Small or medium-scale focused research project (STREP) proposal in FET proactive

ICT Call 8

FP7-ICT-2011-8

Hierarchical Aggregation of Complex Systems

HACS

<u>Small or medium scale focused research project (STREP)</u>
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Work programme topic addressed

9.7 Dynamics of multilevel complex systems

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Proposal abstract
We shall devise new algorithms for computation of properties of complex dynamical systems and to gain understanding of their behaviour, by constructing descriptions at a hierarchy of levels adapted to the system, using variants of hierarchical clustering and hierarchical elimination. We shall analyse their efficiency mathematically. We shall test the algorithms by implementing them in software and applying them to data from a range of large complex dynamical systems, including gene expression, epidemiology, airflow in the lung, formation of quasipatterns in fluid systems, brain images, traffic flow, and the dynamics of social norms.

<u>**Table of contents**</u>

Section 1: Scientific and/or technical quality, relevant to the topics addressed by the call

1.1 Concept and objectives

Background

Stephen Hawking declared: "the 21st century will be the century of complexity" (San Jose Mercury News (23 Jan 2000)). The words *complex system* are now widely used in sciences, from mathematics, physics and computer sciences to chemistry, biology, social sciences and technology. Complex systems are collections of a large number of interacting components, agents or units. They are often the result of an evolutionary adaptive process and show some emergent properties: interactions between units give rise to cooperative macroscopic phenomena, non-trivial patterns and complex dynamics that cannot be simply deduced from the basic microscopic interactions. These collective behaviours can in turn influence the microscopic dynamics. Observations and experiments suggest that some common fundamental principles should indeed govern large classes of complex systems. Among such principles, one finds the *emergence* of non-trivial hierarchical super-structures, which often dominate the system behaviour and cannot be easily traced back to the properties of the constituent entities. These multi-level structures are *robust* against various large-scale and potentially disruptive perturbations, i.e. they possess inherent capacity to *adapt* and maintain their stability.

Scientific Computing is more and more concerned with the efficient computation of large-scale problems in a wide variety of application areas, such as the life sciences, traffic or climate science. All these problem areas can be interpreted as (highly) complex systems, where often simulation is the only tool available to study them in full detail. Scientific computing is therefore a key technology in a number of scientific decision problems, such as in medical applications where diseases and their different treatments can be studied in silico, or in climate research, where simulations can predict which policies have what kind of impact in the future. Although it is true that computational capabilities have increased enormously in the last decade through improved hardware technology, it has also become more and more clear that many applications have a multi-scale structure that makes it impossible to study the full problem down to its finest defining structures. Here aggregation techniques are necessary throughout the complete simulation process, from the modelling aspect itself, to solution techniques for large-scale computational problems.

Clever algorithms are key to efficient computation. For example, "Even more remarkable -- and even less widely understood -- is that in many areas, performance gains due to improvements in algorithms have vastly exceeded even the dramatic performance gains due to increased processor speed" (from: Designing a Digital Future: Federally Funded Research and Development in Networking and Information Technology, President's Council of Advisors on Science and Technology, 2010, page 71), and "But the ingenuity that computer scientists have put into algorithms have yielded performance improvements that make even the exponential gains of Moore's Law look trivial," said Edward Lazowska, a professor at the University of Washington (from http://bits.blogs.nytimes.com/2011/03/07/software-progress-beats-moores-law).

Concept

The technical challenges to be addressed are to speed up computations of the properties of complex systems and to gain understanding of the behaviour to which the interactions at the level of individual units of a complex system lead at higher levels of description. The challenges are highly significant because many complex systems are so large that efficiency of computation is a serious issue and because the behaviour of complex systems often can not be inferred easily from a description of the interactions at the level of individual units. The proposed solution is to develop methods of hierarchical aggregation for complex systems that speed up computation of their properties and generate a description at a hierarchy of levels.

Such methods have been developed in some contexts, for example for shortest route planning in road networks under names like "highway hierarchies" and "multilevel refinement". Another context is large Markov processes, where aggregation methods have been developed since at least the 1960s (H.A.Simon & A.Ando, Aggregation of variables in dynamic systems, Econometrica 29 (1961) 111-138) to speed up computation of the stationary probability distribution and more recently of mean first passage times. Similarly, there is a procedure called "algebraic multigrid" for constructing a hierarchy of operators to solve large sparse problems, but so far it has been developed primarily in the context of solving partial differential equations. There is also "hierarchical incomplete LU decomposition" for large linear algebra problems, and there are hierarchical clustering methods. But even in some of these contexts we believe there is great scope for improvement, and there are many contexts in which analogous methods have not been developed.

The main goal of our proposal is to develop hierarchical aggregation methods that can be applied to complex systems of general structure and dynamical nature, for efficient computation of their properties and a deeper understanding of their behaviour at a hierarchy of levels. The end point will be algorithms to achieve this in the contexts of gene expression, epidemiology, airflow in the lung, formation of quasipatterns in fluid systems, brain images, traffic flow, and the dynamics of social norms, together with mathematical analysis of their properties and software implementation.

The results of the project will be applicable to the stated contexts. The project is expected to open up the development of hierarchical aggregation methods for a wide range of further contexts, e.g. flows in cities, smart energy grids, predicting the socio-economic effects of large infrastructure projects.

Although each particular application is likely to need its own customisation, we believe that we can create a general strategy for hierarchical treatment of complex systems. It will be built on the ideas of "hierarchical clustering" and "successive elimination".

Hierarchical clustering is an established method (e.g. section 11.11.2 of M.E.J.Newman, Networks [Oxford U Press, 2010]), which consists in searching for groups of units that are similar with respect to some measure of similarity, and iterating. The key issue for a given complex system is to decide what is the appropriate notion of similarity. Our idea is to group together nodes that are relatively strongly dependent. In a deterministic dynamic context, this would mean that the dynamics of the chosen units, given typical forcing from the rest of the network, collapse onto a lower dimensional submanifold (or more general attracting set), as has been explored in the PhD thesis of a UoW student for the case of coupled limit cycle oscillators (S.Gin, Aperiodically forced oscillators, Sept 2011). In the stochastic dynamics context, it means that the probability distribution for the behaviour of the group of units is far from being a product over units. There are various metrics on spaces of probability distributions that could be used to quantify this, but one that we advocate as particularly appropriate is "Dobrushin metric" (defined in R.S.MacKay, Robustness of Markov processes on large networks, J Difference Eqns & Applns 17 (2011) 1155-67).

In hierarchical elimination methods, certain units are considered to depend relatively strongly on the rest and so can be eliminated up to redefinition of the properties of the remaining units, and this procedure is iterated. This has been used for example in the study of nearest neighbour chains (e.g. R.S.MacKay, Scaling exponents at the transition by breaking of analyticity for incommensurate structures, Physica D 50 (1991) 71-79).

There are strong links between the two approaches. Elimination methods can be considered as aggregation methods in which the effects of the eliminated units are shared in some way between the retained ones. In one-dimensional nearest neighbour chains, elimination is equivalent to aggregation: the eliminated units can be considered as aggregated into the nearest retained unit on the left (or could choose the right). Also aggregation can always be considered as elimination by choosing to identify each super-unit with one of its member units and eliminating the other member units.

With this proposal we move towards the hardest solvable computational models inside application areas that are very relevant to society, for example the functional description of whole organs. Once a computational model is implemented, we can make 'virtual' ICT (Information and Communication Technologies) experiments. With some further experience and improved ICT infrastructure this could go in the future as far as - for example - modeling the treatment of individual patients even before a treatment has actually started. This could even be done remotely, i.e. again embedded inside an ICT architecture. The project HACS is a necessary step towards such a vision, because most of the relevant systems are multi-level, and we need aggregation methods to speed up such computations, without losing too much accuracy of prediction.

Multi-scale systems are ubiquitous in nature, society and technology. Modeling, simulation and optimization of such systems is of fundamental importance. Contemporary ICT approaches for simulation are quite inefficient, however, because they address complex systems on a single scale. Here, HACS will step forward and provide new algorithms that provide a description of complex systems on different scales, which will allow one to speed up their simulation considerably. The ICT implementation of these algorithms requires the solution of challenging problems such as the combination of discrete (agent-based) and continuous models as well as the development of efficient communication and load-balancing schemes for execution on parallel high-performance computers.

Objectives

- explain why hierarchical structures appear in many dynamical complex systems (WP1)
- formulate principles to design useful hierarchical descriptions of dynamical complex systems (WP1)
- devise algorithms for hierarchical aggregation of dynamical complex systems and appropriate data structures (WP2)
- evaluate the theoretical efficiency of the algorithms (WP2)
- develop an ICT architecture that allows one to implement our algorithms efficiently (WP3)
- customise the methods to a suite of application areas: brain imaging, chronobiology (dynamical gene expression), spread of infectious diseases, airflow in the lung, quasipatterns in fluid experiments, dynamics of social norms, and traffic flow (WP4)
- validate the methods on datasets for each of the above application areas (WP5)
- disseminate our results widely (WP6)
- explore routes for their exploitation (WP6)

Milestones

1. Mathematical framework in outline (M9)
2. Computational Theory in outline (M15)
3. ICT Implementation in outline (M21)
4. Customisation to most of the application areas (M27)
5. Validation on most of the application areas (M33)

Targeted Breakthrough

- **A new, powerful and unifying framework for computation and understanding of the dynamics of complex systems via hierarchical aggregation.**

Long-term vision

Our long-term vision is that our framework, methods, algorithms and software will form the basis for analysis and computation by city planners, medical researchers, material scientists, social policy makers, government departments, pharmaceutical industries, satellite navigation devices, public health authorities, e-commerce and more.

Relevance to the call

Our project will provide new mathematical and computational formalisms for dynamics of multi-level systems, making important steps towards a general theory of complex systems via an international effort looking for a general common theoretical approach. It will develop and validate them on real-world applications involving large and heterogeneous datasets. The proposed application areas present clear ICT challenges and three of them (tasks I,S,T) have a strong social component. The project will produce new ICT-based methods and principles for the management of large-scale systems and a better understanding of structural patterns of complex systems in socio-economic and technological areas. These items are all features of the call and cover most of the features of the call.

1.2 Novelty and foundational character

Novelty

We will bring together the ideas of renormalisation from theoretical physics and hierarchical clustering from computer science, into the domain of dynamics of complex systems and their computation. This can be expected to produce firstly a conceptual step change in understanding of the dynamics of complex systems, analogous to those produced by Kadanoff when he introduced his spin block renormalisation idea into statistical physics in 1965, or by Feigenbaum, Cvitanovic, Coullet and Tresser in 1977 when they introduced the idea of renormalisation into the study of dynamics of one-dimensional maps. Secondly, it can be expected to produce a breakthrough in computation of dynamics of complex systems by streamlining via a description at a hierarchy of levels. One analogy is the invention of the fast Fourier transform (FFT) algorithm, which sped up the computation of Fourier transforms so dramatically that it opened the doors to its practical use in many areas previously prohibited by excessive computing time (its use is essential to digital cameras, for example). Our ambition is stronger, however: not just to speed up computation of dynamics of complex systems, but to create a new and useful type of description at a hierarchy of levels.

Foundational character

Our project will lay the foundations for much future computation of dynamical complex systems and ways of thinking about dynamical complex systems. At the heart is the design of principles (mathematical and computational) for hierarchical representation of the dynamics of complex systems.

1.3 Specific contribution to progress in science and technology

Proposed advances, including Specific contributions to progress in Science and Technology

We will explain why complex systems often exhibit hierarchical structure. We will make a thorough assessment of the merits of all current approaches to hierarchical aggregation. We will propose unifying principles for hierarchical aggregation, extracting the best from all current approaches and adding our own innovations. We will devise algorithms for hierarchical aggregation of dynamical complex systems and appropriate data structures, and evaluate the theoretical efficiency of the algorithms. We will develop an ICT architecture that allows one to implement our algorithms efficiently. We will customise the methods to a suite of application areas: brain imaging, chronobiology (dynamical gene expression), spread of infectious diseases, airflow in the lung, quasipatterns in fluid experiments, dynamics of social norms, and traffic flow. We will validate the methods on datasets for each of the above application areas. We will disseminate our results widely and explore routes for their exploitation, in particular via our Users Group.

State of the art

For background, we summarise various strands of the state of the art.

For linear algebra there are various hierarchical elimination and hierarchical clustering methods, implemented in software, e.g. algebraic multigrid, incomplete LU decomposition and hierarchical incomplete LU decomposition. These include ILUPack, HIPS (Hierarchical iterative parallel solver) and KNN. For example, see www-users.cs.umn.edu/~saad/software. For algebraic multigrid, one reference is A.M.G.Wagner, Introduction to algebraic multigrid, Lecture notes of a course given at Heidelberg, 1998/9. A relevant recent paper by one of our consortium is F.W.Wubs & J Thies, A robust two-level incomplete factorization for Navier-Stokes saddle point matrices, SIAM J Matrix Anal Appl 32 (2011) 1475-99.

For shortest route finding there are various multilevel methods, notably highway hierarchies (e.g. P.Sanders & D.Schultes, Engineering highway hierarchies, in ESA 2006, Lect Notes in Computer Science 4168 (Springer, 2006) 804-816).

In equilibrium statistical mechanics, renormalisation procedures have been developed since the 1960s and the concept is fundamental to all theoretical physicists' thinking, though at the mathematical level the theory remains unclear. The aspect that is relevant here is "real-space renormalisation". For an analysis of its limitations, see A.van Enter, Renormalization group, non-Gibbsian states, their relationship and further developments, RIMS Lecture Notes 1483: Applications of Renormalization Group Methods in the Mathematical Sciences, pp.49-64, 2006.

For Markov chains, there is a large and old literature, e.g. P.J.Schweitzer, A survey of aggregation/disaggregation methods in large Markov chains, in: W.J.Stewart (ed), Numerical solution of Markov chains (Marcel Dekker, New York, 1991) 63-88, but the methods look unsatisfactory to us in that they require a global computation at each step. A recent improvement (but so far implemented as a successive elimination method rather than hierarchical) is D.J.Wales, Calculating rate constants and committor probabilities for transition networks by graph transformation, J Chem Phys 130 (2009) 204111.

Multilevel analysis of traffic flow has been proposed since e.g. J.H.Johnson, The Q-analysis of road traffic systems, Environment and Planning B 8 (1981) 141-189. Similarly, multilevel analysis has been introduced in epidemiology, e.g. D.J.Watts, R.Muhamad, D.C.Medina, P.S.Dodds, Multiscale resurgent epidemics in a hierarchical metapopulation model, PNAS 102 (2005) 11157-62.

In graph theory there are the concepts of "Modular decomposition" (e.g. Ille, P. Indecomposable graphs. Discrete Math. 173, 1-3 (1997), 71–78) and "Agglomerative Clustering" (for which a recent reference is Fränti P, Virmajoki O, Hautamäki V, Fast agglomerative clustering using a k-nearest neighbour graph, IEEE Trans Pattern & Machine Intell 28 (2006) 1875-81).

Much work has been done on observations and potential explanations of scaling in complex systems, e.g. in biological organisms, cities, socio-economic systems, the magnetosphere, and the internet. This all suggests that some appropriate renormalisation procedure could apply and shed light.

Another strand of work that must be mentioned is multiscale analysis, e.g. homogenisation theory. Although much of this treats just two or three scales, there is work of Ben-Arous and Ohwadi concerning infinitely many scales (e.g. H Owhadi & L Zhang, Metric-based upscaling, Communications on Pure and Applied Mathematics 60 (2007) 675–723; Berlyand L, Owhadi H, Flux Norm Approach to Finite Dimensional Homogenization Approximations with Non-Separated Scales and High Contrast, Arch Rat Mech Anal 198 (2010) 677-721). There is also the quasi-continuum method, and work of Schütte.

Another phrase under which related work is performed is "dimension reduction". In this direction there is much work by statisticians, but also by mathematicians like works of Brandt & Kevrekedis and Weinan E & Engquist, e.g. W. E, B. Engquist, X. Li, W. Ren and E. Vanden-Eijnden. Heterogeneous multiscale methods: A review. Comm. Comput. Phys. 2, no. 3, pp. 367-450, 2007; I.G. Kevrekidis and C.W. Gear. Equation-free: The computer-aided analysis of complex multiscale systems, AIChE Journal, vol 50, p 1346 (2004).

1.4 S/T methodology and associated work plan

i) Overall strategy of the work plan

The work will be carried out through the following work packages:
WP1 Mathematical Theory (coordinator Gambaudo (INLN))
WP2 Computational Theory (coordinator Kirkilionis (UoW))
WP3 ICT Implementation (coordinator Bastian (HB))
WP4 Customisation to Applications (coordinator Waalkens (RuG))
WP5 Validation of Methods on Data (coordinator Flache (RuG))
WP6 Dissemination and Exploitation (coordinator MacKay (UoW))
WP7 Management (coordinator Ladwa (QTC))

WP1, 2&3 will develop methods of a generic nature, proceeding from mathematical ideas and analyses, to design and efficiency study of algorithms, and then to their implementation on computers.

WP4&5 will apply the resulting methods to the following list of application areas:
B Brain imaging (mainly UoW + HB); data source via Nichols (UoW)
C Chronobiology (mainly RuG + UoW); data source Beersma (RuG)
I Infectious diseases (mainly UoW); data source via Keeling (UoW)
L Lung flow (HB with UoW & INLN); data source via Chung (UoW) and Gutheil (HB)
Q Quasicrystals & quasipatterns (INLN with UoW & RuG); data source Residori & Rajchenbach (INLN)
S Social norms (mainly RuG); data source Flache (RuG)
T Traffic flow (mainly UoW with RuG & HB); data source Huitema (RuG & TNO)

Each node will be involved in each work package. The work plan is a truly collaborative effort. In particular, in addition to the above indication of responsibilities for WP4 &5, aspects of WPs 1,2 & 3 will be directed by:

WP1 MacKay (UoW), van Enter (RuG)
WP2 Bastian (HB), Wubs (RuG)
WP3 Wubs (RuG), Kirkilionis (UoW)

The workpackages will be linked in a 2-way linear chain from WP1 to WP5. Each will feed ideas to the next, and in return each will provide feedback to the previous one. WP6&7 will connect to all of them.

The division of work between WP 4 & 5 is:

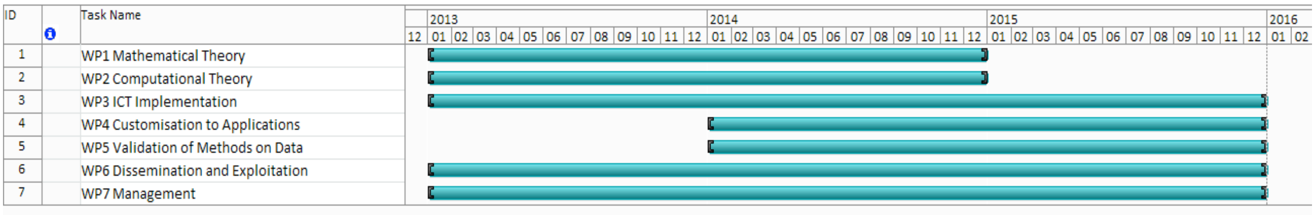
WP 4 develops per area of application the specific tools that we need to hierarchically aggregate lower level units. That is, per area of application / data we will do the following in WP 4:

- Establish what are the appropriate lowest level units to start from. (What can we measure / observe, for which level can we establish similarity / interdependence between units)?
- Decide based on previous steps. Do we need for specific application area deterministic or probabilistic, static or dynamic of model of interdependence (see intro) for this particular application area?
- Analyze how strength of interdependence of units can be operationalised / measured.
- Fine tune measurement instruments.
- Fine tune aggregation methods per area of application: i.e. test aggregation methods for simple / well known sample data sets to assure that “meaningful hierarchical aggregation” results.
- Establish / decide per application area what the outcomes are that we want to model / explain / predict and how we operationalise those (e.g. dynamics of norm compliance, air flow in lung, activation of brain cell…).

