vector Stefan problem, is very time consuming. Optimization of this algorithm is required in order to make the method robust and efficient.

- **Finite element method**: Our method to solve vector Stefan problems is such that the diffusion part of the model uses a finite element method (FEM), whereas the level set approach is based on the finite difference method (FDM). The FEM method can be applied to very general geometries. In order to be able to apply our method to general problems, it is necessary to solve also the level set part with the finite element method. Challenging problems are: which upwind method should be used in order to solve the hyperbolic level set problem, how to extend the interface velocity, how to deal with the reinitialization of the level set function in a finite element framework etc.

- **Various particles**: The influence of various particles with a different composition is in general very important. As an example one can think of the growth of an α particle on a β plate. Or the break up of a β plate due to α particles. This effect can be modelled by using more level set functions. This is a generalization of the known method. However, the occurrence of triple points and how to handle them is in this application the most challenging problem.

- **Diffuse interface models**: Next to so-called sharp interface models (of Stefan type) for particle dissolution and/or growth, we would like to investigate the diffuse interface models based on the phase-field approach (the Allen-Cahn equation) or the Cahn-Hilliard equations. The diffuse interface models allow for a straight-forward implementation of relevant physical phenomena such as a more accurate description of the governing thermodynamics or mechanical loading. These models are nowadays used very often in the materials science community for the beforementioned reasons. However, the computation of their numerical solution is very expensive. Therefore, a numerical challenge is to investigate efficient procedures, such as by local mesh adaptation to have a local fine resolution of the mesh in the interface region. Further, an extension to multi-component alloys is straight-forward and interesting from a materials science point of view.

2.1.5 Track record

Fred Vermolen has developed a number of models and solution methods of increasing complexity to simulate phase transformation in alloys. Currently, he is also active in modeling moving boundary phenomena in wound healing.

Kees Vuik is involved in studying and developing methods for moving boundary problems with the following applications: wet chemical etching, dissolution of multi-component particles, bubbly flow, and optical recording.

2.1.6 Publications

W.O. Dijkstra and C. Vuik and L. Katgerman, *A direct method of solidification for the enhancement of mushy zone network models* Materials Science and Engineering: A, 413-414, pp. 255-258, 2005

C.W. Kuijpers, F.J. Vermolen, C. Vuik, P.T.G. Koenis, K.E. Nilsen and S. van der Zwaag, *The dependence of the beta-AlFeSi to alpha-Al(FeMn)Si transformation kinetics in Al-Mg-Si alloys on the alloying elements* Materials Science and Engineering A, 394, pp. 9-19, 2005

F.J. VERMOLEN AND C. VUIK, *Solution of vector Stefan problems with cross-diffusion* Journal of Computational and Applied Mathematics, 176, pp. 179-201,2005

F.J. VERMOLEN AND C. VUIK AND S. VAN DER ZWAAG, *A mathematical model for the dissolution of stoichiometric particles in multi-component alloys* Materials Science and Engineering, A328, pp. 14–25, 2002

F.J. VERMOLEN AND C. VUIK, *A mathematical model for the dissolution of particles in multi-component alloys* J. Comp. Appl. Math., 126, pp. 233–254, 2000

2.2 Solvers for electro-magnetic field simulations in electronics and optics

2.2.1 Projectleader

Prof. P. Wesseling

2.2.2 Projectgroup

Senior researchers:
Dr.ir. C. Vuik (TUD, 0.3 fte)
Dr.ir. C.W. Oosterlee (TUD, CWI, 0.3 fte)
Dr.ir. M.B. van Gijzen (TUD, 0.3 fte)
Prof.dr.ir. A.P.M. Zwamborn (TNO, 0.3 fte)
Dr.ir. E.S.A.M. Lepelaars (TNO, 0.3 fte)
Junior researchers:
2 PhD students, each 1.0 fte (TUD/CWI/TNO-FEL)

2.2.3 Project description and relevance

The main goal of the proposal is to develop fast, robust, black-box solution methods for important systems of partial differential equations in computational science and engineering. The applications here are related to electromagnetism. Electromagnetic field simulations play an important role in designing electronic devices, and in optics. In a finite element or finite difference analysis an important but time consuming part is the solution of systems of discrete partial differential equations.

In many present day problems, often very small structures of the size of the order of the wavelength are encountered. Nevertheless, due to the vectorial nature of Maxwell's equations and the fact that in many applications metals occur, which should be discretized by very fine grids, the system of discretized equations is often huge. A fast and efficient solution method for general electromagnetic scattering problems, discretized on unstructured grids for example EMC problems in large systems, biological structures and platform design. Unstructured grids are needed to discretize the configurations, which often are very complicated and also to be able to adapt the local coarseness of the grid to the material properties. The problems originate from cooperations with industry.

2.2.4 Research questions and challenges

Currently, optical problems are prominently investigated for efficient biosensors in medical applications and also in new sustainable lighting technologies based on light-emitting diodes (LED). LED lighting will replace conventional light bulbs and tubes in the future. LED's enable spectacular new applications of lighting and if LED's take over the lighting market, energy consumption needed for lighting will drop by 50%. Rigorous electromagnetic modeling is also needed for improving the sensitivity of bio-sensors based on fluorescence. By optimizing the structures the fluorescence yield can be improved considerably. Surface plasmons generated at metal surface can play an important role in increasing high local fields and consequently more efficient fluorescence.

In all these applications the structures are complicated and of the order of the wavelength. Therefore, accurate modeling for the optimization of the devices must be based on the Maxwell's equations. Maxwell's equations are very challenging from Finite Elements numerical point of view. Below we specify these challenges:

- Special curl-conforming FEM elements are needed.
- The computational domain of the radiation or scattering problem must be truncated appropriately. This is not trivial an possible approaches consists by using an integral equation on the boundary or a so-called perfect matching layer.
- Due to the vectorial nature, the discretized system is huge, typically more than 10^6 complex-valued unknowns.
- In most devices metals are used. They require a very fine grid to account for the skin effect. Furthermore, resonance-like phenomena, such as a plasmon surface wave can occur.
- Preconditioning of the iterative solver is necessary.
- There is an FEM code where the preconditioner is based on Saad's ILUT. This preconditioner is relatively robust but at the expense of large memory requirements. This restriction of the current FEM code needs to be eliminated to enhance the industrial applicability of the current code.

Recently, the applicants have been successful in solving the heterogeneous Helmholtz equation at high wave-numbers on structured grids. Project work resulted in a reduction by a factor 100 of computing time for solving wave problems in seismic data processing. Realistic three-dimensional applications involving the Helmholtz equation have become feasible. The work was funded by Shell, Philips and Senter-Novem. A multigrid iteration applied to a specially designed preconditioner for heterogeneous high wavenumber Helmholtz problems, in combination with a Krylov subspace method has led to this impressive improvement. This method, in particular the geometric multigrid method, relies however heavily on a structured grid.

The research team at TNO is heavily involved in Electromagnetic Engineering for years now. Their expertise is to utilize and adapt electromagnetic modelling tools for the design of complex electronic systems such as naval vessels. Also, TNO is involved in the electromagnetic engineering aspects of an IOP-EMVT project on stochastic models to tackle EMC-problems. Internationally know experts on iterative global EM-solvers are working at TNO. By using the lessons-learned encountered during research on global Integral Equations based EM-solvers (see "challenges") in this local Finite Element based numerical research will undoubtedly benefit the quality of the research and generates scientific spin-in/spin-off on high academic level.

The aim of the present proposal is to generalize the successful approach for the Helmholtz equation to Maxwell's equations. Furthermore, a generalization towards unstructured grids is proposed here. For this purpose we need iterative solution methods that are, to a large extent, independent of a given grid. Algebraic multigrid methods, and domain decomposition methods relying on deflation satisfy this requirement. These solvers are the basis of our proposal.

2.2.5 Track record

The research team at TNO is heavily involved in Electromagnetic Engineering. Their expertise is to utilize and adapt electromagnetic modelling tools for the design of complex electronic systems such as naval vessels.

Kees Oosterlee, Kees Vuik and Martin van Gijzen have a long experience with robust iterative methods, which are applied to Helmholtz problems.

2.2.6 Publications

Y. Erlangga, C. Oosterlee, and C. Vuik, *A novel multigrid based preconditioner for heterogeneous Helmholtz problems*, SIAM J. Sci. Comput., 27 (2006), pp. 1471–1492.

J. Frank and C. Vuik, *On the construction of deflation-based preconditioners*, SIAM J. Sci. Comput., 23 (2001), pp. 442–462.

M. Brezina, R. Falgout, S. MacLachlan, T. Manteuffel, S. McCormick, and J. Ruge, *Adaptive algebraic multigrid,* SIAM J. Sci. Comp., 27 (2006), pp. 1261-1286.

R. Nabben and C. Vuik, *A comparison of Deflation and Coarse Grid Correction applied to porous media flow*, SIAM J. Numer. Anal., 42 (2004), pp. 1631–1647.

U. Trottenberg, C. Oosterlee, and A. Schüller, *Multigrid*, Academic Press, London, 2000.

2.3 Next-generation software for seismic hydrocarbon exploration

2.3.1 Project leader

Prof.dr. W.A. Mulder (Shell)

2.3.2 Project group

Senior researchers:
Dr.ir. C.W. Oosterlee (CWI, 0.3 fte),
Dr.ir R. Remis (TUD EM group, 0.3 fte),
Dr.ir. C. Vuik (TUD, 0.3 fte),
Dr. Chuanjian Shen (Shell, 0.3 fte)
Prof.dr. W.A. Mulder (Shell, 0.3 fte),
Dr. R.E. Plessix (Shel, 0.3 fte)
Junior researchers:
1 Post-Doc student, NN, (Shell)
3 PhD students, NN, (TUD/CWI)
(Shell sponsors 75 Keuro/year for a PhD student at TUD)

2.3.3 Project description and relevance

In close cooperation with Shell Rijswijk the consortium will take up the next step in accurate, reliable and modern solution methods in seismic exploration. At the same time, the aim is to incorporate existing academic insights and techniques in an industrial environment. The tasks and novel techniques to include are:

- Prepare the next-generation wave equation software. Issues in this context are:
  - Accurate resolution of small-scale contrasts (structures much smaller than the wavelength, such as boreholes, fractures)
  - Inclusion of topography (mountains, dunes, ice)
  - Drastic enhancement of the performance of the solution methods
  - Inclusion of poro- and visco-elastic effects
- Migration and inversion of seismic data
- Advanced geomechanical modeling
- Improvement on diffusive electromagnetism modeling and inversion.
  Geophysical prospecting with electro-magnetic techniques is not only used for mineral and ore detection, but also for oil and gas exploration. During the last decade, marine applications of controlled-source electro-magnetic methods have become popular. Currents are injected into the sea water by a wire that is towed by a ship. Detectors are placed at the sea bottom and record the horizontal components of the electric and magnetic fields. Because sea-water is fairly conductive and the conductivity contrast with the sediments is not large, it is generally easier to detect resistive or conductive anomalies at sea than on land. For shallow waters, the so-called air-wave may pose problems, just as with measurements on land. This air-wave is the almost static response of the highly resistive air. Important issues in this context are

- Efficient solvers for accurate discretizations of the problem stated in the frequency and in the time domain.
  Accurate and fast modeling and inversion software is required for the interpretation of electro-magnetic measurements. The problem is governed by the Maxwell equations together with Ohm's law. A frequency-domain formulation is attractive because marine data are usually provided at one or a few frequencies.
- Inclusion of medium contrasts
- Accurate representation of details of a source,
- Include the presence of air in the models
- Implementation of relevant boundary conditions

2.3.4 Research questions and challenges

Recently, the applicants have been successful in solving the heterogeneous Helmholtz equation at high wave-numbers on structured grids. Realistic three-dimensional applications involving the Helmholtz equation have become feasible. The work was funded by Shell, Philips and Senter-Novem.

One aim in the present proposal is to generalize the successful approach for the Helmholtz equation to the diffusive Maxwell equations. Another is to enable the use of these techniques in the industrial Shell environment.

2.3.5 Track record

René-Edouard Plessix developed techniques for ray-based velocity inversion of seismic data, rock property inversion, inversion of cross-well seismic data, modelling of seismic and electroseismic data, inversion of magneto-telluric and controlled-source electromagnetic data for exploration.

Wim Mulder has worked on a wide range of problem in scientific computing and applications. He developed methods for the simulation of stationary gas flows and worked on schemes for porous media flow, for wave propagation, and electromagnetic diffusion. Applications include modelling the large-scale structure of our galaxy, flow around air foils, oil and water flow in reservoirs, seismic modelling, imaging, velocity analysis and inversion, and electromagnetic modelling.

2.3.6 Publications

Y. Erlangga, C. Oosterlee, and C. Vuik, *A novel multigrid based preconditioner for heterogeneous Helmholtz problems*, SIAM J. Sci. Comput., 27 (2006), pp. 1471–1492.

W.A. Mulder, *A multigrid solver for 3-D electromagnetic diffusion. Geophysical Prospecting*, in press 2006.

W.A. Mulder and R.-E. Plessix, A comparison between one-way and two-way wave-equation migration, Geophysics, 69 (2004), 1491-1504.

C.D. Riyanti, Y.A. Erlangga, R-E Plessix, W.A. Mulder, C. Vuik and C.W. Oosterlee, A new iterative solver for the time-harmonic wave equation applied to seismic problems. To appear in Geophysics.

U. Trottenberg, C. Oosterlee, and A. Schüller, *Multigrid*, Academic Press, London, 2000.

2.4 Simulation tools for coupled problems in electronic circuits

2.4.1 Project leader

dr. E.J.W. ter Maten (Philips Research)

2.4.2 Project group

Senior researchers:
prof.dr. R.M.M. Mattheij (TU/e, 0.2 fte)
dr. J.M.L. Maubach (TU/e, 0.2 fte)
dr.ir. M.J.H. Anthonissen (TU/e, 0.2 fte)
dr.ir. J.H.M. ten Thije Boonkkamp (TU/e, 0.2 fte)
dr.ir. Th.G.J. Beelen (Philips, 0.2 fte)
dr. E.J.W. ter Maten (Philips, 0.2 fte)
prof.dr. W.H.A. Schilders (Philips, TU/e, 0.2 fte)
dr. B. Tasic (Philips, 0.2 fte)
Junior researchers:
ir. M.F. Sevat (Philips, TU/e)
3 PhD students (Philips, TU/e)

2.4.3 Project description and relevance

Simulations are increasingly important in the electronics industry. The complexity of a VLSI chip has increased from just a few components in the early sixties, to several tens of millions of devices today in Systems on Chip (SoC) and are even integrated at the package level in order to get Systems in Package. Apart from the size problem due to the increase of complexity, a lot of physical effects have to be taken into account, which implies that several couplings have to be taken into account when simulating an electronic circuit:

- Coupling to electromagnetic effects (EMC, Electromagnetic Compatibility).
- Coupling to heat (components are temperature dependent).
- Coupling to detailed semiconductor device equations (to calculate effects that show up at nanoscale).
- Coupling to mechanical devices (stresses) and even fluid devices (in new products).

The combined problems show a large variety in different multiscale dynamics. Also the information has to be passed at frequencies up to a 100 GHz. No existing circuit simulator is yet able to simulate these extreme and coupled problems.
In order to develop new products mathematics must provide the basis, the theory, and the algorithms to obtain new methods for these advanced simulations. These methods have to be applied to real industrial problems to show their relevance in being accurate, efficient, and robust.
The project tackles the problem from the point of view of electronics. However, the eventual applicability of the new methods is expected as much larger. Circuit simulators can be used to simulate flow problems in networks (like for blood circulation), or to simulate mechanical problems, or heat radiation problems. Also here the coupling to include more physical effects becomes of interest (for instance in MRI scanners). High frequency couplings also

occur when simulating coupled systems within an environment of ambient intelligence. Finally, we observe that many results of modern model order reduction methods are formulated in terms of an (abstract) electronic circuit. This makes an (enhanced) circuit simulator a key ingredient in simulating coupled problems.

2.4.4 Research questions and challenges

Physical effects, such as supply noise, voltage drop, and cross-talk have a negative influence on circuit behaviour and require special design solutions. They are examples of deep-submicron effects that put a burden on maintaining circuit performance and robustness. They also have an impact on the simulation tools that are used to study the circuit behaviour. In addition to this the behaviour of most devices degrades when varying temperature. The incorporation of electromagnetic effects or heat flux to electronic circuits leads to the mathematical problem of coupling differential-algebraic equations to partial differential equations. A very elegant way of taking the electromagnetic effects into account is to separately analyse the interconnect structure by means of a Maxwell equation solver, and to summarise the results of these simulations into a compact model which is then integratedly co-simulated with the electronic circuit. Such compact models may be re-used when optimizing the circuit. This approach will form the starting point in the research to tackle couplings.

Several challenges show up and are described in some more detail:

- Increasing complexity (more components are combined on a chip). Extension of model order reduction techniques from linear ordinary differential equations to nonlinear differential-algebraic equations have to be taken into account. Also re-use of building blocks using different parameter values is needed and research started here recently.
- Many different not-ignorable coupling effects (electromagnetic, heat, detailed semiconductor simulation) to the circuits: intrinsic coupling between partial differential equations and differential-algebraic equations. Also coupling to fluids and mechanics are becoming more important: lab-on-chip, MEMS. This requires new sophisticated time integration methods to solve such coupled problems.
- Different multiscale effects, requiring new techniques for multirate time integration (different times steps), and coupling of different simulators using techniques that allow implicit synchronization (for instance properties may change when some additional expression crosses a zero value).
- Different signals from different frequency bands are combined. High frequency signals require much smaller time steps then low frequency signals. Nonlinearity requires to efficiently deal with this in the time domain. The introduction of different independent times offers ways to integrate along characteristics, but this has only been demonstrated on small, simple problems in academic code. The coupling of pulses with analog signals is a new step here to be made. Frequencies up to a 100 GHz have to be taken into account.

2.4.5 Project plan and deliverables

The research program is defined for 4 years, staffed by 4 PhD-students and 2 PostDocs, in which the candidates will spend 50% of his or her time at each institute (TU/e and Philips). Deliverables include journal articles, PhD theses, presentations at key conferences, and simulation software for use at Philips.

2.4.6 Track record

CASA has a large expertise in analysis and numerical simulation of problems that can be modelled as differential equations. In the fields of electromagnetics and circuit simulation, several PhD projects have been successfully completed. This has lead to a large number of articles in scientific journals.

Philips Research currently is involved in the MCA-RTN project COMSON in which first steps are being made to tackle the above problems (Oct. 2005–Oct. 2009). Here a Demonstrator Platform will be built that must allow the simulation of relevant industrial problems. Philips Research recently initiated the MCA-ToK project O-MOORE-NICE (Dec. 2006–Dec. 2009) in which mathematics concentrates on different aspects of Model Order Reduction: parameterization and usage in behavioral modeling; MOR for nonlinear problems; response surface techniques for the purpose of robust design.
For the challenges mentioned in Sections 2.4.3 and 2.4.4 much more effort from mathematics and computational science will be needed than that is covered by the above projects. However these projects offer an environment for international cooperation.

2.4.7 Publications

- Anthonissen, M.J.H., Mattheij, R.M.M., Thije Boonkkamp, J.H.M. ten (2003). *Convergence analysis of the local defect correction method for diffusion equations.* Numerische Mathematik, 95(3), 401-425.
- Houben, S.H.M.J., Maubach, J.M.L., Mattheij, R.M.M. (2003). *An accelerated Poincaré-map method for autonomous oscillators.* Applied Mathematics and Computation, 140(2-3), 191-216.
- Schilders, W.H.A., Maten, E.J.W. ter, Houben, S.H.M.J. (Eds.). (2004). *Scientific Computing in Electrical Engineering (Proceedings of the SCEE-2002 Conference, Eindhoven, The Netherlands, June 23-28, 2002) (Mathematics in Industry, The European Consortium for Mathematics in Industry, 4).* Berlin: Springer-Verlag.
- Tasic, B., Mattheij, R.M.M. (2005). *Explicitly solving vectorial ODEs.* Applied Mathematics and Computation, 164(3), 913-933.
- Mattheij, R.M.M., Rienstra, S.W., Thije Boonkkamp, J.H.M. ten (2005). *Partial Differential Equations: Modeling, Analysis, Computation (SIAM Monographs on Mathematical Modeling and Computation).* Philadelphia: SIAM Press.

2.5 Technical applications of magnetohydrodynamics for propulsion of liquids

2.5.1 Project leader

dr.ir. B. Gravendeel (Technisch Adviesbureau Early Minute)

2.5.2 Project group

Senior researchers:
dr.ir. P.J. van Duijsen (Simulation Research BV, 0.2 fte)
dr.ir. B. Gravendeel (Technisch Adviesbureau Early Minute, 0.3 fte)
prof.dr. R. Keppens (FOM Rijnhuizen, 0.2 fte)
prof.dr.ir. B. Koren (CWI, 0.2 fte)
Junior researchers:
2 PhD students (1 at CWI, 1 at FOM Rijnhuizen)

2.5.3 Project description and relevance

Technical applications of magnetohydrodynamics (MHD) in the propulsion of liquids form a technology of growing future importance. For instance, MHD promises the most efficient propulsion of ships at high speed. It is more effective and efficient to exert body forces on liquids than contact forces, in order to accelerate these. By imposing a magnetic field and by guiding an appropriate electric current through a liquid, a body force, a Lorentz force, is exerted on it. MHD ship propulsion is one example of this emerging MHD technology. The MHD pumping of blood in medical applications is another one. Contact forces in classical hydrodynamic blood pumping may more easily cause damages to blood particles than MHD blood pumping. Still another application is dredging of mud and minerals by Lorentz forces. MTI Holland, a leading research and development institute for dredging, dredge mining and dredging equipment, has interest in the latter.

2.5.4 Research questions and challenges

A difficulty of MHD liquid propulsion is that it may generate a rather strong, unwanted magnetic field outside the propulsion system. The major challenge is to design the channel for the fluid flow, and the magnets and the electrical coils around the channel in such a way that the external strength of the magnetic field is within the limits of acceptability.

2.5.5 Project plan and deliverables

The primary goal of the research is to develop a practical computational simulation tool for MHD liquid propulsion problems occurring in industry. The secondary goal is to also develop design techniques for computing optimal shapes of nozzles, magnets, coils, ... present in these MHD liquid-propulsion problems. At CWI expertise has been built for this in the work of Echeverria, Hemker and Lahaye.

Deliverables at the end of this four-year project will be: *(i)* improved understanding of the physics of the MHD liquid propulsion, and *(ii)* user-friendly software tools enabling the simulation and design of sustainable MHD machines. We plan to have a flying start by using existing software:

- fluid dynamics and electromagnetics software developed at CWI and the TU Delft, and
- MHD software available in the KU Leuven group.

Simulation Research and Early Minute can play a fruitful role in bringing the research results to industrial practice.

2.5.6 Track record

Keppens and Koren have a long-standing experience in the development and application of computational methods for MHD and fluid dynamics in general, respectively.

Van Duijsen and Gravendeel, with their private companies, form a unique bridge to real industrial practice, and are excellent advisers in the electromagnetic aspects of the technical applications. Gravendeel is the Dutch expert on MHD liquid propulsion. He is the ideal leader of the project.

2.5.7 Publications

- G.F. Duivesteijn, H. Bijl, B. Koren and E.H. van Brummelen. On the adjoint solution of the quasi-1D Euler equations: the effect of boundary conditions and the numerical flux function. *International Journal for Numerical Methods in Fluids*, **47**, pp. 987–993 (2005).
- D. Echeverría, D. Lahaye, L. Encica and P.W. Hemker. Optimization in electromagnetics with the space-mapping technique. *COMPEL*, **24**, pp. 952–966 (2005).
- R. Keppens and G. Toth. Using high performance Fortran for magnetohydrodynamic simulations. *Parallel Computing*, **26**, pp. 705–722 (2000).
- G. Toth, R. Keppens and M.A. Botchev. Implicit and semi-implicit schemes in the Versatile Advection Code: numerical tests. *Astronomy and Astrophysics*, **332**, pp. 1159–1170 (1998).
- J. Wackers and B. Koren. A fully conservative model for compressible two-fluid flow. *International Journal for Numerical Methods in Fluids*, **47**, pp. 1337–1343 (2005).

2.6 Solvers for non-polynomial eigenvalue problems in integrated optics

2.6.1 Project leader

Dr. M. Botchev (University of Twente)

2.6.2 Project group

Senior researchers:
Prof.dr. E. van Groesen (University of Twente, 0.2 fte)
Prof.dr.ir. J.J.W. van der Vegt (University of Twente, 0.1 fte)
Dr. Mike Botchev (University of Twente, 0.3 fte)
Dr. G. Sleijpen (Utrecht University, 0.2 fte)
Dr. R. Stoffer(Phoenix BV, 0.5 fte)
Junior researchers:
1 PhD student (University of Twente, daily supervision and promotor Prof.dr. E. van Groesen)
1 PhD student ((Utrecht University and University of Twente, daily supervision Dr. M. Botchev, Dr. G. Sleijpen, promotor Prof.dr.ir. J.J.W. van der Vegt)

2.6.3 Project description and relevance

Integrated optics deals with wave guiding and micrometer devices functioning with nanometer precision for redirection or selection of light. Specific examples of devices are microresonators to select a specific wave length, photonic structures with cavities, and optical sensors for sensing bio-chemical composites or physical changes due to temperature, stress, etc.

Characteristic for all these problems is that the problems are essentially formulated on the unbounded domain in 1, 2, or 3 space dimensions. For numerical calculations, confinement of the domain is essential. This is possible provided suitable boundary conditions on an artificial numerical boundary can be found. In a (for now) limited number of interesting cases this has shown to be possible. These boundary conditions should be "exact" reflecting the physical field in the exterior domain. Consequently the (effective or transmittant) boundary conditions depend on the problem investigated.

Important wave guiding and resonance problems from various applications in integrated optics can be formulated as a linear eigenvalue problem for the physical problem defined on all space. However, when the problem is formulated on the confined domain a complicated (possibly non-selfadjoint) eigenvalue problem arises where, due to the imposed boundary conditions, the eigenvalue also enters the (pseudo-differential) boundary operators. This leads to nonlinear eigenvalue problems of which basic properties are still unknown, just as algorithms for the numerical calculation of such large-scale non-polynomial algebraic eigenvalue problems.

2.6.4 Research questions and challenges

The specific mathematical structure of the continuous and the discrete problem (provided a consistent discretisation is used) reflect the special properties of the physical description by the linear Maxwell equations. This specific structure should be studied in detail and exploited in two ways. First it is essential that the continuous nonlinear eigenvalue problem (the spectral problem for problems with pseudo-differential operators on the boundary) is studied with the primary aim to derive variational a priori bounds on real and imaginary parts of the eigenvalues. Secondly, the specific (skew-) symmetry properties of the matrices entering the discrete eigenvalue problem have to be taken into account in the design of efficient numerical solution algorithms.

The celebrated Jacobi-Davidson method developed in the 90s by Gerard Sleijpen and Henk van der Vorst is nowadays considered as one of the most efficient tools for solving large scale nonlinear eigenvalue problems. For the large-scale non-polynomial eigenvalue problems as occur in integrated optics, we will develop new efficient eigenvalue solvers of the Jacobi-Davidson type. These solvers will be able to naturally handle the nonpolynomial character of the problem and will specifically take into account other characteristic features of the problem, to achieve a high computational efficiency.

We will deal with wave guiding and resonance problems in 1, 2 and 3 dimensions. A non-trivial 1D example is the calculation of states and radiating modes of a defect grating, when efficient boundary conditions are used to simulate an infinite extension of the grating, see [1]. Problems in 2D and 3D will deal with wave guiding structures [2] and with photonic crystal problems [3,4]. For these problems transparent boundary conditions based on Dirichlet to Neumann pseudo-differential equations [5], or so-called Film Mode Matching methods for waveguiding in straight or bent waveguides, lead to the type of nonlinear eigenvalue problems to be studied in this project.

An important problem (which will be dealt with in the project and arises in any integrated optics device) is the connection of a device to the outside world. An optical fiber is used to bring light to the device. Usually, the desired waveguide geometry of the device (that is, the cross-section whose properties with respect to device performance and fabrication error tolerance is optimal) is not suitable for direct coupling to the waveguide; the size or shape of the waveguide mode does not match the fiber mode. Thus, the waveguide must be tapered to a suitable cross-section. These tapers, which have slated faces, should be optimized for loss and length, and the optimization simulations must be done quickly. It may be feasible to use a coordinate transform from the Cartesian system into one in which the slanted faces are straight, the mode calculation of which would again lead to a nonlinear eigenvalue problem.

[1] E. van Groesen, A. Sopaheluwakan & Andonowati, Direct characterization of defect states and modes in defect grating structures, JNOPM 13(2004), 155-173.

[2] H. Uranus, H. Hoekstra & E. van Groesen, Galerkin Finite Element Scheme with Bayliss-Gunzburger-Turkel-like boundary conditions for vectorial optical mode solver, JNOPM 13(2004), 175-194.

[3] A. Sopaheluwakan & E. van Groesen, Calculation of pulse loading and radiative unloading of an optical defect grating structure, submitted Optics Communication.

[4] A. Sopaheluwakan & E. van Groesen, Efficient FEM calculations and a simple low-dimensional model to determine the quality of photonic crystal microcavities, submitted.

[5] J. Nicolau & E. van Groesen, Hybrid analytic-numeric calculation method for light through a bounded planar dielectric, JNOPM 14(2005), 161-176.

2.6.5 Project plan and deliverables

One PhD student will study in particular the continuous formulation of the nonlinear eigenvalue problems and will investigate variational formulations (generalizations of Rayleigh quotients) with the aim to derive a priori bounds for the (real and imaginary part of the) eigenvalues. Another PhD solver will apply this knowledge for numerical solution of the problems and work on development of the Jacobi-Davidson eigenvalue solvers. An outline of a project plan is as follows:

PhD student 1:
Year 1: 1D problem with efficient boundary conditions.
Year 2: 2 and 3D wave guiding problems.
Year 3,4: 2D and 3D photonic crystal cavity problems.

PhD student 2:
Year 1: studying the problem structure and effects of different types of boundary conditions and properties of the exterior domain, application of the standard Jacobi-Davidson schemes to quadratic eigenvalue problems for simple uniform exterior domains.
Year 2: studying the problem structure and designing efficient solution strategies for the Jacobi-Davidson correction equations, selection of a number of representative test cases, their implementation and solution (first, with existing algorithms, later, with the new solvers).
Year 3: implementation and testing the new eigenvalue solvers.
Year 4: writing theses, testing the developed techniques on a number of the selected applications.

Phoenix BV, 1 fte:
- Supply problems which are of direct interest to industry to the both PhD students
- Apply the eigenvalue solvers in Film Mode Matching (or other) straight and bend mode solvers
- Work on the taper issue (fiber-chip coupling), culminating in a tool to design and optimize these components

2.6.6 Track record

The AAMP group has an excellent record of long-term research in the field of mathematical modeling and analytic-numeric calculations for integrated optics. Fruitful collaboration exists with the IOMS Group and with software companies, among which Phoenix BV.

The NACM group, which forms a cluster together with the AAMP group, since recently actively works on computational electromagnetism, focusing on highly accurate adaptive numerical methods (vector and discontinuous Galerkin finite elements, efficient time and frequency domain solvers, aposteriori error estimation).

Within the last decade, the Numerical Analysis group of Utrecht University, until recently headed by Henk van der Vorst, has made several outstanding contributions to the field of numerical linear algebra, which are recognized worldwide.

Phoenix is a company that was founded in 2002, with employees that have excellent experience in modeling in integrated optics; in some cases over 10 years. The company provides database software for clean room management, mask design software, and software for integrated optics simulations.

2.6.7 Publications

H. Uranus, H. Hoekstra and E. van Groesen, Galerkin Finite Element Scheme with Bayliss-Gunzburger-Turkel-like boundary conditions for vectorial optical mode solver, JNOPM 13(2004) 175-194

J. Nicolau and E. van Groesen, Hybrid analytic-numeric calculation method for light through a bounded planar dielectric, JNOPM 14 (2005) 161-176

G.L.G. Sleijpen and H.A. van der Vorst, A Jacobi-Davidson iteration method for linear eigenvalue problems, SIAM J. Matrix Anal. Appl., 17:401-425, 1996.

G.L.G. Sleijpen, J.G.L. Booten, D.R. Fokkema and H.A. van der Vorst, Jacobi-Davidson Type Methods for Generalized Eigenproblems and Polynomial Eigenproblems, BIT, 36:595-633, 1996.

M.A. Botchev, D. Harutyunyan and J.J.W. van der Vegt, The Gautschi time stepping scheme for edge finite element discretizations of the Maxwell equations, Journal of Computational Physics, Vol. 216(2), 2006, Pages 654-686.

3 Complex Flows

3.1 Symmetry-preserving turbulence modelling in aero- and hydrodynamics

3.1.1 Projectleader

dr.ir. R.W.C.P. Verstappen (RuG)

3.1.2 Projectgroup

Senior researchers:
prof.dr. A.E.P. Veldman (RuG, 0.1 fte)
dr.ir. R.W.C.P. Verstappen (RuG, 0.4 fte)
dr.ir. J. Kok (NLR, 0.2 fte)
dr.ir. R.E. Uittenbogaard (WL | Delft Hydraulics, 0.2 fte)
dr.ir. T. Bunnik (MARIN, pm)
Junior researchers:
1 junior researcher (NLR, 0.6 fte)
1 PhD student (RuG)
dr.ir. R. Luppes (Postdoc, RuG, 0.5 fte)

3.1.3 Project description and relevance

Turbulent flow dominates many industrial applications, and in many cases the large scale flow patterns are dependent on small turbulent details. This makes understanding and prediction of turbulence of utmost engineering importance. The project intends to bring turbulence analysis and simulation a major step forward, by using innovative mathematical and numerical concepts (described below).

Specific applications in the maritime area are related to ship design (stern flow and propellor efficiency; hull flow and manoeuvrability) and waterworks (coastal defence systems and safety; spillways; groynes in rivers). The same techniques are applicable in the aerodynamic area, where focus lies on wing design in take-off and landing conditions (optimum lift to increase cargo capacity; reduction of wake vortex to increase runway capacity). The common denominator of these applications is the presence of large regions of recirculating flow, which are highly sensitive to turbulent flow details.

3.1.4 Research questions and challenges

Because of its small flow features, in many practical situations accurate description of turbulent flow in industrial applications is out of reach of 'traditional' simulation methods. Thus far, computational errors are heavily interfering with modelling issues, effectively hampering the design of more accurate turbulence models. Recently, however, a new class of numerical methods has been designed that are based on a novel discretization paradigm, based on preservation of the symmetry of the flow equations, rather than on the traditional minimisation of local truncation error. In this way the discrete convection does preserve energy. Because of the latter property, these methods are found to lead to an increase in efficiency of several orders of magnitude [1, 2]. They have been originally developed and validated for space discretization on DNS (direct numerical simulation) of turbulent flow at moderate Reynolds numbers (around 10^5). Similar ideas, but now applied to time integration methods, have been presented in [3] for hydrodynamic applications.

The same ideas are also applicable in modelling turbulence. In [4] the convective term is remodelled, with some kind of filtering, such that the energy transport to the smaller scales is decreased. The skew symmetry of the convective operator is retained under all circumstances, such that the total amount of (turbulent) energy remains unaffected. The 'filter' is only active in cells that are too coarse to resolve the smaller flow scales. In finer grid cells the method approaches the DNS discretization described above.

The challenge is to extend these new ideas to LES (large-eddy simulation) modelling of turbulent flow at industrial Reynolds numbers (around 10^7). In this way, the industrial applications mentioned above are expected to become accessible at affordable computational cost (comparable to the Reynolds-averaged computations that are currently carried out): LES quality for the price of RaNS.

3.1.5 Project plan and deliverables

The first part of the project focusses on algorithm development: it is devoted to extending the range of application of the new approach towards industrial Reynolds numbers. Algorithmic attention is on refining the design of the convective 'filter', which can also be regarded as a non-linear discretization (similar to the limiters that are used in compressible flow). Preliminary validation of the method will take place with existing, mainly eperimental, data: several flow cases representative for our application area of vastly separated flow (e.g. flow past circular cylinders) haven been extensively measured in the literature. The final validation will be on industrial applications (e.g. with data from the LESFOIL project).