WP 5 then “applies” and “tests” the aggregation methods per area of application. This involves:

- Collect the data and / use existing data sets. That is: collect data on dynamics of individual level units and their strength of similarity, and data on the outcome variables.
- Prepare the data sets (maybe already part of WP 4) for application of aggregation methods.
- For small subsets of the data, run comparison of predictions for behavior of outcome variables obtained with “non-aggregated” and with “aggregated” models of individual level dynamics and their interplay.
- Assess the relative accuracy and efficiency of aggregation method for the data per area of application.
- Fine tune / optimise models for the given data.
- Apply aggregation methods to data sets too large for conventional one-level models. Generate predictions for system behavior at macro level and test predictions at macro level.

ii) Timing of work packages



For work packages containing more than one task, those tasks will be carried out in parallel.

iii) Work Packages

Work package list

Work package No	Work package title	Type of activity	Lead partic no.	Lead partic. short name	Person-months	Start month	End month[5]
1	Mathematical Theory	RTD	4	INLN	106	1	24
2	Computational Theory	RTD	1	UoW	62.6	1	24
3	ICT Implementation	RTD	2	HB	58	1	36
4	Customisation to Applications	RTD	3	RuG	51.5	13	36
5	Validation of methods on data	RTD	3	RuG	54.5	13	36
6	Dissemination and exploitation	MGT	1	UoW	18.5	1	36
7	Management	MGT	5	QTC	16.9	1	36
	TOTAL				367.9		

List of Deliverables

Del. no.	Deliverable name	WP no.	Nature	Dissem. level	Delivery date
D1.1	Answers to 4 of Qs1-7 of T1	WP1.T1	R	PU	M24
D1.2	Workshop on hierarchical aggregation methods	WP1.T2	O	PU	M1
D2	Specification of computational methods	WP2	R	PP	M12
D3	Software to carry out hierarchical aggregation	WP3	O	PP	M30
D4	Reports on customization to at least 4 of the tasks	WP4	R	PU	M30
D5	Reports on validation for at least 4 of the tasks	WP5	R	PU	M36
D6.1	Brochure and poster	WP6	R	PU	M1

D6.2	Project website	WP6	O	PU	M4
D6.3	Publications in high impact journals	WP6	R	PU	M36
D6.4	Socio-economic impact report	WP6	R	PU	M30
D6.5	Symposium	WP6	O	PU	M36
D6.6	Report on patent searching	WP6	R	CO	M24
D6.8	Users Group report	WP6	R	PP	M36
D7.1	Initial management meeting	WP7	O	CO	M1
D7.2	Mid-term Project review	WP7	R	PP	M18
D7.3	Final report	WP7	R	PP	M36

List of Milestones

Milestone number	Milestone name	Work package(s) involved	Expected date	Means of verification
1	Mathematical Framework	WP1	M9	WP2 leader can see how to develop computational theory for it
2	Computational Theory	WP2	M15	WP3 leader can see how to implement it in ICT
3	ICT Implementation	WP3	M21	WP4 task leaders can see how to customize it to their tasks
4	Customisation	WP4	M27	WP5 task leaders can see how to validate it on data
5	Validation	WP5	M33	WP5 task leaders succeed in validating the methods on data

Work Package 1

Work package number	1	Start date or starting event:		M1	
Work Package Title	Mathematical Theory				
Activity Type	RTD				
Participant Number	1	2	3	4	5
Participant Short Name	UoW	HB	RuG	INLN	QTC
Person-months per participant:	40	0	27	39	0

Objectives

This work package has two main tasks. The first is to understand why many dynamical complex systems exhibit hierarchical structures. The second is to formulate principles for designing a useful hierarchical description of the dynamics of a complex system.

Task 1: Hierarchical structures

1a To explain why hierarchical structures are they observed in so many different situations: from the structure of muscle fibres and distribution of cracks in materials, to the discovery of quasi-crystals by D. Schechtman (who received the 2011 Nobel Prize in Chemistry for his findings), or also at a more theoretical level Parisi's distribution of overlaps in the Sherrington-Kirkpatrick spin glass model. In which sense are these structures stable?

1b To understand the formation of hierarchical structures: what is their birth process, is there something like crystal growth theory for hierarchical structures?

1c To understand dynamics on hierarchical structures: once hierarchical structures are created as the result of an evolutionary process, they are often the support of some dynamical process (as models we can imagine systems of oscillators coupled in a way that reflects the hierarchical structure). It is a challenging problem to understand how information, energy, and waves travel in these structures.

Task 2: Theory of hierarchical aggregation methods

To abstract from the wide range of current approaches and our own innovations, general useful principles for choosing which units to aggregate in a complex system, to derive a description at the aggregated level and the connections between the levels of description. To assess the effects of approximations in the process.

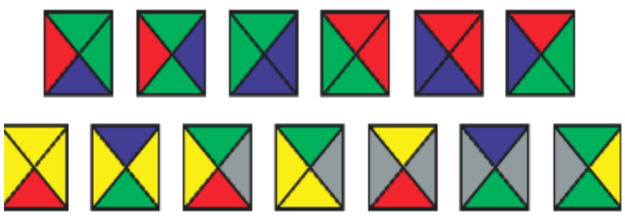
Description of work

Task 1: Hierarchical structures

1a: Ubiquity

Existence: Why do hierarchical structures appear everywhere? Our intention is to show that, in a very broad setting of interacting units, they appear naturally as minimal configurations and play a role that was so far supposed to be the role of spatially periodic configurations. Let us be more precise in the particular context of Wang tilings. A Wang tile is a unit square with coloured edges. Once given a finite collection of Wang tile, one can ask if it is possible to tile the plane with copies of the Wang tiles in the collection in such a Wang that the colours of adjacent edges match.

As shown by Berger in the 60's [Ber], there are examples of collections that can tile the plane but cannot tile it periodically. Such an example, due to Culik [Cul], is given in the following picture.



For such examples, the most "repetitive" ways to tile the plane are hierarchically structured. This means that there exists a finite collection of patches (a patch is a finite collection of the initial squares: a sort of super-polygon) that can tile the plane, and there exists also a finite collection of larger patches made with these super-polygons that can tile the plane and this process can be repeated indefinitely. This nice result can be proved as follows. The set of all admissible tilings of the plane can be equipped with a metrisable topology which makes it compact. The group of translations acts continuously on this set and thus there exists a minimal invariant subset. It is then easy to check that all tilings in this minimal set have a hierarchical structure**.**

Q1. The first question is to state this type of result in its largest general setting, for example for interacting systems of particles.

Stability: It is not because hierarchical structures formally exist that we can see them. Attached to these structures there must be some stability criteria that we have to explore. Clearly a final goal is to give such stability criteria in the general case of interacting particles but so far this goal is out of reach. We turn then to the standard approach of statistical mechanics which consists in modelling this problem for a lattice gas. Consider a finite alphabet A and consider the configuration space C which associates to every point of the integer lattice in dimension d a letter in A. A sub-shift of finite type (SFT) is the set of all configurations that do not contain any of a finite list of "forbidden words". The study of SFT, which is quite easy and useful in dimension $d=1$, turns out to be very delicate in dimension $d>1$. In dimension 2, it is for instance possible to find uniquely ergodic SFT (for the shift action) which do not reduce to a periodic configuration. It follows easily that all the configurations of such an SFT possess a hierarchical structure.

Q2. Equip our space *C* with a translation invariant interaction, can we find an open set (in a suitable space) of interactions for which the ground states are the same uniquely ergodic non-periodic SFT?

There have been nice pioneering works in this direction by Miekisz [Mie] but the global picture is not yet clear and satisfactory. There is a lot to do in this direction.

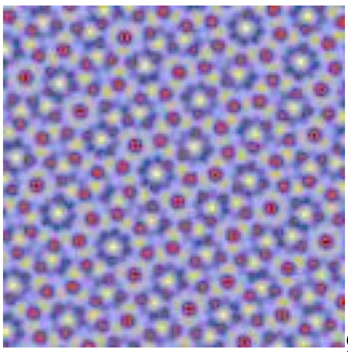
2b: Birth and growth

How do hierarchical structures appear? We will develop 4 approaches which represent 4 different points of view on this question:

1- A thermodynamical approach. Consider (as in Task 1a) a lattice gas on a finite alphabet with a translation-invariant interaction such that the ground states (temperature $T=0$) are configurations of a uniquely ergodic non-periodic SFT (d>1). Consider now the situation when the temperature T is positive and goes to 0.

Q3. How do these hierarchical structures appear in the cooling process. Some works have been developed in this direction [AR] but so far there is no clear answer. How do the Gibbs measures behave as the temperature decreases, is there a phase transition at positive temperature?

2- An experimental approach. Quasi-patterns remain one of the outstanding problems of pattern formation. These are two-dimensional patterns that have no translation symmetries and are quasi-periodic in any spatial direction. These quasi-patterns exhibit some hierarchical structures. They were first discovered in non-linear pattern-forming systems in the Faraday wave experiment [EF], in which a layer of fluid is subjected to vertical oscillations. Since their discovery, they have also been found in non-linear optical systems [HWAALL], shaken convection and in liquid crystals [LD], as well as being investigated in detail in large aspect ratio Faraday wave experiments. We have an experimental group that realizes the Faraday wave experiment as well as the corresponding one for liquid crystals (WP5).


Quasi-patterns for the Faraday experiment (Image J Vinals McGill U.).

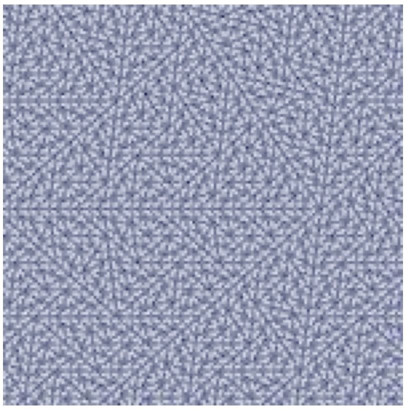
Q4. Explore how, when a parameter varies, hierarchical structures appear or disappear, and model these transitions by partial differential equations.

3- An analytical approach. It turns out that quasi-patterns appear as approximate steady solutions of the simplest pattern-forming PDE, the Swift–Hohenberg equation [IR]. A proof that they are really solutions of this equation is still lacking because of the lack of good analytical tools.

Q5. Proving the existence of these solutions can hopefully be done using techniques developed in [BBG] to prove the gap-labelling conjecture for quasi-crystals.

4- A hierarchical growth approach

Q6. How can local rules create a hierarchical structure? If this question has no general answer so far, in some particular cases it can be done and understood. These cases concern substitution tilings in dimension $d>1$. Consider a finite collection of polyhedra P and assume that there exists a scaling factor $l<1$ such that every polyhedron in P is tiled by (isometric copies of) polyhedra in P. This allows to construct a space of tilings whose elements are tilings equipped with a hierarchical structure. It has been proved [GS] that such tilings can be reconstructed simply by imposing some local rules to the boundaries of the polyhedra in P as soon as the dimension of the polyhedra is greater than one. This strong result that is linked with the way information can travel in a hierarchical system will be the source of a forthcoming strong stream of research.



An example of substitution tiling:

The pinwheel tiling.

1c: Dynamics in hierarchical structures

On the one hand, units of a complex system can cooperate to give rise to a hierarchical structure, on the other hand each unit can carry its own dynamics and in many situations these local dynamics are coupled together. In the last decades a huge amount of work has been devoted to coupled map lattices, with a special emphasis on short range coupling [Kan]. Little is known about coupled systems that preserve or essentially preserve a hierarchical structure, i.e. when the coupling between two units in the same cell of generation n is stronger than the coupling between units in different cells and this at every level of the hierarchy.

Q7. Many questions are still open in this direction as for instance: the synchronization process, self-similar pattern formation, and propagation of instabilities from micro to macro dynamics...

Other tools like deterministic or probabilistic cellular automata can probably be useful for this type of problem.

Bibliography

[AR] D. Aristoff and C. Radin*, Emegent structures in large networks*, arxiv:1110.1912.

[BBG] J. Bellissard, R. Benedetti, J.-M. Gambaudo, *Spaces of Tilings, Finite Telescopic Approximations and Gap-Labelling*, Comm. Math. Phys. 1, (2006), 1–41.

[Ber] R. Berger, *The undecidability of the domino problem,* Mem Am Math Soc 66 (1966), 1–72.

[Cul] K. Culik, *An aperiodic set of 13 Wang tiles,* Discrete Math. 160 (1996), no. 1-3, 245–251.

[EF] W. S. Edwards and S. Fauve, *Patterns and quasi-patterns in the Faraday experiment*. J. Fluid Mech., 278:123–148, (1994).

[GS] C. Goodman Stauss *Matching Rules and Substitution Tilings*, Ann. Math, 147 (1998), 181-223

[HWAALL] R Herrero, EG Westhoff, A Aumann, T Ackemann, YA Logvin, & W Lange. *Twelvefold quasiperiodic patterns in a nonlinear optical system with continuous rotational symmetry.* Phys. Rev. Lett., 82(23): 4627–4630, 1999.

[IR] G.Iooss, A.M. Rucklidge. *On the existence of quasipattern solutions of the Swift-Hohenberg equation*. J. Nonlinear Science 20: 3 (2010), 361-394.
[Kan] Kaneko, K. *Overview of Coupled Map Lattices,* Chaos 2:3 (1992), 279.
[LD] R. Lifshitz and H. Diamant. *Soft quasicrystals: Why are they stable?* Philos. Mag., 87(18-21):3021–3030, 2007.
[Mie] Miekicz *Low Temperature Stability of Nonperiodic Structures*. Physica A, 185: 151-153 (1992).

Task 2: Theory of hierarchical aggregation methods

The task will start with a brainstorming workshop between consortium members and invited external experts on the relative merits of the wide range of current approaches and the new ideas that consortium members are already generating. This will involve members of all participant nodes plus invited externals, which could include C.Maes (Leuven) on spatially extended stochastic dynamics, M.San Miguel (Palma) on social dynamics, P.Sanders (Karlsruhe) on highway hierarchies, K.Briggs (BT) on hierarchical structure in the telecommunications industry, Y.Notay (ULB, Belgium) on aggregation methods.

It will proceed to assess initial possible approaches to the seven application areas of WPs 4 & 5 (some of which were sketched in the position paper by R.S.MacKay for this call). This will ensure that a wide range of contexts is kept in mind for the formulation of general principles.

As an example, we sketch an approach to the context of networks of coupled oscillators, of direct relevance to Task C. By an oscillator let us understand a continuous-time dynamical system with an attracting limit cycle. In a network of oscillators there may be a group of n oscillators which synchronise together. This means that in their joint state space there is not just an attracting n-torus but the dynamics on this n-torus has an attracting periodic orbit. Or there could be partial synchronisation, meaning that the dynamics on the n-torus has an attracting m-torus for some $1 < m < n$. This does not suffice as an aggregation procedure, however, because the group of oscillators in general has inputs from others. Thus the way to look at an oscillator is in extended state space, with the addition of time to take into account input functions of time. Instead of being a limit cycle, an oscillator is an attracting cylinder for each set of input functions of time. A group of n oscillators subject to input functions of time produces an attracting n-torus cross time. The dynamics on this n-torus cross time may possess an attracting m-torus cross time for some $0 < m < n$, in which case we say the group synchronises (partially if $m > 1$). In the case $m = 0$ one says the group synchronises to its inputs.

Q: Can one formulate an aggregation process consisting in recognising groups of oscillators that are likely to synchronise in the presence of inputs in some expected class, making a rigorous verification that they do have a lower dimensional attracting submanifold, and then replacing them by the lower-dimensional submanifold?

Work in this direction has been done at UoW (see the PhD thesis of S.Gin, Aperiodically forced oscillators, Sept 2011) using normal hyperbolicity theory. The same ideas could apply to more general dynamics than oscillators, where some dimension reduction can occur.

Next, general principles will be formulated for the design of aggregation methods for the description and analysis of dynamical complex systems.

A key aspect to be addressed is the effect of approximations. It may be useful to make some approximations in the description at a higher level. Then error bounds need to be derived.

Deliverables (brief description and month of delivery)
D1.1: Answers to at least 4 of Qs 1-7 (M24)
D1.2: Initial workshop on hierarchical aggregation methods (M1)

Work Package 2

Work package number	2	Start date or starting event:	M1	
Work package title	Computational Theory			
Activity type	RTD			
Participant number	1	2	3	4	5
Participant short name	UoW	HB	RuG	INLN	QTC
Person-months per participant	26	12.6	24	0	0

Objectives

The main overall objective of this work package is to find for every mathematical model used in this project a computational (discretised) version of the same model, possibly an approximation (in case some parts of a model are not formulated as discrete objects or events) which can be implemented and simulated on a digital computer. We will in particular achieve the following goals:

- Develop a computational theory that allows us to consider various combinations of multi-level complex systems, partly formulated as discrete and continuum objects, and either formulated in discrete or continuum time (in case a dynamic process is considered).
- Formulate numerical discretisations and algorithms adapted to describe a large class of complex systems in the context of aggregation. Whenever feasible, the computational method should in fact be analogous to the aggregation procedure developed in work package 1, moreover deliver error estimates when possible.
- Test the computational theory by way of real-world case studies inside the consortium.

In this work package we will work inside the following general problem themes, but eventually focus on some aspects within these themes which are most relevant to us and which should be feasible to solve in time within the project. All these general themes are considered to be highly relevant for any efficient simulation in many if not all scientific applications:

- What fine-level structures or temporal processes of a simulation model can be aggregated during the modelling process without changing the solution too much, or inside a well-defined error bounds? The solution will be defined on a relatively coarser scale of observation.
- How does the aggregation method change the simulation model when another scale of observational resolution is chosen?
- Once the computational model is implemented it will typically incorporate a mix of discrete objects (such as lower-dimensional manifolds defining the boundaries of computational sub-domains) and temporal processes (such as transport processes) defined on these structures. In order to gain more accuracy of the solution, refinements of the computational grid at all these defining structures have to be made. Can aggregation methods help to determine when grid refinements (including those in time) lead to a change of the computational model defined on relative micro-structures?

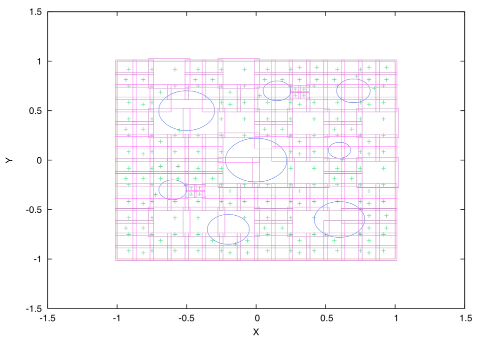


Figure: A simple example of a computational domain with obstacles (holes). Also shown is a computational grid, in this case a cover using overlapping patches (‘partition of unity’). See [6].

- In case the computational domain is very heterogeneous (such as in porous media), the multi-scale character of the computational domain should be exploited in order to find an iteratively convergent and stable solution algorithm. One successful class of algorithms are the Algebraic Multi-Grids (AMG) [1], [2] which in a broad sense rely on stochastic sampling and aggregation on different scales of the problem. Can we define similar methods efficiently on computational domains with a mix of random and non-random structures, such as multi-scale transport networks?

- An overall question is whether complex multi-scale systems can be simulated in a stable way, using the latest advances in software methodology? There are many issues involved, such as the interplay of domains and surfaces in such problems, interaction with discrete objects such as obstacles in different dimensions etc. Any such multi-scale structure imposes severe difficulties on the discretisation part of an algorithm, i.e. the construction of the computational grid at different scales.
- In complex systems theory, but also in economics and finance, so-called **agent-based models** [5] are frequently used. They can be implemented on digital computers directly, because (a) they are based on discrete objects (the agents), and (b) their updates in state (such as their 'opinion' or 'strategy') are following a discrete event statistics. It is clear that combinations of PDE (Partial Differential Equations) based models with agent-based models make perfect sense. Just think for example of agents that are acting in some kind of field (of 'information', or of a 'force') influencing their state, and that this field is having different effects than interaction with other agents. Such models will allow to model more advanced social systems, and are also occurring in reaction systems where some of the molecules are large enough in order to be described as discrete objects. We will aim at finding a basis for a computational theory combining numerical analysis with agent-based modelling.
- Often aggregation of a mathematical model induced by time-scaling can change the computational 'type' of the model. A good example is agents or molecules modelled by discrete states with the help of Markov Chains. In case the agents' switching behaviour between discrete states is on a faster scale than their interaction with their continuum environment one can collapse the discrete state dynamics to the invariant measure of the Markov Chain, i.e. their states' equilibrium distribution. Under this assumption one can reduce a reaction system (also if modelled in space) to a pure 'weighted' continuum model. [6]
- A computational theory of hierarchical modelling and aggregation must account for compatibility between aggregation methods and respective data structures. The aggregation method is essentially a compression of algorithmic speed or increase of efficiency. This triggers usually at the same time a data compression where the data structure itself becomes of structured type.

References

[1] P. Bastian, M. Blatt, and R. Scheichl. Algebraic multigrid for discontinuous Galerkin discretizations. *Numer. Linear Algebra Appl.*, 2011, accepted.

[2] M. Blatt: A Parallel Algebraic Multigrid Method for Elliptic Problems with Highly Discontinuous Coefficients. Dissertation, Universität Heidelberg, 2010.

[3] Eigel, M., George, E., and Kirkilionis, M. 2008. The Partition of Unity Meshfree Method for Solving Transport-Reaction Equations on Complex Domains: Implementation and Applications in the Life Sciences. Meshfree Methods for Partial Differential Equations IV. Springer-Verlag Berlin and Heidelberg.

[4] Eigel, M., George, E., and Kirkilionis, M.: 2009. A Meshfree Partition of Unity Method for Diffusion Equations on Complex Domains. IMA J. Num. Math. doi:10.1093/imanum/drn053, p. 1-25.

[5] Miller, H and Page, S.: Complex adaptive systems. An introduction to computational models of social life. Princeton University Press, 2007.

[6] Kirkilionis, M. and Sbano, L.: 2010. An averaging principle for combined interaction graphs – connectivity and applications to genetic switches, Adv Complex Sys 13(3), pp. 293-326.