A substantial part of the project is dedicated to the implementation of the new modelling approach in the industrial simulation methods in use at the participating GTI's: ENFLOW at NLR, DELFT3D at WL|Delft Hydraulics, and COMFLOW at MARIN.

3.1.6 Track record

The projectleader has a long-year experience in developing efficient simulation methods for turbulent flow. The improvement of our novel discretisation paradigm has been demonstrated at various workshops on LES and DNS flow simulation [1, 2]. In the mean time, they have received quite some outside interest. As an example, a first version has been implemented successfully in the NLR aerodynamic flow solver ENFLOW [5].

The COMFLOW method (for simulating free-surface flow) has been developed at RUG, in close cooperation with MARIN and NLR [6,7].

3.1.7 Publications

1. R.W.C.P. Verstappen and A.E.P. Veldman: Spectro-consistent discretization: a challenge to RANS and LES. *J. Engng. Math.* 34 (1998) 163–179.

2. R.W.C.P. Verstappen and A.E.P. Veldman: Symmetry-preserving discretisation of turbulent flow. *J. Comp. Phys.* 187 (2003) 343–368.

3. J.J.A.M. van Os and R.E. Uittenbogaard: Towards the ultimate variance-conserving convection scheme. *J. Comp. Phys.* 197 (2004) 197–214. .

4. Roel Verstappen: Conservative smoothers for turbulent convection: an alternative simulation shortcut. In: J.A.C. Humphrey, et al. (eds.), *Turbulence and Shear Flow Phenomena 4* (2005) 859–864.

5. J.C. Kok: Symmetry and dispersion-relation preserving high-order schemes for aeroacoustics and aerodynamics. *Proc. ECCOMAS 2006*, Egmond aan Zee, 2006.

6. J. Gerrits and A.E.P. Veldman: Dynamics of liquid-filled spacecraft. *J. Eng. Math.* 45 (2003) 21–38.

7. K.M.T. Kleefsman, G. Fekken, A.E.P. Veldman, B. Iwanowski and B. Buchner: A Volume-of-Fluid based simulation method for wave impact problems. *J. Comp. Phys.* 206 (2005) 363–393.

3.2 Hydrodynamic loading on coastal protection systems and offshore platforms

3.2.1 Projectleader

prof.dr. A.E.P. Veldman (RuG)

3.2.2 Projectgroup

Senior researchers:
prof.dr. A.E.P. Veldman (RuG, 0.25 fte)
dr.ir. T. Bunnik (MARIN, 0.1 fte)
dr.ir. M. Borsboom (WL | Delft Hydraulics, 0.1 fte)
Junior researchers:
dr.ir. R. Luppes (Postdoc, RuG, 0.5 fte)
1 PhD student (RuG/MARIN/WL, 1 fte)

3.2.3 Project description and relevance

Heavy storms, generating large waves, can be threatening to coastal areas behind the shore line, as well as to fixed and floating structures operating at mid ocean. Thus, coastal protection systems (dikes, spillways, groynes) have to be designed to withstand the forces of nature even in extreme weather situations. The same applies to offshore platforms and FPSO's (floating production storage and offloading platforms). Loss of lives and economic damage has to be prevented. In the project sophisticated models for the description of extreme water waves and their impact forces will be developed. The project is based on the ComFLOW method, developed by RUG and MARIN in a number of international projects (in cooperation with the worldwide offshore industry) [1–4].

3.2.4 Research questions and challenges

Prediction of the forces of nature is highly challenging because of their non-linear character. Linear models (based on potential-flow theory) have been around for quite some time, but they cannot describe the non-linear physics of more extreme waves in coastal areas; also non-linear shallow-water models lack sufficient physics. Thus, it appears necessary to resort to a full Navier–Stokes model; however, such a model is computationally expensive. Moreover, the description of the free water surface in extreme-wave conditions requires considerable care and effort; of special concern during impact are cushioning effects of entrapped regions of (compressible) air.

3.2.5 Project plan and deliverables

The first part of the project focusses on algorithm development. Basis is the in-house ComFLOW method [2]. Originally, this method used a one-phase model: only the water motion is calculated. Currently, the model is extended with a second phase, describing the motion of the air. In this way the cushioning effects of air-entrapment and aeration can be included [4]. This modelling will be further refined. Especially the sharpness of the liquid-air interface requires attention, as interfaces that are smeared out over several cells (which is the case for many existing methods) will underpredict impact forces. Moreover, in the coastal areas the bottom morphology plays an important role in wave propagation; this aspect also will receive attention in the project. Further, the influence of turbulence on the flow wil be studied. The method will be validated with a series of experiments, to be carried out at MARIN and WL|Delft Hydraulics.

3.2.6 Track record

The project leader has long-time intensive contacts with the participating GTI's. He is currently an advisor of the Directory Boards of NLR and MARIN. The ComFLOW method (for simulating free-surface flow) has been developed under his supervision in close cooperation with both NLR and MARIN. Through the latter cooperation in several PhD projects (funded by MARIN, EU and STW, respectively), ComFLOW is currently in use at various offshore industries worldwide. Further, the WL|Delft Hydraulics method Skylla is based on a predecessor of ComFLOW [5].

3.2.7 Publications

1. K.M.T. Kleefsman, G. Fekken, A.E.P. Veldman, B. Iwanowski and B. Buchner: A Volume-of-Fluid based simulation method for wave impact problems. *J. Comp. Phys.* 206 (2005) 363–393.

2. K.M.T. Kleefsman: *Water impact loading on offshore structures - a numerical study.* PhD thesis, University of Groningen (2005).

3. B. Buchner, T. Bunnik and A.E.P. Veldman: The use of a Volume of Fluid (VOF) method coupled to a time domain motion simulation to calculate the motions of a subsea structure lifted through the splash zone. In: *Proc. 25th Int. Conf. Offshore Mech. Arctic Eng.,* Hamburg, Germany (2006) paper OMAE2006-92447.

4. R. Wemmenhove, E. Loots and A.E.P. Veldman: Hydrodynamic wave loading on offshore structures simulated by a two-phase flow model. In: *Proc. 25th Int. Conf. Offshore Mech. Arctic Eng.,* Hamburg, Germany (2006) paper OMAE2006-92253.

5. M.R.A. van Gent: *Wave interaction with permeable coastal structures.* PhD thesis, TU Delft (1995).

3.3 Numerical simulation of efficient ship stern flow

3.3.1 Projectleader

Dr.ir. F.W. Wubs (RuG)

3.3.2 Projectgroup

Senior researchers:
Dr.ir. A. van der Ploeg (MARIN, 0.1 fte)
Dr.ir. F.W. Wubs (RuG, 0.3 fte)
Dr.ir. K.W.A. Lust (RuG, 0.15 fte)
Junior researchers:
1 PhD student (RuG, 1.0 fte)

3.3.3 Project Description and relevance

Dredgers have undergone drastic changes during the last decades due to changing demands of the owners. Not only the loading capacity has increased, but also the operation range and the maximum speed. Besides, more stringent requirements on the comfort for the crew are imposed nowadays. Hence, the design has become critical. Especially in shallow water conditions, optimizing the hydrodynamical behavior of dredgers is becoming increasingly important. Shallow water conditions occur, for example, during cleaning polluted delta areas, gaining new land from the sea, or the construction of dams and dikes to protect land from incursion from the sea.
The design of cruise vessels and of single-screw, relatively full-block ships are other areas in which numerical simulations are very useful: they can be used to minimize the viscous resistance and to make sure that a reasonable inflow for the propellor is obtained, a necessary condition for the avoidance of vibration problems.

Both measurements and Computational Fluid Dynamics (CFD) are nowadays used in the design process of ships. CFD is more flexible, can be used at full-scale and gives a more complete picture of the flow and therefore gives more insight into the physics. However, a drawback of CFD versus model testing is that it is still very hard to predict resistance sufficiently accurate. To improve the accuracy of the numerical simulation, more details of the ships geometry have to be taken into account (e.g. rudders, struts and propeller shafts), requiring more economical simulation techniques. Such techniques will help in designing ships that can compete with the ships designed abroad and hence will give MARIN, but also the Dutch ship-building industry, a stronger position in the world.

3.3.4 Research questions and challenges

Viscous flow computations are already very useful in many areas of ship hydrodynamics, for example in optimizing bare hull forms without the appendages mentioned above. However, they are still insufficiently developed for complex flows including three-dimensional turbulent separation regions and the resulting unsteady vortical flow patterns within these regions. Such complicated flows are likely to be generated near ships operating in shallow water or at a drift angle, especially at the sterns of full ships and behind transom sterns. In addition, the application of viscous flow computations to manoeuvring and seakeeping is not mature yet due to obstacles from unsteady flows, complex environment (e.g. bubbly flow, incident waves, wave breaking) and ship motions. The challenge is to improve the efficiency of the software such that computation of these complex flows comes into range.

3.3.5 Project plan and deliverables

This project proposal aims at improving the accuracy and efficiency in the viscous flow computation around ships. Improvements of both accuracy and efficiency are expected from high-order discretisation techniques [2] quaranteeing that the discretized and linearized system of equations has a coefficient matrix of which the symmetric part is positive real, irrespective of the (ir)regularity of the grid. Efficiency gains are expected to be obtained from a more advanced handling of the nonlinearity and by application of incomplete LU decompositions using special ordering techniques developed at the RuG [1].

The deliverable is a new version of Parnassos capable of handling complex flows

3.3.6 Track Record

MARIN has extensive experience in hydrodynamics, both in advanced experimental testing and numerical simulations. The company serves a wide range of customers around the world. The code PARNASSOS, developed at MARIN, is a workhorse in designing modern ships.

The numerical analysis and computational mechanics group at the university of Groningen has much experience in solving large nonlinear problems in Fluid Dynamics using numerical techniques. Advanced codes for solving turbulent flows by direct numerical simulation, free surface flows (COMFLO) and linear systems (MRILU) have been developed.

A cooperation with MARIN exists already for more than a decade.

3.3.7 Publications

1. E.F.F. Botta and F.W. Wubs, Matrix renumbering ILU: An effective algebraic multilevel ILU preconditioner for sparse matrices. *SIAM J. Matrix Anal. Appl* 20(4) (1999) 1007–1026.

2. R.W.C.P. Verstappen and A.E.P. Veldman, Symmetry-preserving discretisation of turbulent flow. *J. Comp. Phys.* 187 (2003) 343–368.

3. K.W.A. Lust, D. Roose, A. Spence, and A.R. Champneys, An adaptive Newton-Picard algorithm with subspace iteration for computing periodic solutions. *SIAM J.Sci. Comput.* 19(4) (2003) 1188–1209.

4. H.C. Raven, A. van der Ploeg and A.R. Starke, Computation of free-surface viscous flows at model and full scale by a steady iterative approach. *25th Symposium on Naval Hydrodynamics*, St. John's, Newfoundland, Canada, August 2004.

5. A. van der Ploeg, M. Hoekstra and L. Eça, Combining accuracy and efficiency with robustness in ship stern flow computation. *23rd Symp. Naval Hydrodynamics*, Val de Reuil, France, 2000.

3.4 Numerical simulation of extreme waves in wave basins

3.4.1 Project leader

Dr.ir. O. Bokhove (University of Twente)

3.4.2 Project group

Senior researchers:
Prof.dr.ir. J.J.W. van der Vegt (University of Twente, 0.15 fte)
Dr.ir. O. Bokhove (University of Twente, 0.3 fte)
Dr. F. Izsak (University of Twente, 0.3 fte)
Dr. ir. T. Bunnik (MARIN, 0.3 fte)
Dr. ir. J.H. Westhuis (Gusto Engineering, 0.1 fte)
Junior researchers:
1 PhD student, 1 Postdoc (University of Twente, both 1.0 fte)

3.4.3 Project description and relevance

Offshore constructions and ships frequently must operate under severe weather conditions. Recently, this was highlighted again by the tremendous damage caused by Hurricanes Katrina and Rita. Accurate predictions of the impact of wind, waves and current on floating and fixed structures using model tests and numerical simulations are therefore essential for their design and save operation.

This project aims at improving the accuracy in predicting wave conditions in wave basins by integrating model tests and numerical simulations as a precursor for the simulation of wave impact and load on offshore structures. For this purpose numerical simulation techniques will be developed which aim i) to improve our understanding and control of the wave generation process in a model basin, in particular the effects of wave-current interaction, bottom topography and beaches, and ii) to investigate the effects of the tank boundaries on the generated waves.

The numerical techniques will be based on the space-time frame work which allows the use of moving and deforming meshes necessary to follow large free surface motions. Different levels of wave models will be used, viz. a coupling between potential flow and shallow water equations, which aims at modeling the complete MARIN Seakeeping Basin and Offshore Basin, and a computationally more expensive model based on the Euler/Navier-Stokes equations, which will allow the study of wave-current interaction. By combining this technique with a level set method and using the two-fluid element technique recently developed in NACM, also breaking waves can be modelled.

The numerical simulation model will be implemented using the *hpGEM* finite element toolbox under development in NACM which will provide much of the finite element software necessary to construct the wave simulation models.

3.4.4 Research questions and challenges

Numerical simulations of large amplitude steep waves require the use of moving and deforming meshes to accommodate for the motion of the free surface. It is, however, not trivial to maintain accuracy on these dynamic meshes. In particular, realistic wave simulations require minimal dissipation and dispersion errors in the wave motion for long simulation times. This accuracy requirement is frequently counteracted by the need for a sufficiently robust and stable numerical discretization.

In order to meet these requirements, this project aims at developing space-time discontinuous Galerkin finite element methods for the different types of flow models used in this project, e.g. potential flow, shallow water equations and the Euler/Navier-Stokes equations. The space-time technique is well suited for problems which require moving and deforming meshes and can obtain high order accuracy, even on unstructured meshes. Within NACM this technique has been applied to a large variety of fluid flow problems, including waves described by potential flow and the shallow water equations. The aim will now be to develop these techniques into robust and accurate models for large amplitude wave motion. In particular, maintaining numerical stability under extreme wave conditions is a challenge, which we aim to address by developing stabilization operators based on variational multi scale techniques.

Also the calculated pressures and velocities under the wave field will be compared with other numerical approaches such as a VoF method.

The second topic which will be addressed is the interaction between waves and current. In general it is difficult to completely control the current in a model basin and more insight into the mechanisms of the interaction between waves and current will be very useful for model experiments. This requires the modelling of the flow field using a space-time discretization for the Euler/Navier-Stokes equations in combination with the nonlinear free surface boundary conditions. A particularly complicated task is to compute overturning and breaking waves which we will address by combining a level set technique with two-fluid elements which can accurately track moving interfaces.

The numerical models will be implemented using the general purpose finite element toolbox *hpGEM*. Since numerical models of a complete wave basin require a large number of elements special attention will be given to obtain very efficient solution techniques for the nonlinear algebraic equations in the FEM discretization. This will be addressed using fast iterative solvers and also parallel computing will be necessary to ensure reasonable computing times.

Extensive verification and validation using experiments and theoretical results will be conducted. In particular, the simulation results will be compared with the data sets of extreme waves measured at MARIN.

3.4.5 Project plan and deliverables

Ph.D. Student:

Yr 1: Study space-time DG methods for potential flow and the shallow water equations.

Yr 1/2: Become familiar with the *hpGEM* package and implement the potential flow and shallow water equation into the package for two- and three-dimensional problems. Test the computer program on model problems.

Yr 2/3: Study nonlinear stability of the space-time discretization and further improve the computational efficiency using fast iterative solvers. Apply the simulation model to compute the wave field in the MARIN Seakeeping Basin. Investigate the modelling of the beaches.

Yr 3/4: Study the accuracy of the numerical discretization using theoretical techniques and by comparison with detailed experiments.

Yr 4: Writing thesis

PostDoc:

Yr 1: Develop space-time DG model for nonlinear waves described by the Euler equations and implement the algorithm in a two-dimensional pilot code.

Yr 1/2: Test computer program on model problems and investigate the effect of current on the wave motion. Analyze the accuracy of the numerical discretization, in particular the dissipation and dispersion error in the wave motion.

Yr 2/3: Use two-fluid elements in combination with a level set technique to model breaking waves. Investigate nonlinear stability of the algorithm.

Yr 3: Conduct simulations of extreme waves and compare with experiments.

Contribution MARIN:

Yr 1-3 Contribution in kind of 0.90 fte

Yr 1-3 Data from extreme wave generation experiments, measuring the evolution of extreme waves over a large horizontal domain. (100 kEuro)

3.4.6 Track record

The Maritime Research Institute (MARIN) has extensive experience in conducting model tests and numerical simulations to predict the wind, wave and current loading and motions of fixed and floating offshore constructions and ships. For this purpose MARIN has some of the most advanced experimental facilities in the world and MARIN has a unique position to serve the offshore industry world wide. The extensive network of MARIN with the offshore industry will guarantee a fast application of the techniques developed in this project in industry and further strengthen the position of MARIN.

The numerical analysis group NACM at the University of Twente has an extensive experience on discontinuous Galerkin methods for a wide range of applications, consisting of compressible, incompressible and two phase flows and electromagnetic problems. The research in NACM covers the whole range from algorithm development, theoretical analysis including error estimation, applications and software implementation. In particular, Dr. Bokhove (NACM) is an expert in both theoretical and numerical techniques to model various types of waves models and has applied them to a variety of wave problems, in particular waves in the near coastal region.

3.4.7 Publications

- V.R. Ambati and O. Bokhove, "Space-time finite element shallow water flows". Accepted J. Comp. Appl. Math. 2005.
- V.R. Ambati and O. Bokhove, "Space-time finite element shallow water flows". Submitted J. Comp. Phys., 2006.