Description of work

Task 1 Initial workshop: Workshop on computational theory. This will bring together members of all participant nodes plus invited external experts, to assess the state of computational theory for hierarchical aggregation. External experts include Bollhöfer (Braunschweig), C.Simo (Barcelona), Schultes (Karlsruhe), van den Eijnden (Courant), Beal (MIT), Scholtes (Zürich), Tessone (Zürich). (all partners)

Task 2: Computational modelling of large-scale traffic networks. This is largely a similar setting as the lung transport network, again a transport phenomenon mostly restricted to a (planar) branching network across several scales. We will however aggregate small-scale traffic to a diffusion process on the domain into which the transport network is embedded on larger scales. (HB and UoW)

Task 3: Computational modelling of large-scale social and epidemiological networks. In this application we will combine PDE discretisations with agent-based modelling. (HB and UoW)

Task 4: Mathematical and computational modelling of the human lung. The human lung is a paradigm example of a biological multi-scale transport network. The endless branching of the transport tubes (glottis -> trachea -> bronchi -> bronchioles -> alveoli) down to the cellular level is adapted to an efficient exchange of oxygen from the air into the blood stream. The exchange rate of oxygen into the blood is depending on two fundamental different periodic events, breathing and heart beat. Moreover this exchange rate is of course dependent on the effective surface of oxygen exchange, defined on the cellular level. Breathing effectively establishes a basic push and pull mechanism, which will create different types of directed turbulent air motion in the lung's transport network, at least inside the larger branches such as the trachea and bronchi. (HB and UoW)

Outputs

2.1: (M6) Specification of a general class of multi-level complex systems that incorporates all examples considered inside the consortium. Outline of a computational theory for this class of models.

2.2: (M12) Algorithmic outlines of computational aggregation methods considered inside the project.

2.3: (M18) Specification of a transport test example to be implemented in WP 3, incorporating transport equations implemented on an underlying computational domain, and coupling with event-driven discrete objects.

2.4: (M24) Computational modelling of the epidemiological/opinion formation model.

Deliverables

D2: Specification of computational aggregation methods (M24)

Work Package 3

Work package number	3	**Start date or starting event:**		M1	
Work package title	ICT Implementation				
Activity type	RTD				
Participant number	1	2	3	4	5
Participant short name	UoW	HB	RuG	INLN	QTC
Person-months per participant	28	27	2	1	0

Objectives

The main overall objective of this work package is the efficient ICT implementation of complex system simulation on high-performance computers. We will in particular achieve the following goals:

- Develop a general ICT architecture that allows us to implement various aggregation methods developed in WP 1.
- Use respective numerical discretisations and algorithms adapted to describe a large class of complex systems in the context of aggregation, as developed in WP 2.
- Test the ICT architecture by way of real-world case studies inside the consortium.
- Prepare the ICT implementation for dissemination to end-users.

Complex systems arise in different flavours. In this project we seek to combine the more general description of the system as interacting agents (and other discrete structures, such as networks) with the description of the system by a partial differential equation (PDE). After discretization (with e.g. the finite element method and using time-stepping and/or iterative solvers for the arising linear systems) any PDE simulation can be viewed as an agent-based simulation on a very large graph with a regular nearest neighbour structure. However, this may not be the most efficient way to implement and carry out such large-scale simulations. We therefore seek to combine state-of-the-art approaches for PDE-based simulation with the state-of-the-art in agent-based and discrete event simulation.

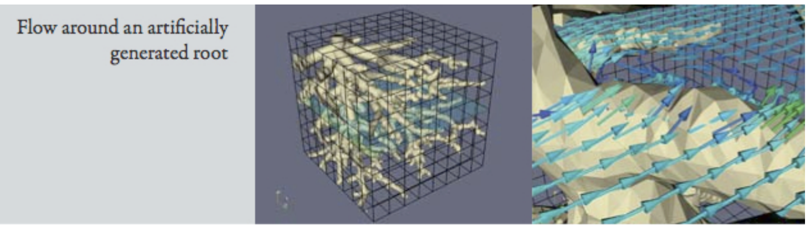


Image: Example of combination of discrete structure with PDE coupling: a flow around a plant root system.

The PDE simulation will be based on the Distributed and Unified Numerics Environment (DUNE)[8] that has been developed for ten years in several groups in Germany and at the University of Warwick. DUNE provides a framework for the implementation of a large class of numerical schemes for the grid-based numerical solution of PDEs including high-order finite element schemes, adaptive mesh refinement as well as multi-level and domain decomposition solvers [5,6,7]. DUNE combines flexibility and high performance by separating algorithms and data structures using generic programming techniques in C++.

Hierarchical aggregation techniques were explored in DUNE with an algebraic multigrid solver [1,3,6,7]. The technique developed there scales very well on high-performance computers and enabled us to solve systems with up to 147 billion unknowns on 287496 cores of BlueGene/P [2]. We propose that these techniques can be carried over to more general aggregation techniques in the context of complex systems.

The combination of PDE-based simulation with event-based has been developed in DUNE in the context of the simulation of networks of neurons [9]. The individual neurons are represented by the solution of a diffusion-reaction system on a detailed neuron morphology while the interaction between different neurons is realized by discrete firing events. In this project we will provide an abstract framework for general agent-based complex systems where the individual agents may be realized by the solution of a PDE. The agent-based part will use Charm++ [11,12] as the underlying framework for communication and load balancing. Charm++ is a mature parallel programming environment that has been used for a variety of different applications, including event-based simulation. Charm++ won the HPC challenge award competition in 2011. The challenges with this approach will lie in an efficient integration of both frameworks and in the development of efficient load balancing techniques.

References

[1] P. Bastian, M. Blatt, and R. Scheichl. Algebraic multigrid for discontinuous Galerkin discretizations. *Numer. Linear Algebra Appl.*, 2011, accepted.

[2] O. Ippisch and M. Blatt. Scalability test of mf and the parallel algebraic multigrid solver of DUNE-ISTL. In B. Mohr and W. Frings, editors, Jülich Blue Gene/P Extreme Scaling Workshop 2011, 2011. Technical Report FZJ-JSC-IB-2011-02.

[3] M. Blatt: A Parallel Algebraic Multigrid Method for Elliptic Problems with Highly Discontinuous Coefficients. Dissertation, Universität Heidelberg, 2010.

[4] P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klöfkorn, M. Ohlberger, and O. Sander. A generic grid interface for parallel and adaptive scientific computing. part I: abstract framework. *Computing*, 82(2-3):103-119, 2008.

[5] P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klöfkorn, R. Kornhuber, M. Ohlberger, and O. Sander. A generic grid interface for parallel and adaptive scientific computing. part II: implementation and tests in DUNE. *Computing*, 82(2-3):121-138, 2008.

[6] Markus Blatt and Peter Bastian. C++ components describing parallel domain decomposition and communication. *International Journal of Parallel, Emergent and Distributed Systems*, 24(6):467-477, 2009.

[7] P. Bastian and M. Blatt. On the generic parallelisation of iterative solvers for the finite element method. *Int. J. Computational Science and Engineering*, 4(1):56-69, 2008.

[8] DUNE : http://www.dune-project.org

[9] NeuroDUNE : http://www.neurodune.org/

[11] CHARM++ : http://charm.cs.illinois.edu/

[12] L.V. Kale and S. Krishnan. CHARM++: A Portable Concurrent Object Oriented System Based on C++. In A. Paepcke, editor, Proceedings of OOPSLA'93, pages 91{108. ACM Press, September 1993.

[13] Laxmikant V. Kale, Anshu Arya, Abhinav Bhatele, Abhishek Gupta, Nikhil Jain, Pritish Jetley, Jonathan Lifflander, Phil Miller, Yanhua Sun, Ramprasad Venkataraman‡, Lukasz Wesolowski, Gengbin Zheng. Charm++ for Productivity and Performance - A Submission to the 2011 HPC Class II Challenge, Parallel Programming Laboratory, Department of Computer Science, University of Illinois, 2011.

Description of work

Task 1 Initial workshop: This will bring together members of all participant nodes plus invited external experts and potential users, to discuss specific aspects of the ICT implementation. (all partners)

Task 2: Specification of interfaces: (a) event-based simulation and PDE, (b) discrete structures (mainly networks) and transport processes described by PDE, (c) discrete event-based objects acting in a field described by a PDE (application to social systems, opinion formation and epidemiology) (HB & UoW)

Task 3: Implementation of test applications: (a) neuronal activity, (b) air transport in human lungs, (c) regional traffic flow. (team from HB and UoW)

Task 4: Testing the efficiency of the ICT implementation in the different test applications (HB & UoW)

Task 5: Testing the novel ICT frameowork for usage with end users. (all partners and external end-users).

Outputs

3.1: (M6) Specification of ICT interfaces, describing effectively the class of complex systems that can be described and implemented with the ICT framework. The framework will be based on DUNE, and Charm++.

3.2: (M12) Implementation of a test example, transport equations implemented on both graphs and the underlying computational domain, with coupling of the two structures.

3.3: (M18) Implementation of a test example, transport equations implemented on an underlying computational domain, and coupling with event driven discrete objects.

3.4: (M24) Implementation of the lung application.

3.5: (M30) Implementation of the traffic flow application.

3.6: (M36) Implementation of the epidemiological/opinion formation model.

Deliverables

D3: Software to carry out hierarchical aggregation (M30)

Work package 4

Work package number	4	Start date or starting event:	M13	
Work package title	Customization to Applications			
Activity type	RTD			
Participant number	1	2	3	4	5
Participant short name	UoW	HB	RuG	INLN	QTC
Person-months per participant	22.2	6.5	15.8	7	0

Objectives

The overall goal of the proposal is to develop universal approaches based on hierarchical aggregation to tackle complex systems. As these approaches are sought to be not just of theoretical value but applicable to real world problems it is important to test their applicability to concrete problems.

The main objective of WP4 is therefore to facilitate and coordinate the application of the mathematical and computational theory developed in WP1 and WP2 and their ICT implementation in WP3 to concrete and typical examples of complex systems, and in return give stimuli to WP1-3 through demands faced in real world applications. To this end the following seven application areas are chosen:

B Brain imaging (mainly UoW + HB)
C Chronobiology (mainly RuG + UoW)
I Infectious diseases (mainly UoW)
L Lung flow (HB with UoW & INLN)
Q Quasicrystals and quasipatterns (mainly INLN with UoW & RuG)
S Social norms (mainly RuG)
T Traffic flow (mainly UoW with RuG & HB)

The application areas are chosen in such a way that they exhibit typical features and challenges that one faces with complex systems. The application areas B,I,L,S and T have an emphasis on computations and in the upward direction are mainly linked to WP 2+3 whereas C and Q have a stronger emphasis on theory and accordingly are mainly linked to WP 1. All seven areas are directly linked to WP5 in the downward direction by providing models, schemes to analyse and key questions to look at in application area using the data to validate theoretical and computational approaches developed in WP 1-3.

Different nodes will be involved in different application areas to stimulate the interaction between the different areas and to exchange ideas. As problems and their solutions are often discussed separately in isolated communities despite of the fact that the nature of the problems and solutions have much in common we expect a fruitful cross-fertilization by bringing these communities together.

Description of work

B Brain imaging (mainly UoW + HB)

In the last 10 years brain-imaging research has moved swiftly from a focus on functional segregation, mapping the brain regions that support different behaviors, to functional integration, understanding how different regions work together to support behavior and cognition (Friston, 2011). Essential for understanding functional integration are network models. While Structural Equation Models and related methods (McIntosh, A. R., & Gonzalez-Lima, 1994) were popular initially, they are limited to very small graphical structures based on highly distilled data, typically from 5 or fewer brain regions. Attention is now focused on mapping brain-wide connectivity with graph theory methods (see, e.g., Bullmore & Sporns 2009), but this work is also based on distilled data, typically using only about 100 fixed anatomical region of interests (ROIs) derived from the 100 000-voxel full-resolution brain data.

The goal of this task is to develop computationally tractable hierarchical aggregation methods based on probabilistic models. While community detection is a highly active area (Fortunato & Castellano, 2007; Porter & Onnela, 2009) relatively little of the work is based on hierarchical, overlapping classes of nodes (Section XII of Fortunato, 2010). Also, with a few notable exceptions (Daudin, et al., 2007; Newman & Leicht, 2007) the methods are algorithmic, based on heuristics with no generative stochastic model. We will extend the existing non-hierarchical probabilistic approaches, make them computationally tractable for the imaging setting, and consider the incorporation of imaging-specific information (i.e. spatial adjacency; other temporal association characteristics aside from correlation).

Friston, K. J. (2011). Functional and effective connectivity: a review. *Brain Connectivity*, *1*(1), 13-36. doi:10.1089/brain.2011.0008
McIntosh, A. R., & Gonzalez-Lima, F. (1994). Structural Equation Modeling and Its Application to Network Analysis in Functional Brain Imaging. *Human Brain Mapping*, *2*(1-2), 2-22. doi:10.1002/hbm.460020104
Bullmore, E. T., & Sporns, O. (2009). Complex brain networks: graph theoretical analysis of structural and functional systems. *Nature reviews. Neuroscience*, *10*(3), 186-98. doi:10.1038/nrn2575
Fortunato, S., & Castellano, C. (2007). Community Structure in Graphs. (R. A. Meyers, Ed.)*Networks*, *814*(2005), 42. Springer. Retrieved from http://arxiv.org/abs/0712.2716
Porter, M., & Onnela, J. (2009). Communities in networks. *Notices of the AMS*, *56*(9). Retrieved from http://www.ams.org/notices/200909/rtx090901082p.pdf
Fortunato, S. (2010). Community detection in graphs. *Physics Reports*, *486*(3-5), 75–174. Elsevier. Retrieved from http://linkinghub.elsevier.com/retrieve/pii/S0370157309002841
Daudin, J.-J., Picard, F., & Robin, S. (2007). A mixture model for random graphs. *Statistics and Computing*, *18*(2), 173-183. doi:10.1007/s11222-007-9046-7
Newman, M. E. J., & Leicht, E. A. (2007). Mixture models and exploratory analysis in networks. *Proceedings of the National Academy of Sciences*. doi:10.1073 pnas.0610537104.
Cordes, D., Haughton, V. M., Arfanakis, K., Carew, J. D., Turski, P. a, Moritz, C. H., Quigley, M. a, et al. (2001). Frequencies contributing to functional connectivity in the cerebral cortex in “resting-state” data. *AJNR. American J neuroradiology*, *22*(7), 1326-33. From http://www.ncbi.nlm.nih.gov/pubmed/11498421
Niazy, R. K., Xie, J., Miller, K., Beckmann, C. F., & Smith, S. M. (2011). *Slow Brain Oscillations of Sleep, Resting State and Vigilance*. *Progress in brain research* (Vol. 193, pp. 259-76). Elsevier. doi:10.1016/B978-0-444-53839-0.00017-X

C Chronobiology (mainly RuG + UoW)

The behaviour of most organisms shows clear aspects of periodicity. In the context of 24-hour periodicities animals alternate between sleep and wakefulness and some plants open and fold their leaves. In an annual context some animal species alternate between active episodes and hibernation and many plant species between episodes in which they grow branches and leaves and episodes in which they shed their leaves and have reduced growth. These periodicities are clear adaptations to fluctuations in their external environment. However, they are usually not just direct responses to the environment. Over millions of years of evolution many organisms developed internal clocks that maintain periods near 24 hours even in the absence of the light-dark stimulus or Zeitgeber. This allows them to predict environmental changes in advance, and to prepare appropriate internal changes at the right time. A major question in circadian biology is how the internal clock synchronizes with or entrains to an external Zeitgeber. This does not only include adjustment of period, but also of phase. Obviously, if hibernation serves avoiding the harsh conditions of winter, it is not sufficient for an animal to show periodic alternations between hibernation and euthermia with a period of one year. In addition hibernation should occur in winter, not in summer. For many organisms, the daily cycle of light and darkness to which the organism is exposed is the major signal to entrain the circadian clock, and the changes of the daily light-dark cycle across the year are of major importance to entrain annual rhythms.

For mammals, the internal clock is formed by neurons or pacer cells in the hypothalamic tissue which resides above the optic chiasm. These neurons (typically of the order of 10 000 in number) can be viewed as a collection of interconnected two-state (active/inactive) phase oscillators. Experiments indicate that in the internal clock not every individual pacer cell is entrained but the internal clock emerges from the collective behavior of the ensemble of pacer cells. The main subject of this research is to understand the mechanisms that lead to the emergence of the collective behavior of the pacer cells and its ability to synchronize with or entrain to an external Zeitgeber. In collaboration between mathematicians and biologists, models of pacer cells, their mutual interactions and response to external Zeitgebers will be developed which on the one hand show the characteristic features observed in nature, and which on the other hand allow to distill key mechanisms. It is to be expected that the collective behavior of an ensemble of such cells can be analyzed and understood from the perspective of hierarchical aggregation, namely the spatial and temporal formation of clusters of pacer cells which synchronize or entrain in a hierarchical manner.

From a mathematical point of view the pacer cells are oscillators with a circular state space. Together they form a network of such oscillators. The state space is accordingly a high-dimensional torus. Because of the high dimensionality the dynamics on the torus is too complex to be studied as a whole. In particular the dynamics of each individual oscillator is not directly relevant for the emergence of the internal clock that rather is a property of the network as a whole. Hierarchical aggregation now comes into play by viewing the emergence of entrainment or synchronization of the network as a process in which the interactions between individual oscillators together with their response to a periodic external stimulus like the light-dark cycle leads at first to clusters of entrained or synchronized oscillators. The state space of such a cluster of oscillators is then a lower dimensional torus and the entrainment or synchronization implies the existence of a limit cycle on this lower dimensional torus. The limit cycle of each such cluster can now be viewed as a new "cluster" oscillator. The number of the cluster oscillators is then smaller than the number of oscillators in the original network, i.e. the dimensionality has been reduced. This process can now be iterated, i.e. the cluster oscillators of one generation again form through their effective interaction and the external periodic stimulus entrained or synchronized clusters on a higher level. Iterating this process one finally ends up with a fully entrained or synchronized network of oscillators. The study of such a hierarchical aggregation process requires one to understand the stability and formation and break up of tori on different scales. The interest of chronobiologists to understand seasonal changes in the responses of the pacer network to corresponding alternations in the shape of the light-dark cycle adds another layer of complexity to this problem. We want to understand annual changes in the phase distribution of pacers in the network.

The questions studied are relevant for many other application areas and the main goal is to develop general principles. For example, periodic stimulation naturally occurs in climate research in the form of seasonal or tidal forcing. The research in this application area is directly linked to the general questions in WP1 on the formation, stability, and transport in hierarchical structures.

As a diagnostic tool for studying dynamical aggregation we want to use and further develop computational methods from time-frequency analysis based on wavelets. This allows one to distract the instantaneous frequencies of a system from the ridges of the time-frequency landscape of trajectories. This has recently been recognized as a strong tool to detect trappings and transitions between resonances and to study the underlying phase space structures.

The research will be carried by a core team formed by mathematicians from the Dynamical Systems and Mathematical Physics group at the Johann-Bernoulli Institute in Groningen and biologists from the Chronobiology Department at the University of Groningen, in collaboration with the Centre for Complexity Science in Warwick (MacKay), the group of Gambaudo in Nice and other nodes.

The research team at RuG includes D.G.M.Beersma (Biology; Chronobiology), H.W.Broer (Mathematics; Dynamical Systems & Mathematical Physics), J.B.T.M Roerdink (Computer Science; Scientific Visualizations & Computer Graphics), G. Vegter (Mathematics; Computational Geometry), H.Waalkens (Mathematics: Dynamical Systems and Mathematical Physics).

References:

D.G.M. Beersma, H.W. Broer, K. Efstathiou, K.A. Cargar and I. Hoveijn, Pacer cell response to periodic Zeitgebers, Physica D 240 (2011) 1516-1527

Beersma DG, van Bunnik BA, Hut RA, Daan S. Emergence of circadian and photoperiodic system level properties from interactions among pacemaker cells. J Biol Rhythms. (2008) 23:362-373.

C. Baesens, J. Guckenheimer, S. Kim, R.S.MacKay, Three coupled oscillators: mode-locking, global bifurcations and toroidal chaos, Physica D 49(3):387-475, 1991.

H.W. Broer, G.B. Huitema, F. Takens, and B.L.J. Braaksma, Unfoldings and bifurcations of quasi-periodic tori. Mem AMS 83(421), American Mathematical Society, 1990.

H.W. Broer, Resonance and Fractal Geometry. ACAP 2012, to appear.

H. W. Broer, S. J. Holtman, G. Vegter, and R. Vitolo, Dynamics and Geometry Near Resonant Bifurcations. Regular and Chaotic Dynamics, 16(1-2): 39–50, 2011.

H.W. Broer and M.B. Sevryuk, KAM Theory: quasi-periodicity in dynamical systems. In H.W. Broer, B. Hasselblatt, and F. Takens, eds., Handbook of Dynamical Systems. North-Holland, pages 249–344, 2010.

H.W. Broer and F. Takens, Dynamical Systems and Chaos. Appl. Math. Sc. 172, Springer, 2011.

H.W. Broer, K. Efstathiou, and E. Subramanian (2008) Robustness of unstable attractors in arbitrarily sized pulse-coupled systems with delay. Nonlinearity, 21:13–49, 2008.

H.W. Broer, K. Efstathiou, and E. Subramanian (2008) Heteroclinic cycles between unstable attractors. Nonlinearity, 21:1385–1410, 2008.

A.E. Sterk, R. Vitolo, H.W. Broer, C.Simó, and H.A. Dijkstra, New nonlinear mechanisms of midlatitude atmospheric low-frequency variability. Physica D, 239(10):702–718, 2010.

S. Sosniyenko, R.A. Hut, S. Daan, A. Sumová. Influence of photoperiod duration and light-dark transitions on entrainment of Per1 and Per2 gene and protein expression in subdivisions of the mouse suprachiasmatic nucleus. Eur. J. Neurosci. (2009) 30:1802-1814.

C.Chandre, S.Wiggins & T.Uzer. Time-frequency analysis of chaotic systems. Physica D 181 (2003) 171-96.

L.V.Vela-Arevalo and J.E.Marsden. Time-frequency analysis of the restricted three-body problem: transport and resonance transitions. Class. Quantum. Grav. (2004) 21:351-375.

I Infectious diseases (mainly UoW with HB)

Epidemiology and the study of infectious diseases has been quick to embrace the range of new techniques derived from complex systems. In fact, models of disease spread are often used as motivating examples in the study of many complex phenomena. In addition, predicting the spread of infectious diseases and how they can best be controlled is a fundamental problem where mathematics can have a strong positive benefit on public health (Keeling and Rohani 2008). Fully understanding the spread of infection brings together multiple scales of interaction, from within-host dynamics that govern the rates of onward transmission, to localized clustering and network structure of social contacts which determine the immediate transmission, while longer-range movements of infected individuals enable the disease to spread through the wider population.

Many of the novel mathematical and computational advances proposed in this project have direct application to the spread of infectious diseases. Three particular examples are given below:

For many infectious diseases, spread within the household, school classroom or workplace dominate transmission. The use of so-call household models allows us to capture the strong transmission within a social clique (home, school workplace) together with weaker transmission between such cliques. While many results can be rigorously proved about the final outbreak size both in the entire population and within cliques (Ball 1999, Ball & Lyne 2001), the transient dynamics are best captured as a large set of ODEs:

$$\dot{x} = \mathbf{Q}x + (x \cdot I)\mathbf{Z}x$$

Here the vector x captures the probability of a clique being in each possible configuration of infective states, the vector I gives the total level of infection associated with each state, while the sparse matrices $\mathbf{Q}$ and $\mathbf{Z}$ determine the transitions through the state space due to within clique dynamics and infection from outside the clique (Ross, House, Keeling 2010). Techniques for dealing efficiently with such sparse systems of coupled ODEs would provide a major break-through in the types of problem that can be addressed (Keeling and Ross 2008, 2009). This is particularly the case when more realistic infection dynamics are modeled such that each individual moves through multiple latent and infectious classes; this greatly increases the dimension of the problem and hence the need for more refined and efficient computational tools.

Secondly, network structure is now seen as a fundamental element in understanding how diseases spread and how reality deviates from the random mixing models of the 1980s. While some headway has been made in developing approximations for these dynamics (Keeling 1999, Dangerfield, Ross and Keeling 2009), stochastic (Markovian) simulations remain the standard approach. Therefore, developments in Markovian simulations and understanding network structures will be exploited to better inform disease simulation dynamics (Danon et al 2011). The ability to simulate very large stochastic populations can be vitally important when attempting to validate deterministic approximation models, while being able to simulate many network realizations rapidly has clear implications for parameter inference.

Finally, the applied work on social norms (S) and traffic flow (T) will have direct impact on the study of disease spread. The movement of individuals (who act as hosts of infection) inevitably leads to the movement of infection; understanding the driving factors that affect an individual’s decision of where to travel to (eg choosing between competing venues based on time and distance) has implications for how widely an infection will be transmitted. The work on social norms has direct parallels to individuals’ willingness to conform to good health-care practices. Traditional work on vaccination, hand-washing, or self isolation generally assume a fixed proportion that comply, whereas more recently epidemiological models have begun to realize the compliance is conditional on the behaviour of others, the perceived risks and the media coverage (Funk, Salathe and Jansen 2010).

References

Ball F (1999) Stochastic and deterministic models for sis epidemics among a population partitioned into households. Math Biosci 156: 41–67.

Ball F, Lyne O (2001) Stochastic multitype sir epidemics among a population partitioned into households. Adv App Prob 33: 99–123.

Dangerfield C, Ross J, Keeling M (2009) Integrating stochasticity and network structure into an epidemic model. J Roy Soc Interface 6: 761–774.

Funk, S., Salathe, M. and Jansen, V.A.A. (2010) Modelling the influence of human behaviour on the spread of infectious diseases. *J. Roy. Soc. Interface.* **7** 1247-1256.

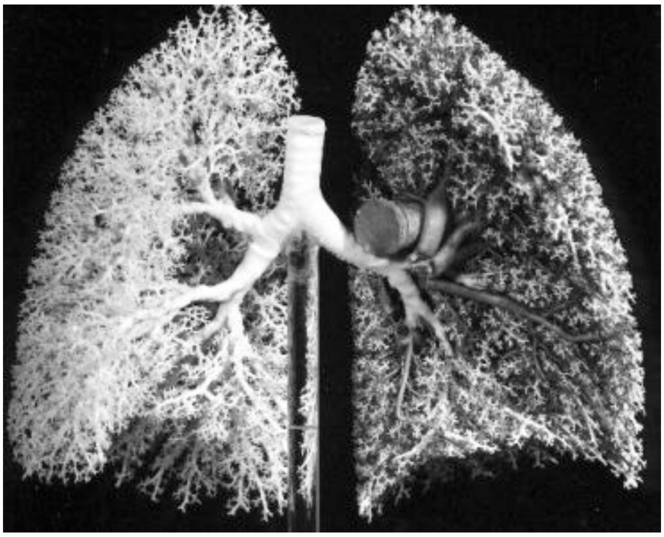
Keeling, M.J. (1999) The effects of local spatial structure on epidemiological invasions. *Proc. Roy. Soc. Lond. B.* **266** 859-867.

Keeling, M.J. and Rohani, P. (2008) *Modeling Infectious Disease in humans and animals*. Princeton U Press.

Keeling, M.J. and Ross. J.V (2008) On methods for studying stochastic disease dynamics. *J. Roy. Soc. Interface.* **5** 171-181

Keeling, M.J. and Ross, J.V. (2009) Efficient methods for studying stochastic disease and population dynamics. *Theo. Pop. Biol.* **75** 133-141
Ross, J.V., House, T.A. and Keeling, M.J. (2010) Calculation of Disease Dynamics in a Population of Households. *PLoS ONE* **5** e9666

L Lung flow (HB with UoW & INLN)
The human lung is a paradigm example of a biological multi-scale transport network. The endless branching of the transport tubes (glottis -> trachea -> bronchi -> bronchioles -> alveoli) down to the cellular level is adapted to an efficient exchange of oxygen from the air into the blood stream. The exchange rate of oxygen into the blood depends on two fundamental different periodic events, breathing and heart-beat. Moreover this exchange rate is of course dependent on the effective surface of oxygen exchange, defined on the cellular level. Breathing effectively establishes a basic push and pull mechanism, which will create different types of directed turbulent air motion in the lung's transport network, at least inside the larger branches such as the trachea and bronchi.



The goal is to develop a hierarchical computation scheme for the airflow in the lung. Aspects of this have been described already in WP2 and 3, so we will not repeat them here.

Q Quasicrystals and quasipatterns (mainly INLN with UoW & RuG)
Quasiperiodic patterns, which have a hierarchical structure, appear in many contexts, e.g. quasicrystals, experiments on Faraday waves and on liquid crystals. Our aim is to understand why. For this we have several dynamical approaches which include the study of quasicrystal growth, the stability of pde solutions that generate quasipatterns, and the variation of Gibbs measure when temperature goes to zero for lattice gas systems. The task here is to provide a computational link between the mathematical studies of WP1 and the experiments of WP5 task Q.

S Social norms (mainly RuG)
Whether individual actors comply with social norms and what the content of the norms is that emerge in a community is the outcome of the interplay of social influence processes between multiple individual actors, organized in partially constructed social units (e.g. departments in an organizations) and partially emergent ones (e.g. clusters in friendship networks) at various levels of aggregation. In recent years, social scientists increasingly employ formal modelling techniques to cope with the complexity of such dynamics, e.g. the formation of cultural groups (e.g. Axelrod 1997; De Sanctis & Galla 2009; Flache & Macy 2011a) or of opinions (e.g. Hegselmann & Krause 2002; Maes, Flache & Helbing 2010, Flache & Macy, 2011b). In addition, researchers increasingly collect the data and develop the statistical tools – mostly based on based on complex models which can only be estimated using simulation methods - that allow to address the interdependent dynamics of the formation of networks of social relations (e.g. friendships) that convey influence and the individual behaviours (e.g. opinions, norm compliance) that exert influence and are influenced in social interaction (Steglich, Snijders, West, 2006; Snijders, van de Bunt, Steglich, 2010; Robins et al. 2007).

Formal models of the dynamics of social influence and social relations are typically computationally highly demanding because they model interaction at the inter-individual level. Simulation studies therefore usually involve not more than several hundreds to thousands individual nodes. This is not sufficient to address the dynamics of opinion and norm formation in large-scale social communities as they arise for example in online interactions. The main objective in this application area is applying the aggregation methods developed in the core part of the project to assess to what extent and under what conditions the dynamics of norms, opinions and networks in large scale online communities can be modelled more efficiently and still be predicted with reasonable accuracy when inter-individual interactions are aggregated into interactions between larger scale units. For example, to predict how the average political opinion about a given political issue evolves in a network of interconnected political blogs, it may be sufficient to model influence processes between the aggregate opinions of each of the blog-communities rather than the inter-individual influence processes between all individual bloggers in the overall network.

T Traffic flow (mainly UoW with RuG & HB)
An idealised model for traffic flow is that each driver chooses its route to minimise some notion of cost, but the cost depends on the amount of traffic encountered along the route and any tolls. As satellite navigation becomes more sophisticated, incorporating real-time traffic information, this ideal is becoming realised more closely, not just in a statistical sense.

A department for transport may wish to determine tolls or speed limits in real time or determine the likely benefits or otherwise of proposed changes to the road network, like new traffic signals or bypasses or one-way systems. Restrict attention for the moment to the steady situation and to the case of a sum of edge costs only. Even this requires a massive calculation of the Nash-Wardrop flows for a massive database of origin-destination flow rates and of the road network (e.g. T.Roughgarden, The price of anarchy, MIT Press, 2005).

It is highly desirable to have an efficient method of calculation of the Nash-Wardrop flows and one for which the effects of changes in one region do not require recomputation of the whole network from scratch.

Our proposed solution is a hierarchical computation. Parts of the network can be solved for presumed flows between their external edges, from internal origins to external edges, and from external edges to internal destinations. Each such part can be represented as a super-node. The only difference from a node in the edge-costs-only model is that a super-node incurs "junction-costs", i.e. costs for going from one edge to another that depend on the flows between all pairs of edges adjacent to the super-node. Although this sounds a major step up in complication, it is not significantly harder than edge-cost-only models, and it is much closer to reality as in any case junctions impose significant costs that should be included from the start.

This project will build on results for the transformation rules for aggregating a selected part of a road network with junction costs into a super-node with junction costs by the group of MacKay. The main steps that need to follow are to decide which groups of nodes to aggregate, to implement the method in software, to analyse its efficiency, and to test the method on real data.

Outputs
For the computational aspects of the application areas, the outputs are
4.1: (continuously) Development and fine-tuning of models (determination of appropriate lowest level units, and operationalisation of aggregation; criteria for similarity and model of interdependences)
4.2: (M18) Identification of coherent requests and demands in the application areas on computational means to be developed in WP2-3
4.3: (M24) Test runs on small data sets and feedback to WP2-3 on performance of algorithms
4.4: (M24) Establish/decide per application area what the outcomes are that we want to model / explain / predict and how we operationalise those

For the theoretical aspects, the outputs are mainly feedbacks to WP1 on
4.5: (continuously) the question of ubiquitous occurrence of hierarchical structures,
4.6: (continuously) the formation of hierarchical structures,
4.7: (continuously) transport in hierarchical structures, and
4.8: (continuously) the stability of hierarchical structures.

Deliverables
D4 Reports on customisation to at least 4 of the tasks (M30)

Work Package 5

Work package number	5	Start date or starting event:	M13	
Work package title	Validation of methods on data			
Activity type	RTD			
Participant number	1	2	3	4	5
Participant short name	UoW	HB	RuG	INLN	QTC
Person-months per participant	22.1	6.5	17.1	8.7	0

Objectives

The main objective of this work package is to validate the new algorithms developed in WP 1,2 and 3 on data from a range of application areas (gene expression, epidemiology, airflow in the lung, formation of quasipatterns, brain images, traffic flow, and the dynamics of social norms). For this, the work package will draw upon the customizations of the algorithms to the various application areas that have been elaborated in WP 4. That is, WP4 has established what are per application area the properties of the system that are to be modeled and how they can be measured. WP 4 has also established what in the specific application area the relevant individual level units are, how their properties can be measured and how the degree of their interdependence or similarity can be assessed for the purpose of constructing descriptions at a hierarchy of levels adapted to the system.

Building on this, WP5 has as main goals per area of application:

Objective 1: the collection of data on both the system level properties of interest as well as the interrelated properties of the meso- and individual level units of the system,

Objective 2: for sufficiently small subsets of the data: comparison of the accuracy and efficiency of prediction of system level and individual or meso-level behavior between (1) conventional models that describe the interaction of individual units only at the lowest level of hierarchy, and (2) models simplifying the system by making use of our newly developed methods for hierarchical aggregation,

Objective 3: for datasets too large to be addressed with conventional non-hierarchical models: testing predictions of system level behavior derived from models using hierarchical aggregation against data on observable macro-level behaviour of system.

Description of work

In order to attain the goals, we need per area of application to conduct a number of tasks. The areas of application and the division of labor and data sources between partners in the application tasks has been described in the overall work strategy under 1.4.

For every area of application, the work in WP 5 involves the following **tasks**:

Task 5.1: collect the data and / or use existing data sets. That is: collect data on dynamics of individual level units and their strength of similarity, and data on the outcome variables.

Task 5.2: Compare hierarchical aggregation models vs. non-aggregated models vs. data. Run non-hierarchically structured models for subsets of the data that are small enough for this. Run for comparison "hierarchically structured" models of same data. Compare predictions of both sets of models for behavior of outcome variables at macro / meso and micro level of the system.

Task 5.3: Assess relative performance of hierachical aggregation models. Assess for these datasets (task 3) the relative accuracy and efficiency of methods of hierarchical structuring for the data per area of application.

Task 5.4: Fine tune / optimize hierarchical aggregation methods for the given data based on results of task 5. Go through task 3 / task 4 / task 5 loop until sufficient gain of efficiency at tolerable loss of accuracy has been obtained.

Task 5.5: Apply fine-tuned methods to model large data sets. Address data sets too large for conventional one-level models. Use hierarchical structuring to generate predictions for system behavior at macro level and test predictions at macro level against observable system-level behavior.

Here follows a more specific description of the data to be collected and the methods of data collection per area of application.

B – Brain imaging: For brain imaging, there are two types of motivating data, functional connectivity data and structural connectivity data, both obtained from MRI scans. For functional connectivity we use resting-state Functional MRI (fMRI) data, where a subject is imaged in an awake, restful condition over 5-10 minutes. With no variation from an experimental task, these data are ideal for identifying the local and long-range correlations in typical brain activity. Of interest is the relationship in brain activity between pairs of single voxels (volume elements) or regions of interest (ROIs), usually summarised with the Pearson's correlation coefficient. For structural connectivity we use gray matter images obtained from T1-weighted MRI scans. Gray matter does not change over the time-span of minutes, so intra-subject temporal correlations are not feasible; instead cross-sectional correlations are computed, measuring the similarity of gray matter between different voxels/ROIs over subjects. The data will be obtained from the Human Connectome Project [http://humanconnectome.org/], a 5-year US$30m project to acquire and distribute state-of-the-art functional and structural connectivity data on 1200 subjects. Dr. Nichols is a co-investigator on the Connectome project and will have early and complete access to the data collected.

Data preparation. Original functional & structural connectivity data will require some standard preprocessing (head motion correction, registration to a standard atlas space) with standard freely available software (FSL, http://www.fmrib.ox.ac.uk). The full, preprocessed data in atlas space has 228 453 spatial elements. To compare the methods developed in this grant with established methods, we will produce connectivity data (i.e. intra-subject temporal correlations for function, inter-subject correlations for structure) for ROI's of different resolutions. We will use a hierarchical ROI atlas we have used in previous work (Vounou et al, 2010). The end result of this fundamental task is data prepared and ready to be used with the methods proposed in WP1-3

Evaluation of methods. Evaluation of network methods for brain connectivity data is particularly challenging, as there is no gold standard. Hence we consider the stability and replicability of the methods developed in WP1-3 and customized in WP4. For connectivity based on fMRI we have two approaches, one based on intra-subject data-splitting, and one based on inter-subject comparisons; for structural connectivity, we only have inter-subject cross-validation. For fMRI, we can compute a network twice, once based on the first half and once based on the second half of each subject's time-series data. Using partition similarity metrics (like Minkowski distance, adjusted Rand index or mutual information; see Handl et al., 2005) we can compare the two sets of partitions, and see if their similarity is better or worse than reference methods. Possible reference methods include purely-anatomically-defined networks, or simple hierarchical agglomerative clustering methods; in both cases we can roughly match the number partitions in the proposed and reference methods. For inter-subject evaluations we can compare all (or a random subset of all) possible pairs of subjects, and measure similarity of graph partitions between subjects. While we expect substantial inter-subject variability, among non-degenerate methods we favor those that give the most consistent results over subjects.

Vounou, M., Nichols, T. E., & Montana, G. (2010). Discovering genetic associations with high-dimensional neuroimaging phenotypes: A sparse reduced-rank regression approach. *NeuroImage*, *53*(3), 1147-59. Elsevier B.V. doi:10.1016/j.neuroimage.2010.07.002

Handl, J., Knowles, J., & Kell, D. B. (2005). Computational cluster validation in post-genomic data analysis. *Bioinformatics*, *21*(15), 3201-3212. doi:10.1093/bioinformatics/bti517

C – Chronobiolology: Data on electrical activity of the pacer network (provided in various publications by the group of Joke Meijer (Meijer e.a. 2010; Rohling e.a. 2011, 2006a, 2006b, van der Leest e.a. 2009) at the University of Leiden) will be used to estimate the distribution of phase of the pacer ensemble in real life situations. They form the background to validate the results of the modeling efforts. In these studies, recordings have been made from SCN (suprachiasmatic nucleus) tissue. Sometimes the SCN was isolated from animals and kept alive in a dish, sometimes recordings were from otherwise intact animals. Mostly electrical activity was recorded extracellularly. Action potentials were examined and sorted by size. Action potentials of large size are infrequent and assumed to be generated by one cell. This provides information about single cells. The sum of all recorded action potentials gives a good impression of the behaviour of the ensemble of neurons in the SCN. So the system level is SCN level here, and the individual level is single cell level. To assess the interdependence and similarity between cells when modelling the system in terms of coupled and driven oscillators, the background theory of dynamical systems provides globally emerging characteristics in terms of dimension, measure, entropy, Lyapunov exponent, etc. to describe the system at a higher hierarchical level.

Meijer JH, Michel S, Vanderleest HT, Rohling JH. Daily and seasonal adaptation of the circadian clock requires plasticity of the SCN neuronal network. Eur J Neurosci. (2010) 32:2143-2151.

Rohling JH, van der Leest HT, Michel S, Vansteensel MJ, Meijer JH. Phase resetting of the mammalian circadian clock relies on a rapid shift of a small population of pacemaker neurons. PLoS One. (2011) 6(9):e25437
Rohling J, Meijer JH, Van der Leest HT, Admiraal J. Phase differences between SCN neurons and their role in photoperiodic encoding; a simulation of ensemble patterns using recorded single unit electrical activity patterns. J Physiol Paris. (2006a) 100:261-270.
Rohling J, Wolters L, Meijer JH. Simulation of day-length encoding in the SCN: from single-cell to tissue-level organization. J Biol Rhythms. (2006b) 21:301-313.
van der Leest HT, Rohling JH, Michel S, Meijer JH. Phase shifting capacity of the circadian pacemaker determined by the SCN neuronal network organization. PLoS One. (2009) 4(3):e4976.