- E. Bernsen, O. Bokhove, and J.J.W. van der Vegt, "A (dis)continuous finite element model for generalized 2D vorticity dynamics". J. Comp. Phys. 212, 719-747, 2006.
- O. Bokhove, "Flooding and drying in finite-element Galerkin discretizations of shallow-water equations. Part I: One dimension". J. Sci. Comput. 22, 47-82, 2005.
- O. Bokhove and E.R. Johnson. "Hybrid coastal and interior modes for two-dimensional flow in a cylindrical ocean". J. Phys. Ocean. 29, 93-118, 1999.
- O. Bokhove, M.D. Patterson, and D.H. Peregrine, "Breaking shallow water wave simulations in the surf and swash zone". In: 27th International Conference on Coastal Engineering, Reston ASCE, Sydney, Ed. Billy L. Edge, ISBN: 0-7844-0549-2, 2000.
- C.M. Klaij, J.J.W. van der Vegt and H. van der Ven, "Space-time discontinuous Galerkin method for the compressible Navier-Stokes equations", in print and on line available Journal of Computational Physics, February 2006.
- P. Tassi, O. Bokhove, and C. Vionnet, "Space discontinuous Galerkin method for shallow water flows —kinetic and HLLC flux, and potential vorticity generation—". Submitted to Advances in water resources, 2006.
- J.J.W. van der Vegt and H. van der Ven, "Space-Time Discontinuous Galerkin Finite Element method with dynamic grid motion for inviscid compressible flows I. General Formulation", Journal of Computational Physics, Vol. 182(2), pp. 546-585, 2002.
- J.J.W. van der Vegt and S.K. Tomar, "Discontinuous Galerkin method for linear free-surface gravity waves", Journal of Scientific Computing, Vol. 22-23, pp. 531-567, 2005.
- J.J.W. van der Vegt, F. Iszak,and O. Bokhove, Error analysis of a continuous-discontinuous Galerkin finite element model for generalized 2D vorticity dynamics. Applied mathematics memorandum 1759. Submitted Siam J. Num. Anal., 2005.
- J.J.W. van der Vegt and J.J. Sudirham, A space-time discontinuous Galerkin method for the Time-Dependent Oseen Equations, submitted to Applied Numerical Mathematics, March 2006.

3.5 Numerical simulation of the dynamic behavior of risers

3.5.1 Project leader

Dr. R.M.J. van Damme (University of Twente)

3.5.2 Project group

Senior researchers:
Prof.dr.ir. J.J.W. van der Vegt (University of Twente, 0.2 fte)
Dr. R.M.J. van Damme (University of Twente, 0.40 fte)
Dr. F. Izsak (University of Twente, 0.15 fte)
Ir. J.J. de Wilde (MARIN, 0.3 fte)
Ir. F. Lange (Heerema Leiden, 0.1 fte)
Dr.ir. J.H. Westhuis (Gusto Engineering, 0.1 fte)
Junior researchers:
1 PhD student, 1 Postdoc (University of Twente, both 1.0 fte)

3.5.3 Project description and relevance

The increasing demands for oil and gas production require offshore exploration and production at continuously greater water depths and poses tremendous technological challenges. One of the central problems is the occurrence of vortex induced vibrations of risers (VIV), which is caused by the interaction of periodic vortex shedding and the slender elastic structure with lengths of over two kilometers. Limiting these flow induced vibrations is crucial for a safe operation of oil and gas production and to reduce fatigue damage. Present technology is, however, insufficient to guarantee a safe operation already in the design stage and frequently serious delays are encountered during actual operation. Also, no efficient strategies are available which enhance the lifetime of a riser. Accurate prediction tools for the dynamic behaviour of risers can therefore result in saving large expenses.

The key problem in predicting VIV is that it is sensitive to small details in the flow and geometry and the extreme length to diameter ratio of the construction. This makes it extremely difficult to measure at the proper model scale and also semi-empirical techniques are generally insufficient.

This project aims at improving the prediction of vortex induced vibrations by an integrated program of developing advanced numerical solution techniques and detailed experiments. For this purpose a space time discontinuous Galerkin finite element discretization of the incompressible Navier-Stokes equations will be developed and coupled with a model to compute the elastic vibrations of the construction [5,7]. The space time DG approach allows the use of deforming elements which is essential to deal with the elastic deformation of the riser, but also to compute the mutual interaction of several risers in close vicinity of each other.

The numerical simulation model will be implemented using the *hpGEM* finite element toolbox under development in NACM, which will provide much of the finite element software necessary to construct the numerical model [7].

The computational model will be supported with detailed experiments on cylinders mounted in springs and free to oscillate under the influence of vortex shedding. The experiments consist of flow visualization, force and pressure measurements and recording of the cylinder motion.

3.5.4 Research questions and challenges

The full problem of computing the behaviour of an array of risers in deep ocean is an immense and challenging task.

We can distinguish the following aspects within this problem:

1 The flow around a bluff object gives rise to turbulence, in particular periodic vortex shedding. The resulting vortex induced vibrations are essentially three dimensional and time dependent phenomena.

2 The flow induces movement of the riser itself, which in turn will affect the flow, and this effect is by no means negligible.

3 The problems as described above hold for a single riser. In reality in offshore industry one wants the solve the same problem, but now for a group of risers which are all in each others vicinity and interact.

Choice of numerical method

It is clear that any solver of the problem (three-dimensional, time accurate) will have to be very efficient and flexible. This method must also, amongst others, be able to handle moving domain boundaries. The physics of the problem demands that in certain regions we must use very fine grids due to boundary layers, especially near the separation points – the same holds for the regions of the vortices. However, as all these regions of interest are also moving in time, it is evident that the numerical method must also allow adaptivity.

It is for these reasons that a space time discontinuous Galerkin method is an obvious choice. It is very flexible and allows *hp*-adaptivity [9]. Moreover, an ALE version of this space time discontinuous Galerkin method has the eminent capacity to cope with deforming elements, as shown in, e.g. [8,9,10]. Within the NACM group an extensive experience on discontinuous Galerkin methods for a wide range of applications has been built up. For this same reason this gives also a head start to the project. Namely, implementation can be performed within the *hpGEM* toolbox [7]. This is the standard framework within NACM to build and maintain the discontinuous Galerkin software.

Some other minor choices follow quite naturally:

- In order to use equal order polynomials for incompressible flows the space time discontinuous Galerkin discretization requires stabilization to satisfy the inf-sup condition. The stabilization operator developed in a previous project [1,2,3] provides a mathematically well founded choice.
- The STDG discretization results in a large system of non-linear algebraic equations. An excellent choice to solve this system, while preserving the locality of the DG discretization, hence its suitability for adaptation and parallel computing, is to use the pseudo-time integration method in combination with multigrid techniques developed in NACM [4,6,11] instead of the commonly used Newton method.

Choice of sub tasks

The activities can be divided into three main parts:

1. **Construction and validation of a space-time discontinuous Galerkin solver**

   a **Fixed riser section.** The simplest subproblem is the flow around a fixed riser section, modelled as a cylinder. To this end use can be made of software currently being developed in the NACM group and based on the *hpGEM* toolbox. This software will be extended to improve both its computational efficiency and suitability for riser simulations. Initial tests will be conducted at relatively low Reynolds numbers which can be used to verify the numerical method and its performance.

   b **Fluid structure interaction.** The modelling of the coupling between a riser and the fluid has to be incorporated as well. The actual model can be kept simple. The principle problem in this step is not the implementation of this interaction, but the effect it has on the flow field and the solver. As a consequence this solver must be able to cope with deforming meshes.

   c **Comparison with experiments.** In order to validate the model a detailed comparison must be made with experiments conducted at MARIN on a cylinder mounted in elastic springs. Both cylinder motion, lift and drag forces will be considered. Also, the flow field will be compared with flow visualization experiments.

2. **Improvements in modelling of Von Karman vortex street**

   a Since the Von Karman street of vortices is turbulent it will not be possible at higher Reynolds numbers to capture all relevant flow structures with a direct numerical simulation. Modelling the turbulence with a RANS model is, however, not feasible due to the unsteady nature of the flow and the limitations of RANS modelling in unsteady separation regions and concentrated vortices. In order to extend the capabilities to compute high Reynolds number flows a Large Eddy Subgrid (LES) model will be added. This model can be based on the extensively tested subgrid models in the NACM group.

   b Since the vortices move in time and are strongly localized structures, a significant accuracy improvement can be obtained using adaptive schemes, see e.g. [4]. The discontinuous Galerkin method allows for both local mesh refinement and adjustment of the polynomial order and can significantly increase the capability to capture vortical structures and improve the prediction of unsteady lift and drag forces.

   c **Outflow boundary conditions.** As the computational domain is necessarily finite and the Von Karman vortex street is much longer, vortices will have to leave the computational domain. This will cause a disturbance on the vortex street, since the vortex leaving the domain will influence nearby vortices in the domain, unless proper boundary conditions are imposed.

3. **Model reduction**

a **Multiple risers** In practice more than one riser section needs to be considered and the wake of nearby risers strongly influences the dynamic behavior. A sensible reduction in complexity can be achieved by considering one cylinder standing in its own backstream flow. In other words, by taking the flow to be periodic in the streamwise direction the problem of several risers can be mimicked. Variations on this same theme will be worked out in this context.

b **Treatment of vertical direction.** Risers can be kilometers long whereas the diameter generally is less than a meter. This third space dimension is essential in the problem. Still its effect is of a completely different nature. A significant savings in computing time can be obtained by using a Fourier spectral method in the direction along the riser. This limits the flexibility to deal with geometric changes along the riser, but greatly enhances the capability to consider longer riser sections and to investigate the size of the correlation length in the vertical direction.

3.5.5 Project plan and deliverables

Ph.D. Student:

Yr 1: Getting acquainted with the space time DG method and the *hpGEM* toolbox and code. Develop code for fixed riser section.

Yr 1/2: Fluid-structure coupling for a single riser and comparison with experiments conducted at MARIN for low Reynolds numbers.

Yr 2/3: Test the adaptive strategies developed by the PostDoc/van Damme to efficiently capture vortices. Include the LES subgrid model. Comparison with experiments conducted at MARIN for higher Reynolds numbers.

Yr 3: Extend space time discontinous Galerkin method to a combination of riser sections including deforming meshes. Improve efficiency of the algorithm and code.

Yr 3/4: Work on genuine three dimensional problems, including risers in an array. The probably necessary simplifications for this full three problem are part of the collaboration between the PhD, the PostDoc and Van Damme throughout the whole project.

Yr 4: Writing thesis.

PostDoc:

Yr 1/2: Develop efficient *hp*-adaptive methods suitable for unsteady flows and improved LES turbulence modelling for vortical flows.

Yr 2/3: Treatment of vertical direction using a Fourier spectral method and investigation of the effect of the correlation length in the direction of the riser. Semi analytic approaches and model reduction techniques, that may help in finding suitable approximations making the step to three dimensions more feasible.

Contribution MARIN:

Yr 1-3 Results of detailed 3C-2D PIV Experiments on a forced oscillating and free moving cylinder.(150kEuro)

Yr 1-3 Contribution in kind 2.0 fte. total

3.5.6 Track record

The Maritime Research Institute (MARIN) has extensive experience in conducting experiments to determine the flow features and dynamic behaviour of cylindrical structures used in risers and other offshore structures. This ranges from model tests on cylindrical sections to complete models of complicated riser bundles. For this purpose MARIN has some of the most advanced experimental facilities in the world, including a deep offshore basin in which waves and currents can be generated. This gives MARIN a unique position to serve the offshore industry world wide. The extensive network of MARIN with the offshore industry will also guarantee a fast application in industry of the techniques developed in this project and further strengthen the position of MARIN.

The numerical analysis group NACM at the University of Twente has an extensive experience on discontinuous Galerkin methods for a wide range of applications, consisting of compressible, incompressible and two phase flows and electromagnetic problems. The research in NACM covers the whole range from algorithm development, theoretical analysis including error estimation, applications and software implementation. In particular, extensive experience in Discontinuous Galerkin methods is available in the group.

3.5.7 Publications

1 M. Polner, J.J.W. van der Vegt and R.M.J. van Damme, "Analysis of stabilization operators for Galerkin least-squares discretizations of the incompressible Navier-Stokes equations", Computer Methods in Applied Mechanics and Engineering, Vol. 195, pp. 982-1006, 2006.

2 M. Polner, "Galerkin least-squares stabilization operators for the Navier-Stokes equations –A unified approach", PhD thesis, November 17, 2005, University of Twente.

3 M. Polner, L. Pesch and J.J.W. van der Vegt, "A unified formulation of stabilization operators for Galerkin least-squares discretizations of the Navier-Stokes equations", submitted to Computer Methods in Applied Mechanics and Engineering, April 2006.

4 C.M. Klaij, J.J.W. van der Vegt and H. van der Ven, "Space-time discontinuous Galerkin method for the compressible Navier-Stokes equations", in print and on line available Journal of Computational Physics, February 2006.

5 J.J.W. van der Vegt and H. van der Ven, "Space-Time Discontinuous Galerkin Finite Element method with dynamic grid motion for inviscid compressible flows I. General Formulation", Journal of Computational Physics, Vol. 182(2), pp. 546-585, 2002.

6 C.M. Klaij, J.J.W. van der Vegt and H. van der Ven, "Pseudo-time stepping methods for space-time discontinuous Galerkin discretizations of the compressible Navier-Stokes equations", accepted for publication Journal of Computational Physics , April, 2006.

7 L. Pesch, A. Bell, W.E.H. Sollie, J.J.W. van der Vegt, V.R. Ambati, O. Bokhove, "hpGEM - A software framework for discontinuous Galerkin finite-element methods", submitted to ACM Transactions on Mathematical Software, 2006.

8 J.J. Sudirham, J.J.W. van der Vegt and R.M.J. van Damme, "Space-time discontinuous Galerkin method for advection-diffusion problems on time-dependent domains", Applied Numerical Mathematics, in print and on line available, January 2006.

9 J.J. Sudirham, "Space-time Discontinuous Galerkin for Convection-Diffusion Problems – Application to Wet-Chemical Etching", PhD thesis, December 8, 2005, University of Twente.

10 J.J.W. van der Vegt and J.J. Sudirham, A space-time discontinuous Galerkin method for the Time-Dependent Oseen Equations, submitted to Applied Numerical Mathematics, March 2006.

3.6 Hydrodynamics of industrial bubble columns

3.6.1 Project leader

Prof.dr.ir. B.J. Geurts (UT and TU/e)

3.6.2 Project group

Senior researchers:
Prof.dr.ir. B.J. Geurts (UT and TU/e, 0.2 fte)
Prof.dr.ir. R.M.M. Mattheij (TU/e, 0.1 fte)
Dr.ir. J. ten Thije Boonkkamp (TU/e, 0.15 fte)
Prof.dr.ir. Ch. Hirsch (NUMECA, 0.25 fte)
Junior researchers:
1 PhD student (UT, 1.0 fte), 1 PhD student (TU/e, 1.0 fte)

3.6.3 Project description and relevance

Examples of the industrial use of bubble columns are found in organic waste-water purification or the synthesis of hydro-carbons. The complex hydrodynamics at high bubble-phase concentrations seriously complicates the control of such reactors. To avoid some of the costly experimental set-ups and pilot plants to support the industrial up-scaling, the use of computational fluid dynamics becomes more and more important. Presently, continuum multi-fluid models are frequently adopted, involving a number of phenomenological modeling steps and 'tuning' parameters. However, this type of modeling is found not sufficiently accurate for heterogeneous situations and high bubble fractions such as arise inside stirred reaction-columns.

In the proposed research a 'first principles' discrete bubble approach is selected to provide an alternative to available computational multi-fluid strategies. A multi-block Navier-Stokes solver for the macroscopic flow will be coupled to a viscous nonlinear Stokes solver for the flow on bubble scales. This multiscale, multi-resolution strategy involves the development of a high order symmetry preserving finite volume discretization, boundary element methods and local defect correction. Such an integral approach has the potential to treat all dynamically relevant phenomena in a transparent manner, from the large scales of the size of the vessel, down to the mesoscopic scales of individual deformable bubbles. It relies on computationally resolving the primary dynamic processes at all scales.

In much of the chemical industry in the Netherlands, computational fluid dynamics is based on commercial software. The proposed development of computational multiscale modeling for bubble columns will yield a dedicated boundary element/local defect correction (BEM/LDC) solver for the complete meso-scale dynamics of the bubbles. This module can be directly coupled to a commercial Navier-Stokes solver as used in industry. Following this strategy, the research-findings can be directly translated into a form suitable for potential users.

3.6.4 Research questions and challenges

The aim of this project is the development of a *computational multiscale modeling* applicable to the simulation of bubbly flow in reaction vessels at high bubble volume-fractions. Chemical industry makes extensive use of bubble columns for reactions between gases and liquids. The present operational control and efficiency of these reaction vessels is limited, especially at high bubble fraction. Anisotropic conditions, e.g., near vessel walls and under strong stirring, pose particular challenges in view of the significant heterogeneity of the bubble mixture and the high turbulent fluctuation levels. A more precise control of the complex hydrodynamics requires the modeling and simulation of the dispersed bubble-liquid mixture, capturing the large range of length- and time-scales present in the flow inside these reactors.

The computational multiscale modeling exploits the separation of scales that exists between the macroscopic turbulent flow and the mesoscopic viscous flow at the bubble-level. The new computational approach allows simulating the dynamic formation and disintegration of extensive bubble-clusters while accounting for the precise flow between the bubbles, as well as the bubble deformations. We propose to develop a simulation strategy based on the integration of

(i) Dispersed viscous Stokes flow, to represent the collective motion on the smallest scales. This will involve the development of the local defect correction method and its comparison with a boundary integral formulation.

(ii) Macroscopic Navier-Stokes flow to describe the global transport in the bubble column. Direct- and large-eddy simulation based on finite volume discretization will be included.

The coupling between the macro- and mesoscopic levels will rely on explicit simulation at all scales, which is a unique element of the proposed research. Rather than following a continuous multi-fluid approach, the relevant dynamical processes of the dispersed bubble- and liquid phases will be solved explicitly, taking momentum exchange and convective sweeping into account. Special attention will be given to anisotropic flow that is present near vessel walls and due to intense large-scale time-dependent stirring. The deformable bubble approach will be compared with point-particle models for the dispersed phase. This contributes to our understanding of the flow-modulation and induced self-organization in complex fluids which is of central importance to improve the operational control of industrial bubble columns.

3.6.5 Project plan and deliverables

A prototype coupling between the macro- and meso-scale computational models will be developed, involving a generic Navier-Stokes solver that was developed at the University of Twente. In a later stage, this expertise may be translated in an implementation involving a commercial Navier-Stokes solver. A close connection with industrial partners is essential in this respect. This is further stimulated in the context of the European COST-Action 'LES-Advanced Industrial Design' in which the research team participates.

The successful completion of the research requires a number of steps. Restricting to the primary aspects only, an outline of the planned work is as follows:

Year 1

- PhD1: The LDC method will be developed and applied to a number of benchmark problems to verify the method as well as to optimize the implementation.
- PhD2: The three-dimensional implementation of BEM will be updated and a parallel processing will be constructed and tested for single bubbles and periodic dispersions.

Year 2

- PhD1: The LDC method will be analyzed and used to study deformation, break-up and coalescence of bubbles as well as to collective flow properties in periodic dispersions. LDC will be compared with BEM, available from PhD2.
- PhD2: The coupling of the mesoscale stress field to turbulent flow in periodic flow-domains and in a mixing layer will be studied. Both DNS and LES will be investigated and LDC will be compared with BEM.

Year 3

- PhD1: Non-linear Stokes flow will be implemented using LDC. The rising of a large number of bubbles and the precise hydrodynamic interactions will be investigated. The Stokes formulation for flow in a channel will be developed and applied, focusing on effects due to boundary layer flow.
- PhD2: Two-way and four-way coupled point-descriptions for the bubbles will be compared with the Stokes formulation, in turbulent flow. Particular attention will be given to turbulent channel flow, concentrating on the turbulence modulation that arises in the boundary layer.

Year 4

- PhD1/PhD2: In the final year of the PhD-projects time will be reserved for completing the theses and to address specific research-issues that will have arisen as a result of the developments in the first three years. The integration of the LDC module with commercial flow solving software will be investigated.

A strong connection between the two sub-projects is facilitated by the involvement of the PI who holds a part-time chair for Anisotropic Turbulence at the Physics Department of Eindhoven University of Technology as well as a chair for Multiscale Modeling and Simulation at the Mathematics Department of the University of Twente. The developing Federation of the three Universities of Technology in the Netherlands will also contribute to a close collaboration, to the benefit of the proposed research.
Contribution NUMECA:

The contribution of NUMECA consists of the participation of senior research-staff to this project to an amount of 0.25 fte. The NUMECA support will be directly available to the PhD students. Contacts with NUMECA will be used to promote the integration of the multi-resolution modeling approach into commercial software. Access will be given to NUMECA software for this purpose.

3.6.6 Track record

The researchers involved in the team are each productive scientists, publishing regularly in international journals on topics of direct relevance to the proposed research. In addition, members of the team are regularly invited to deliver keynote lectures at international venues. Moreover, they are involved in the organization of a number of international workshops and conferences and are incorporated in the recently established Dutch center of excellence 'Fluids and solids: Multiscale problems'. For instance, the PI is chairman of COST Action P20: LES- Advanced Industrial Design and coordinates the special interest group DLES of ERCOFTAC, the European Research Council on Flow, Turbulence and Combustion. R. Mattheij is former president of ECMI and member of a variety of (European) institutions devoted to industrial mathematics.

The Twente group is involved in a number of STW and FOM projects. In addition, the PI supervises PhD students and Postdocs in Eindhoven and Twente, supported by FOM, working on fundamental aspects of turbulence modulation and numerical modeling. The Eindhoven group is currently involved in three STW projects. Moreover there are a number of other mostly externally funded PhD's (ASML:2, Philps:2, EU:2). The Scientific Computing Group has ample experience in the modeling and numerical simulation of engineering problems, examples being the numerical simulation of turbulent flow in turbines, laminar flames in domestic burners or the production process of glass. Common to many of these problems is the application of LDC as numerical simulation technique.

3.6.7 Publications of the research-team in 2006

1. Bos, F. van der, Geurts B.J.: 2006. Computational turbulent stress closure for large-eddy simulation of compressible flow. *J. of Turbulence*, **7** (9)

2. Kuczaj, A.K., Geurts, B.J., Lohse, D.: 2006. Response maxima in time-modulated turbulence: Direct numerical simulations, *Europhys. Lett.*, **73** (6), 851-857

3. Geurts, B.J., Holm, D.D.: 2006. Leray and NS-α modeling of turbulent mixing, *J. of Turbulence*, **7** (10), 1 - 33.

4. Geurts, B.J., Holm, D.D.: 2006. Commutator errors in large-eddy simulation, *J. Phys.A: Math. Gen.*, **39**, 2213-2229.

5. Minero, R., Anthonissen, M.J.H., Mattheij, R.M.M.: 2006. A local defect correction technique for time-dependent problems, *Numer. Methods Partial Differential Eq.* **22**, 128-144.

6. Minero, R., Anthonissen, M.J.H., Mattheij, R.M.M.: 2006. Solving parabolic problems using local defect correction in combination with the finite volume method, *Numer. Methods Partial Differential Eq.*, in press.

7. Swart, J.A.M. de, Groot, G.R.A., Oijen, J.A. van, Thije Boonkkamp, J.H.M. ten, Goey, L.P.H. de: 2006. Detailed analysis of the mass burning rate of stretched flames including preferential diffusion effects, *Combust. Flame*, **145**, 245-258.

8. Geurts, B.J., Vreman, A.W.: 2006. Dynamic self-organization in particle-laden channel flow, To appear: *International Journal of Heat and Fluid Flow*

9. Kuczaj, A.K., Geurts, B.J.: 2006. Mixing in manipulated turbulence. To appear: *J. of Turbulence*

10. Geurts, B.J.: 2006. Interacting errors in large-eddy simulation: a review of recent developments, To appear: *J. of Turbulence*

11. Sizov, M., Anthonissen, M.J.H., Mattheij, R.M.M.: 2006. Analysis of the local defect correction and high order compact finite differences, *Numerical Methods for Partial Differential Equations*, **22**, 815-829.

12. Allaart-Bruin, S.M.A., Linden, B.J. van der: 2006. Modeling the glass press-blow process, in: Progress in Industrial Mathematics at ECMI 2004 (A. Di Bucchianico, et al. eds.), Springer, 351-355.

3.7 Robust solver design for CFD packages used in industry

3.7.1 Projectleader

Prof.dr.ir. P. Wesseling (TUD)

3.7.2 Projectgroup

Senior researchers
Dr.ir. C. Vuik (TUD, 0.3 fte)
Ir. A. Segal (TUD, 0.10 fte)
Dr. D. Hegen (TNO Science and Industry, 0.4 fte)
Junior researchers
1 PhD student (TUD and TNO, 1.0 fte)

3.7.3 Project description and relevance

The main goal of the proposal is to develop simulation tools for multi-phase flow possibly combined with chemical reaction (CVD, combustion, flow with solidification). It appears that multiple time and length scales makes the problems very hard to solve in a robust and efficient way. The aim in this research is to bridge the gap between solver technology known at universities and the application of these solvers in CFD packages used in industry.

3.7.4 Research questions and challenges

For relatively simple flow problems it is possible to use general purpose CFD packages to simulate the flow. For more challenging problems: complicated 3 dimensional problems, many chemical reactions, sharp fronts and multi-phase flow, current methods used in these packages can not be used. The reason is that many different time and length scales are involved. These problems can only be solved by stable time integration methods, combined with local grid refinement and robust iterative solvers. Below some of these research questions are specified in more detail:

- **3D Navier Stokes equations**: For a robust method it is necessary to use implicit methods. In these methods, the coupled velocity and pressure equations should be solved. A lot of research is done at universities to invent methods, which convergence is independent of: number of grid points, size of the Reynolds number, and high aspect ratio of the discretization cells. Application of these methods to unstructured grids is another challenge.
- **Multi-phase flow**: In a number of industrial applications melting of solids and solidification of fluids are important. A coupling between fluid flow and phase transformations is a hard problem, because the fluid flow, combined with the temperature (and latent heat) are coupled and involve moving interfaces. A number of new mathematical methods to solve moving boundary problems are developed recently: level set methods, phase field methods and discontinuous integration methods. Coupling these methods with fluid flow in industrial applications is a new and challenging development.
- **Model order reduction**: Most of the problems mentioned above are difficult due to coupling of various 'basic' equations. Solvers are available for these basic equations,

the challenge is to use these building blocks in order to solve the coupled equations. It seems that model order reduction can be an important tool to address these problems. A typical feature of model order reduction is that the complete coupled problem is solved on a carefully selected small subspace of the solution space. This implies that the small problem is much cheaper to solve but the characteristic properties of the coupled problem are conserved. This technique coupled with the aforementioned building blocks seems to be a very promising method to solve a large class of coupled problems with large differences in time and length scales.

3.7.5 Track record

Dries Hegen is an expert in the solution of flow problems coming from industries. He is involved in flow simulations in the food industry and the production of glass products (bottles, monitors etc.).

Kees Vuik and Guus Segal have a long experience in solving the discretized Navier-Stokes equations. Their work involve solution of industrial flow problems (with moving boundaries), robust solvers for the incompressible Navier-Stokes equations and the stability of seawater circulation of the oceans.

3.7.6 Publications

S.P. van der Pijl, A. Segal, C. Vuik, and P. Wesseling, *A mass-conserving Level-Set method for modelling of multi-phase flows* International Journal for Numerical Methods in Fluids, 47, pp. 339–361, 2005

C. Li and C. Vuik, *Eigenvalue analysis of the SIMPLE preconditioning for incompressible flow*, Numerical Linear Algebra with Applications, 11, pp.511-523, 2004

C. Vuik and J. Frank and A. Segal, *A parallel block-preconditioned GCR method for incompressible flow problems*, Future Generation Computer Systems, 18, pp. 31–40, 2001

J. van Kan and C. Vuik and P. Wesseling , *Fast pressure calculation for 2D and 3D time dependent incompressible flow*, Num. Lin. Alg. with Appl., 7 pp. 429-447, 2000

C. Vuik and A. Saghir and G.P. Boerstoel, *The Krylov accelerated SIMPLE(R) method for flow problems in industrial furnaces*, International Journal for Numerical methods in fluids, 33 pp. 1027-1040, 2000

4 Bio(techno)logy and Health

4.1 Simulation of human tissues exposed to electromagnetic fields

4.1.1 Project leader

dr.ir. D.W. Harberts (Philips Applied Technologies)

4.1.2 Project group

Senior researchers:
dr.ir. D.W. Harberts (Philips Applied Technologies, 0.3 fte, to be seconded at CWI)
prof.dr.ir. B. Koren (CWI, 0.2 fte)
dr.ir. G. Peeren (Philips Medical Systems, 0.1 fte)
Junior researchers:
1 PhD student (CWI, 1.0 fte)

4.1.3 Project description and relevance

There is a growing concern about possibly harmful effects of electromagnetic fields (EMFs) on human beings, due to the increasing presence of electrical devices in daily life. Worldwide, possible adverse health effects are actively being studied and are often topic of emotional debate. The effects on human bodies depend on the frequencies and the strengths of the fields. Known effects are heating of human tissue at microwave frequencies and muscle contraction at lower frequencies.

Scientific research provides an effective means to address the public concern about possible adverse health effects of EMFs generated by all kinds of apparatus. The ideal situation is that in the design phase of these apparatus, compliance with the EMF requirements can be demonstrated through computations.

4.1.4 Research questions and challenges

The main goal of the project is to develop accurate and efficient numerical algorithms for the simulation of the direct physical effects of EMFs on human tissues, e.g., local dissipation (specific absorption rates) and ultimately temperature rise through heat capacity models. The interaction of external EMFs with medical implants (a pacemaker, e.g.) will be used as a special project carrier. It is expected that the number of people receiving medical implants will grow while at the same time the exposure to EMFs will increase.

The simulation of the thermodynamics of human tissue may require the solution of poroelastic equations coupled to the Maxwell equations (a mathematical challenge) Concerning the electromagnetic aspects: the permittivity of human tissue depends on frequency, and the conductivity is highly anisotropic. Human nerves have a high and anisotropic conductivity and are in general not resolved by the grid. Homogenization techniques (another mathematical challenge) are needed to model microscopic effects on the computational grid.

4.1.5 Project plan and deliverables

The discretization methods for the mathematical model describing the EMF – human-tissue interaction will build upon methods as: *(i)* the scalar-potential finite-difference technique, *(ii)* the finite-integration technique, and *(iii)* the boundary-element method. The large differences in spatial dimensions are a complication for the currently available computational approaches. For accurately and yet efficiently resolving regions of interest in the human body, subgridding approaches are therefore necessary.

The following deliverables of the research activities are anticipated:

- accurate human-body models relying upon realistic high-resolution voxel models and accurate models for the electromagnetic sources in space and time, and
- efficient numerical simulation tools that support designers of electrical and electronic equipment *(i)* to minimize the exposure of persons to EMFs and *(ii)* to assess compliance with legal EMF requirements.

4.1.6 Track record

With his vast experience and good overview over electromagnetic compatibility, Harberts is the ideal project leader. The secondment of Harberts from Philips at CWI will guarantee a direct transfer of the outcomes of this research to industrial practice of Philips. The same holds for the participation of Peeren, gradient chain architect in the development of MRI systems at Philips Medical Systems. Koren has a long-standing experience in the development and application of computational methods for science and engineering. Benefit is also expected from the promised collaboration with Dr. De Gersem (TU Darmstadt) and Dr. Oosterlee (CWI and TU Delft), experts in computing the interaction of EMFs and human tissues, and scientific computing in general, respectively.

4.1.7 Publications

- A. Barchanski, M. Clemens, H. De Gersem and T. Weiland. Efficient calculation of current densities in the human body induced by arbitrarily shaped, low-frequency magnetic field sources. *Journal of Computational Physics*, **214**, pp. 81–95 (2006).
- D. Lahaye, H. De Gersem, S. Vandewalle and H. Hameyer. Algebraic multigrid for complex symmetric systems. *IEEE Transactions on Magnetics*, **36**, pp. 1535–1538 (2000).
- J.J.H. Miller, G.I. Shishkin, B. Koren and L.P. Shishkina. Grid approximation of a singularly perturbed boundary value problem modelling heat transfer in the case of flow over a flat plate with suction of the boundary layer. *Journal of Computational and Applied Mathematics*, **166**, pp. 221–232 (2004).
- U. Trottenberg, C. Oosterlee and A. Schüller. *Multigrid*. Academic Press (2001).
- R. Wienands, F.J. Gaspar, F.J. Lisbona and C.W. Oosterlee. An efficient multigrid solver based on distributive smoothing for poro-elasticity equations. *Computing*, **73**, pp. 99–119 (2004).

4.2 Patient-specific simulation for improved stroke prediction

4.2.1 Projectleader

Dr. ir. E.H. van Brummelen (TUD/LR))

4.2.2 Projectgroup

Senior researchers:
Ir. Maribel Adame (Medis BV, 0.3 fte)
Dr. ir. Bob Goedhart (Medis BV, 0.2 fte)
Dr. ir. Freek Reinders (Medis BV, 0.3 fte)
Dr. ir. Frank Gijsen (Erasmus MC, 0.4 fte)
Dr. Rob Krams (Erasmus MC, 0.4 fte)
Dr. ir. Jolanda Wentzel (Erasmus MC, 0.4 fte)
Dr. ir. Harald van Brummelen (TUD, 0.5 fte)
Dr. ir. Miguel Gutiérrez (TUD, 0.25 fte)
Consultants:
Dr. Diederik Dippel M.D. (Erasmus MC, 0.05 fte)
Dr. Aad van der Lugt M.D. (Erasmus MC, 0.05 fte)
Dr. Rini de Crom (Erasmus MC, 0.05 fte)
Prof. dr. ir. Rene de Borst (TUD, 0.1 fte)
Prof. dr. ir. Ton van der Steen (Erasmus MC, 0.05 fte)
Prof. dr. Johan H.C. Reiber (Medis/LKEB, 0.05 fte)
Junior researchers:
8.0 fte (2 Medis, 3 Erasmus MC, 3 TUD)

4.2.3 Project description and relevance

Cerebro vascular accidents (stroke) are the leading cause of disability in the Netherlands, claiming approximately 100 victims daily. In addition to the great personal tragedy that CVA causes to its victims, it imposes a significant economic loss: stroke-related health-care costs alone add up to over one billion euro annually[1].

The aim of this research project is to develop a computer-simulation environment that enables a reliable patient-specific prediction of stroke, within clinically feasible time constraints. Such computer simulations can form an invaluable instrument in preemptive treatments. The simulation environment consists of three complementary components. First, fast and automated segmentation and mesh-generation techniques are required to construct a geometric model of the lumen and the arterial wall, including information on the biomechanical structure of the arterial tissue. Second, reliable biomechanical models are necessary to establish the mechanical behavior of sclerotic arteries and to assess the susceptibility of vulnerable plaques to rupture. Third, efficient, robust and automatic numerical solution methods serve to compute the fluid-solid interactions in sclerotic arteries and to compute the potential occurrence of rupture in vulnerable plaques. Clinical time lines stipulate that the entire sequence of operations, from scanning and imaging to solving the numerical model, transpires in 24 hours. Furthermore, the numerical results must be adequately validated versus experimental results and patient control groups to ensure clinical acceptance.

[1] source: RIVM.

4.2.4 Research questions and challenges

Successful development and implementation of the aforementioned computer-simulation environment requires advancement of the following technologies:

1. **Fast and automated segmentation and mesh-generation methods.** This technology delivers the patient-specific geometry and biomechanical data for the subsequent computational modeling. To enable automated mesh-generation without expert intervention, unstructured meshes will be used. The critical exponents in this subproject are the generation of quality meshes on the basis of imaging data and the identification and segmentation of the mechanical microstructure of the arterial wall. The lumen of the blood flow needs to be automatically segmented out of the MRA image data. The composition of the arterial wall and artherosclerotic plaque is to be determined from MR vessel wall imaging data. The latter includes so-called tissue classification, viz., the assignment of mechanical properties to individual components of the arterial wall. Moreover, the merger of the lumen data obtained by MRA and the biomechanic data obtained by MR requires a matching procedure, referred to as registration, as these data are obtained at different instances in time.