I: Infectious diseases. For testing models of the dynamics and hierarchical structure of the spread of infectious diseases, a wide range of epidemiological data is available. These data will be used to validate and infer parameters for the models developed. Data collected during the 2009 H1N1 influenza pandemic provides very high resolution information on detected cases during the early stages of the epidemic; although it should be noted that only a proportion of cases are detected. Such data will be ideal for exploring household models in more detail, as information (and serological swabbing) is often collected from entire households. Similar data exist for other outbreaks and much of this information is in the public domain. In addition, serological and lesion dating information from the 2007 foot-and-mouth outbreak in the UK can be used with household data in the same manner, but with the farm playing the role of the household. Together the 2009 H1N1 pandemic and the two outbreaks of Foot-and-Mouth disease in the UK (2001 and 2007) provide a wealth of examples of localized transmission, longer-scale spread (potentially by networks) and the social response to risk. The other key means of validating results developed in this part of the project is via a comparison of approximation models to the results of full stochastic simulations, or a comparison to limiting cases where exact results can be found. For example, network models should converge to specific and well-understood limits when the population size is large and the network is randomly connected; while the final number of cases within a household and the number of secondary households infected are both well characterised in the early stages of an epidemic.

L – Lung flow: This subproject focuses on modeling how flow rate and flow resistance in the human lung at the system level relate to the lung geometry at the level of meso-level and individual-level units. The exchange rate of oxygen into the blood is depending on two fundamental different periodic events, breathing and heart beat. Moreover this exchange rate is dependent on the effective surface of oxygen exchange, defined on the cellular level. Breathing effectively establishes a basic push and pull mechanism, which will create different types of directed turbulent air motion in the lung's transport network, at least inside the larger branches such as the trachea and bronchi We will reconstruct and analyselarge airways (typically, first 6-8 generations) using 3D CFD (computational fluid dynamics). Typically, this 3D airway model will contain 50-100 bronchioles. We calculate the pressure, velocity and turbulent intensity at each section of this airway model. The resistance of the lung as well as the total gas flow rate can be calculated.

To supplement this 3D model, the entire lung airways are also constructed using a simple 1D model (so called the Weibel mode). In this 1D model, the pressure and velocity in the entire lung airways including alveoli are calculated. Physiological lung properties such as the elasticity of the lung tissue are also considered using mathematical as well as empirical models. Aggregation methods can be applied by making use of the similarity between airways, in particular smaller airways can share many similarities with each other, but larger airways can have different sizes and angles. To prepare the actual modeling of empirical data making use of hierarchical aggregation methods, the bifurcation of the lung geometry will be analysed.
Lung geometry has a series of bifurcation; a branch divides into two sub-branches with a certain angle between them. This bifurcation can be modelled as symmetric or asymmetric.

Q – Quasi crystals and quasi patterns: The theoretical approaches will be supported by exploring experiments (Faraday and liquid crystals) to be conducted at INLN. Here is an outline of the liquid crystal experiments.

Experimental investigation of optical hierarchical structures

Hierarchical structures will be investigated in a nonlinear optical setup consisting of a liquid crystal light-vale, LCLV, with optical feedback. The LCLV is made of a thin layer of liquid crystals in between a glass wall and a photoconductor substrate over which a mirror is deposited. An externally applied voltage induces an electric field, in the direction of which molecules tend to orientate. The photoconductive side of the

LCLV modulates the voltage across the liquid crystal layer as a function of the impinging light intensity and, as a consequence, a reorientation of the liquid crystal molecules, which induces on the reflected light a phase retardation proportional to the light intensity. By this mechanism the LCLV converts light intensity modulations into phase modulations of the reflected beam, while the free propagation inside the optical loop converts phase into intensity modulations. A positive feedback sets in so that a self-consistent spatial distribution of the light intensity is selected at each round-trip and a spontaneous spatial self-structuring occurs over the transverse section of the light beam [1]. Figure 5.1 below describes the experiment.

In the LCLV with optical feedback two-dimensional crystals and quasi-crystals have been observed and selected by imposing suitable symmetry breaking conditions in the optical loop [2], as well as hierarchical structures of the super-lattice type, which have been shown to be metastable configurations of the complex spatiotemporal dynamics characterizing the system [3]. More recently, it has been shown that suitable, and arbitrary, optical potentials can be superimposed on the nonlinear medium by placing a spatial light modulator, SLM, in the path of the input beam. By this method we can control the phase and amplitude profile of the light entering the optical loop. By imposing appropriate grid profile on the phase of the input beam the control of localized structures has been demonstrated [4], while grid intensity profiles have permitted to study bistable regimes and front dynamics, demonstrating a large pinning effect of the front [5] and allowing a careful characterization of the homoclinic snaking diagram of localized structures [6].

In the HACS project optical hierarchical structures will be created in the LCLV experiment and will be studied in conjunction with suitable optical potentials. The growth of the hierarchical structures will be investigated first by characterizing the spontaneous evolution and then by exploiting the optical potential method for influencing and controlling the hierarchy of the patches and their appearance. Local rules will be tested by characterizing the tiling as a function of different boundary conditions and by letting the evolution to take place over different symmetries of the background potential. The dynamical behaviors will be characterized and modeled on the basis of generalized Swift-Hohenberg models.

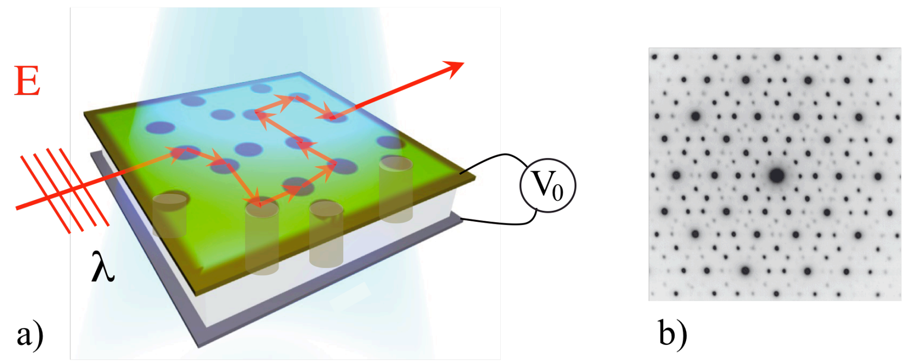


Figure 5.1 Light propagation in photo-induced quasi-crystal potentials. a) Experimental scheme showing the light propagating inside the liquid crystal layer and the photoconductive wall of the cell addressed with a quasi-crystal light intensity distribution, as shown in b).

Moreover, we plan in the HACS project to setup optical experiments where the light will propagate longitudinally inside the liquid crystal layer and the hierarchical structures will be superimposed by means of a controlled photo-addressing over the photoconductive wall of the LCLV. During its propagation, the light will experience the presence of the superimposed hierarchical structure, hence, will be diffracted accordingly, giving rise to complex field distributions. The propagation will be, first, studied and modeled in the linear regime, then, nonlinearity could be introduced by exploiting the orientational nonlinearity of the liquid crystals. The nonlinear regime will be investigated experimentally and will be modeled by using the nonlinear Schrödinger equation, from which universal behaviours are expected.

1. S. Residori, Phys. Rep. **416**, 201 (2005).
2. E. Pampaloni, P.L. Ramazza, S. Residori, F.T. Arecchi, Phys. Rev. Lett. **74**, 258 (1995).
3. E. Pampaloni, S. Residori, S. Soria, F.T. Arecchi, Phys. Rev. Lett. **78**, 1042 (1997).
4. U. Bortolozzo, S. Residori, Phys. Rev. Lett. **96**, 037801 (2006).
5. F.Haudin, R.G.Elias, R.G.Rojas, U.Bortolozzo, M.G.Clerc, S.Residori, Phys Rev Lett **103**, 128003 (2009)
6. F. Haudin, R.G. Rojas, U. Bortolozzo, S. Residori, M.G. Clerc, Phys. Rev. Lett. **107**, 264101 (2011)

S - Compliance with social norms: a large-scale dataset on the dynamics of compliance with social norms will be collected from an online community that is partly self-organized, complex, and easily accessible for analysis of the structure and content of interactions with regard to specific norms. Using existing expertise on online data collection (Stadtfeld) data will be collected from the Wikipedia community on the extent to which members indicate violations of the rules emanating from the "five pillars" of the community (http://en.wikipedia.org/wiki/Wikipedia:Five_pillars) about how to write and edit entries in the encyclopedia. Since the community was set up, about 15 million registered users have joined, they have created about 25 million pages, and c. 500 million page edits have occurred (http://en.wikipedia.org/wiki/Special:Statistics), many accompanied by background discussions in which explicitly the obedience with the five pillars was addressed. The work in this subproject will be conducted in 6 steps. (1) Data will be collected on e.g. the relative frequency with which authors refer in background discussions to these five pillars, or to which monitors mention on sites suspected violations of the five pillars. Such data can and will be extracted from crawling the publicly available information on the site. This will result in statistics and a data set on change and frequency of discussions about norm violations in Wikipedia, broken down by subcommunities, topical areas and other meaningful distinctions. (2) In addition, data on relations between community members (e.g. online referrals, editing on the same articles, joint participation in other related community) will be obtained to assess the interdependent dynamics of behaviour and network relations. Here, the aim is to generate data sets on (change of) online network relations. Following recent developments (see Stadtfeld e.a. 2011), this data set can contain an event-based representation of the pattern of social interactions in the community. (3) On basis of the data collected in steps 1 and 2, the aggregation methods developed WP 1-3 of HACS will be used to obtain possible aggregations of the overall community of users that we observe. This will result in a proposal for the identification of subcommunities and higher order hierarchical structures in the overall community, possibly broken down by subcommunities, topical areas and other meaningful distinctions. (4) Drawing on previous research by the team members (Flache 2011a,b; Maes e.a. 2010; Van Duijn 2011, Stadtfeld, 2011) formal models of the interdependent dynamics of norm-related behaviour and network relations of the community members will be developed and tested on the inter-individual data for a subsets of the community that are large enough to be coped with. The aim is to generate models and simulations of the dynamics of norm obedience and norm violations for conditions (e.g. initial network structures, number of nodes) reflecting the empirical case of various subsets of Wikipedia community. Building on this work, we will then, in step (5), compare the predictions and predictive accuracy of these models to alternative models for the same subset of data that focus on modelling the interactions between the aggregated units above the level of inter-individual social influence dynamics. This will help to assess the relative predictive accuracy of aggregation models vs. inter-individual models of the dynamics of norm compliance and network change in Wikipedia. Finally, in step (6), we will use the models based on aggregation methods to address dynamics in the community as a whole that can otherwise not be coped with (using non-hierarchical models of opinion and network dynamics). We aim to test predictions of such models on observable macro-level outcome such as the overall level of participation in the online community activities, obedience with and violations of community rules, change of the network structures (e.g. clustering). This should result in testable predictions and scenario analyses for past and future dynamics of norm compliance and network change in Wikipedia. Eventually, it is aimed to give a tentative answer to the question whether obedience with the key norms of the community can be expected to be sustainable in the long run and what conditions (e.g. which subcommunities, which possible institutional regulations and monitoring systems) will foster norm compliance.

Stadtfeld, Christoph & Andreas Geyer-Schulz. 2011. Analyzing event stream dynamics in two-mode networks: An exploratory analysis of private communication in a question and answer community, Social Networks, Volume 33, Issue 4, October 2011, Pages 258-272.

Flache, A., & Macy, M.W. (2011a). Local Convergence and Global Diversity: From Interpersonal to Social Influence. *Journal of Conflict Resolution* 55.6: 968 - 993. DOI: 10.1177/0022002711414371.

Flache, A., & Macy, M.W. 2011b. Small Worlds and Cultural Polarization. *Journal of Mathematical Sociology* 35.1. Pp. 146-176 in Marcel A. L. M. van Assen, Vincent Buskens, and Werner Raub (eds.). Special triple issue: "Micro-Macro Links and Micro-Foundations".

Mäs M, Flache A, Helbing D. 2010. Individualization as Driving Force of Clustering Phenomena in Humans. *PLoS Computional Biology* 6(10): e1000959. doi:10.1371/journal.pcbi.1000959

Van Duijn, M.A.J. & Huisman, M. (2011). Statistical Models For Ties and Actors. In: J. Scott and P.J. Carrington (Eds.). *The SAGE Handbook of Social Network Analysis*. London: Sage.

T: Traffic Flow: To test the aggregation methods on data, Huitema of the RuG node, and also employed at TNO, will organize access to a number of road pricing pilots that have been conducted in the Netherlands, prior to the planned introduction. In 2007, the Dutch Ministry of Infrastructure and the Environment legislated the implementation of road pricing by 2011, and nationwide by 2016. In 2010, the Dutch road pricing project was put on indefinite hold owing to political changes, but data from pilots and ongoing-developments in research labs are available for HACS.

TNO specified an ICT-architecture for running the related business processes from registration of vehicle movements and collection of traffic data up to the invoicing of the users. The project was called "Paying differently for mobility" (Anders Betalen voor Mobiliteit). An important part of the introduction of road pricing is the handling of privacy. Hoepman, Jaap-Henk, George Huitema, Privacy Enhanced Fraud Resistant Road Pricing, IFIP Advances in Information and Communication Technology, pp 202-213, 2010.

Several commercial pilots were held proving the maturity of the involved GPS and On Board Equipment technology. Generically the collected traffic data contains of sets of records containing: vehicle-id, starting point, way points on the route, destination, and timestamps. In the back office the records are enriched with pricing data. The km-price will vary according to time, place and environmental effects.

There are two pilots that can be used by HACS. First, NXP and IBM conducted a road pricing trial which demonstrated that with the help of technology, drivers can be motivated to change their driving behavior, reducing traffic congestion. The six-month road pricing trial, conducted in the city of Eindhoven was overwhelmingly successful, with 70 percent of drivers changing their behavior to avoid rush-hour travel when presented with the right incentives. More than 200.000 test kilometers were logged. The second pilot was the Dutch Road Pricing Trial on the accuracy and reliability of distance-based measurement and determination of Tariff for Kilometre Pricing (KMP) performed by TRL (Transport Research Laboratory). Three identical test vehicles were fitted with highly accurate location and distance measurement equipment. The routes, tests and analysis were designed to create equally challenging situations. The test vehicles were driven around the test routes in convoy, over a period of four weeks. Each route was repeated a number of times to ensure the results were statistically significant, with each test vehicle covering approximately 5000 km. The research evidence suggested that GPS-based road pricing technologies were sufficiently accurate, reliable and cost-effective to support the Netherlands' desire to introduce the first national (all roads, all vehicles) GPS-based road charging system (based on time, place and distance driven). In HACS, we will use hierarchical aggregation methods to devise efficient models of traffic flow and effects of road pricing on it, aggregating traffic flow patterns from models of individual road choice behavior which, in turn, are fitted to and based upon the data collected in the pilots.

Outputs for each application area:

1. **Data sets** containing the key variables needed for testing models. *Ready month 18.*
2. **Test reports** per application area of performance hierarchical models vs. non-hierarchical models on performance in describing data for subsets of overall data sets. *Ready month 21.*
3. **Comparison report:** summary of assessment of relative performance and efficiency of models on selected data sets. *Ready month 24*.
4. **Report on optimisation of aggregation methods** (parameter selection for aggregation algorithms) per application area. *Ready month 27*
5. **Predictions and macro-level tests for large-scale data sets.** *Ready month 36*

Deliverables

D5 Reports on validation for at least 4 of the application areas (M36)

Work Package 6

Work Package No.	**6**	Start date or starting event		Month 1	
Work package title	Dissemination and Exploitation				
Activity type	MGT				
Participant No	1	2	3	4	5
Participant short code	UoW	HB	RuG	INLN	QTC
Person-months per participant	16	0.5	0.5	0.5	1

Objectives: The objectives of this work package are to make the essential arrangements for protection of knowledge achieved in this project through patent applications. We also aim to disseminate knowledge to the wider scientific community as well as the public, which will include a non-specialist audience. This will be achieved by setting up of a website. We will publish material in peer reviewed international journals, carry out poster presentations at relevant conferences and hold a symposium at Warwick University. A detailed study on the socio-economic impact of the project will be carried which will also include market penetration and the different routes to market.

Description of work:

Task 6.1.Preparation of project presentation material, including a project brochure and a project poster (UoW).

Task 6.2. HACS website for the dissemination of the project results to a wider community (UoW).

Task 6.3. Dissemination activities including publications in peer reviewed international journals such as the SIAM journals, the Royal Society (of London) journals and Proceedings of the National Academy of Science of the USA, and symposia. Attendance at major exhibitions and conference presentations will be made such as the annual European Conference on Complex Systems, the biennial European Future Technologies conference and the 4-yearly European Congress on Computational Methods in Applied Sciences and Engineering (all).

Task 6.4. A major study will be carried out on the socio-economic impact of the project (all).

Task 6.5. Warwick University will hold an ***International Symposium*** to disseminate knowledge by inviting leading scientists, young academics, industry, and the EC before completion of the project. This dissemination role will be supported by Warwick University and will allow partners to present material at the conference through talks and poster presentations. We will invite world leaders and young scientists who will be given an opportunity to present findings of their own research (UoW).

Task 6.6. Patent searches will be carried out during the duration of the project and if required patent applications will be made (all).

Task 6.7. Preparation of a final plan for Dissemination of Knowledge & project results (all).

Task 6.8. Summary report of Users Group on problems to address and routes to exploitation (all).

Deliverables

6.1	One-page brochure/poster detailing the objectives of the project and supplied to the EC (M1)
6.2	A project website for the dissemination of project results to the wider community (M4)
6.3	Publication of results in at least 2 high impact journals (M36)
6.4	A report on the socio-economic impact of the project (M30)
6.5	Symposium at the University of Warwick (M36)
6.6	A report on patent searching (M24)
6.8	Users Group report (M36)

Work Package 7

Work package no.	**7**		**Starting date or event**	M1	
Work package title	Project Management				
Activity type	MGT				
Participant No.	1	2	3	4	5
Participant Short code	UoW	HB	RuG	INLN	QTC
Person-months per participant	4	0.3	0.3	0.3	12

Objectives

To provide a link between the Consortium and the European Commission

To ensure the smooth running and organization of the HACS project

To ensure that the technical objectives of the HACS project are fully met within the allocated budget

Ensure that all commitments with respect to dissemination and exploitation are fully met.

Description of work and role of partners

Effective project management is essential for the smooth running of the HACS project and this will include:

- Detailed and up-to-date knowledge of the progress of each work package
- Monitoring of the overall progress of the project against the contract
- Taking any necessary action to keep the project on track
- Recognising failings that impact on the aims of each work package and introducing contingency plans if necessary to ensure correct re-alignment
- Report project progress and any decisions made at the Project Management Committee meetings to the Commission.

Task 7.1 Financial and Administrative Coordination and Communication with the Commission
Task leader: WARWICK UNIVERSITY
Participant: QTC

WARWICK UNIVERSITY will receive and manage all payments for the consortium and will ensure the transfer of appropriate funding to each partner according to the EU contract. WARWICK UNIVERSITY will also be responsible for:

- Collating and preparing the periodic financial reports which will include reporting on the use of financial resources
- Submitting all documentation (e.g. contract preparation forms, reports, cost statements etc) to the Commission
- Requesting the Commission's permission for publication/travel outside of Europe and for significant changes to the budget distribution or the work programme
- Informing the Commission of any changes to designated names, project partners, patent applications and any significant delays likely to affect progress of the project.

WARWICK UNIVERSITY will prepare the Consortium Agreement between all partners and obtain sign off of this document. It will also manage any changes to this agreement throughout the lifetime of the project.

Task 7.2 Project Management Committee Meetings and Industrial Advisory Board Meetings
Task Leader: QTC
Participant: WARWICK UNIVERSITY

The Project Management Committee will meet quarterly and will be focused on ensuring the project is on track both from a technical and financial viewpoint. The Industrial Advisory Board will meet twice per year and this will provide the forum for communication of information on the progress of the project as a whole. QTC will be responsible for organising and facilitating these meetings.

Task 7.3 Communication between Members of the Consortium
Task Leader: QTC
Participant: WARWICK UNIVERSITY

QTC will be responsible for establishing clear methods of communication between all members of the consortium. To ensure efficient and effective communication across the consortium, collaborative software meetings (e.g. using Webex or FlashMeeting) will be used on a regular basis to ensure an uninterrupted flow of information and discussion between partners.

WARWICK UNIVERSITY will be responsible for notifying the contracting parties of any circumstances affecting the project.

Task 7.4 Undertake Efficient and Regular Management of the Project
Task Leader: QTC
Participant: WARWICK UNIVERSITY

Quotec will lead on this task and some examples of the type of activities that will be undertaken are outlined below:

- Collection of internal reports from partners
- Providing quarterly updates to the coordinator assessing technical progress and related partner costs in each of the previous 3 months activity
- Providing monthly progress updates to the coordinator, monitoring the input of the core group at monthly intervals
- Collation, organisation and monitoring of all deliverables against the work plan
- Reviewing partners' performance, interaction and progress of the work packages against plan
- Track and report on gender equality in the project
- Manage a risk register.