2. **Reliable multiscale mechanical models of atherosclerotic plaque tissue.** Accurate models of atherosclerotic tissue are presently unavailable because of its complex plaque composition at different scales. Atherosclerotic plaques that are susceptible to rupture and cause stroke, are in general characterized by the presence of a large lipid pool covered by a thin fibrous cap, which is surrounded by matrix tissue. Moreover, at an even smaller scale, infiltration of the fibrous cap by certain cell types and the presence of networks of micro vessels are also associated with a more rupture-prone plaque phenotype. Present mechanical models do not properly describe the complexity of the atherosclerotic vessel wall. Mechanical models will be developed with increasing complexity: from fluid structure interaction models towards rupture models. To guide the development of the multiscale mechanical models, atherosclerotic plaque tissue, containing all various components at different scales, will be characterized applying mechanical tests to individual plaque components and the intact tissue.

3. **Efficient space/time finite-element methods and fast and robust solution methods for hemodynamic flows.** Concurrent computational techniques are essentially incapable of delivering sufficiently accurate numerical solutions for the blood flow within acceptable time constraints. The computation of accurate solutions within clinically-relevant time bounds prompts the development of reduced-basis techniques and state-of-the-art computational methods. In particular, solenoidal-basis finite-element methods offer the prospect of delivering optimal computational efficiency for incompressible flows. The finite-element method must be of space/time-type, to accommodate the movement of the arterial wall and, moreover, it must be able to operate on unstructured meshes, in compliance with the requirements set by the automatic segmentation and meshing methodology. To accelerate the computation, reuse of computational information must be fully exploited, which is enabled by the many levels of recursion in fluid-solid-interaction computations. In addition, precomputing is required, i.e., a priori generation of computational primitives based on generic information.

4. **Efficient iterative coupling techniques for strongly-coupled fluid-solid interaction problems.** Fluid-solid interaction in arterial systems induces a strong mechanical coupling between the blood flow and the arterial wall. The strength of the coupling emanates from the incompressibility and the relatively high density and viscosity of blood, in combination with the flexibility of the arterial wall and, in particular, of vulnerable plaques. To solve such a strongly-coupled fluid-solid interaction problem within the prescribed time frame, we must appeal to extremely efficient and robust iterative solution techniques, such as multigrid and interface GMRES. Moreover, it is to be anticipated that the coupling algorithm must handle incompatible fluid and solid meshes, on account of the fact that the fluid and solid meshes have been generated separately on the basis of distinct imaging modalities with different resolutions.

5. **Computational sensitivity analysis and model adaptivity.** The tremendous complexity of the fluid-solid interaction and rupture processes is further compounded by the multiscale mechanical behavior of sclerotic arteries. To guide the development of microscale biomechanical models and to quantify the uncertainty induced by, for instance, limitations on the resolution of imaging and segmentation, macroscale computational models can be used to identify the sensitivity of rupture behavior to modeling assumptions.

Moreover, embedding of the simulation environment into clinical practice stipulates:

6. **Validation of the multiscale-mechanical and rupture models and of their capacity to improve the prediction of clinical events.** Validation of the used models are of crucial importance to get the multiscale mechanical models accepted in the clinical community. Current invasive and non-invasive imaging techniques allow imaging of the local vessel geometry including the vessel wall, its components and strain values. Based on these images and methods to segment these images developed under project 1, numerical simulations can be performed and validated against the measured strain values. We will perform such techniques in atherosclerotic mice and patients with atherosclerotic plaque in the carotid arteries. In addition, the atherosclerotic material will be processed by histological techniques so that the local plaque composition can be assessed. Similarly, the rupture models will be validated by studying the rupture behavior of the tissue as a result of increments in pressure. In order to study the capacity of the multiscale mechanical models to improve prediction of stroke, the carotid artery of a group of patients, which had minor symptoms, will be imaged. Based on these images, the patient specific geometry of the carotid artery is derived and the mechanical parameters calculated. By following the patients over time, the accuracy of multiscale mechanical models to improve risk prediction will be evaluated.

4.2.5 Project plan and deliverables

The long-term deliverable of this project is a computer-simulation environment for patient-specific prediction of stroke eventualities, including protocols and workflow descriptions for implementation of the technology in clinical practice. The primitives of this computational environment and the intermediate deliverables are concisely detailed in the provisional project plan below.

Subproject {1} Selection and adaptation of an 'off the shelve' unstructured lumen-meshing algorithm based on provisional MRA imaging data (yr. 0-1, cf. subproj. {3}). Development and implementation of techniques for automatic lumen-detection and segmentation from MRA images (yr. 0.5-2.5). Implementation of registration technique to match lumen and vessel-wall data (yr. 2.5-4, cf. {2}).

Subproject {2} Selection and adaptation of an 'off the shelve' unstructured vessel-wall-meshing algorithm based on provisional MR imaging data (yr. 0-1, cf. subproj. {5}). Development and implementation of techniques for automatic tissue and plaque identification from MR data (yr. 0.5-2.5) and tissue classification (yr. 2-4, cf. {6,7}).

Subproject {3} Implementation of an unstructured space/time finite-element discretization with solenoidal bases for incompressible flows (yr. 0-1, cf. {1} for meshing algorithm). Development and implementation of a Krylov/multigrid iterative solution process (yr. 0.5-2.5). Investigation of reuse of approximate inverses (yr. 2-4).

Subproject {4} Implementation of a partitioned iterative solution method for fluid-solid interaction with compatible fluid-solid meshes (yr. 0-0.5). in this phase a rudimentary solid model will be used. Extension of the method to incompatible meshes and to the base-line mechanical model (yr. 0.5-1.5, cf. {1,2,4}). Implementation of the interface-GMRES method (yr. 1.5-2). Extension and implementation of multigrid for fluid-solid interaction (yr. 2-4).

Subproject {5} Implementation of an unstructured discretization of a base-line mechanical model for arterial tissue and plaque (yr. 0-1.5, cf. {1,2,5}). Implementation of the dual problem for sensitivity analysis (yr. 1.5-2.5, cf. {2,6,7}). Assessment of modeling errors and implementation of an improved mechanical model (yr. 2.5-4, cf. {5}).

Subproject {6} Assessment and implementation of existing macro-scale mechanical models for diseased arterial tissue and investigation of its limitations(yr. 0-1, cf. {5}). Development of a sequence of increasingly advanced arterial-wall models, which allow for more complex plaque composition and which account for the presence, position, strength and interaction of load bearing structures (yr. 1-4, cf. {5,7} and also {2}).

Subproject {7} Validation of the model with its increasing complexity as being developed under {6} (in close collaboration with the tissue classification from {2} and the sensitivity analysis from {5}). Atherosclerotic arterial tissue will be harvested from laboratory animals or patients and will be imaged in vivo or ex vivo to allow application of the developed models of the intact tissue (yr. 0-2.5). Subsequently, methods are developed to assess the mechanical behavior of the tissue under different loading conditions in vivo and ex vivo, so that the models with its increasing complexity can be evaluated (yr. 0.5-3). Furthermore, tests will be applied to gain knowledge on the fracture behavior of the atherosclerotic material (yr. 2.5-4).

Subproject {8} Validation of the computational model developed under subproject {1-7}. The stress distribution and the prevalence of high stress peaks will be evaluated and its value for risk prediction will be assessed by following a patient group over time. Setup of protocol (yr. 0-1). Collection of patient data (yr. 1-3). Feedback to {1-7} (yr. 2-3.5). Evaluation of results (yr. 3-4).

4.2.6 Track record

Ir. Isabel M. Adame's field of expertise is the post-processing of MR images of vascular structures, automated contour detection of vessel wall boundaries and plaque characterization in atherosclerotic vessels. Her work has been supported by a Marie Curie grant (2002-2004). In 2003 she received the second prize of the ESMRMB Young Investigators Award for young researchers in magnetic resonance imaging.

Dr. ir. Bob Goedhart holds a Ph.D. in computer science and image processing from Delft University of Technology. He was scientific researcher in the medical domain at the Leiden University Medical Center from 1994, and has switched to industrial software engineering at Medis medical imaging systems in 1998, where he currently fulfill the position of R&D director.

Dr. ir. Freek Reinders has a Ph.D. in computer science and visualization from Delft University of Technology. He entered industrial software engineering at Medis medical imaging systems in 2001, where he currently fulfill the position of project manager of the Vascular MR-CT applications group of Medis.

Dr. ir. Harald van Brummelen has an established record in computational methods for free-boundary problems, in particular fluid-structure-interaction problems. In 2001, he received the Bill Morton prize for young researchers in computational fluid dynamics. The excellence of his work is supported by a VENI grant in the innovational-research programme of the Netherlands Organization for Scientific Research (NWO).

Dr.ir. Miguel A. Gutiérrez is a leading expert in stochastic finite-element methods and failure mechanics. Dr. Gutiérrez obtained his PhD (cum laude) in 1999 at Delft University of Technology, on the simulation of material failure by means of stochastic finite element methods. He is currently appointed as associate professor of Engineering Mechanics at the Faculty of Aerospace Engineering of Delft University of Technology. In 2001 he received the Vreedenburgh award. In 2003 he received a VIDI innovational-research grant from the Netherlands Organization for Scientific Research (NWO) for his work on computational methods for simulation of coupled electrochemical- mechanical damage of metals.

Dr. Krams is associate professor at Erasmus MC. The primary focus of his work is the application of biomechanics to patient related disease, by means of a combination of biomechanics and genomics. This approach allows to understand shear stress related gene expression and to develop new therapies or new imaging related to biomechanics. Dr. Krams is an established investigator of the Dutch Heart Foundation. He is author of more than 120 papers and over 500 abstracts.

Dr. ir. J.J. Wentzel's research over the past decennium has been devoted to the influence of biomechanical parameters on the generation and progression of atherosclerotic plaque formation and restenosis after percutaneous treatment in human coronaries. She received the ErasmusMC fellowship and the Dutch Atherosclerosis Society fellowship, supporting her work over the past 5 years. Her work has resulted in more than 30 peer-reviewed papers in highly ranked scientific journals and 7 book chapters and/or conference proceedings.

Dr.ir. Frank Gijsen received his PhD from the Eindhoven University of Technology for his thesis on the numerical and experimental analysis of non-Newtonian blood flow in large arteries. After his PhD he served on the board of the newly-founded department of

Biomedical Engineering as assistant director research, where he was responsible for setting up new research lines. He returned to doing research by accepting a position at the department of Biomedical Engineering at the Thoraxcenter in Rotterdam, where his main focus is application of image based advanced computational fluid and solid mechanics to study atherosclerosis in patients.

4.2.7 Publications

1. I.M. Adame, P.J.H. de Koning, B.P.F. Lelieveldt, B.A. Wasserman, J.H.C. Reiber, and R.J.van der Geest, *An integrated automated analysis approach for vessel stenosis and plaque burden from carotid mr images: combined post-processing of mra and vessel wall mr*, STROKE ((in press)).

2. I.M. Adame, R.J. van der Geest, D.A. Bluemke, J.A.C. Lima, J.H.C. Reiber, and B.P.F. Lelieveldt, *Automatic vessel wall contour detection and quantification of wall thickness in in-vivo mr images of the human aorta*, JMRI ((in press)).

3. I.M. Adame, R.J. van der Geest, B.A. Wasserman, M. Mohamed, J.H.C. Reiber, and B.P.F. Lelieveldt, *Automatic segmentation and plaque characterization in atherosclerotic carotid artery mr images*, Magnetic Resonance Materials in Physics, Biology and Medicine **16** (2004), 227–234.

4. E.H. van Brummelen and R. de Borst, *On the nonnormality of subiteration for a fluid-structure interaction problem*, SIAM J. Sci. Comput. **27** (2005), 599–621.

5. E.H. van Brummelen, K.G. van der Zee, and R. de Borst, *Space/time multigrid for a fluid-structure-interaction problem*, Tech. Report DACS-06-004, Delft Aerospace Computational Science, 2006 (submitted for publication). Available at `http://www.em.lr.tudelft.nl/downloads/DACS-06-004.pdf`.

6. C. Cheng, D. Tempel, R. van Haperen, A. van der Baan, F. Grosveld, M.J. Daemen, R. Krams, and Crom R.de, *Atherosclerotic lesion size and vulnerability are determined by patterns of fluid shear stress*, Circulation **113** (2006), 2744–2753.

7. F.J.H. Gijsen, R.M. Oortman, J.J. Wentzel, J.C.H. Schuurbiers, K. Tanabe, M. Degertekin, J.M. Ligthart, A. Thury, P.J. de Feyter, P.W. Serruys, and C.J. Slager, *Tissue regression in sirolimus-eluting stents in human coronary arteries is localized and correlates with shear stress*, Am. J. Cardiol. **92** (2003), 1325–1328.

8. F.J.H. Gijsen, J.J. Wentzel, F. Mastik, J.A. Schaar, J.C.H. Schuurbiers, P.J. de Feyter, A.F.W. van der Steen, and P.W. Serruys, *Shear stress predicts distribution of high strain spots on plaques in human coronary arteries*, (submitted for publication).

9. M.A. Gutiérrez, *Size sensitivity for the reliability index in stochastic finite element analysis of damage*, Int. J. Fract. **137** (2006), 109–120.

10. M.A. Gutiérrez and R. de Borst, *Simulation of size-effect behaviour through sensitivity analyses*, Engng. Fract. Mech. **70** (2003), 2269–2279.

11. M.A. Gutiérrez and K. Steen, *Stochastic finite element methods*, Encyclopedia of Computational Mechanics (E. Stein, R. de Borst, and T.J.R. Hughes, eds.), vol. 2, John Wiley & Sons, 2004, pp. 657–681.

12. R. Krams, G. Bambi, F. Guidi, F. Helderman, A.F. van der Steen, and P. Tortoli, *Effect of vessel curvature on doppler derived velocity profiles and fluid flow*, Ultrasound Med. Biol. **31** (2005), 663–671.

13. C. Michler, E.H. van Brummelen, and R. de Borst, *Error-amplification analysis of subiteration-preconditioned GMRES for fluid-structure interaction*, Comput. Methods Appl. Mech. Engrg. **195** (2006), 212–2148.

14. J.H.C. Reiber, G. Koning, A. Dijkstra, J. Wahle, B. Goedhart, and F.H. Sheehan, *Angiography and intravascular ultrasound*, Medical Image Processing and Analysis (J.M. Fitzpatrick M. Sonka, ed.), SPIE Press, 2001, pp. 711–808.

15. J.H.C. Reiber, G. Koning, J.C. Tuinenburg, A. Lansky, and B. Goedhart, *Quantitative coronary angiography*, Coronary Radiology (M. Oudkerk, ed.), Springer-Verlag, 2004, pp. 43–58.

16. C.J. Slager, J.J. Wentzel, F.J.H. Gijsen, Schuurbiers J.C.H., A.C. van der Wal, A.F.W. van der Steen, and P.W. Serruys, *The role of shear stress in the generation of rupture-prone vulnerable plaques*, Nat. Clin. Pract. Cardiovasc. Med. **2** (2005), 401–407.

17. C.J. Slager, J.J. Wentzel, F.J.H. Gijsen, A. Thury, A.C. van der Wal, A.J. Schaar, and P.W. Serruys, *The role of shear stress in the destabilization of the vulnerable plaque and its therapeutical implications*, Nat. Clin. Pract. Cardiovasc. Med. **2** (2005), 456–464.

18. A.G. Ten Have, F.J. Draaijers, E.B. Gijsen, J.J. Wentzel, C.J. Slager, P.W. Serruys, and A.F. van der Steen, *Influence of catheter design on lumen wall temperature distribution in intracoronary thermography*, J. Biomech. (2006), (in press).

19. Wentzel JJ Slager CJ van der Steen AF ten Have AG, Gijsen FJ, *Temperature distribution in atherosclerotic coronary arteries: influence of plaque geometry and flow (a numerical study)*, Phys Med Biol. **49** (2004), 4447–4462.

20. J.J. Wentzel, F.J.H. Gijsen, J.C.H. Schuurbiers, R. Krams, P.W. Serruys, P.J. De Feyter, and C.J. Slager, *Geometry guided data averaging enables the interpretation of shear stress related plaque development in human coronary arteries*, J. Biomech. **38** (2005), 1551–1555.

21. J.J. Wentzel, E.H. Janssen, J. Vos, J.C.H. Schuurbiers, R. Krams, P.W. Serruys, P.J. de Feyter, and C.J. Slager, *Extension of increased atherosclerotic wall thickness into high shear stress regions is associated with loss of compensatory remodelling*, Circulation **108** (2003), 17–23.

4.3 Algorithms and software for hybrid (bio)chemical modelling

Algorithms and software for molecular and mesoscale simulations

4.3.1 Projectleader

Dr. Joanne Klein Wolterink (Culgi BV)

4.3.2 Projectgroup

Senior researchers:
Dr. Joanne Klein Wolterink (Culgi BV, 0.6 fte)
J.G. Blom (CWI, 0.5 fte)
Dr.ir. J.E. Frank (CWI, 0.2 fte)
Dr. G.J.A. Sevink (UL, 0.3 fte)
Prof.dr.ir. J.G.E.M. Fraaije (UL/Culgi BV, p.m.)
Prof.dr. M.A. Peletier (TU/e, p.m.)
Prof.dr. J.G. Verwer (CWI/UvA, p.m.)
Junior researchers:
2 Postdocs (Culgi BV, 3 year)
2 PhD student (one at CWI and one UL, both 1.0 fte)

4.3.3 Project description and relevance

CULGI (Chemistry Unified Language Interface, `www.culgi.com`) is a general purpose environment for molecular and mesoscale simulations. One of the major goals of Culgi BV is to bring the modeling concepts from different length scales into a single modeling environment to be used in an industrial soft matter chemistry setting. This fits very well with the work done at CWI within the framework of the Silicon Cell Consortium (`www.cwi.nl/projects/SiliconCell`). Although the application is not the same, basic modeling concepts and the algorithms used have a considerable overlap. One of these concepts is the dynamic density functional theory or DDFT which is developed by the Soft Condensed Matter (SCM) group at Leiden University (`wwwchem.gorlaeus.net/scm`).

In this project the consortium will cooperate with Culgi BV and the SCM group to address some of the most pressing issues with respect to reliability and speed of simulations by developing and implementing novel numerical algorithms for

- dynamic density functional models that describe at a mesoscale soft condensed matter like copolymers or a biological membrane
- 3D field methods (DDFT/hybrids) that describe systems with particular molecular chain properties like chain stiffness - extending the simulation-functionality to a new class of systems with liquid crystalline properties, like short surfactant membranes
- hybrid free energy computation - ODE/PDE models that describe (macro)molecular systems like surfactants in a polymer/solvent or proteins in a membrane
- machine learning a.o. to fit a computational model to possibly noisy data

4.3.4 Research questions and challenges

Although modeling at a mesoscale level is a step forwards to simulate microscale phenomena at realistic time-scales it is still computationally quite expensive. The training of a 'learning machine' based on a realistic cost function is likewise a computationally complex problem, especially when the task is to fit a complicated mathematical model to noisy experimental results. More specific research questions are

- In the DDFT model the potential field is given implicitly and requires the computation of a path integral, i.e. integrals of high space dimension. This results in a computationally expensive, implicit system of PDEs with a strong non-local character for which efficient implicit solvers need to be developed. Since the solutions have intrinsically steep gradients that evolve and move in time through the domain it will be necessary to use a discretization with a variable resolution in space, like an adaptive-grid method. In these field methods that are based on a microscopic Hamiltonian, any change that is made in the representation on the chain level (for instance, stiffness or microscopic interactions) will not only increase the computational expenses of the path integral and the number of PDEs to be solved, but also requires the development of appropriate quadrature rules (stencils) for the new path integral. It will be necessary to precondition the iterative solvers. A possible route is considering 'physical' information derived from alternative phenomenological liquid-crystal free energy expressions;

- Developing a framework for hybrid (free) energy computation in a dynamic system is a challenge in itself. In these so-called multiscale models for molecular and mesoscale molecular simulations, a mixed dynamic system consists of particle and fields that interact together. In one such hybrid hyrdodynamic model, proprietary to Culgi BV, one can mix physical representations of polymers, surfactants, colloids and molecules. The coupling free energy that provides the interaction between the separate models is mapped to a very high dimensional set of coupled SDEs (particles) and PDEs (fields). Since these coupled models are completely new, but nevertheless already very successful commercially and scientifically, the currently used integration methods are only first order approximations. It is challenge to develop new integration strategies that can cope with the intrinsically multiscale character of the system. In particular the challenge is to develop integration methods that are both robust, can operate on parallel computers and can be extended easily. Such integrator can also immediately be used for other particle-field hybrid methods that are of relevance for Culgi, for example as integrator for a mixed quantum-molecular model;

- In many industrial soft materials research problems, recourse is made to a robot operated throughput screening device that optimizes materials behavior by trial and error. In such method, until now a materials model was irrelevant. In a newly developed method proprietary to Culgi BV, methods from statistical learning are combined with sophistical multiscale models, that act as a hybrid between the trial and error robotic methods and advanced physical models. In this case, from a mathematical perspective the task is to optimize a compound function, given a set of (imprecise) experimental data, and a specified multiscale physical model. Not only a global search is required through the parameter space to fit parameters to possibly noisy data, but also indications should be provided whether the model is overspecified or whether in certain regions of time-space extra measurements are necessary to make it possible to fit the model.

4.3.5 Project plan and deliverables

The projectmanagement lies with Culgi BV. The PhD students will follow the standard approach of literature study, algorithm development, implementation and writing the PhD thesis. Workpackages:

- SCM/UL and MAS/CWI: incorporation of liquid crystallinity in a general-purpose field simulation tool; development, implementation and simulation of biological membrane model;
- Culgi BV and MAS/CWI: hybrid free energy computation;
- Culgi BV and MAS/CWI: parameter identification.

Deliverables: extension and improvement of the CULGI environment, general purpose software, PhD theses.

4.3.6 Track record

Culgi BV is a fast growing, young, dynamic and international computational chemistry company. In traditional computational chemistry, modeling tools are developed with focus on a specific length scale. In Culgi, we understand that in an advanced materials laboratory, materials of various length scale coexist, and our focus is to integrate the modeling concepts of various length scales to replicate the laboratory environment into a software model of materials. The flagship product of Culgi is the Chemistry Unified Language Interface (CULGI) software library. The Culgi library is unique in the way it integrates molecular, mesoscopic and statistical modeling approaches in one hybrid simulation environment. The Culgi team is composed of physical chemists, computational scientists and software engineers. The leaders of the company are world-class recognized researchers in molecular and mesoscopic modeling with many years of experience in industrial computational chemistry and an extensive international industrial network. Moreover, Culgi has collaborative partnership with academic institutes, industry, government agencies and a qualified group of computational chemistry consultants. Culgi customers include midsize to large multinational companies and government agencies in the areas of personal and health care products, pharmaceuticals, plastics, petrochemicals and space research.

The SCM/UL group is internationally leading in mesoscopic field-theoretic modeling of pattern formation in polymer systems. The parallel MesoDyn (DDFT) software was developed as a HPCN project within a European ESPRIT Program and commercialized by Accelrys Ltd. In the past the group collaborated with G. Goldberg-Wood, Cambridge University, UK (2D DDFT for liquid crystalline polymers). Long-term collaborations exist with experimentalists prof. G. Krausch, Bayreuth University, Germany (thin films, electric fields) and T. Russell, Amherst, USA (electric fields).

The research group at MAS/CWI has a long-term expertise in the analysis and computation of time-dependent PDEs, including the design and implementation of efficient numerical algorithms. Within the Silicon Cell program the group collaborates extensively with biologists from the VU (Westerhoff group) and the UvA (van Driel group), with computer scientists from SCS/UvA (Kaandorp group; a.o. on parameter identification), and with Peletier from CASA/TU/e on membrane models.

4.3.7 Publications

1. J.G. Blom and M.A. Peletier. A continuum model of lipid bilayers. European Jnl of Applied Mathematics, 15:4:487–508, 2004.

2. Hamm M, Goldbeck-Wood G, Zvelindovsky AV, Sevink GJA, Fraaije JGEM. Dynamic mean-field model for the mesoscale morphologies of liquid crystalline polymers. Macromolecules 34 (23), 8378-8379, 2001.

3. Knoll A, Lyakhova KS, Horvat A, Krausch G, Sevink GJA, Zvelindovsky AV, Magerle R. Direct Imaging and Mesoscale Modelling of Phase Transitions in a Nanostructured Fluid. Nature Materials 3, 886-890, 2004.

4. Sevink GJA, Zvelindovsky AV. Self-assembly of complex vesicles. Macromolecules 38, 7502-7513, 2005.

5. Jordi Vidal Rodríguez, Jaap A. Kaandorp, Maciej Dobrzyński, and Joke G. Blom. Spatial stochastic modelling of the phosphoenolpyruvate-dependent phosphotransferase (PTS) pathway in Escherichia coli. Bioinformatics, 2006.

5 Sustainable World (climate, energy, ecology)

5.1 Numerical and stochastic simulation for climate and weather prediction

5.1.1 Project leader

Dr. J. E. Frank (CWI)

5.1.2 Project group

Senior researchers:
Dr. D. T. Crommelin (CWI, 0.3 fte)
Dr. J. E. Frank (CWI, 0.2 fte)
Dr. W. T. M. Verkley (KNMI, p.m.)
Dr. J. Barkmeijer (KNMI, p.m.)
Dr. O. Bokhove (U. Twente, p.m.)
Junior researchers:
Postdoc (KNMI, 1.0 fte 3 years, matching in cash)
2 Ph.D. Students (CWI, 2.0 fte)

5.1.3 Project description and relevance

The most fundamental feature of flows in the atmosphere and ocean, and the most confronting challenge to their numerical simulation, is the intrinsic coupling across spatio-temporal scales. This project addresses two topics in inter-scalar numerical modelling of geophysical flows:

- *Discretization on variable-resolution grids in numerical weather prediction models.* There is a great impetus in numerical weather prediction to develop 'unified models' for which short-term, mesoscale local-area predictions and long-term, macroscale global simulations are combined into a single code. At the global scale, this provides increased resolution, either statically at geographic locations of greater interest (e.g. populated areas), or dynamically where the fluid structure demands greater resolution (e.g. near instabilities). In contrast, at the mesoscale, the global coupling allows more realistic treatment of the boundary of the local model.
- *Stochastic sub-grid modeling in simulations of atmospheric and oceanic flow.* The effect of micro-scale motions on properties of large-scale atmospheric and oceanic flow is enormous. This creates a major challenge for numerical modeling, where spatial resolution is limited by computer power and computational costs. Eddies that are too small to be resolved by the spatial resolution of a numerical atmosphere or ocean model nevertheless significantly alter flow characteristics such as effective dissipation and diffusivity. Commonly used methods to deal with this problem, like biharmonic viscosity and a constant eddy-diffusivity tensor, are deterministic in nature, and cannot account for the randomness and irregularity of motions at sub-grid scales. We propose to use stochastic rather than deterministic models for sub-grid scale parameterizations, which will enable us to represent the stochasticity of small-scale turbulence. This allows for more realistic simulations, and should lead to improved models for applications such as weather prediction, climate change studies and tracer transport problems.

5.1.4 Research questions and challenges

- A promising discretization approach for mesoscale inclusion is based on the use of finite element methods on geodesic grids, derived by (locally) recursive tiling of regular geometric polyhedra, such as the icosahedron. A challenge is the construction of methods that conserve energy and other implicit structure under local refinement. Recent work by Frank, Moore & Reich (2006) has identified a class of collocation methods that preserves the sign of group velocity, at least for linear wave equations in one dimension. As a result, energy always flows in the right direction, and internal reflections due to abrupt changes in grid spacing are impossible. Much work is yet to be done however, if such methods are to be used in weather codes: these results must be extended to 2 and 3 dimensions, the 'correct' generalization to triangular meshes must be understood, the local refinement in higher dimensions is nontrivial, and the generalization of the concept of 'group velocity sign' must be developed in higher dimensions.

- The main scientific questions to be addressed in the case of stochastic microscale modelling are the synthesis of the stochastic numerical model and the validation of the resulting method. Both questions will be investigated by introducing stochastic parameterizations in a hierarchy of models, ranging from idealized 2-dimensional flow to realistic multi-layer models with spherical geometry. A natural starting point for the formulation of a stochastic sub-grid model is a stochastic generalization of known, deterministic parameterization schemes. The properties of the involved stochastic processes will be inferred from physical theory (such as turbulence closure theories) or from data generated by (limited-domain) high resolution models. The approach to the formulation of a stochastic numerical model will be guided by several notions: importance of state-dependent (multiplicative) noises; use of available data, where possible, through inverse modeling and/or data assimilation techniques; availability of computationally efficient methods for stochastic systems. The feasability and practical computability of the algorithm(s) in high-dimensional model situations is a key concern, as the transfer of modeling techniques from simple/idealized to complex/realistic settings is often a non-trivial problem.

[NPSC topics: all topics]

5.1.5 Project plan and deliverables

The project will assume the form of a 3-year postdoc fellowship, housed at KNMI and addressing the first topic, a 4-year Ph.D. research program, housed at CWI and also focusing on the first topic, and a 4-year Ph.D. research program, housed at CWI and focusing on the second topic. Deliverables include journal articles, Ph.D. theses, and numerical prediction software for use at KNMI.

5.1.6 Track record

Dr. Barkmeijer studied mathematics in Groningen where he received his PhD in 1988 on a subject in dynamical systems. In 1989 he decided to change direction and chose KNMI to work on predictability issues. During 1995-2002 he joined the European Center for Medium-Range Weather Forecasts (ECMWF) in England, where he became involved in the design of the ECMWF Ensemble Prediction System. He returned to KNMI in 2002 to work in Climate Variability department. His interests are incorporating data-assimilation techniques and model uncertainty in construction ensembles.

Dr. Bokhove obtained his Ph.D. degree at the University of Toronto in 1996 at the Department of Physics on Dynamic Meteorology with specialization in Theoretical Meteorology and Hamiltonian geophysical fluid dynamics. He has been een Royal Netherlands Academy of Arts and Science (KNAW) scholarship holder till recently on discontinuous Galerkin finite element models of coastal flows in complex domains.

Dr. Crommelin is an expert in applied dynamical systems theory, model reduction, statistical and stochastic methods. He has held positions as postdoctoral fellow and Courant Instructor at the Courant Institute, New York University.

Dr. Frank's expertise is in geometric integration of partial differential equations, with a focus on applications to geophysical fluid dynamics and wave equations. He is currently leader of two Ph.D. research projects and co-supervisor for a third project in this subject area. He was the recipient of an NWO Vernieuwingsimpuls (Veni) grant for the period 2002–2006.

Dr. Verkley studied Theoretical Physics in Amsterdam and received his PhD-thesis, on atmospheric blocking, in 1989. The PhD-work was carried out at the Royal Netherlands Meteorological Institute (KNMI). His stay at KNMI was followed by post-doctoral positions in the Space and Atmospheric Physics Group at Imperical College in Londen and at the Royal Netherlands Insitiute for Sea Research (NIOZ). From 1992 onwards he is a staff member of the Climate Variability Research Section at KNMI. He works on several topics concerning the dynamics of weather and climate.

5.1.7 Publications

1. J. Barkmeijer, T. Iversen and T.N. Palmer, Forcing singular vectors and other sensitive model perturbations, *Quart. J. Royal Meteorolol. Soc.*, **129** (2003) 2401–2423.

2. E. Bernsen, O. Bokhove and J.J.W. van der Vegt, A (Dis)Continuous Finite Element Model for Generalized 2D Vorticity Dynamics, *J. Comp. Phys.* (2006) **212** 719–747.

3. D.T. Crommelin, E. Vanden-Eijnden, Reconstruction of diffusions using spectral data from timeseries *Comm. Math. Sci.*, (2006) to appear.

4. J. Frank, B. Moore and S. Reich, Linear PDEs and numerical methods that preserve a multi-symplectic conservation law, *SIAM J. Sci. Comput.*, **28** (2006) 260–277.

5. W.T.M. Verkley, A spectral method for two-dimensional incompressible fluid flow in a circular basin, I. Mathematical formulation and II. Numerical examples, *J. Comput. Phys.*, **136** (1997) 100–131.

5.2 Coupling climate models to phytoplankton models

5.2.1 Project leader

Dr. L.R.M. Maas (NIOZ)

5.2.2 Project group

Senior researchers:
Prof. dr. H. de Baar (NIOZ, 0.25 fte)
Dr. L.R.M. Maas (NIOZ, 0.4 fte)
Dr. J. E. Frank (CWI, 0.2 fte)
Dr. B.P. Sommeijer (CWI, 0.25 fte)
Prof. dr. J. Huisman (UvA, 0.15 fte)
Dr. P. M. Visser (UvA, 0.15 fte)
Prof. dr. H.E. de Swart (UU/IMAU, p.m.)
Junior researchers:
1 Postdoc (4 yr, Dr. U. Harlander, NIOZ, 1.0 fte)
1 Ph.D. Student (NIOZ, 1.0 fte)
1 Ph.D. Student (UvA and CWI, 1.0 fte)

5.2.3 Project description and relevance

This project consists of two subtopics:

- *Coupling climate models to phytoplankton models.* During recent years much progress has been made in modelling phytoplankton dynamics in oceans. Such studies are of utmost importance since phytoplankton is on the basis of the marine food web and, moreover it has a significant impact on the climate by sequestration of CO_2 from the atmosphere. As a result of this research, insight in the phytoplankton behaviour in reaction to light and nutrients limitation has considerably improved. However, marine ecosystems are definitely not isolated mechanisms; as a matter of fact, they are strongly influenced by climate changes. Hence, the next step to arrive at a better understanding of ecosystems as a whole, is to add more realism to the physical part by coupling the phytoplankton models with climate models. This comprises aspects like (turbulence in) ocean flows, mesoscale upwelling processes, changing environment, in particular the influence of global warming, biodiversity, etc.

- *Wave induced mixing.* Perhaps due to the interest in global climate change, numerical ocean models tend to have a bias toward resolving only the largest scale. Limited computing resources preclude fully resolved simulations, at the expense of precise determination of small scale phenomena such as baroclinic eddies, waves and turbulence. Attempts are of course made to provide a proper parametrisation of these unresolved processes, or to use adaptive grids, but in most cases it is questionable if these expedients are sufficient. Not only will the large scale circulation, through instabilities, develop small scale features with concomitant wave generation, but for some time it has been emphasized that there may also be an important reverse effect: the large scale circulation of the atmosphere (and ocean) may for a large part actually be driven by waves. Here we propose to improve on this by studying a particular combined two-scale problem, in which the waves that are generated will affect the mean field (at the large scale) and the mean field (together with the geometry) will affect the wave field (and ensuing mixing) at the small scale.

5.2.4 Research questions and challenges

- Obtaining better insight into the living conditions on our planet is obviously a major scientific challenge. Since the (climate) changes on earth have a dramatic speed nowadays, the lack of scientific understanding is increasing. To reduce this gap, a considerable investment in scientific computing is necessary. The extended (i.e., coupled) models will be based on an Eulerian approach (described by partial differential equations). Apart from large and fast computers, much gain is to be expected from 'fast and intelligent solvers'.

- For the second topic, at the large scale, a low-order slow-time model captures the dynamics of the mid-latitude ocean on an f-plane in terms of the dynamics of the centre-of-mass vector(Maas 1994, 2004; van der Schrier and Maas, 1998, 2000), and can be coupled to an active atmosphere. This model is presently driven by differential buoyancy (insolation, rain, evaporation etc) and momentum (wind stress) fluxes. In the present study we will add complexity by developing a dynamic representation of the mixing underlying the diffusion and viscosity tensors. The mixing will be due to internal waves focused onto wave attractors. Depending on the degree and orientation of the stratification, the shape of the wave attractor can be inferred on the fast time scale (Maas 2005) and can be used to represent the diffusion and viscosity magnitudes. We anticipate that simpler wave attractors lead to stronger focusing and mixing. The amount of mixing will thus differ and will lead, on the longer time scale, to an adjustment of the density and momentum fields. Due to the fractal dependence of the shape on the stratification rate, we expect to see an interesting feedback through the varying mixing coefficients on the large scale. It is a challenge to see if these interactions can in fact also be incorporated in a numerical model that resolves the largest scale. Additional challenges are found in correctly representing the internal wave paths, as they are influenced by the combination of stratification, rotation, and sheared current profiles.