Deliverables	
D7.1	Kickoff management meeting (M1)
D7.2	Midterm Project review (M18)
D7.3	Final report to the EC (M36)

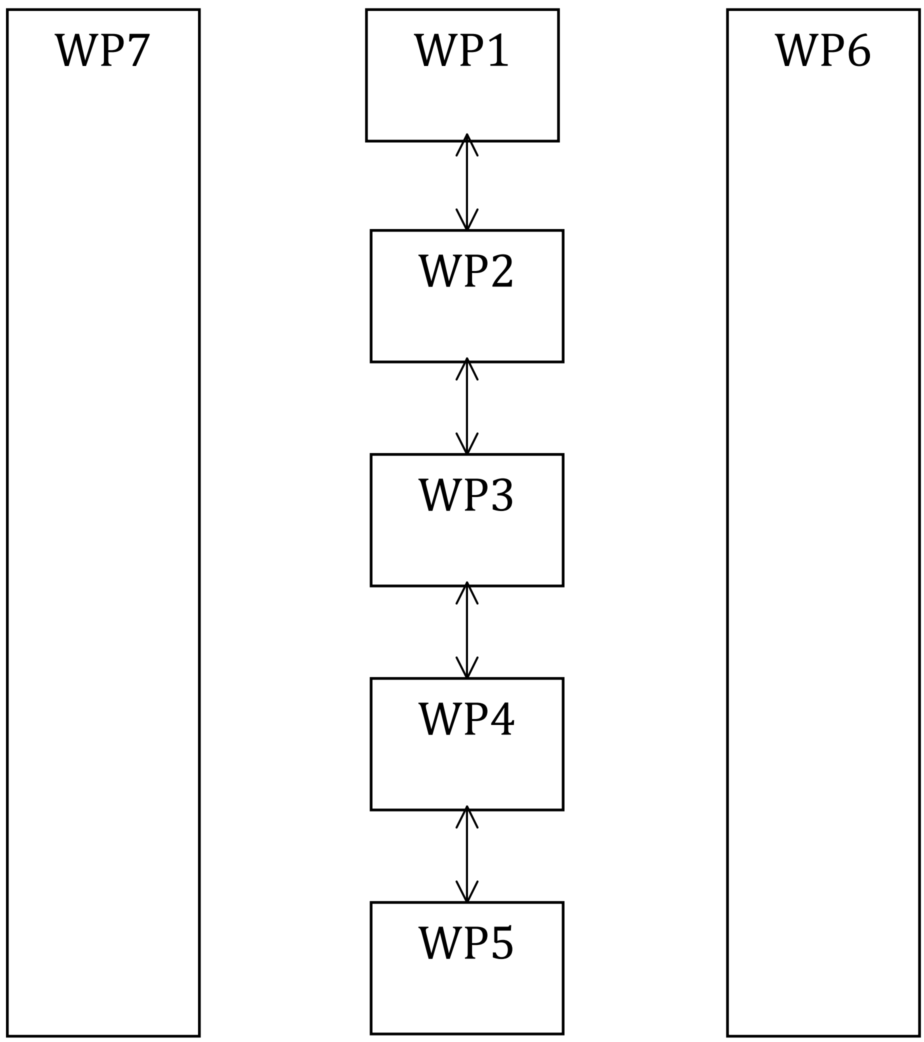
Summary of effort

A summary of the effort is useful for the evaluators. Please indicate in the table number of person months over the whole duration of the planned work, for each work package by each participant. Identify the work-package leader for each WP by showing the relevant person-month figure **in bold**.

Partic. no.	Partic. short name	WP1	WP2	WP3	WP4	WP5	WP6	WP7	Total person months
1	**UoW**	40	26	28	22.2	22.1	16	4	158.3
2	**HB**	0	12.6	27	6.5	6.5	0.5	0.3	53.4
3	**RuG**	27	24	2	15.8	17.1	0.5	0.3	86.7
4	**INLN**	39	0	1	7	8.7	0.5	0.3	56.5
5	**QTC**	0	0	0	0	0	1	12	13
Total		106	62.6	58	51.5	54.4	18.5	16.9	367.9

iv) Interdependencies of the components

The PERT chart below shows the interdependencies between the work packages. HACS has been divided into 7 work packages with WP1, WP2 &WP3 based on theory and WP4 and WP5 based on applications. WP6 is devoted to dissemination of the project results and will run throughout the duration of the project. WP7 is focused on the management of the project and will similarly run throughout the project.



v) Risks and Contingency Plans

Risk	Contingency Plan
We will not come up with a truly general approach	We will develop different methods for different classes of problem
The approaches may turn out to be difficult to implement efficiently	We will make some judicious approximations
Data may turn out not to be obtainable on time or in a suitable form for validation*	We will seek alternative data
The work may take longer than planned	We will seek further funding for the project

*An explicit example for Task B: The Human Connectome Project may run late in its planned acquisition of subjects, delaying the work of this project. If this happens, we will instead use data from the already-existing "1000 Connectomes" project [http://fcon_1000.projects.nitrc.org/]; this data is freely available, and will adequately serve the goals of the project (though it is more heterogeneous than the Human Connectome Project data).

Risk management is addressed again towards the end of section 2.1.

2. Implementation

2.1. Management Structure and Procedures

To meet the objectives of this project the expertise and competence of the individual partners needs to be combined in a successful and effective European consortium. The management of the consortium takes advantage of each partner's expertise, while also involving all of the partners in the decision making process through meetings at regular intervals. A key requirement for the successful completion of the project will be an efficient and accurate exchange of information and decisions between the partners and the Coordinator. There will be a procedure for the collection and handling of the data in a central database, which will be setup during month 1 of the project by Quotec Limited (QTC). This procedure will respect publication rights and the protection of intellectual property.

The consortium for the proposed research is composed of five participants. Four participants are research Universities and one an SME company. The coordination will need to direct the various groups to act in a synergistic and iterative way so that the results from one group are available to the other in a timely manner. The Coordinator will thus be responsible for the integrative, cross-disciplinary issues of the project, for planning and communication between the research partners, industrial partners and the European Commission. Where science permits, we shall adhere as closely as possible to the work plan and milestones outlined in the proposal, but reserve the right to respond flexibly to scientific developments in the field. Each Work Package leader will be responsible for developing a project plan for their work package and keeping it updated during the course of the project.

The Project Coordinator

The project coordinator will be the University of Warwick and the principal contact will be Professor Robert MacKay. Warwick University will be responsible for tasks such as:

- Ensuring the EC grant agreement is signed
- Being the interface to the EC
- Receiving, distributing and accounting for monies from the EC
- Reviewing reports to verify consistency with project tasks
- Monitoring compliance of project partners with grant obligation.

MacKay will represent the partnership in all scientific matters related to the project work. This function also involves supervision of the partners' performance, interaction and progress of the work packages. Crucially he will be charged with the coordination of the partners and the decisions on the movement of deliverables and information from one work package to another. As part of the process, MacKay may call meetings or wider workshops on an ad hoc basis as required. He will organise any electronic meetings that are required in order to make swift and decisive decisions. He will collect and prepare all scientific material to be presented and reviewed by the Project Management Committee. MacKay will also ensure that the work programme is kept to schedule and that the project meets the objectives, deliverables and milestones. Additionally he will oversee the monitoring of the input of the partners at monthly intervals and ensure that the consortium is meeting the deliverables within each work package. MacKay will also use his skills and experience to ensure that the required inputs for specific tasks are forthcoming from each partner and integrated to achieve a positive outcome.

Administrative/Consortium Management

This project has very challenging objectives and the work packages require close monitoring and integration to ensure a successful outcome. Quotec will provide expert project management assistance to the Coordinator to undertake the project management tasks and ensure that a subset of the administrative aspects of the project are undertaken and delivered in line with European-funded project requirements. Dr Mitesh Ladwa from Quotec will be responsible for this activity and he has successfully delivered administrative project management support to previous projects funded under the Framework Programme. He will work very closely with MacKay and other Warwick University staff. This approach will allow MacKay to focus his attention on the scientific and technological challenges of the project.

The project coordination function is a single function and the roles of the partners responsible for it are set out in the Table below.

Indicative Division of Management Responsibilities

University of Warwick	Quotec Limited
Warwick University is the project coordinator with the reporting relationship to the EC. *Summary of Main Responsibilities* Manage interface with the EC Lead on contract negotiation/funding agreement Manage payments and submit claims Responsible for Consortium Agreement and amendments.	Quotec provides project management support to the project coordinator *Summary of Responsibilities on behalf of the Coordinator:* Manage and implement the project procedures for ensuring delivery Monitor progress against plan and spend Monitor and manage systems for ensuring quality of deliverables.
Detail of Main Responsibilities ✓ Manage the development of the consortium agreement and any subsequent changes ✓ Development of the payment schedule ✓ Resolution of any contractual issues with the Commission ✓ Coordinating payments and distribution of money across the consortium ✓ All communication with the EC ✓ Submission of the periodic management reports.	*Detail of Main Responsibilities* ✓ Organisation of project management meetings ✓ Communications between consortium members ✓ Oversight of the Quality Assurance system, ensuring deliverables are of the highest quality ✓ Reviewing partners' performance, interaction and progress of the work packages against plan. Matching deliverable reports against the work plan ✓ Quarterly updates with the coordinator assessing technical progress and related partner costs in each of the previous 3 months activity ✓ Monthly progress updates with the coordinator/monitoring the input of the core group at monthly intervals ✓ Track and report on gender equality in the project ✓ Manage risk register ✓ Organisation of Project Management Committee meetings

The Project Management Committee

The project will be controlled by the Project Management Committee (PMC), comprised of one senior representative from each of the partners and chaired by the Coordinator's principal contact, MacKay. The PMC will have overall responsibility for the direction of the project. The principal tasks of the PMC include:

- Monitoring and updating (if required) the Consortium Agreement
- Assessing the scientific progress
- Assigning priority and resources to Tasks on the critical path
- Reviewing deliverables before submission to the EC
- Resolution of problems
- Ensuring compliance with legal and ethical obligations.

Project Management Structure

This activity is led by the Project Coordinator with support from the other partners.

- **Coordinator** Professor Robert MacKay, University of Warwick, will lead on communications inside the consortium, as well as motivation, dispute handling and resource management.
- **Project scientific manager** Dr. Markus Kirkilionis, University of Warwick will take responsibility for identifying and solving technical problems across the partnership and work packages.
- **Administrative/Consortium Manager** Dr Mitesh M Ladwa, Quotec Limited will be responsible for the administration component of the project.

- **Exploitation Manager** Dr Shum Prakash, Warwick Ventures (UoW), will take responsibility for IPR protection and licensing as well as knowledge transfer.
- **Dissemination Manager** The Knowledge Centre, UoW, will take responsibility for the broadcasting of the project results to the public and end-users widely across the EU.
- **Work package leaders** have been chosen based on the relevant technical expertise and management skills they bring to the project

The PMC will meet every three months to review the progress made by each of the partners and to agree in detail the actions for the next period. These meetings will be held at the same time as quarterly project meetings and will involve formal presentations from each of the partners who are actively working on tasks at that time. It is anticipated that most of these meetings will be physical but, where appropriate, virtual conferencing will be considered. The quarterly meetings will also include reviews of exploitation and dissemination activities.

Every quarter each work package leader will submit progress reports on each of the tasks in their work package. Partners will also submit reports on the resources they have used on each task during the quarter. These reports will be collated by Quotec. A progress report for the project will be generated by MacKay from these inputs and will be circulated to each of the partners in advance of the quarterly project meetings. The minutes and a summary of the quarterly meetings will be sent out to all the partners. The summary will include a table indicating the partner effort during each quarter on each task. The work plan, the deliverables and the milestone table will be used to measure progress.

In addition to the formal three-monthly meetings, the partners will also set up a number of working party meetings to focus on particular aspects of the work packages as required.

The task leaders will prepare brief monthly status reports on technical progress against plan for the Coordinator and the work package leader. The Coordinator will collate and review the monthly reports to track progress and identify any problems or deviation from the plan at the earliest opportunity. The Coordinator will also identify information that needs to be distributed to other partners within the consortium that may not be directly involved in a particular task but need the results to progress subsequent or parallel tasks.

Project Reviews with the Commission

Project Review meetings will be organised at M18 and M36 by the Coordinator with the support of Quotec. The Project Management Committee members will attend the Annual Project Reviews and the scientific officer of the EC responsible for the project will also be invited but may be represented by independent experts who shall be subject to confidentiality agreements. The coordinator will agree with the EC the date, the agenda and the participants of the meeting in advance of the meeting. The principal objectives of the Project Review meetings will be:

- To assess the extent to which the project is likely to meet its objectives as stated in the contract;
- To assess the possible impact of the project from both a scientific and a socio-economic point of view;
- To determine any reorientation of the project that may be required.

Communication Strategy

Communication will take place within the project on several levels. The Coordinator will control and gather information from the partners such that Warwick University will be the single point of contact with the Commission. During its quarterly meetings, the PMC will review the milestones and actions for the next period whilst the exploitation issues will be raised by the partners with the work-package leader responsible for Dissemination and Exploitation (WP6) for discussion during the meeting. The Work Package and Task Leaders will be responsible for communicating any necessary working party meetings between task groups, such that technical aspects can be clearly communicated between task participants from different consortium members. Individual researchers will communicate with their task leaders with regard to resource planning and periodic delivery of reports and results. As and when required, task participants will take advantage of workshops, brainstorming and technical media such as e-mail or videoconferencing, to ensure clear communication. In addition, a project web based document management system will be set up so that all members of the consortium can access all project documentation, such as meeting minutes, reports, pictures, presentations, results, agreements and drawings. There will also be a website which will act as a key dissemination and exploitation tool for the partnership, where conference notes, seminar agendas and other event information will be displayed. The communications within the project will take place on several levels that will support internal monthly and quarterly reporting on project progress.

Progress monitoring will require partner and research site visits by MacKay and by the task leaders, although not necessarily co-incidentally. To ensure that project results are accurate and correctly reported, the Coordinator will ask all the proposers to keep detailed experimental records using log books or a similar system. A project management software tool (such as Microsoft Project) will be utilized to plan and track progress on the project. In conjunction with the quarterly resource reporting it is envisaged that this will make it easier to ensure that each partner is delivering the effort to each task that they have committed to in the proposal and that the various tasks are started on time and the correct personnel and competences identified as necessary for each task are being utilized. Ensuring the information on project progress and resource allocation is reported and shared is a key tool to enable the integration of the various tasks across the project consortium.

Dissemination and exploitation will include communication with the members of the Users Group, for advice on key problems to address and on routes to exploitation.

Conflict Resolution

In the event of a dispute arising between two or more of the partners, the partners involved will enter into good faith discussions to resolve the dispute amicably and in a timely fashion. If, following this, the dispute remains unresolved then the said partners will engage in mediation in accordance with the procedures of the Centre for Effective Dispute Resolution by one or more mediators appointed in accordance with the said procedures. If, following this, the dispute remains unresolved, it shall finally be settled under the Rules of Arbitration of the International Chamber of Commerce by one or more arbitrators appointed in accordance with the said Rules.

Project Risk Management

We have an ambitious project with a tight budget and a multinational partnership. It consequently carries a high level of risk that will need managing effectively. The risk management roles have been split into two: the Coordinator's principal contact (Professor Robert MacKay) will oversee the technical risk management; Quotec (Mitesh Ladwa) will oversee management risks. The Work Package Leaders will identify and evaluate the risks (ranking in terms of likelihood and impact) in each of their work packages. Mitigation measures to address the risks will be described and a risk register for the project will be prepared. Risk reviews will be part of the quarterly project review process and also of the individual work package and task project meetings. The risk register will be updated to take account of any changes to the project plan and will be maintained by Quotec on behalf of the Project Coordinator.

Monthly reporting

The status of technical progress will be reported monthly by the Task leaders to Work Package leaders and the Coordinator using a short standard template. The monthly reporting will ensure that any issues arising are identified and dealt with at the earliest opportunity.

Task leaders assess the overall progress and summarise the progress made against each task. They will collect this information from each of the project partners and send the template report back to the Work Package leader and the Coordinator.

The WP Leader will review any problems with the Task Leader(s) and recommend actions for discussion with the Coordinator.

Coordinator is sent a summary of each of the tasks to review monthly technical progress. The coordinator will discuss the results with the WP leaders and put into place actions if the project is behind plan.

Quarterly Reporting

Every quarter each partner will complete a template report recording project expenditure and technical progress for each of the tasks that it is involved with. The partners will send the quarterly report to the Work Package leaders and to Quotec. The work package leaders will provide technical progress summaries at the Work Package level and Quotec will provide a summary of the project expenditure against plan. This information will be used by the coordinator for quarterly meetings with the PMC and the partners, and to build up the six-month progress reports. Reports will be available to all partners.

Partners complete a template report detailing project expenditure and technical progress. This report is sent to the Work Package Leader and to Quotec.

WP Leader receives a quarterly summary from each of the active partners and with input from the task leaders prepares a quarterly status report of the work package and sends this to Quotec.

Quotec receives the quarterly reports from the partners and the work package leaders and collates the input for review with the Coordinator. Quotec prepares a summary of the project expenditure against plan.

The Coordinator prepares a brief summary of the technical progress status at the project level and identifies key issues to be addressed.

Summary of Project Reporting and Interactions

	Year 1	**Year 2**	**Year 3**
Monthly summary from Task leaders	1-12	13-24	25-36
PMC meetings	3, 6, 9, 12	15, 18, 21, 24	27, 30, 33, 36
Quarterly Project Reviews	3, 6, 9, 12	15, 21, 24	27, 30, 33
Publicity Brochure	3		
Project Website	3 onwards		
Periodic Reports to EC		18	36
Distribution of monies and reports of transfers	1 and then according to consortium agreement		
Signed consortium agreement	Before project start		
Kick Off Meeting	1		
Project Reviews		18	36

Quarterly project reviews and PMC meetings will be at the same time as the Project Reviews in M18 and M36 respectively.

2.2 Individual participants

The University of Warwick (UoW) is a leading higher education establishment in the UK. Its research in Mathematical Sciences is particularly highly regarded worldwide. In the UK Research Assessment Exercise 2008, UoW was ranked 2nd in the country in pure mathematics, 1st equal in applied mathematics for the proportion of its research awarded the top rating, and 2nd in statistics and operational research. Its Mathematical Interdisciplinary Research programme has spawned a string of research centres including Scientific Computing, Systems Biology, Complexity Science, and Discrete Mathematics. Its mathematical scientists are well connected internationally, in particular playing key roles in the Complex Systems Society, the EC project ASSYST (Action for the Science of complex SYstems and Socially intelligent icT), and the EC network of excellence on Internet Science (EINS), and coordinating an Erasmus Mundus Masters Course in Complex System Science.

It will coordinate the project overall and WPs 2&6. It will play a major role in WP1 and in the tasks I, B & T of WPs 4&5. It will also play a significant role in WPs 2&3.

The main individuals who will undertake or direct the work are:

R.S.MacKay, Professor of Mathematics, Director of the Centre for Complexity Science and of Mathematical Interdisciplinary Research at Warwick: dynamics of complex systems, renormalisation theory, mathematics of hierarchical aggregation (coordinator of the project and of the UoW team)
M.A.Kirkilionis, Mathematics: dynamics of complex systems, scientific computation, chronobiology
M.J.Keeling, Mathematics & Life Sciences: spread of infectious diseases
T.Nichols, Statistics & Warwick Manufacturing Group: brain imaging
Y.Chung, Engineering: computational fluid dynamics of airflow in lung
D.Barkley, Mathematics: scientific computing and dynamical systems.

When appropriate we will also make use of the expertise of others like Rand (chronobiology and renormalisation), Czumaj (algorithms), Nazarenko (computational fluid dynamics), Roemer (hierarchical LU decomposition), Kotecky (statistical mechanics), House (epidemiology), Dedner (Scientific Computing), Ortner (Multiscale analysis), Baesens (dynamical systems and applications).

Both MacKay and Kirkilionis have deep experience of coordinating European Commission research projects (MacKay coordinated the Research & Training Network "LOCNET" from 2000-4, and Kirkilionis coordinated the NEST network "UNINET" 2005-8).

Prof. MacKay FRS has long expertise in hierarchical aggregation procedures for Frenkel-Kontorova chains, starting with the minimum energy configurations (R.S.MacKay, A renormalisation approach to invariant circles in area preserving maps, Physica D 7 (1983) 283-300), then extending to the slow dynamics (R.S.MacKay, Scaling exponents at the transition by breaking of analyticity for incommensurate structures, Physica D 50 (1991) 71-79), the classical statistical mechanics (R.S.MacKay, The classical statistical mechanics of Frenkel-Kontorova models, J Stat Phys 80 (1995) 45-67), and the quantum statistical mechanics (N.R.Catarino, R.S.MacKay, Renormalization and quantum scaling of Frenkel-Kontorova models, J Stat Phys 121 (2005) 995-1014). He wrote a position paper for this call and taught a graduate course Oct - Dec 2011 on Aggregation for Complex Systems.