(NPSC topics: fast, robust and intelligent solvers; adaptivity and error bounds; model reduction techniques)

5.2.5 Project plan and deliverables

The project encompasses two Ph.D. research programs (1 each at NIOZ and UvA) and one postdoc fellowship (NIOZ). Two PhD students are requested for the first topic, and the postdoc will focus on the second topic. Deliverables include journal articles, Ph.D. theses, and numerical prediction software for use at NIOZ.

5.2.6 Track record

Dr. Frank's expertise is in geometric numerical integration methods for partial differential equations, with a focus on applications to geophysical fluid dynamics and wave equations. He is currently leader of two Ph.D. research projects and co-supervisor for a third project in this subject area. He was the recipient of an NWO Vernieuwingsimpuls (Veni) grant for the period 2002–2006.

Dr. Harlander's expertise is in meteorology and oceanography with an emphasis on wave processes in geophysical fluids. He has studied Rossby, internal gravity and inertial wave dynamics, and is an expert on the use of ray dynamics.

Dr. Maas is an oceanographer with an interest in fundamental fluid dynamical problems. He has worked on observations and models of surface and internal tides, simple models of the ocean wind-driven and meridional overturning circulation, and, both theoretically as well as experimentally, on wave attractors. He is co-supervisor of two Ph.D. research projects in this subject area.

Dr. Sommeijer's expertise is numerical solution of PDEs, with accent on time integration aspects. He successfully led several PhD/Postdoc research projects, and is editor of *J. Comput. Appl. Math.*

5.2.7 Publications

1. J. Frank, Conservation of wave action under multisymplectic discretizations, *J. Phys. A: Math. Gen.*, **39** (2006) 5479–5493.

2. U. Harlander and L. R. M. Maas, On quasigeostrophic normal modes in ocean models, *J. Phys. Oceanogr.* **34** (2004) 2086–2095.

3. J. Huisman, N.N. Pham Thi, D.M. Karl, B.P. Sommeijer, Reduced mixing generates oscillations and chaos in the oceanic deep chlorophyll maximum, *Nature* **439** (19 January 2006) 322–325.

4. L.R.M. Maas and F.-P. A. Lam, Geometric focusing of internal waves, *Journal of Fluid Mechanics*, **300** (1995) 1–41.

5. N.N. Pham Thi, J. Huisman, B.P. Sommeijer, Simulation of 3D phytoplankton dynamics: competition in light-limited environments, *J. Comput. Appl. Math.* **174** (2005) 57–77.

5.3 Simulation tools for the next generation off-shore wind farms

5.3.1 Projectleader

Ir. H. Snel (ECN)

5.3.2 Projectgroup

Senior researchers:
ir. H. Snel (ECN, 0.3 fte)
Dr.ir. S. van der Pijl (ECN, 0.3 fte)
Ir. A. van Garrel (ECN, 0.3 fte)
Ir. D. Winkelaar (ECN, 0.5 fte)
Ir. J. G. Schepers (ECN, 0.2 fte)
Ir. J. de Boer (Aerotortechniek, 0.3 fte)
Di.ir. E.J.Lingen (Habanera,0.3 fte)
Prof.dr.ir.drs. H. Bijl (TUD, 0.3 fte)
Prof.dr.ir. G.A.M. van Kuik (TUD, 0.1 fte)
Ir. A.H. Van Zuijlen (TUD, 0.3fte)
Prof.dr.ir. H. Hoeijmakers (UT, 0.2fte)
Junior researchers:
Developers (Aerotortechniek, 0.5 fte)
PhDs and Postdocs (TUD, 3 fte)
PhDs and Postdocs (UT, 1 fte)

5.3.3 Project description and relevance

For the next generation offshore wind farm energy production costs can be immensely reduced by

1. new rotor concepts for large turbines, including aerodynamic and distributed control
2. new wind farm concepts aiming at maximization of annual energy output and minimization of additional fatigue loads.

1. New rotor concepts demand more detailed dynamic flow simulations
Wind turbines undergo an ongoing up-scaling, needed for the economy of offshore wind parks. The use of present design methods for the design of larger and larger wind turbines, will lead to heavy machines, partly due to the needed conservatism in the safety factors. Higher risks by lower safety factors are unacceptable because of the significant investment even in the large turbine prototypes. Hence there is an urgent need for more reliable methods for aerodynamic loads prediction and the related Fluid Structure Interaction (FSI). At the same time, to mitigate load fluctuations and reduce costs, new rotor concepts need to be (and are being) developed for large turbines, including aerodynamic and distributed control. These concepts cannot be designed adequately with the crude - but fast aerodynamic simulation methods currently used in industry and need much more detailed calculations.

2. New wind farm concepts demand more accurate wake simulations
The wind farms offshore will be very large sized, comprising of 100 to 200 wind turbine each

rated 5 MW or more. The capital cost of such farms amounts up to billions of Euros. The need for an accurate prediction of both the mechanical loading and the energy output is evident for such projects. Furthermore, due to missing physics details in the present models, these are not suitable for evaluating new farm concepts aiming at reduced wake effects. Several ideas for new farm concepts exist but remain in need of a reliable quantification, as in industry no suitable models exist. These ideas include yaw misalignment in the first rows, reduced axial loads in the first rows, and 3D spacing, e.g. different tower heights. The wind speed deficit and the added turbulence in wind parks are presently calculated with relatively simple aerodynamic models. Comparisons with measurements show significant deviations in the predicted wind speed deficit and turbulence level. Furthermore, phenome na are observed in reality, which cannot be explained with present models. Hence an urgent need exists for more reliable modeling of wind turbine wakes.

State-of-the-art academic flow solvers need to be extended and speeded-up
Both at Delft University of Technology and at Twente University state-of-the-art flow solvers have been developed. These simulation tools incorporate more accurate aerodynamic models than those in industry. Currently, these solvers are extended to facilitate dynamic simulations of fluid-structure interactions. In addition, they can be further developed to simulate the complex interactions of wakes of different turbines in a farm. However, the complexity comes at a cost. Typically these solvers are orders of magnitude slower than the simple aerodynamic models. Moreover, in some crucial cases the accuracy of current simulation techniques does not suffice either, due to inaccurate turbulence models. This leads to uncertainties in the simulation results. Therefore, careful validation and uncertainty estimation is of the utmost importance.

5.3.4 Research questions and challenges

This project aims at bridging the gap between the speed of industry and the accuracy of university simulation tools to facilitate development of next generation offshore wind farms. Joining the forces of TUD, UT, ECN and AERotortechniek we can make a quantum leap in simulation techniques for offshore wind farms. The following challenges are foreseen:

1. Increase efficiency of academic solvers.
   Further development of Navier-Stokes solvers, including FSI capabilities, for rotating lifting systems. These methods must include the wake flow, as the wake development and the flow in the rotor-plane are strongly coupled through the vorticity distribution in the wake. Time scales are small, Reynolds numbers are large (order of 107) and Mach numbers are small to moderate (inflow maxima excepted offshore are of 0.4, for onshore applications smaller due to related noise production), so that the calculation demands of these solvers will be enormous. Therefore, we intend to develop new techniques to increase the efficiency by two orders of magnitude. Key words are: a coupling shell to facilitate FSi simulations, high order time integration methods, output-based adaptive mesh techniques in space and time and new combination of highly efficient iterative solvers.

2. Increase accuracy of industrial solvers.
   Development of efficient more accurate solvers, based on potential flow, strongly coupled with boundary layer and wake vorticity descriptions. These methods can possibly

be two orders faster than the first category, but are not as complete in the description of the physics. Therefore, we intend to improve the accuracy of the simple models using results from the academic solvers in two ways: a) the more accurate, unsteady results of the academic solvers will lead to increased physical insight, which can be used to deign better simple models and b) the results of the academic solvers can be collected into databases which may be directly used by the simple models. Due to the high computational speed, it may be expected that these improved methods will find their way into design practice much sooner than the academic ones.

3. Proper validation and uncertainty quantification.
   Apart for the development of the aforementioned methods, validation is very much needed, both from real size measurements and from the wind tunnel (relatively low Re) controlled environment. Some material is available (NREL-NASA Ames) or will hopefully become available in the EU project Mexico experiments. Validation data activities include

   - use of ECNs full scale research wind farm (5 Nordex N80 turbines) and its database of measurements,
   - NSW-MEP (data of the near shore wind farm at Egmond),
   - ECNs future scale wind farm with variable geometry,
   - and possibly wind tunnel research.

   In addition, the effect of unknown model parameters on the simulation results, both in the industrial solvers and in the turbulence model of the academic solvers, will be investigated. Hereto, the highly accurate and efficiency uncertainty quantification techniques for flow and FSI simulations developed in Delft will be extended and applied to crucial wind turbine cases.

5.3.5 Project plan and deliverables

This project boosts the wind energy community by actual knowledge development, sharing, and direct cooperation of universities, research institute and company.

1. Increase efficiency of the academic solvers : 3 fte of the junior researchers. Deliverable: Orders of magnitude faster solver. This solver is applied to simulate a variety of flow and fluid-structure problems of existing rotors, as well as new rotor concepts. In addition, it can be applied to wake interaction problems of wind farms.

2. Increase accuracy of industrial solver : 3 fte of the junior researchers. Deliverable: More accurate solver, especially for separated flow and wake interaction cases, which will be used for the design of new rotor concepts.

3. Validation and uncertainty quantification: 3 fte of the junior researchers. Deliverable: Thorough validation of both the academic and industrial codes for a wide variety of relevant cases. Benchmark with experimental data and simulation results of others. In addition, efficient uncertainty quantification methods are developed, and for relevant cases the uncertainty in the load prediction resulting from uncertainties in model parameters is quantified.

5.3.6 Track record

ECN, TUD and UT coordinate and are partners in various EU projects. For example: the EU project Mexico (Detailed rotor aerodynamic measurements in the DNW tunnel), the EU IP project Upwind (Focusing at R&D for the large wind turbines of tomorrow) and Downwind (Demonstration of two REpower 5M turbines in 45 m deep water east of Scotland, and studies of economic and technical feasibility of a 1000 MW wind park at that location). ECN and TUD also are consortium partners in the EOS-LT program Innwind and are involved in many other projects funded by Senter Novem. Prof.dr.ir.drs. Bijl is projectleader of various NWO and STW projects, ao the VIDI project "Uncertainties in unsteady flow and fluid-structure interactions applied to wind turbines at sea", "Computational non-linear aeroelasticity" and "A flexible coupling shell for the computation of fluid-structure interactions".

5.3.7 Publications

H. BIJL, M.H. CARPENTER, V.N. VATSA, C.A. KENNEDY, Implicit time integration schemes for the unsteady Navier-Stokes Equations, J Comp Phys 2002.

H.BIJL, M.H. Carpenter, Iterative solution techniques for unsteady flow computations using high order time integration schemes, Int J Num Meth Fl 2005.

H.BIJL, A.H. VAN ZUIJLEN, A. VAN MAMEREN, Validation of adaptive unstructured hexahedral mesh computations of flow around a wind turbine airfoil, Int J Num Meth Fl, 2005.

A.H. VAN ZUIJLEN, H.BIJL, Implicit and explicit higher order time integration schemes for structural dynamics and fluid-structure interaction computations, Comp & Struct 2005.

A.VAN GARREL, Development of a wind turbine aerodynamics simulation model, ECN-C–03-079, 2003.

D.WINKELAAR, DOWEC 6MW pre-design in PHATAS, ECN-CX–01-135, 2002.

J.G.SCHEPERS, Final report of the Annexlyse project: Analysis of aerodynamic field measurements on wind turbines ECN -C-050064, 2005.

J.G. SCHEPERS. Endow: Validation and improvement of ECNs wake model, ECN-C-03-034. 2003

H. SNEL, Application of a modified Theodorsen model to the estimation of aerodynamic forces and aeroelastic stability. Proceedings of the 2004 EWEC Conference, London, November 2004, also ECN-RX–04-120, Nov. 2004

6 Finance and Business

6.1 Numerical solution of high dimensional problems in option pricing

6.1.1 Projectleader

Dr. R.P. Stevenson (UU)

6.1.2 Projectgroup

Senior researchers:
Dr. ir. C.W. Oosterlee, (CWI, 0.3 fte),
Dr. R.P. Stevenson (UU, 0.3 fte),
Dr. R.M. Elkenbracht (ABN AMRO, 0.2 fte)
Dr. G.L.G. Sleijpen (UU, 0.2 fte)
Dr. J.H. Brandts (UvA, 0.2 fte)
Junior researchers:
3 PhD students (ABN AMRO, UU, CWI, 1.0 fte);
(two of them will be sponsored for 50% by ABN AMRO)

6.1.3 Project description and relevance

Nowadays, there is an increasing interest in the numerical solution of PDEs posed in n space dimensions, with n being larger than 3. We mention only mathematical finance (e.g. pricing of derivative contracts on baskets of n assets), multi-scale problems (elliptic homogenization problems with n separated length scales), stochastic PDEs (the computation of n-point correlation functions for random solutions), quantum dynamics (with n being three times the number of electrons), molecular biology (n being the number of substances that interact in a cell). When solving such PDEs with standard numerical methods, the convergence rate in terms of the number N of degrees of freedom is inversely proportional to n (known as the *curse of dimensionality*), meaning that an infeasible large N is needed to get an acceptable accuracy.

6.1.4 Research questions and challenges

Our main focus will be on high-dimensional problems in option pricing. The problem of interest is the basket option, whose payoff typically depends on the value of more than one asset. To price these options, high-dimensional partial differential equations from computational finance may need to be solved, as each asset gives rise to an extra space dimension. An accurate resolution of the hedge parameters, i.e., derivatives of the numerical solution, is of high interest in the financial industry. Nowadays, option pricing problems between five and fifteen dimensions occur frequently, but the interest from the financial industry may reach up to 60 dimensions! For low-dimensional problems (fewer than four dimensions) well-known classical discretization techniques are an obvious choice for solving the partial differential equations with methods from numerical mathematics. Derivatives can then be straightforwardly computed by numerical differencing. For higher dimensions, Monte Carlo simulations are in principle adequate, but they are relatively slowly converging and not very accurate for the representation of the solution's derivatives.

The aim of this project is to circumvent the curse of dimensionality, that is, to develop methods that converge with rates that are (nearly) independent of n and to provide accurate solution derivatives. Fortunately, high dimensional problems are usually posed on product domains. Therefore, one can apply so-called hyperbolic cross or sparse grid approximation. With that, one obtains nearly n independent rates, under smoothness conditions on the mixed derivatives. Recently, it was demonstrated that, at least theoretically, these conditions can be relaxed to realistic ones, when *adaptive* sparse grid approximations are considered. In this project we want to use, and where necessary, extend this theory to construct a practical method for solving these high dimensional problems within the required tolerances.

6.1.5 Project plan and deliverables

The project plan comprises the following 3 PhD projects:

One PhD student (supervision Oosterlee) will continue the research in the STW project DWI.6322 "Multi-asset options in computational finance, combining early exercise and high dimensional partial differential equations". Here, the sparse grid technique serves as the basis for the high dimensional discretization and solution method. The aim here is to go up in the dimensions by means of parallelization and adaptivity.

A second PhD student (supervision Stevenson) will work on adaptive wavelet methods for solving PDE's in high dimensions. Here the aim is to construct an iterative method that realizes a convergence rate that is equal to that of the best N-term approximation in the tensor product wavelet basis. It is known that the latter rate is independent of the space dimension n, and is not restricted by the regularity of the solution of the problem.

The third PhD student will develop a hybrid method, in which the standard sparse grid technique is combined with stochastic approaches of Monte Carlo type.

Tackling the problems from different sides, the primary goal of the project as a whole is to solve the concrete problems concerning option prize and interest rate models that are of interest for the bank.

6.1.6 Track record

Elkenbracht is co-head of the Product & Transaction Analysis group at ABN AMRO bank.

Oosterlee is project leader of STW project DWI.6322 "Multi-asset options in computational finance, combining early exercise and high dimensional partial differential equations" dealing with similar research questions. He is co-author of a book called "Multigrid" and associate editor of SIAM's J. Sci. Computing.

Stevenson is holder of an innovation impulse project "Wavelets for solving operator equations", funded by NWO from 2001-2006. Recently, he made important contributions in the field of adaptive wavelet and finite element discretizations. He has an ongoing collaboration with Prof. Ch. Schwab (ETH Zürich) on the solution of high dimensional PDE's.

Sleijpen is (co)author of more than 70 refereed papers in the field of numerical linear algebra, a number of them being highly cited. He was involved in the supervision of 18 PhD students. A recent project concerned numerical techniques in Quantum Chromo Dynamics, a subject related to the proposed project.

Brandts has been studying computational geometrical aspects of finite element methods in moderately more than three space dimensions with co-authors Prof. M. Křízek (AVCR

Prague) and Dr. S. Korotov (HUT Helsinki) and is associate editor for SIAM's J. Lin. Alg. Appl.

6.1.7 Publications

C.C. W. Leentvaar and C.W. Oosterlee, 'Pricing multi-asset options with sparse grids and fourth order finite differences', Proceedings Enumath conference 2005, Santiago de Compostella, Spain.

H. bin Zubair, R. Wienands, C.W. Oosterlee *Multigrid for high dimensional elliptic partial differential equations on nonequidistant grids*, Technical Report TU Delft, submitted for publication.

Ch. Schwab, R.P. Stevenson, *Adaptive Wavelet Algorithms for Elliptic PDE's on Product Domains*, Preprint Department of Mathematics, Utrecht University, May 2006. Submitted.

T. Gantumur, H. Harbrecht, R.P. Stevenson, *An optimal adaptive wavelet method without coarsening of the iterands*, To appear in *Math. Comp.* 2006.

J. van den Eshof, G.L.G. Sleijpen, M.B. van Gijzen, *Iterative linear solvers with approximate matrix-vector products*, In QCD and Numerical Analysis III, the Proceedings of the Third International Workshop on Numerical Analysis and Lattice QCD, Edinburgh, 2003.

J.H. Brandts, S. Korotov, M. Křížek, Dissection of the path-simplex in $\mathbb{R}^n$ into n path-subsimplices Linear Algebra and its Applications, submitted, 2006.