Dr. Markus Kirkilionis is a mathematician educated at the University of Heidelberg (Germany) specialised on mathematical modelling and simulation. During most of his career he was and is especially interested in modelling biological systems, but since several years has widened his interest to applications of complex systems theory to both natural science and the humanities. His role in the consortium will be to support mathematical modelling in all application areas, and to transform the multi-level problems into a computationally implementable form, by both discretisation and aggregation methods. He is a member of the Warwick Centre for Complexity Science, and Chair of the Conference Committee (European Conference on Complex Systems, ECCS) of the Complex Systems Society (CSS). He was involved in several European projects, like being coordinator of UniNet (as mentioned above), and with the complex systems coordination actions GIACS and ASSYST. Moreover he is in the editorial board of several journals in the area of complex systems (Springer Series in Complex Systems, Advances in Complex Systems). Recent publications:

Kirkilionis, M., & Kepes, F.: Introduction to special issue ECCS'09 in Theory in Biosciences. *Theory Biosci*, *130*(3), 153, 2011.

Kirkilionis, Markus, and Sbano, Luca. "An Averaging Principle for Combined Interaction Graphs. Part I: Connectivity and Applications to Genetic Switches." Advances in Complex Systems, 13 (2010) 293-326.

Kirkilionis, M.: Exploration of Cellular Reaction Systems. Review article, invited contribution, Briefings in Bioinformatics, Vol II, No I: 153-178, 2010.

Bouchekhima, A.-N., Frigerio, L., & **Kirkilionis, M. A.**: Geometric Quantification of the Plant

Endoplasmatic Reticulum. Journal of Microscopy, 234(2):158-72, 2009.
Eigel, M., George, E., and **Kirkilionis, M.** "A Meshfree Partition of Unity Method for Diffusion Equations on Complex Domains." *IMA Journal of Numerical Analysis,* doi:10.1093/imanum/drn053, 1-25, 2009.

Prof. Keeling has considerable experience of working at the cutting-edge of mathematical models predicting the transmission of infectious diseases, in both theoretical and applied contexts. Particular interests are how spatial densities of organisms affect disease spread and control (Keeling *et al* (2001) Dynamics of the 2001 UK Foot and Mouth Epidemic: Stochastic Dispersal in a Heterogeneous Landscape. *Science* **294** 813-817), how infection spreads through networks (Keeling (1999) The effects of local spatial structure on epidemiological invasions. *Proc Roy Soc Lond B* **266** 859-867; Danon, L., et al.(2011) 'Networks and the epidemiology of infectious disease' *Interdisciplinary Perspectives on Infectious Diseases* **2011** (284909), (1687-708X)), and how the partitioning of the population into households can impact on transmission (Ross, J.V., House, T.A. and Keeling, M.J. (2010) Calculation of Disease Dynamics in a Population of Households. *PLoS ONE* **5** e9666).

Dr. Nichols is a statistician who has focused solely on brain imaging data for the past 19 years. He is known for his work in neuroimaging inference, producing sensitive detection methods that control false positive risk over the brain (see, e.g., Nichols & Holmes, 2001; Genovese et al, 2002; Nichols & Hayasaka, 2003; Nichols et al, 2005). More recently he has focused on modelling connections between different brain regions, from an exhaustive comparison of existing Bayes Net & related methods using realistic resting-state fMRI simulations (Smith et al, 2011) to a novel graph inference method for comparing populations of weighted undirected graphs (Ginestet et al, 2011). He is the imaging genetics expert on the US$30m Human Connectome Project [http://humanconnectome.org/], which will collect state of the art structural and functional connectivity MRI data on 1200 subjects, and will thus be able to apply the methods of the HACS project to the unique Human Connectome data.

References

Genovese, C. R., Lazar, N. A., & Nichols, T. E. (2002). Thresholding of Statistical Maps in Functional Neuroimaging Using the False Discovery Rate. NeuroImage, 15(4), 870-878.
Ginestet, C. E., Nichols, T. E., Bullmore, E. T., & Simmons, A. (2011). Brain Network Analysis: Separating Cost from Topology Using Cost-Integration. PLoS ONE, 6(7), e21570.
Nichols, T. E., & Hayasaka, S. (2003). Controlling the familywise error rate in functional neuroimaging: a comparative review. Statistical Methods in Medical Research, 12(5), 419-446.
Nichols, T. E., & Holmes, A. P. (2001). Nonparametric permutation tests for functional neuroimaging: A primer with examples. Human Brain Mapping, 15(1), 1–25.
Nichols, T. E., Brett, M., Andersson, J., Wager, T. D., & Poline, J.-baptiste. (2005). Valid conjunction inference with the minimum statistic. Neuroimage, 25(3), 653–660.
Smith, S. M., Miller, K. L., Salimi-Khorshidi, G., Webster, M., Beckmann, C. F., Nichols, T. E., Ramsey, J. D., et al. (2011). Network Modelling Methods for FMRI. NeuroImage, 54(2), 875-891.

Dr. Chung has expertise in high performance computing, in particular unsteady computational fluid dynamics of complex systems, with the main research interest in multi-scale analysis of airflow in human lung. Recent work also includes the flow control for aircraft drag reduction (Y. M. Chung, T. Talha, Effectiveness of active flow control for turbulent skin friction drag reduction, Physics of Fluids 23 (2011) 025102), the thermal oscillation in a liquid metal nuclear reactor (S. Chacko, Y. M. Chung, et al., Large-eddy simulation of thermal striping in non-isothermal triple jet. Int. J. Heat and Mass Transfer 54 (2011) 4400-4409), and the mixing behaviour in a micro combustor (T. S. Park and Y. M. Chung, Turbulent flow and scalar mixing of a coaxial injector having two fluid jets. Numerical Heat Transfer Part A-Applications 60 (2011) 197-211).

Prof. Barkley's interest is in high-performance computing and nonlinear phenomena. He teaches graduate-level computing courses including a highly successful short course on Core Algorithms in High Performance Scientific Computing, which trains users of HeCTOR (UK national supercomputer service). He has studied many different physical, chemical, and biological systems. He is particularly interested in the large-scale structure and dynamics of turbulence and its connection to statistical phase transition.

D. Barkley and L.S. Tuckerman,``Computational study of turbulent-laminar patterns in Couette flow",
Phys. Rev. Lett. 94, 014502 (2005);
D. Moxey and D. Barkley, ``Distinct largescale turbulent-laminar states in transitional pipe flow",
PNAS 107, 8091-8096 (2010);
K. Avila, D. Moxey, A. de Lozar, M. Avila, D. Barkley, B. Hof, ``The Onset of Turbulence in Pipe Flow",
Science 333, 192-196 (2011).

Universität Heidelberg (HB) is one of the leading and internationally top-ranked German universities. It is one out of nine universities of excellence funded by the federal and state governments for its innovative future concept.

The Interdisciplinary Center for Scientific Computing (IWR, www.iwr.uni-heidelberg.de) is a central institution of the university founded in 1987 to promote interdisciplinary research in mathematical and computational methods for science and technology; it comprises 37 main research groups and 13 independent junior research groups with about 550 researchers (professors, junior group leaders, post-docs and doctoral students). Each research group is rooted both at the IWR and an institute of one of the seven faculties `Mathematics and Computer Science', `Physics and Astronomy', `Chemistry and Earth Sciences', `Biosciences', `Philosophy', `Modern Languages' or the `Medical Faculty in Mannheim'.

This horizontal cross-faculty structure of the IWR is the cornerstone of the research and the doctoral education within the Heidelberg Graduate School for Mathematical and Computational Methods in the Sciences (HGSMathComp) as it ensures that method development and applications fertilize each other. The IWR has a proven record of collaborative research (former Special Research Centers 123 and 359) and research training groups (RTG 13 `Scientific Computing in Mathematics and the Natural Sciences' established 1992, international RTG 710, RTG 850, RTG 1653) which culminated in the foundation of the HGSMathComp in 2007. External evaluations by its International Scientific Advisory Board in 2004 and the State of Baden-Württemberg in 2001 have confirmed the international reputation and unique interdisciplinary profile of IWR.

The IWR will design and implement generic software for the simulation of complex systems based on hierarchical aggregation algorithms developed within the consortium. Special emphasis will be laid on the efficient use of high-performance computing resources available at IWR and elsewhere.

Peter Bastian is professor for Scientific Computing at IWR and the Institute for Computer Science of the University of Heidelberg. His research activities are in the numerical solution of partial differential equations including efficient and accurate discretization methods as well as fast solvers, in particular algebraic multigrid methods, parallel high-performance computing and application of these methods to simulation of multiphase flow and transport processes in porous media. Dr. Bastian is one of the developers of the Distributed and Unified Numerics Environment (DUNE, www.dune-project.org), a general software framework for the numerical solution of partial differential equations.

Dr. Olaf Ippisch's research field is modeling and simulation of flow and transport in porous media. In particular he concentrates on highly heterogeneous media, multiphase flows and flows on the landscape scale. He also did very large-scale simulations on Germany's biggest supercomputer in Jülich recently.

Dr. Johannes Schönke is a physicist by training, did his Ph.D. in astrophysics and works now in the field of computational neuroscience. His research interest is to model and simulate signal propagation in the extra-cellular space of the brain on the mm-scale and up. This is the basis to understand and interpret local field potential measurements from neurophysiologists.

Recent publications

Peter Bastian, Christian Engwer, Jorrit Fahlke, Olaf Ippisch. An unfitted Discontinuous Galerkin method for pore-scale simulations of solute transport. *Mathematics and Computers in Simulation*, 81 (2011) 2051-61.

P. Bastian, M. Blatt, and R. Scheichl. Algebraic multigrid for discontinuous Galerkin discretizations. *Numer. Linear Algebra Appl.*, 2011. To appear.

Markus Blatt and Peter Bastian. C++ components describing parallel domain decomposition and communication. *International Journal of Parallel, Emergent and Distributed Systems*, 24(6):467-477, 2009.

H.-J. Vogel and O. Ippisch. Estimation of a critical spatial discretization limit for solving Richards equation at large scales. *Vadose Zone Journal*, 7(1):112-114, 2008.

H.-J. Vogel, A. Samouëlian, and O. Ippisch. Multi-step and two-step experiments in heterogeneous porous media to evaluate the relevance of dynamic effects. *Adv. Water Res.*, 31(1):181-188, 2008.

Rijksuniversiteit Groningen (RuG) enjoys an international reputation as one of the oldest and leading research universities in Europe. It is ranked among the world's top 120 universities (QS World University Rankings 2010). In 2010, it hosted over € 118 million in contract research, with over € 14 million attracted from the attracted from the EC framework programme for University of Groningen projects. In the Netherlands, the RuG has the highest score for ERC starting grants.

The RuG offers degree programmes at Bachelor's, Master's and PhD levels in virtually every field, many of them completely taught in English. It has 8 Erasmus Mundus master programmes. The total number of students is approximately 30 000 with about 450 professors and 1500 PhD students. Every year more than 5,000 research publications go to print and 374 PhD students were awarded their PhD degree in 2010. The university is utilizing its academic heritage to generate innovation, with the help of cutting-edge facilities. The degrees awarded are all internationally acknowledged.

The University of Groningen is organised into nine faculties that offer programmes and courses in the fields of Humanities, Social Sciences, Law, Economics and Business, Spatial Sciences, Life Sciences, and Mathematics and Natural Sciences. Each faculty (cf., College in the USA or School in Europe) is a formal grouping of academic degree programmes, schools and institutes, discipline areas, research centres, and/or any combination of these drawn together for educational purposes. Each faculty offers Bachelor's, Master's, PhD, and Exchange programmes, while some also offer short certificate courses.

The RuG will coordinate WP4 (H. Waalkens, who is also node leader for RuG) and WP5 (A. Flache), and will lead the work on tasks C (Chronobiology) and S (Social norms). Moreover the RuG will be involved in WP1-3 through A.C.D. van Enter and F.W. Wubs, and in task T through G.Huitema.

The main RuG personnel to work on the project are:

- H.W. Broer: nonlinear dynamical systems, bifurcation theory, periodic and quasi-periodic dynamics, resonances, applications in physics, biology and meteorology;
- A.C.D. van Enter: statistical mechanics, interacting particle systems and Gibbs measures;
- G. Vegter: computational geometry, applications of singularity theory, dynamical systems, applications in astronomy;
- H. Waalkens: Hamiltonian systems, applied dynamical systems theory, semiclassical quantum mechanics;
- F.W. Wubs: numerical mathematics, sparse systems, discretization of PDEs, fluid flow computations, bifurcation analysis.
- G.Huitema: traffic flow
- J.B.T.M. Roerdink: multiresolution visualization, in bioinformatics and astronomy., neuroimaging,
- D. G. M. Beersma: chronobiology experiments.
- A. Flache: modeling of norms and networks.
- Maritje van Duijn: Statistical modelling of networks
- Christoph Stadtfeldt: event-based modelling of online social network data

Andreas Flache (1963) is professor of Sociology, in particular modelling norms and networks, at the Department of Sociology of the University of Groningen. His main research areas are social norms and social integration. He applies computational agent-based modelling, game theory, laboratory experiments, survey research and network research. Flache was research fellow of the Royal Netherlands Academy of Arts and Sciences (KNAW) 1999-2002 and received in 2004 an Innovational Research Incentive (VIDI) grant from NWO. He published in, e.g., Proceedings of the National Academy of Sciences, American Journal of Sociology, PloS Computational Biology, Journal of Conflict Resolution.

Publications and/or Patents:

D.G.M. Beersma, H.W. Broer, K. Efstathiou, K.A. Cargar and I. Hoveijn, Pacer cell response to periodic Zeitgebers, Physica D 240 (2011) 1516-1527

Flache, A., & Macy, M.W. (2011a). Local Convergence and Global Diversity: From Interpersonal to Social Influence. Journal of Conflict Resolution 55.6: 968 - 993.

Flache, A., & Macy, M.W. 2011b. “Small Worlds and Cultural Polarization.” Journal of Mathematical Sociology 35.1. Pp. 146-176 in Marcel A. L. M. van Assen, Vincent Buskens, and Werner Raub (eds.). Special triple issue: “Micro-Macro Links and Micro-Foundations”.

Mäs M, Flache A, Helbing D. 2010. “Individualization as Driving Force of Clustering Phenomena in Humans.” PLoS Computional Biology 6(10): e1000959. doi:10.1371/journal.pcbi.1000959

Macy, M.W. & Flache, A. 2009. Agent Based Modelling: Social Order from the Bottom Up. pp. 245-268 in Hedström, P. & P. Bearman (eds). *The Oxford Handbook of Analytical Sociology* (Oxford University Press).

Flache, A & Mäs. 2008. How to get the timing right. A computational model of the effects of the timing of contacts on team cohesion in demographically diverse teams. *Computational and Mathematical Organization Theory* 14.1:23-51.

Institut Non Linéaire de Nice Sophia Antipolis (INLN) was created in 1991 as a multi-disciplinary research Institute. It is a joint research laboratory of the Centre National de Recherche Scientifique (CNRS) of France with the University of Nice Sophia-Antipolis. Its director is Jean-Marc Gambaudo who is node leader for INLN in this HACS project.

It gathers researchers from different background from mathematics to theoretical and experimental physics. Its domains of interest essentially cover:

- Modeling and analysis of networks and complex systems;
- Bifurcation and dynamical systems;

- Statistical mechanics;
- Fluid mechanics;
- Spatio-temporal dynamics and optical systems;
- Experimental approach of out-of-equilibrium phenomena;
- Mesoscopy with cold atoms.

It hosts 26 permanent researchers and around 15 Ph.D students and postdocs.

From the scientific point of view, it is strongly connected to the other physics laboratories of the campus (LPMC and CHREA) and the mathematics department (LJAD). Currently these 4 labs work together in a "federation" (Doeblin) that organises workshops and gives funding to pluridisciplinary projects. It also benefits from the proximity of the INRIA Sophia Antipolis laboratory.

The INLN will contribute to the HACS program by conducting research on hierarchical structure, offering to HACS visitors all the facilities of the lab and by hosting the realisation of experiments on the occurrence of hierarchical structures in optical devices.

The team for the project is:

- Méderic Argentina (Assistant professor), Laboratoire J.-A. Dieudonné (LJAD), Université de Nice;
- Umberto Bortolozzo (Assistant professor) Institut Non Linéaire de Nice (INLN) (liquid crystals),
- Jean-Marc Gambaudo, (DR cnrs) INLN, team leader.
- Lionnel Gil (CR cnrs) INLN;
- Jean Rajchenbach (DR cnrs), Laboratoire de physique de la matière condensée (LPMC) (Faraday);
- Stefania Residori (DR cnrs) INLN (liquid crystals).
- Benjamin Mauroy (CR cnrs) LJAD, works on hierarchical structures in lungs.
- Bruno Marcos (Assistant professor) LJAD, works on hierarchical structures in cosmology.
- Denis Talay, INRIA, Scientific computation

Quotec Limited is a UK based company focused on supporting organisations with all aspects of technology strategy and technology management from basic research to the marketplace, working largely in the UK and Europe for multinational and UK clients. The company was founded in 1984 as a technology consultancy specialising in assisting materials and engineering companies to exploit the benefits of new and improved technologies. Quotec started to manage technology programmes and to develop innovation tools for the public sector in the late 1980s. In 2000, Quotec was acquired by CSIR, Africa's largest knowledge intensive technology organisation, giving it direct access to the technical expertise of 2500 researchers, working in a wide range of technical specialist areas, and the management support of a large, international organisation. The delivery of high quality project management services for technology projects is one of Quotec's key business areas.

Quotec have been approached by Warwick University to support the consortium with managing this highly complex project. Quotec will use methods they have developed to efficiently assist with tracking the technical progress made by partners.

Quotec will solely be involved in WP7 (though with some implied activity in WP6) and will be responsible for working with the project coordinator and the project partners to ensure that the project stays on course both financially and technically for the duration of the project.

Quotec does not expect any benefit from the output of the project such as commercialisation and IP.

Dr Mitesh M Ladwa is a Senior Consultant at Quotec Limited. Dr Ladwa has over 10 years' experience managing EUFP6 and EUFP7 projects both technically, and financially, to the end of the project. He has organised partners to deliver technically and performed administrative duties, and also been the Principal Investigator of an EU FP6 project. He has over 10 years' experience of supporting organisations with the dissemination and exploitation of results from nationally and internationally funded projects. Dr Mitesh M Ladwa achieved his PhD in synthetic organic chemistry from Kings College, University of Aberdeen.

Amy Skinner is a Prince 2 qualified consultant with Quotec, with over 9 years experience supporting, delivering and managing projects for government and the private sector. Most recently Amy has provided project management support for Department of Health (DH) i4i Programme, monitoring the financial aspects of the funding programme. Amy also managed the central portal for the DTI Knowledge Transfer Networks, maintaining the website, developing new content and orchestrating online events. Amy has overall responsibility for the development and maintenance of Quotec's Quality systems (ISO 9001) and for the Quotec IT systems and website and has used her in-house experience to help develop client websites. Amy achieved her BEng in Materials Science, Engineering and Business Management at Brunel University. Prior to joining Quotec, Amy worked at a consultancy managing a project to set up a European networking group of SAP users.

2.3 Consortium as a whole

The HACS project gathers a multidisciplinary consortium. On the one hand, we have a theoretical team (mathematics, statistical mechanics, non-linear physics, computer science) that is able to deal with all the different models that are involved in the description of hierarchical structures and the design and analysis of hierarchical aggregation schemes. On the other hand, we have experimental teams (liquid crystals, hydrodynamics, chronobiology), data gatherers (social norms) and access to other databases (brain images, infectious diseases, lung data, traffic flow) that give us a wealth of example of complex dynamical systems exhibiting multilevel structure. We strongly believe that this interaction between theory and data will be as fruitful as it was some decades ago for the birth of chaos theory.

The participants each have mathematical, computational and complex systems expertise. They have individual strengths in specific relevant areas, e.g. HB in algebraic multigrid, INLN in the theory of quasicrystals and experiments on quasipatterns, UoW in spread of infectious diseases and in brain imaging, RuG in social science data and in chronobiology. Thus they are well matched. They are all committed to the project and by working together can achieve the project objectives.

WP1 will be coordinated by INLN, with task 1 carried out by INLN in collaboration with RuG, and task 2 by UoW in collaboration with INLN and RuG.

WP2 will be coordinated by UoW in collaboration with HB and some input from RuG and INLN.

WP3 will be coordinated by HB in collaboration with UoW and some input from RuG and INLN.

WP4&5 will be coordinated by RuG with the work on the tasks carried out by

B: UoW with input from HB
C: RuG with input from UoW
I: UoW with input from HB
L: HB with input from UoW and INLN
Q: INLN with input from RuG and UoW
S: RuG
T: UoW with input from RuG and HB

WP6 will be coordinated by UoW with input from all partners

WP7 will be coordinated by QTC with input from UoW and the project management committee (which contains representatives for all partners).

The results of the work packages will be integrated by:

- regular reports, as specified in section 2.1
- overlap in personnel, e.g. the same members of HB and UoW will work on general computational theory for WP2, ICT implementation for WP3, customization for task L of WP4 and validation on data for task L in WP5; the same members of INLN with some input from UoW and RuG will work on general mathematical theory for WP1, its customization for task Q of WP4 and validation of data for task Q in WP5. Similarly, some of the research staff to be engaged for the project will work on more than one work package, e.g. one PhD student to be engaged at RuG will start on WP1 and then move to task C of WP4&5, the other student to be engaged at RuG will start on WP2 and move to task S of WP4&5.
- consortium meetings

Industrial/commercial involvement

To ensure exploitation of the results and to benefit from advice on the directions of research, the consortium will form a Users' Group, consisting of relevant invited businesses or research organisations. In particular the Users' Group already includes:

TNO (Netherlands Organisation for Applied Scientific Research, Delft, NL): Huitema will provide data on traffic flow, and Kotterink on large-scale social network datasets

Almende (Rotterdam, NL): Salden will advise on requirements for agent-based software for formation and coordination of communication and collaboration across evolving networks of humans and ICT infrastructures (social networking, swarm robotics, emergency response, logistics).

Innaxis (Madrid, ES): Alvarez will advise on modeling and simulation of large socio-technical systems (e.g. air transport, urban mobility, energy, social patterns)

RAND Europe (Cambridge, UK): Cave will advise on research and analysis to improve policy and decision-making, notably on information security in networked systems and cloud computing, internet regulation, and use of radio-frequency identification technology in eHealth.

HPA (Health protection agency) (UK): Ian Hall will advise on health protection issues.

Others invited:
IBM (Warwick, UK): Robinson to advise on smart cities
Veolia (Paris, FR): Morvan to advise on smart cities
COMSOL (Cambridge, UK): to advise on the market for software
Microsoft Research (Cambridge, UK): Key to advise on algorithms for networks
BT (Martlesham, UK): Briggs to advise on the telecommunications industry

2.4 Resources to be committed

This is an extremely ambitious project that will require all the resources that it can get for its execution. The resources requested from the EC are presented here in two ways: firstly by work package and secondly by participant. A list of contributions to the running of the project from elsewhere is given at the end of the section.

Resources requested, by work package

WP1. 2 PhD student years (RuG), 3 postdoc years (INLN), 2 postdoc years (UoW), 1 research workshop, travel for collaboration

WP2. 2 PhD student years (RuG), 1 postdoc year (UoW), 1 postdoc year (HB), 1 research workshop, travel for collaboration

WP3. 1 postdoc year (UoW), 2 postdoc years (HB), computing equipment, travel for collaboration

WP4. Task
- B 0.5 postdoc year (UoW)
- C 0.5 PhD student year (RuG)
- I 0.5 postdoc year (UoW)
- L 0.5 postdoc year (HB)
- Q 0.5 postdoc year (INLN)
- S 0.5 PhD student year (RuG)
- T 0.5 postdoc year (UoW)
- + travel for collaboration for each task

WP5. Task
- B 0.5 postdoc year (UoW)
- C 0.5 PhD student year (RuG)
- I 0.5 postdoc year (UoW)
- L 0.5 postdoc year (HB)
- Q 0.5 postdoc year (INLN)
- S 0.5 PhD student year (RuG)
- T 0.5 postdoc year (UoW)
- + travel for collaboration for each task

WP6. 1 final conference (travel, accommodation, secretarial support 40kE), travel to disseminate results particularly at conferences (c. 30kE), Users Group meetings for routes to exploitation (20kE), patent filing fees (50kE), professional website development (12kE), publication page charges (12kE), dissemination fees for UoW Knowledge Centre (5kE), secretarial support (3 years 1/3-time)

WP7. 6 face-to-face management meetings (alternating with 6 to be held by videoconference), Users Group advisory meeting, consumables, administrator salary

Resources requested, by participant

UoW

MacKay	3 postdoc years (WP1 + Task T) + 20% salary (for management of the whole project, leading WP6, research on WP1 and Task T)
Kirkilionis	2 postdoc years (WP2&3) + 15% salary (for management including leading WP2 and for research on WP1 and Task L)
Nichols	1 postdoc year (Task B) + 10% salary (for leading Task B and research on WP1)
Keeling	1 postdoc year (Task I) + 10% salary (for leading task I and research in WP1)

Computing equipment (WP3), two workshops (WP1 & 2) (2x12kE), final conference (40kE), Users group meetings (10kE), patent filing fees (10kE), website development (12kE), publication page charges (12kE), Knowledge centre fee for dissemination (5kE), Travel to disseminate and for collaboration with the partners, high performance computing access charges, 3 years of 1/3-time secretary [some of these items are on behalf of the whole consortium but have to be based with the coordinating institution]

Note that the secretarial support is essential to assist MacKay with the dissemination and exploitation.

HB
Bastian 4 postdoc years (WP2&3+TaskL)
Travel, consumables

RuG
Waalkens 3 PhD years (WP1 + Task C) + 10% salary (for leading WP4 and task C)
Flache 3 PhD years (WP2 + Task S) + 10% salary (for leading WP5 and task S)
Travel to collaborate (28kE), consumables, a computer (2kE)

INLN
Gambaudo 3 postdoc years (WP1) + 10% salary (for leading WP1 and task Q in WP4)
Residori 1 postdoc year (Task Q) + 10% salary for years 2&3 (for leading task Q in WP5)
Experiments for Task Q of WP5: equipment 10.5kE (calibrated stage for temperature control for liquid crystal cells, arbitrary signal/function generator, oscilloscope), consumables 6.5kE (optics and mountings, liquid crystals, polymers, chemical materials, photoconductive substrates)
Computing equipment 5kE
Travel 52.5kE

QTC
Management 84KE (12 person-months)
Other direct costs 21KE (inc. 16KE travel)

Contributions to the project be funded from elsewhere

Time of Peter Bastian (HB) to coordinate WP3 and task L.
Some PhD student time in the Centre for Complexity Science (UoW) (36 months has been included in the tables, shared between WP1,2&3).
Time of some others at each of the partners, e.g. van Enter (RuG), van Duijn (RuG), Wubs (RuG), Nazarenko (UoW), House (UoW), Chung (UoW), Barkley (UoW), Dedner (UoW), Ortner (UoW), Ippisch (HB), Argentina (INLN), Bortolozzo (INLN)…
Use of library, basic computing resources, etc at all partners
HB already has the computing equipment it needs for this project.
Related projects that have been funded from other sources can be expected to benefit this one, e.g. Sloan Foundation project on Management of complex systems at UoW (Jan 2012-Dec 2013).

Section 3. Impact

3.1 Transformational impact on science, technology and/or society

Introduction

The aim of the project is to devise new algorithms for computation of properties of complex dynamical systems and to gain understanding of their behaviour, by constructing descriptions at a hierarchy of levels adapted to the system. We recall our targeted breakthrough:

- A new, powerful and unifying framework for computation and understanding of the dynamics of complex systems via hierarchical aggregation.

Benefits

This will benefit a huge range of areas of science, technology and society. The specific application areas to which we will customise our methods and on which we will validate them are

- Brain imaging
- Chronobiology (the dynamics of gene expression)
- The spread of infectious diseases
- Airflow in the lung
- Quasipatterns in fluid systems
- The dynamics of social norms, and
- Traffic flow

Here are some of the ways in which our research will benefit these areas. It will help brain imaging by extracting a hierarchical description of the images, which can be expected to have clinical significance and aid in diagnosis. It will identify tactics for a social (human or animal) system to prevent the spread of infectious diseases. It will aid in the understanding of respiratory diseases, in particular asthma, which affects millions. It will aid in the design of road pricing systems.

Our approach is expected to be crucial for advancement of many other important socio-economic goals like

- Prediction of the effects of large infrastructure projects
- Strategies for evacuation of large cities in case of an earthquake
- Design of real-time pricing of electricity for the coming era of the smart grid
- Agricultural ecology
- Satellite image analysis
- Demographic flows

Strategy for Impact

To ensure that the results of our project have a transformational effect, we will

- Promote the results on our seven application areas to stakeholders in these areas, e.g. hospitals, health protection agencies, departments for transport
- Work with our Users Group (section 2.3) to identify opportunities for impact and routes for exploitation
- Link up with related research projects, notably FuturICT, EINS, and to the other DyM-CS projects via the coordination action for this DyM-CS call (see section 3.2)
- Dissemination via conferences and publications
- Submit proposals to organise additional workshops on the topics of the project at international venues, e.g. Lorentz Centre (Leiden, NL), Centre International de Recherche Mathematique (Luminy, FR), Isaac Newton Institute (Cambridge, UK)
- Submit exhibits for popular exhibition events like the UK Royal Society summer exhibition and worldwide events for Mathematics for Planet Earth 2013.

3.2 Expected impacts listed in the work programme

Referring to the DyM-CS call for proposals,

- We will make progress towards a general theory of complex systems.
- We will develop new ICT-based methods and principles for the management of large-scale systems.
- We will develop a better understanding of structural patterns of complex systems in socio-economic and technological areas (e.g. resilience and sensitivity to failure).

We will achieve these impacts by:

- WP1 will provide progress on understanding the emergence of hierarchical structure in many complex systems and to construct hierarchical descriptions to aid understanding
- WP3 will produce new ICT-based methods and principles for the computation of dynamical complex systems, which will be useful for their management
- WP1 will develop a better understanding of hierarchical structure in complex systems

All three impacts will be supported by the validations of the methods on data (WP5), and all other parts of the project are required to achieve this.

European Approach

We will combine the skills from four different European research institutions to achieve results which none of us could achieve on our own, and to make a diverse base (both geographically and in terms of subject expertise) from which to cross-fertilise and promote our results. The partners have individual strengths in specific relevant areas, e.g. HB in algebraic multigrid, INLN in the theory of quasicrystals and experiments on quasipatterns, UoW in spread of infectious diseases and in brain imaging, RuG in social science data and in chronobiology.

Each institution will use its national and other networks to enhance its performance in this project. For example, the UoW team leads a UK network on Complex System Dynamics and a Sloan Foundation project on Management of Complex Systems.

Contribution to previously funded EU projects

We will build on and contribute to the work of other EU research projects, of which we list several examples here.

The COSI-ICT programme supported research on complex systems for socially intelligent ICT via four integrated projects:

CYBEREMOTIONS: Collective emotions in cyberspace
EPIWORK: Developing the framework for an epidemic forecast infrastructure
QLECTIVES: Quality collectives: socially intelligent systems for quality
SOCIONICAL: Complex socio-technical system in ambient intelligence
And one coordination action
ASSYST: Action for the science of complex systems for socially intelligent ICT

They will come to an end early in 2013 (and already in Feb 2012 for ASSYST), but our project will build on their results. Our project will differ somewhat from them by its emphasis on general mathematical and computational foundations. Thus although our project contains work addressing seven application areas, the over-riding theme is to synthesise common features from these to design a powerful new general framework to speed up computations of dynamical complex systems and to make conceptual advances in understanding their behaviour.

Our project will play a vital supporting role to the proposed Flagship FuturICT, currently in pilot phase (to Apr 2012), but anticipated to continue. One of the major issues it faces, as made clear in its Living Earth Simulator meeting on 13 Jan 2012 (in which MacKay participated) is how to perform large-scale computations of social systems. We believe our hierarchical approach is the answer.

Our project with play a significant role in EINS (Network of excellence in Internet Science) that just started in Dec 2011.

There are various other current EU projects to which we could contribute, e.g. CRISIS on systemic instabilities in the economy, and HIPERDNO on smart distribution network operation.

Contributions to EU policy

We support the headline conclusion of the Expert Consultation Report on Complex Systems Science (Dec 2009) to the FET-proactive programme: “The science of complex systems is essential to establish rigorous scientific principles on which to develop the future ICT systems that are critical to the well-being, safety and prosperity of Europe and its citizens”.

There are several areas of EU policy to which our project could contribute:

- Digital agenda for Europe
- Animal diseases (under Agriculture, Fisheries and Food)
- Impact assessment (under Cross-cutting policies)
- Social and demographic trends (under Employment and social rights)
- Trans-European networks (under Energy and natural resources)
- Trans-European networks (under Transport and travel)
- Civilian crisis management (under External relations and foreign affairs)

3.3 Dissemination and/or exploitation of project results, and management of intellectual property

The partnership will follow the policy of sharing the research results that the project generates with external parties. Our proposal has a work package that contains a first objective to disseminate and explain findings to various stakeholders, such as public authorities and industry. This will be done by the setting up of a website, by the production and dissemination of scientific dossiers of findings to explain results to different stakeholders and by the organisation and the presentation of data at appropriate conferences.

The partners are committed to the publication of their results in prestigious journals such as the Society for Industrial and Applied Mathematics journals and Proceedings of the National Academy of Science of the USA, and to give presentations at appropriate conferences and exhibitions such as the annual European Conference on Complex Systems and the biennial European Future Technologies conference and exhibition. The project management committee will also encourage scientists in the project to publish their results in appropriate prestigious international refereed scientific journals. Not later than the first report, the co-ordinator will provide to the commission a publishable poster targeted at a non-specialist audience and summarising the main features of the entire project. In addition, the coordinator shall provide for the same date a one-page publishable summary of the project that can be disseminated and distributed to the public.

Dissemination will take place through the following identified routes.

- We will disseminate findings of our research through publication in International fully peer-reviewed medical and scientific journals such as: the SIAM journals, the Royal Society of London journals, the Proceedings of the National Academy of the USA, etc
- We will submit abstracts for conferences such as the European Conference on Complex Systems, the European Future Technologies conference and exhibition and the European Congress on Computational Methods in Applied Sciences and Engineering meeting and any other relevant conferences/symposia as identified by the consortium.
- We will link up with other projects on related themes, notably via the proposed coordination action COSMOS (or other that the EC may support) for this FET-proactive Dynamics of Multi-level Complex Systems call, and to the FuturICT Flagship project where hierarchical computation is probably essential to achieve the challenges it aims to address, like predicting social unrest, the socio-economic effects of large-scale infrastructure projects, or designing appropriate responses to a new virus or evacuation strategies for large cities in case of an earthquake.
- A public website will be designed allowing a non-specialist audience such as the public population to access findings of the project and improve their awareness of general problems on complex systems. The website will contain information on complex systems and findings of the project which will provide an education to society.
- The University of Warwick will hold an International Symposium to disseminate knowledge by inviting leading scientists, young academics, industry, and the EC before completion of the project. This dissemination role will be supported by the University and will allow partners to present material at the conference through talks and poster presentations. We will invite world leaders and young scientists who will be given an opportunity to present findings of their own research.
- Dissemination will also take place through publication in magazines such as the Institute of Mathematics and its Applications' Mathematics Today.
- Communication to those in national and European government with responsibility for public policy, for example in the UK via the Parliamentary Links days (MacKay will attend on 15 March 2012 when the topic is "Mathematics matters") and interaction with the government's Chief Scientific Advisors and other leading figures.

A dissemination manager will manage this specific role and will co-ordinate the following activities:

- Absorption of the results by the participants
- Dissemination of the knowledge beyond the consortium
- Activities promoting the exploitation of the results
- Activities that will promote or enable synergies with education
- Dissemination of knowledge to the public population and a non specialist audience.

The proposed project is both innovative and technically demanding and as a result will involve a number of highly innovative developments. Consequently a variety of foreground intellectual property rights (IPR) is likely to be developed during this project including patents, designs (registered and unregistered), copyright and know how. The responsibility for filing and protecting this IPR will be assigned by the consortium partners to the designated Exploitation Manager (Dr Prakash). All patent applications will be processed through the Patent Cooperation Treaty (PCT) route to allow global and ensure maximum exploitation potential.

The main potential items of intellectual property to be generated by this project are publications and software. The rights to publications will in general be assigned to the publisher, in accordance with their standard requirements. The rights to software will in general be waived, as we believe in free open source software for maximum benefit to science and humanity.

Management of Intellectual Property

The main considerations regarding the management of intellectual property and dissemination are stated within this part of the proposal. Specific restrictions and specifications (i.e. time-limits, specific measures, or exceptions) will be elaborated in the consortium agreement. Any alterations regarding intellectual property (background or foreground) after signing the consortium agreement will need approval from all the partners.

In principle each participant undertakes to use all necessary and reasonable endeavours and resources to ensure the efficient implementation of the project, and fulfil all of its obligations under the project in a manner of good faith. If a participant feels that its back- or foreground is severely affected by a decision of a consortium body during the project, all participants involved shall make every effort to resolve the matter to the general satisfaction of all participants.

Dissemination

Specific rules regarding dissemination will be stated within the consortium agreement, however in general a participant may not publish or communicate foreground generated by another participant of background of any participant, without its approval.

Exploitation Strategy

The exploitation plan will be included within the Consortium Agreement between the consortium partners, describing what the plan is intended to achieve and under what time frame. This agreement will cover the consortium's joint policy concerning IP ownership, defence of IP, exploitation rights and the licensing arrangements. An **exploitation plan** will be developed with the partners that will be consistent with the Consortium Agreement. The agreement will take into account all aspects of IP such as background and foreground and will be updated during the course of the project. The exploitation **manager** will be in place and will be responsible for generating and managing the formal exploitation plan that will detail vital elements such as product development and validation, IPR strategy, commercial approach etc. The exploitation manager will maintain a draft version of the exploitation plan and ensure it is updated and disseminated to appropriate parties in a timely manner.

IPR ownership

The principles of IPR ownership have been agreed between all main consortium partners. At the outset all background IPR in existence prior to the Consortium Agreement will remain the property of the originating party or parties. The terms under which the said background IPR is made available to the HACS project will be detailed in the Consortium Agreement. Ownership of the IPR generated by the HACS project (Foreground IP) will be defined by the Consortium Agreement and no one company will derive unfair advantages in relation to the exploitation of another. All rights with respect to ownership and exploitation of the foreground IPR will be defined and agreed between each of the consortium partners in accordance with the Consortium Agreement which will be in a manner consistent with the foregoing. The Consortium Agreement will also formalise the exploitation strategy, exploitation rights, licensing arrangements and protection of IPR.

IPR management

The management of all IPR whether Foreground or Background IPR will be the responsibility of the Exploitation Manager as part of the overall Exploitation Strategy. The responsibility includes oversight of the commercial assessment and protection of any foreground IP generated by the HACS project and negotiation of license agreements to allow for the transfer of technology outside the consortium for exploitation purposes. Dr Prakash will direct the consortium partners in recruiting the services of a European Patent Attorney when prosecuting patents and design-rights.

Section 4. Ethical Issues

Task S of WP5 indirectly involves adult healthy volunteers, human data collection and processing of personal data and will be conducted at the Department of Sociology of RuG (Netherlands). For this research, but the plan is to use solely Wikipedia material from contributions individual authors provided to content and discussion of Wikipedia sites. Wikipedia contributors have consented that their contributions are publicly available data (informed consent). Moreover, all material to be used in the research is published under the regulations of the Wikipedia privacy policy (http://wikimediafoundation.org/wiki/Privacy_policy). This implies that the material does not allow the researchers to link content and contributions to the individual authors. Moreover, the researchers also will not make any attempt to establish such a link and will store and process data only in strictly anonymous manner, following the principles of privacy-preserving data mining.

To assure proper compliance with ethics standards, the research plan will be submitted for ethical review to the ethics committee of the department that operates under the principles of academic integrity that are described in the Dutch Code of Conduct for Scientific Practice drawn up by the Association of Universities in the Netherlands (VSNU) to which RuG is committed. This code has been approved by the Dutch Data Protection Authority (DPA. College Bescherming Persoonsgegevens), an independent authority that the Dutch legislator has authorized to supervise the compliance with acts that regulate the use of personal data, in accordance with Article 28 of the European Privacy Directive 95/46/EC.

ETHICAL ISSUES TABLE

	YES	PAGE
Informed Consent		
Does the proposal involve children?	N	
Does the proposal involve patients or persons not able to give consent?	N	
Does the proposal involve adult healthy volunteers?	Y	
Does the proposal involve Human Genetic Material?	N	
Does the proposal involve Human biological samples?	N	
• Does the proposal involve Human data collection?	Y	
Research on Human embryo/foetus		
Does the proposal involve Human Embryos?	N	
Does the proposal involve Human Foetal Tissue / Cells?	N	
Does the proposal involve Human Embryonic Stem Cells?	N	
Privacy		
Does the proposal involve processing of genetic information or personal data (eg. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)	Y	
Does the proposal involve tracking the location or observation of people?	N	
Research on Animals		
Does the proposal involve research on animals?	N	
Are those animals transgenic small laboratory animals?		
Are those animals transgenic farm animals?		
Are those animals cloned farm animals?		
Are those animals non-human primates?		
Research Involving Developing Countries		
Use of local resources (genetic, animal, plant etc)	N	
Impact on local community	N	
Dual Use		
Research having direct military application	N	
Research having the potential for terrorist abuse	N	
ICT Implants		
• Does the proposal involve clinical trials of ICT implants?	N	
I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL		