Applied Analysis and Synthesis of Complex Systems

Proceedings of the IIASA - Kyoto University Joint Seminar, June 28 – 29, 2004

Kazuo Tsuchiya, Tetsuo Sawaragi and Marek Makowski Editors





The 21st Century COE Program for Research and Education on Complex Functional Mechanical Systems, Kyoto University

a n d

International Institute for Applied Systems Analysis, Laxenburg, Austria

Applied Analysis and Synthesis of Complex Systems

Proceedings of the IIASA - Kyoto University Joint Seminar, June 28 – 29, 2004

Kazuo Tsuchiya, Tetsuo Sawaragi and Marek Makowski Editors



International Institute for Applied Systems Analysis www.iiasa.ac.at



The 21st Century COE Program for Research and Education on Complex Functional Mechanical Systems, Kyoto University[†]

[†] Kyoto University Graduate School of Engineering Departments of Mechanical Engineering, Precision Engineering, Engineering Physics & Mechanics and Aeronautics & Astronautics Graduate School of Informatics Dept. of Applied Analysis and Complex Dynamical Systems International Innovation Center

International Institute for Applied Systems Analysis, Laxenburg, Austria

Interim Reports on work of the International Institute for Applied Systems Analysis receive only limited review. Views or opinions expressed herein do not necessarily represent those of the Institute, its National Member Organizations, or other organizations supporting the work.

Preface

This two-day seminar aimed at introducing the new development of the COE by Kyoto University to IIASA and discussing general modeling methodologies for complex systems consisting of many elements, mostly via nonlinear, large-scale interactions. We aimed at clarifying fundamental principles in complex phenomena as well as utilizing and synthesizing the knowledge derived out of them.

The 21st Century COE (Center of Excellence) Program is an initiative by the Japanese Ministry of Education, Culture, Science and Technology (MEXT) to support universities establishing discipline-specific international centers for education and research, and to enhance the universities to be the world's apex of excellence with international competitiveness in the specific research areas. Our program of "Research and Education on Complex Functional Mechanical Systems" is successfully selected to be awarded the fund for carrying out new research and education as Centers of Excellence in the field of mechanical engineering in 2003 (five-year project), and is expected to lead Japanese research and education, and endeavor to be the top in the world.

The program covers general backgrounds in diverse fields as well as a more in-depth grasp of specific branches such as complex system modeling and analysis of the problems including; nonlinear dynamics, micro-mesoscopic physics, turbulent transport phenomena, atmosphereocean systems, robots, human-system interactions, and behaviors of nano-composites and biomaterials. Fundamentals of those complex functional mechanical systems are macroscopic phenomena of complex systems consisting of microscopic elements, mostly via nonlinear, large-scale interactions, which typically present collective behavior such as self-organization, pattern formation, etc. Such phenomena can be observed or created in every aspect of modern technologies. Especially, we are focusing upon; turbulent transport phenomena in climate modeling, dynamical and chaotic behaviors in control systems and human-machine systems, and behaviors of mechanical materials with complex structures.

As a partial attainment of this program, IIASA and Kyoto University have exchanged Consortia Agreement at the beginning of the program in 2003, and this seminar was held to introduce the outline of the COE program of Kyoto University to IIASA researchers and to deepen the shared understandings on novel complex system modeling and analysis, including novel climate modeling and carbonic cycle management, through joint academic activities by mechanical engineers and system engineers. In this seminar, we invited a distinguished researcher in Europe as a keynote speaker and our works attained so far in the project were be presented by the core members of the project as well as by the other contributing members who participated in the project. All IIASA research staff and participants of YSSP (Young Scientist Summer Program) were cordially invited to attend this seminar to discuss general modeling methodologies for complex systems.

Marek Makowski (IIASA) and Tetsuo Sawaragi (Kyoto University)

Seminar Organizers

LIST OF CONTENTS

Preface	i
I. OVERVIEW OF HASA	
Overview of IIASA's Research Leen Hordijk	1
II. OVERVIEW OF COE	
Program Overview Kazuo Tsuchiya	7
Research Program for Complex Fluid Mechanics Research Group Satoru Komori	11
Research Program for Complex System Control and Design Group <i>Tetsuo Sawaragi</i>	16
Properties of Materials with Complex Structure <i>Takayuki Kimatura</i>	22
III. INDIVIDUAL WORKS OF THE COE	
Research Topics in Complex Mechanical Systems Engineering Kazuo Tsuchiya	26
Some Factors Affecting the Air-Sea Gas Transfer Satoru Komori	29
Dynamical and Complex Behaviors in Control Systems and Human-Machine Co-Adaptive Systems <i>Tetsuo Sawaragi</i>	41
Momentum and Heat Transport Mechanisms of Fluid Motion in a Rota Annulus	ting
Phan Vinh Long and Masato Nagata	51
Bone Functional Adaptation by Remodeling through Hierarchical Mechanical Systems from Cell to Tissue Taiji Adachi	58
From "Function Designing" to "Bio-Environment Designing" Naohide Tomita	65
Structural Topology Optimization for the Design of Novel Mechanical Structures <i>Shinji Nishiwaki</i>	72
Design of an Adaptive Control System by Modular Learning: Flight Control of an Autonomous Unmanned Helicopter Hiroaki Nakanishi	80

IV. CONTRIBUTIONS FROM IIASA

An Overview of the Structured Modeling Technology Marek Makowski	_ 88
A Robust Stabilization Technique for Uncertain Models of Global Carbon Cycle Arkady Kryazhimskiy and Nikolai Melnikov	100
V. EVALUATIONS OF THE SEMINAR	
Report on IIASA - Kyoto University First Joint International Seminar on Applied Analysis and Synthesis of Complex Systems <i>Gunnar Johannsen</i>	106
Comments on IIASA - Kyoto University First Joint International Seminat on Applied Analysis and Synthesis of Complex Systems <i>Martin Buss</i>	r 109
APPENDIX Agenda	111
List of Participants	<u>114</u>

Overview of IIASA's Research

Leen Hordijk

Director International Institute for Applied Systems Analysis (IIASA)

The International Institute for Applied Systems Analysis (IIASA) was founded in 1972. It is a non-governmental research organization based in Laxenburg, near Vienna, Austria. The institute conducts inter-disciplinary scientific studies on environmental, economic, technological and social issues in the context of human dimensions of global change. It is sponsored by its National Member Organizations in Africa, Asia, Europe, and North America.

IIASA researchers study environmental, economic, technological, and social developments. In doing so, they generate methods and tools useful to both decision makers and the scientific community. The work, based on original state-of-the-art methodology and analytical approaches, links a variety of natural and social science disciplines.

Societies and decision makers everywhere are being confronted with unprecedented change – to the societies themselves, to their economies, to the environment. In order for national policies to be effective in dealing with global change, national leaders must understand the complex problems associated with them. And equally importantly, they must recognize the interrelationships among the problems. This is precisely the mission of IIASA – to provide science-based insight into complex global problems.

IIASA's work combines methods and models from the natural and social sciences in analyses that provide policy insight on global change issues for decision makers, the scientific community and the public worldwide. Since 2000, the Institute's research is carried out within three core themes: *Energy and Technology; Environment and Natural Resources; and Population and Society.* In addition to its policy-relevant findings, the Institute has made significant contributions to the methodologies of assessment and decision support, as well as the development and refinement of global databases and analytical models. The Institute's staff publishes regularly in prestigious scientific journals such as Nature and Science.

Within the three themes listed above are programs, which define the major research areas in which IIASA does it work. These are relatively stable designations and comprise mostly the research areas for which IIASA is well-known, Energy, Forestry, Population, Technology, Air Pollution, Land-Use, Risk, and Mathematical Modeling. Within these program areas are individual projects; research activities of set duration with specific expected outcomes. However, because of the complexity of the issues studied there is close collaboration among the programs. In addition, there is currently one major cross-cutting activity that draws on the expertise and interests of several programs: the *Greenhouse Gas Initiative*.

1 ENERGY AND TECHNOLOGY

1.1 Dynamic Systems (DYN) Program

Systems analysis is multidisciplinary and mathematical modeling is an integral component. The DYN Program's activities are presently distributed among three major tasks: (1) uncertainty assessment of aggregated models of environmental and economic dynamics; (2) model-based equilibrium analysis of large-scale technological projects; and (3) optimization of models of integrated technological growth.

Specialized mathematical models of dynamics and control are key instruments of the Dynamic Systems Program. Global dynamical optimization principles are at the core of the analysis of models of technological changes, knowledge absorption, and the investment and allocation of economic resources. The competition of firms on markets of new technologies, rational market behaviors, market equilibria, and sustainable techno-economic trajectories are being explored.

The program's environment-oriented studies deal with problems of pollution control and risk assessment. Focus is on the approaches to the estimation of losses due to large-scale catastrophes (earthquakes, forest fires, explosions) and the optimization of preventive counter-measures via governmental and insurance regulation.

1.2 Environmentally Compatible Energy Strategy (ECS) Program

About two billion of the world's six billion people are without access to commercial energy. Before the end of the century, world population is likely to peak around ten billion, and another five to six billion people will need to be "connected". Yet already today, world energy usage is seriously damaging our environment. Can we accommodate future generations and meet the development aspirations of present energy consumers without destroying our planet? Certainly not without new, cleaner and safer sources of energy.

Thus the objective of the ECS Program is to develop and disseminate long-term global energy-economic-environmental scenarios that synthesize advances made throughout the project in: (1) Advancing the state-of-the-art in modeling technological change within energy models; (2) Expanding the existing long-term global energy modeling framework to include sinks and non-CO2 greenhouse gases; (3) Tracing the evolution of energy infrastructure within energy models in order to assess alternative long-term investment strategies, and (4) Maintaining and expanding extensive, accessible databases of technologies and resources in order to support research on technology dynamics, grid evolution, and their incorporation in energy models with an emphasis on hydrogen technologies, in particular fuel cells.

1.3 Transitions to New Technologies (TNT) Program

More than ever, new technologies are demonstrating their potential for transforming society. IIASA's TNT program, launched at the end of January 2000, is concentrating on innovations in the fields of information, communication, transportation and in energy production. The program is analyzing possible diffusion patterns and interlinkanges among cutting-edge technologies as well as the economic and societal impacts that are likely to result if they are widely adopted. In

this context, TNT investigates how various combinations of new technologies might fundamentally affect human activities, and the institutional and organizational changes that would result.

The strategic goal is to develop models that implement concepts of innovation and diffusion dynamics pioneered at IIASA. This includes phenomenological and agent-based models, endogenous treatment of uncertainty, increasing returns and heterogeneity. The models consider impact assessments of the potential economic and societal effects of pervasive diffusion and adoption of new technologies, as well as combinations of new technologies that could lead to fundamentally new human activities. From an interdisciplinary perspective, the strategic goal is to improve the representation of technological change in environmental policies and instruments, particularly in climate change.

2 ENVIRONMENT AND NATURAL RESOURCES

2.1 Adaptive Dynamics Network (ADN) Program

The ADN program works on the development of adaptive dynamics theory, perhaps the most versatile tool currently available for linking the ecological and evolutionary consequences of environmental change. The program attracts a constant flow of international scientists who apply the techniques of adaptive dynamics theory to their own research questions while contributing to the systematic extension of the theory.

The three main facets of the programs work are (1) Work on the theory of cooperation that has shown how the evolution of indirect reciprocity and reputation schemes can explain stable patterns of cooperation observed in human and animal populations; (2) New insights into the formation of biodiversity through processes of adaptive speciation that address one of the most fundamental questions of all biological research; (3) Opening new avenues for simplifying spatial complexity in ecological systems, a step urgently needed for instilling greater realism into tractable ecological models.

ADN has launched a new application of adaptive dynamics theory to questions of fisheriesinduced adaptive change. The project has documented for the first time in an oceanic stock that intensive fishing has led to evolutionary adaptations in the exploited population. In close collaboration with the Institute of Marine Research in Bergen, Norway, ADN has analyzed an extensive database on the maturation dynamics of Northeast Arctic cod, one of the commercially most important stocks worldwide. ADN's investigation has revealed that, beyond the so-called "compensatory response" (increased individual growth rates resulting from diminished stock biomass, an effect long discussed among fisheries scientists), an additional, residual effect was hiding. This finding must be of particular concern to fisheries managers, as the underlying evolutionary change in the stock's genetic makeup is expected to be difficult and slow to revert. Detailed investigations in three other stocks now have corroborated the wide relevance of these findings.

2.2 Transboundary Air Pollution (TAP) Program

The TAP Program has pioneered bridge building between scientific research and policy making on air pollution. It has developed the RAINS model that brings together information on economic and energy development, emission control potentials and costs, atmospheric dispersion characteristics, and environmental sensitivities towards air pollution. With this work, TAP provides the scientific basis for the ongoing revision of the Gothenburg Protocol of the Convention on Long-range Transboundary Air Pollution. Further, the Commission of the European Union has established the Clean Air for Europe (CAFÉ) program that will conduct a systematic and holistic review of all EU legislation related to air quality and will use the RAINS model as the central integrated assessment tool. Further work is focused on understanding the linkages between control measures for different atmospheric pollution problems with different spatial and temporal scales (such as air pollution and climate change).

The long-term vision of TAP is to expand on the recently identified linkages between air pollution and climate change and develop new tools for practical decision making about emission controls that integrate both aspects. This work will address, inter alia, the role of aerosols in climate change and local pollution and will explore the multiple benefits of methane controls on radiative forcing and as an important precursor that determines background concentrations of tropospheric ozone.

2.3 Forestry (FOR) Program

The overall theme of the FOR Program is Global Change and Forests, addressing the question of how to manage the forest sector to harmonize geo- and biospheric functions with socioeconomic development. The overall objective is to carry out science that supports policy issues of interest to research, governmental and industry communities.

Within this overall theme, the FOR Program develops policy recommendations on such topics as uncertainty and verification of greenhouse gases (GHG) in the earth's biogeochemical cycle, and impacts of new information technology on the forest sector

In the former case, FOR has developed a unique framework (information base and methodology) for full GHG accounting for temperate and boreal landscapes. In the latter case, the FOR Program leads an international task force that studies the challenges and opportunities for the global forest sector created by the emergence of new information technologies. IT will play an important role in the paper and woodworking industries but also further downstream to the management of forest resources and environmental values

Additional research themes are the role of forests and land resources in climate risk management, and analyses of institutions of the forest sector in specific countries.

2.4 Modeling Land-Use and Land-Cover Changes (LUC) Program

Land-use and land-cover change are significant to a range of themes and issues central to the study of global environmental change. Alterations in the earth's surface hold major implications for the global radiation balance and energy fluxes, contribute to changes in biogeochemical cycles, alter hydrological cycles, and influence ecological balances and complexity. Through these environmental impacts at local, regional and global levels, land-use and land-cover changes driven by human activity have the potential to significantly affect food security and the sustainability of the world agricultural and forest product supply systems.

Two examples of the LUC Program's work are briefly mentioned here. The first is CHINAGRO (Policy Decision Support for Sustainable Adaptation of China's Agriculture to Globalization), and it addresses a range of policy questions that are at the core of ongoing trade liberalization following China's accession to the World Trade Organization. The second example is MOSUS (Modeling Opportunities and Limits for Restructuring Europe towards Sustainability). The MOSUS study integrates measures of sustainable development, competitiveness, globalization and international trade of EU countries with greenhouse gas emissions from their material flows. The study will provide a consistent database on environmental inputs to European economies.

2.5 Radiation Safety of the Biosphere (RAD) Program

As a result of the production of nuclear weapons and accidents at nuclear enterprises, vast quantities of radioactive waste and numerous radioactively contaminated sites have accumulated in several countries. The United States and the former Soviet Union, as the producers of the largest nuclear arsenals in the world, also face the largest environmental consequences of nuclear weapons production. Efforts to assess and clean up contaminated areas have begun, with billions of US dollars already spent in the United States alone.

The impact of the operation and decommissioning of the world's nuclear navies is an environmental concern because of the ecologically sensitive nature of the oceans. The RAD Program's work on this topic has resulted in the publication of a well-received book on the nuclear legacy of the Soviet Union and, more recently, a report on the potential impact of Russian Pacific Fleet operations on neighboring countries.

3 POPULATION AND SOCIETY

3.1 World Population (POP) Program

The POP Program plays a leading role in the fields of population/environment analysis, and methods of population forecasting. This has made IIASA the only global change research institute with a significant in-house population research capacity. The main research objective is to analyze and forecast the dynamics of global population change in its interactions with changing social, economic and environmental conditions. Special emphasis is placed on quantitative assessments of uncertainty and on capturing population heterogeneity that goes beyond age and sex by further distinguishing by level of education and location.

3.2 Processes of International Negotiation Network (PIN) Program

The PIN Program develops knowledge that is useful to facilitate or support international negotiations either to prevent or cope with dispute and conflict or to develop and establish effective ad-hoc solutions or international regimes for long-term government. The ambition of PIN is to enhance its capacity for such decision support by well-targeted research and effective communication across the boundaries between social and natural science as well as between theory and practice. It seeks to complement the solutions of substance developed in other IIASA programs.

3.3 Risk, Modeling and Society (RMS) Program

The RMS Program has two major objectives. The first is to develop and implement methodologies and policy processes for reducing vulnerability of disaster prone regions and countries to extreme weather and other catastrophic risks through loss mitigation and burden sharing. RMS is developing participatory methods that combine computer models with stakeholder processes that recognize value differences and concerns about fairness in sharing risk burdens. RMS has also developed software tools that use advanced methodologies to assess the socio-economic dimensions of disaster risks and reduce financial vulnerability. These tools have been applied to several case studies in developing and transition countries.

The second objective is to provide advanced modeling support for ever-more complex problems for which general-purpose modeling tools are inadequate. This requires efficient modelbased support, which in turn can only be achieved by a combination of interdisciplinary collaboration, combined with expertise in relevant modeling methods and tools.

Over the years, many of the activities within IIASA and its collaborating institutions have required nonstandard methods and tools for model generation and analysis. To achieve this, applied mathematicians collaborated with various teams at different stages of the modeling process. In order to provide adequate support, a host of widely recognized advances have been made. These advances include novel modeling paradigms for adequate representation of complex problems, effective treatment of uncertainty and risk, tools to support the whole modeling cycle, analysis and the management of huge amounts of data, and specialized algorithms for solving various types of computational problems. The advanced methods and software developed at IIASA have been applied to several widely used in-house models, including management of regional water quality, land use, energy planning, and several versions of the RAINS model.

4 CROSS-CUTTING ACTIVITY

4.1 Greenhouse Gas Initiative (GGI)

The GGI is an inter-program research effort on climate change, its anthropogenic driving forces and possible response strategies. The objective is to develop a new modeling and decision support framework to assess robust policy responses to the challenges of climate change, its driving forces and possible response strategies from local and national to international levels. The special goal is to assist policy makers who act within national and short- to medium-term policy perspectives in including the global and long-term climate change challenges and response strategies in their polices. To achieve these aims, GGI intends to carry out three related activities: (1) Scenario Development: develop a range of global long-term, integrated scenarios that stabilize atmospheric concentrations of greenhouse gasses and other radiatively active substances in accordance with Article 2 of the UN Framework Convention on Climate Change; (2) National Assessment: develop an integrated modeling framework to help individual countries analyze medium-term global scenarios; and (3) Policy Assessment: assess, for selected regions and individual countries, the near to medium-term mitigation and adaptation measures that are consistent with selected long-term stabilization scenarios.

Program Overview

Kazuo Tsuchiya

Project Leader of the COE Department of Aeronautics & Astronautics Graduate School of Engineering, Kyoto University

1 MISSION AND SCOPE OF THE PROGRAM

The 21st Century COE (Center of Excellence) Program is an initiative taken by the Japanese Ministry of Education, Culture, Science and Technology (MEXT), aiming at supporting universities to establish international centers for education and research and to enhance to be the world's apex of excellence in the specific research areas.

Our program of "Research and Education on Complex Functional Mechanical Systems" is awarded the grant for carrying out advanced research and education as Centers of Excellence in the field of mechanical engineering in 2003 (five-year project), and is expected to be a leader in research and education both in Japan and worldwide.

Our objective in research is modeling, analysis, and control of phenomena and design theory geared specifically for complex mechanical systems, and is to form the basis of a novel field of study to be known as "Complex Systems Mechanical Engineering".

Our objective in education is to foster and develop innovative young researchers that will become leaders in these novel fields of study. The COE program provides significant opportunities for such development on the job, promoting these young scientists' broad perspectives, creativity, and a strong will in preparation for their entrance into the global research community.

To this end, we will establish high-level joint teams combining specialized scientists and engineers from the four departments of Graduate School of Engineering (Department of Mechanical Engineering, Department of Engineering Physics and Mechanics, Department of Precision Engineering, and Department of Aeronautics and Astronautics), one department of Graduate School of Informatics (Department of Applied Analysis and Complex Dynamical Systems), and Kyoto University International Innovation Center. Research will be conducted using the facilities of the five departments on Yoshida campus, and it will also be carried out at Katsura Intec Center, our interdisciplinary joint research facility.

2 RESEARCH AND EDUCATION OBJECTIVES

2.1. Introduction

Mechanical Engineering concerns modeling and analysis, and the control and design of mechanical systems. It is traditionally thought of as a mature field; however, there remain within it, and at its intersections with other fields, a number of questions that remain unresolved. One such field of study is Complex Mechanical Systems. In our COE program, we have applied novel methods for analyses and recent discoveries regarding pattern formation and the emergence of function acquired in Complex Systems Science to study and explore complex mechanical systems. By determining universal laws that govern phenomena and emerge on complex mechanical systems and principles that control behaviors of complex mechanical systems, we aim to gain a deeper understanding of complex mechanical systems as well as to form the basis for the novel field of "Complex Systems Mechanical Engineering".

Here, "complex mechanical systems" refer to mechanical systems that comprise a number of complex non-linear interacting elements, and form a variety of structures under the influence of the external environment. At present, in many fields with which Mechanical Engineering is associated, there are urgent demands, both explicitly and implicitly, to study complex mechanical systems. The recent trend of global warming has demanded the development of a model for an atmosphere-ocean system that enables the long-term prediction of global climate change. To be comprehensive and highly reliable, such models must be designed based on an explicit, comprehensive theory. The elementary processes that play crucial roles in this model have been well studied in Mechanical Engineering. For example, in the field of Fluid Mechanics, research on heat transfer through turbulent structures has been a focus of interest, resulting in numerous significant findings. This turbulent convective heat-transfer phenomenon is exactly what plays an essential role in processes such as long-term climate change. Building a model of an atmosphereocean system based on such knowledge is an important research subject for this Complex Systems Mechanical Engineering. With such a phenomenon as global climate change, new difficulties arise in regard to the uncertainty in prediction that naturally accompanies such a large system. Development of new analytical and modelling procedures to deal with these problems is an important item on the COE's agenda.

Nonetheless, Mechanical Engineering has traditionally sought to maximize efficiency, precision and speed progressively; however, these paradigms have shifted and expanded, such that the field is becoming increasingly concerned with how machines can function in concert with its environment. However, such machines cannot be made in the context of conventional rigid, inflexible mechanical systems, but instead require the development of soft and flexible mechanical systems that can change their structure according to the external environment. In the field of control engineering, we target mechanical systems that have complex internal structures and that exhibit a variety of behaviors in response to external environment and elucidate control principles and formulate design theories.

In our COE program, we aim to create a novel field of Mechanical Engineering, "Complex Systems Mechanical Engineering" by elucidating laws that govern the way in which large numbers of interacting components generate the behavior of such complex mechanical systems, and by developing design methods that can control them.

As always, education is a top priority at Kyoto University. Through guidance on-the-research training framework, which has long been a staple of the education system here, we will develop

young researchers with profound prospective, broad vision, and highly specialized skills who will actively create novel research fields and continue to work at the frontiers of science.

2.2. Research program

Systems with a great deal of element and non-linear characteristics that include self-organization, fractal and chaos upon interaction with the environment, are known as complex systems. Such systems have been the focus of much of the recent research in all fields of science. These studies have made it clear that complex systems spontaneously form coherent structures under the influence of the external environment; as a result, such systems can perform higher function through these ordered structures. We believe that novel methods for analyses and recent discoveries regarding pattern formation and emergence of function acquired in the field of Complex Systems Science will become important tools and concepts in the study of complex mechanical systems; to this end, we have engaged in modeling and analysis, and control and design of complex mechanical systems by establishing an effective joint research team comprising of both mechanical engineers and complex systems scientists. The following is an overview of the program's goals.

Modeling and analysis of universal laws governing the dynamic behaviors of natural and artificial complex mechanical systems

We develop novel methods of analysis, fractal analysis, etc., for phenomena that conventional methods cannot treat due to their large size and structural complexity, and analyze the dynamic behaviors of basic physical processes such as thermal diffusion over fractal structure and wave propagation. The modeling of the atmosphere-ocean system has long relied upon phenomenological methods. We plan to develop a new model that is faithful to phenomena, comprehensive, and highly accurate. To that end, we have analyzed turbulent structures and formulated an accurate model of turbulent convective transfer, an important element of the atmosphere-ocean system, based on an analysis of a structural organization of turbulence, and then used a constitutive procedure to model the atmosphere-ocean system. We model and analyze the mechanical characteristics of materials that have complex structures with the aim of applying them to practical use; a fine example material is bone. By constructing a mathematical model based on physiological data of adaptive processes undergone by bone in response to a dynamic environment, we are likely to develop more lifelike artificial bones.

To elucidate and formulate control principles which make possible the practical application of complex systems

A complex system comprises a number of unstable elements with non-linear characteristics and interactions; thus, conventional control theories cannot treat it adequately. For such systems, we aim to develop novel control methods based on dynamical systems theory and autonomous distributed systems theory. We have revealed that flow fields of a certain type of turbulence are governed by an unstable limit cycle, and based on these discoveries we aim to develop a control algorithm of turbulence by the use of chaos control theory. We aspire to develop mechanical systems that have complex internal structures and that exhibit a variety of behaviors in response to external environment and elucidate control principles and formulate design theories.

2.3 Education program for young researchers

One of the primary roles of the 21st Century COE Program is to develop superior young researchers in those fields. In this program, we will employ Kyoto University's tradition of on-the-research training to develop young researchers with broad perspectives and highly specialized skills who possess the ability and courage to act as trailblazers in a novel field of study. Various new systems and programs will be prepared for this purpose.

Joint Interdisciplinary research program

To improve the research capabilities of those in the doctoral course, instead of a traditional education style of unidirectional communications relying on lectures, we will prepare and broaden a system to promote education as a joint act of the teacher and student in conducting research, examining a variety of viewpoints, and deciding upon experimental objectives and procedures. In addition to the joint research that has occurred in the past under the tutelage of a single instructor, a new system designated as the Apprenticeship program is being established. In this system, a student is allowed to participate in joint research unrelated to the department or course to which he or she belongs, including overseas research projects, for a set period of time. In addition, the student will be given opportunities to interact with instructors in other disciplines and participate in their research.

Fellowship program

Young researchers, post-doctoral research fellows and graduate school doctoral students, will be provided with comprehensive support for their research activities, including expenses for research, travels associated with joint study, and domestic and international conferences, so that they will be able to focus on their high-level research as independent researchers.

Public education program

The field of Mechanical Engineering is currently undergoing a paradigm shift, from mechanical systems that emphasize efficiency alone, to those that take a balance between harmony with environments and high productivity. Thus, engineers are now being asked to understand mechanical engineering in the context of complex systems. The COE will offer a recurrent course, open to the public, entitled "Complex Systems Mechanical Engineering." This course will be offered in several cities throughout Japan. The courses will present a simple description of Complex Systems Mechanical Engineering, and provide training opportunities for researchers and engineers who are struggling with relevant problems and seeking a systematic new understanding of mechanical engineering. This program will collaborate with the alumni organization for mechanical systems courses, which have long been active in community outreach.

Research Program for Complex Fluid Mechanics Research Group

Satoru Komori

Complex Fluid Mechanics Group Leader Department of Mechanical Engineering Graduate School of Engineering, Kyoto University

Abstract

Our fluid-mechanics group aims to develop reliable models for describing turbulent transport phenomena appearing in atmosphere and oceans in order to improve the reliability of predictions for global warming. In particular, it is of importance to precisely estimate heat and mass exchange rates between atmosphere and oceans by clarifying the mechanism of heat and mass transfer across the air-sea interface, since very rough sub-models that never reflect the physical heat and mass transfer processes have been used in conventional general circulation models (GCM). This kind of research on the atmosphere-ocean system is also a very challenging subject for our mechanical engineers who have professional expertise in fluid mechanics and thermal engineering. This talk will introduce our experimental and numerical approaches for clarifying turbulent CO2 transfer mechanism across the sheared wavy air-water interface and for estimating CO2 exchange rate between atmosphere and oceans. In addition, some factors affecting the CO2 transfer across the air-sea interface will be discussed together with laboratory measurements in a wind-wave tank.

1 INTRODUCTION

We live in an environment surrounded by fluids and encounter a variety of fluid flow phenomena on a daily basis. The scales of these fluid flows vary widely in the range from microns, as seen in the blood flow of living organisms, MEMS (Micro Electromechanical System) or microreactors, to meters in industrial equipment, and to km in the atmosphere or ocean. These fluid flows are caused not only by pressure force, but also by buoyancy, gravitation, centrifugal force, electromagnetic force and other external forces. In most fluid flows, not only momentum transfer, but also heat and mass transfer, chemical reactions and various other factors are involved, which make the fluid flow phenomena highly complex. Accordingly, to understand fluid dynamics in practical flow fields and develop useful fluid technology, we have to identify each of the various factors that constitute complex fluid phenomena and study their basic properties.

Our fluid mechanics research group in the 21st century COE program "Mathematical Modeling and Design Theory of Dynamic Functional Mechanical Systems," involves eight laboratories which belong to three different departments, Mechanical Engineering, Physics and

Mechanical Engineering and Aeronautics and Astronautics, and our group together forms a collaboration devoted to the study and modeling of complex fluid flow phenomena. Each member of the group promotes unique fundamental research on complex fluid phenomena and publishes his/her research results through international leading journals and academic exchange. The group also develops two research projects, Turbulence Control System and Atmosphere-Ocean System, related to complex fluid flow phenomena that go beyond the framework of conventional fluid and thermal engineering research. Such themes are most challenging for our mechanical engineers who have a deep knowledge of simultaneous transfer of momentum, heat and mass in fluids. Both researchers in this core group and other visiting researchers from Japan and abroad will take parts in the exciting projects

2 OBJECTIVES OF THE COMPLEX FLUID MECHANICS RESEARCH GROUP

2.1 Building a true sense of COE for complex fluid mechanics research

Our fluid mechanics research group is not simply a group of researchers engaged in special research projects. Our ultimate objective is to become a legitimate internationally recognized center of excellence for fluid mechanics research that retains a high level of researchers or scientists and provides the latest advanced information of fundamental researches to the world, as well as to invite many excellent researchers from both Japan and abroad. To attain this objective we set the following three targets:

- 1. We will actively engage in fundamental researches on complex fluid flow phenomena and present these results in leading international peer-reviewed journals. In this context, we will focus especially on the development of young excellent researchers, nurturing them in the global research community and helping them to get grants to support their researches.
- 2. We will host international conferences, invite foreign researchers and dispatch our researchers, to organize collaborations and other international exchange projects to strengthen complex fluid mechanics research, and we will provide new findings to the international community.
- 3. In order to establish an interdisciplinary fundamental fluid mechanics research body in our university, we will collaborate with researchers from the Advanced Institute of Fluid Science and Engineering which involves more than 30 staffs in 6 departments of our graduate school of engineering, Kyoto University. We intend to increase the international visibility of Kyoto University complex fluid mechanics research group, aiming that it is recognized as a leader in the international academic field of fluid mechanics.

Research projects of the complex fluid mechanics research group

Current research subjects of the eight laboratories that belong to the complex fluid mechanics research group are summarized as follows:

- 1) Molecular gas dynamics and its application to complex flows with phase transition (Profs. Aoki & Takada)
- 2) Complex two-phase flows by the lattice Boltzmann method (Profs. Inamuro & Ohwada)
- 3) Plasma-surface interactions on planar and microstructural feature surfaces in space and industrial plasma environments (Profs. Ono & Setsuhara)

4) Dynamical roles of elementary vortices in heat and mass transfer in turbulence (Profs. Kida & Hanazaki)



Figure 1. Research project on turbulence control system

- 5) Turbulent transport phenomena in environmental and industrial flows (Profs. Komori & Nagata)
- 6) Transition to turbulence in shear flows. Analysis on complex thermal convection in rotating systems and its application to turbulence control (Profs. Nagata & Kawahara)
- 7) Complex fluid phenomena with thermal radiation and/or phase changes (Profs. Makino & Matsumoto)
- 8) Complex thermofluid phenomena in microthermal systems (Profs. Yoshida & Iwai)

To exploit maximally the research specialties of each laboratory, our group has focused on two subjects: 1) development of turbulence control system, and 2) modeling of atmosphere-ocean system. These two projects are briefly introduced below

2.3 Development of turbulence control system

For the optimum design of transportation machines such as airplanes, vehicles, and ships and energy equipment such as gas turbines and chemical reactors, it is important to fully understand the turbulence structure near the wall and to develop technology for controlling this turbulence. Particularly important are reduction of the friction drag acting the transportation machines, the efficient promotion of mixing and reaction in reactors, and the control of heat exchange rate in combustors. Resolution of these issues requires clarification of complex fluid flow phenomena associated with heat and mass transfer. Furthermore, surface treatment of the wall at the nanolevel may be required to reduce friction drag or to promote heat and mass transfer. Accordingly, the main focus of our project is on the elucidation of these complex turbulence phenomena and integration of all the information obtained through such investigations, to provide knowledge useful for developing turbulence control technology. Therefore, this project is clearly distinct



from the empirical trial and error researches currently used to develop such systems. Figure 1

Figure 2. Research project on atmosphere-ocean system

illustrates the specific aspect of turbulence control system which some members of our fluid mechanics research group are focusing.

2.4 Modeling of atmosphere-ocean system

Global warming is mainly caused by carbon dioxide (CO2) generated in the course of fossil-fuel burning. It is an important issue for environmental researchers to precisely forecast the greenhouse effect, resulting in the promotion of large-scale national projects such as the "Earth Simulator". This global warming forecast has been conducted using a General Circulation Model (GCM), composed of various sub-models that represent the complex turbulent transport phenomena associated with heat, mass and momentum transfer occurring in atmosphere and oceans. The numerical simulation by the GCM based on the sub-models provides future scenarios on global warming. This simulation method can be used not only for this application, but also for forecasting several unusual climate changes such as localized torrential downpours, droughts, heat island and so on. However, the specific physical sub-models used for the current GCM have not been fully examined, and so there remains a risk of significant errors in forecasting global warming and local climate changes. The reliability of the sub-models for estimating heat, mass and momentum transfer at the air-sea and air-land boundaries is especially poor. When we look at the method used in the GCM for estimating exchange rate of mass (CO2, etc.) between the atmosphere and ocean, for example, heat and mass flux is expressed simply by the product of concentration difference between the atmosphere and ocean and the mass transfer velocity (referred to as the mass transfer coefficient in engineering field). The mass transfer velocity is, however, strongly influenced by several factors, including the turbulence structure near the airsea interface, the density stratification, the entrained air bubbles and dispersed droplets due to intense wave breaking, surface contamination and others. If the transfer velocity model does not accurately express these effects, an estimate of mass exchange rate between the atmosphere and ocean may easily result in the error of about 1 PgC per year. That is, even if we integrate the local

mass flux over the whole ocean surface and evaluate the global mass exchange rate between the atmosphere and ocean, the predicted scenario for global warming will be far from reality, unless the sub-models used as their bases are reliable. Furthermore, to estimate the mass exchange rate between the atmosphere and land is even far more difficult than that between the atmosphere and ocean, due to the influence of land-based vegetation. We can only indirectly estimate the land uptake by taking the mass balance of carbon between ocean uptake and absorption into atmosphere. Therefore, it is of great importance to precisely estimate the atmosphere-ocean flux, in order to accurately forecast the global warming.

Currently, researches related to such global warming forecasts are considered to fall under the category of atmospheric or marine science, and only geophysicists who specialize in meteorology or oceanography are conducting such studies. However, complex fluid transport phenomena in atmospheric and oceanic turbulence are important research subjects that can and should be addressed by mechanical engineers, who can easily treat simultaneous momentum, heat and mass transfer. A number of phenomena, including heat and mass transfer between atmosphere and ocean and between atmosphere and land, turbulent heat and mass transfer with evaporation and radiation in the atmosphere and ocean, the effects of clouds, rain and aerosols on heat and mass transfer, the density stratification effects on turbulent eddy motions in the atmosphere and ocean, interact with one another, together composing the complex atmospheric and oceanic system. Our fluid mechanics group members are specialized at investigating these complex fluid flow phenomena. To create a reliable model for this atmosphere and ocean system, we will study in detail the underlying turbulence and transport phenomena using the most advanced techniques available in the present thermal and fluid engineering. The first two or three years of our project will be devoted to the study on the heat and mass transfer mechanism between the atmosphere and ocean. The project developing component models on which a more reliable climate model can be built is clearly distinctive in comparison to the current research underway, which only conducts global numerical forecasts based on unreliable component sub-models. Figure 2 illustrates the elemental fluid flow phenomena in the atmosphere and the ocean system that individual laboratories of our complex fluid mechanics research group can treat.

Research Program for Complex System Control and Design Group

Tetsuo Sawaragi

Complex System Control and Design Group Leader Department of Precision Engineering Graduate School of Engineering, Kyoto University

Abstract

Fundamentals of complex functional mechanical systems are macroscopic phenomena of complex systems consisting of microscopic elements, mostly via nonlinear, large-scale interactions. Such phenomena can be observed or created in every aspect of modern science/technology. They typically present collective behavior such as self-organization, pattern formation, learning etc., which does emerge out of interactions among individuals with an ability of creating variabilities. Our group aims at clarifying fundamental principles in such phenomena as well as utilizing and synthesizing the knowledge derived out of them to realize the adaptability of the mechanical artifacts to the environmental disturbances. In this lecture, a number of our group's ongoing works are presented including the design and analysis of novel control mechanisms for autonomous robots, biological systems, mechanical artifacts and more general human-in-the-loop systems.

1 INTRODUCTION

The focus of research on a future mechanical system needs to be changed from the machine itself as an entity that is highly accurate and highly efficient to a whole integrated system, which involves the environment that surrounds the machine and a human who operates it. In general, there are limited numbers of systems in which entire functions are accomplished by machines alone. In most cases, the interactions between human and the external environment accomplish the original functional purposes of mechanical systems; however, the theory for its system design and control has yet to be established.

Essentially, autonomous and proactive processes, typically seen in living systems, are not steered only by external forces. Instead, they can autonomously change the relationships among the internal elements that constitute themselves, while taking in external disturbances and adapting themselves to them. In this way, the internal dynamics of each element and the interactions among these elements form a mutual feedback system. Our research group will perform mathematical and experimental analysis of these adaptation processes of internal dynamic systems, and develop a system design theory using those process models. To this end, we have focused on the following three key subjects:

- 1. To elucidate adaptive system structure and dynamics;
- 2. To elucidate adaptive system structure principles; and

3. To develop an adaptive system.

We will cope with the problems inherent in a design of autonomous mobile robots, a design of man-machine systems and a systemic functional emergence arising from the interactions among organic cells and non-linear material elements. We will carry out our research through active and progressive collaboration among all the group members, focusing on the following three subjects (Figure 3) and seeking the possibility of fusion and integration between these disparate research topics:

- 1. Design of autonomous mobile robots that adaptively generates behaviors through physical interactions with the environment;
- 2. Analysis and design of dynamical human-machine interactions and its interface design; and Environmental design for a pattern formation out of interactions among elements.

2 OBJECTIVE: TO ESTABLISH THE CONCEPT OF CONTROL DESIGN BASED ON DYNAMICAL SYSTEM THEORY

Complex mechanical systems can be defined as mechanical systems that consist of multiple elements with their complex interactions and that form a variety of structures and behaviors being affected by an external environment. Each element has its own internal dynamics, and these internal states encounter the competition between two contradicting trends: "stability," which is associated with the extent of autonomy maintained inside, and "adaptability," which represents plasticity for adaptation to the environment and surrounding elements. Furthermore, interactions between the elements underlie a further level of dynamics that allows the evolution of complex behavior, and at the same time, a rational functional design is realized by selecting a nominal option, while other versatile options are suppressed.

Our group aims to clarify the principles with which systems dynamically and autonomously form orders and emerge new functions, and apply our findings to the design of mechanical systems in which functional elements constituting the system transform their nature in response to their environment. This innovative approach to mechanical system design is rooted in the



autonomous mobile mechanical systems dynamical human-machine interactions

Figure 3. An overview of the group

evolutionary and adaptive principles found in life systems that are characterized by its nature of plasticity and loose-couplingness present among components and their interactions. Since complex systems are defined not by any fixed relationships, but by the evolving interactions between its constituent elements, conventional analytical methods are insufficient. We augment them by using constructive approaches, in which we develop a simulation model, and compare its dynamics with experimental observations (Figure 4). In other words, we build up our understanding of a phenomenon by combining several basic processes using an elementary model, aiming to acquire a constructive understanding of nature. Although quantitative forecasts



Figure 4. Constructive approach

will be difficult to make using such analytical methods, this approach will play a significant role in the qualitative prediction and comprehension of phenomena of universal behavior classes. In this way, we hope to make complex subjects comprehensible and applicable for practical development.

3 OUTLINE OF RESEARCH PROGRAMS OF INDIVIDUAL SUBJECTS

In this section, we briefly explain our group's research programs.

To design an environmentally adaptive autonomous mobile mechanical systems that exploits versatility

The stability of motion in multi-dimensional dynamical systems represents a mechanism in which their behaviors are compressed into low dimensional dynamics through interaction among their constituent elements. In autonomous mobile mechanical system design, the degree of freedom is compressed in the manner that even involves a degree of freedom of the environment in addition to that intrinsic to the robot, which creates qualitative stability (isomorphism) of motion patterns. At the same time, by generating versatility within, adaptation to the environment is created. Alternate repetition of the order-structure-formation phase and collapse phase underlies the adaptation of an autonomous mobile mechanical system, which we consider to represent a complex system.

The group of Tsujita and Aoi (the Tsuchiya laboratory) carries out research on the control and design theory of biped robots, taking self-organization and phase transition by control parameters as the principle of motion control. In this research, the nervous system, which is capable of generating voluntary activity patterns related to locomotion, draws in and strongly couples the actions while interacting with a body that is in physical contact with the environment. This results in a mechanism that can generate versatile and adaptive walking motions. The group designs quadruped and biped robots that incorporate this motion control system, which autonomously forms and affects four types of locomotion patterns (walk, trot, bounce, and pace) according to changes in its environment, such as floor inclination, walking speeds and loads. The group develops this mechanism further into one that can create voluntary movements. As an example, the group has shown that by demonstrating the robot's motion and posture control when turning to an intended direction over various turning radii.

Nakanishi studies the design of systems that would dynamically control adaptation in response to complex changes in dynamic characteristics, in order to deal with unanticipated changes in an environment or in a model. In this research, he uses an unmanned helicopter to explore control system design using a neural network as an adaptive component. By combining off-line learning on a simulator and on-line learning in the actual environment, he demonstrated robust adaptation to the problems encountered by actual machines such as model learning errors, changes in environment such as ground effects and gusts, and changes in dynamic characteristics. As a control method with versatility, he adds multiple modules that can adapt to environmental changes and pursue control system design in which individual modules selectively learn adaptations to complex environmental changes and function together as a coherent system.

For social robots that perform social interactions with people using body motions, motion learning is an important technical issue for a robot to enhance its autonomy by adaptively organizing its pre-existing internal structures and to elicit human responses. However, true social behavior in robots is probably not possible, given the limitations on abilities to construct and use an objective external environment model to forecast accurately the behavior of other people. Learning should be focused on the process of transforming the robot itself, rather than model the environment. Through its interaction with others and its internalization, robots define a new reality, then constantly change and optimize their behavior. Taniguchi in the Sawaragi laboratory studies the ability of face robots to trace moving objects. He has proposed an adaptive organization mechanism that allows the robot to organize tracing motions intrinsically, without external instruction signals in learning in the sensorimotor system. In this way, the robot can trace and keep an object in its line of vision by way of adaptive body movement, and learn new strategies for doing so through experience.

To analyze man-machine dynamics and design its interface

Complex phenomena generally occur at interfaces where antagonistic heterogeneous effects coexist. At the interface of man-machine systems, multiple peripheral influences interact and interfere with intrinsic properties to generate such complex phenomena.

Such behaviors often exceed design specifications. For example, on a footbridge, the rhythm of a human and that of the rolling oscillations of the bridge interact with each other, and human rhythm unconsciously synchronizes with the movement of the bridge and thus the rolling becomes amplified. The research group of Utsuno in the Matsuhisa laboratory carries out research on the interaction of such rolling oscillations of bridges with body motion governed by the nervous system that works as a rhythm generator. They analyze these complex behaviors observed at the time of human locomotion on a light and flexible structure such as a pedestrian bridge. They have found that this phenomenon of entrainment of a human's walking pace can be experimentally reproduced by the use of a trapezoid pendulum model, and have also performed mechanical model analysis of the dynamics of the interactions involved in the synchronization.

Yokokoji and Saida in the Yoshikawa laboratory describe the importance of coherence of vision and tactile sense at vision-tactile sense interface to the virtual environment. Specifically, they are investigating a bi-directional motion transfer based on the concept of mechano-media, where a mechanical system takes charge for mapping of human action beyond spatial and temporal aspects. This knowledge, they hope, will enable the design of robots that perform these motions with human-like flexibility, with all the multiple degrees of freedom they entail. Furthermore, through the analysis on the velocity profile of hand and finger movement in grasping motion on a virtual platform, they aim to elucidate the general principles on the selection and combination of degrees of freedom depending on the object type, as well as the segmentation of motions.

Horiguchi in the Sawaragi laboratory conducts studies based on an assumption that the interactions occurring in a human-robot collaboration and the strength of their global association are determined by a specification of an interface design connecting these autonomies. The group has found that these properties manifest themselves in the dynamics of both autonomous and collaborative behavior of human and robot. Often, they have observed that mutually adaptive behaviors become coordinated, thus optimizing the work output of a human-machine combination. Finally, the group has been investigating interface design for tele-operation robot, which is intended to promote the bi-directional exchange of intentions by equivalent and semi-independent parallel loops between a human and a robot, and to share "isomorphism of tasks" through mutual adjustment of their individual behavior.

Environmental design for pattern formation of element groups in the interaction field

To understand the behavior of a living organism, it is essential to elucidate the organic behavior of aggregated as well as single cells. In a life system, there is inherent diversity at the individual level, but at the group level, there is also an inherent mechanism that becomes increasingly more stable and deterministic. It is an extremely important challenge to elucidate the dynamics governing the process in which a macroscopic order emerges and disintegrates controlling the degrees of freedom in such an organization or group consisting of multiple elements. Such knowledge may be utilized for the design of a dynamic and functional mechanical structure system.

Yamamoto, in the Tomita laboratory, studies medical engineering focusing dynamics of organisms and their environments in terms of hierarchy in a biological system in the context of interactions among cells and between cells and tissues. In an initial experiment to observe the structure and function of cartilage cells and tissues without imposing any dynamic environment conditions, ES cells did not differentiate into cartilage cells; however, the group aims to confirm that, when a dynamic state of the environment is altered, morphology and function are enhanced to organize and adapt to the environmental changes. To investigate the dynamics of this system further, specifically the functional and structural adaptations that constituent units undergo, the group has developed an ES cell-cartilage regeneration simulation model using cellular automata.

In order to create microstructures that simulate living organisms, the emergence of hierarchies in the interaction fields, and the pattern formation mechanism in view of topological changes of such functions ought to be elucidated. Compliant mechanisms that actively exploit the structural flexibility of a mechanical structure can realize the mechanical function as the structure itself by adding required flexibility to an appropriate position within the structure. It is, therefore, suitable for structures that cannot be composed entirely of rigid structures. Nishiwaki, in the Yoshimura laboratory, investigates new topological design optimization in structure design of compliant mechanism. To date, this type of optimization has only been conducted empirically; this group intends on studying it analytically, and is focusing especially on vibrating structures. They also have developed this theory into multi-stage design optimization with the intention of designing a method of the functional mechanical structure system for multi-physics phenomenon that deals with the physical coupling phenomena.

Properties of Materials with Complex Structure

Takayuki Kitamura

Materials Group Leader Department of Engineering, Physics, and Mechanics Graduate School of Engineering, Kyoto University

Abstract

Mechanical behaviors of materials are highly dependent on the structures, which possess multiscale hierarchy. We have mainly two directions for the investigations; the ones on biomaterials and on nano-/micro- components. In terms of the latter topics, I will introduce our fundamental research works on the materials from the electronic structure (Microscopic structure), which brings about various natures, to the process/assembly of small components such as dot, wire and film (Macroscopic structure), which endows peculiar characteristics to mechanical systems.

1 INTRODUCTION

From the viewpoint of conventional "complex science", the subject of our group may give a feeling that something does not in a place. Among four groups in the COE program, fewest research works have been done on the mechanical behavior of materials in terms of the conventional "complex science". However, the "modeling of materials" requires the concept of "complexity" because the rich behavior stems from its "compound understructure". In this program, we will discuss the modeling of materials on the basis of "complex science in a broad sense". We do not confine our activity in the conventional research subject on the materials behavior in the mechanical engineering in order to reconstruct the fundamentals for future development in the materials science.

2 MATERIALS SCIENCE IN MECHANICAL ENGINEERING

The study targeted here is centered on the modeling of materials system (including behavior based on the quantum mechanics), which gives the fundamental idea on the design, production, service, and disposition (recycling) of "machine".

In this COE program, "the complex machine systems" are defined as:

(A) Systems that constitute numerous elements with complex interaction, and/or

(B) Systems that shows various structures under environmental influences.

In other words, "complexity" can be construed as various phenomena and structures that arise through interaction of numerous elements under an external environment. Generally, materials that constitute a machine have their own internal structures. Therefore, in the "complex science", material is regarded as a system made up with "elements forming an internal structure" and through "interaction of the elements".

Figure 5 shows research subjects on materials behavior in the mechanical engineering. The subjects are classified into 4 levels, (1) atomic, (2) lattice, (3) cell (grain), and (4) structure levels, according to the dimension of elements. While the basic behavior is illustrated in the upper column, the fabrication process and function of components are shown in the lower column. Although the focus is put on the mechanical strength in the conventional mechanical engineering, other physical properties (piezoelectric, magnetic, electric ones and so on) become important in the development of advanced machines and devices. Our group is investigating the multi-physical aspects of materials behavior. Since the variety of the behavior stems from the understructures, the material itself should be understood as a complex system consisted of multiple elements (microstructures). In view of the rapid progress in computers in recent years, fundamental knowledge obtained by experiments and analyses is integrated in the modeling of system, which gives us insight of not only scientific information but also wisdom for the design and control of industrial products.

As pointed out by the project leader, to comprehend the "complexity" consists of two processes, to identify the elements and to make clear their interaction. Focusing on the atomic level, the modeling and simulation based on the concept are briefly explained below.

At the atomic level, the element is an atom, and the interaction is governed by the quantum mechanics. The active research works are conducted on the low-dimensional nano-structured components such as nano-dot, nano-wire, and nano-film. The numerical simulation are conducted by the methods of molecular dynamics, molecular orbital, Metropolis (Monte Carlo) on the basis of the first principle. The large-scale simulation based on empirical interatomic potential is included in this level.



Figure 5. Research activities on materials behavior



Figure 6. Researchers in frontier research project

As the reader can understand from the example of atomic level, the key point in this project is to understand the complex substructure from the viewpoint of the elements and their interaction. This clearly contributes to enhance the multi-scale understanding of materials.

3 RESEARCH PLAN

As mentioned above, a complex materials study has a wide range of themes. If all the themes are targeted in this program, it may cause desultory results. Therefore, considering the future of mechanical engineering and the past specialization areas of members in the group, the subjects are selected.

The major frontier in the mechanical engineering can be found in the nano- and micro-meter scales. In this program, therefore, we will focus on the research works at the atomic, and cell levels. Table 1 and Figure 6 summarize the young researchers selected and their subjects in 2003 fiscal year supported by the frontier research program. It clearly shows the key areas of this program. This year, we focus on:

- (1) Analysis of mechanical strength and physical properties on the atomic level;
- (2) Formation of functional thin film and its application to structure;
- (3) Analysis of mechanical strength of composite materials.

The emphasis on (3) will be reduced next year and the emphasis will be shifted to

(4) Biomechanics and regenerative medicine.

Accordingly, in the entire program (five years), the main targets will be (1), (2) and (4) in the diagonal line from the upper left to the lower right of the figure. Every year the researchers and themes for the frontier research will be evaluated. Furthermore, as the program progresses, meetings to exchange information in the materials group are planned, and should develop joint research and cooperative relationships among researchers. Cooperation beyond fields and scales is expected e.g. piezoelectric materials -> Formation of thin film -> Structure -> Application to living organisms.

On the other hand, to strengthen cooperation with foreign researchers, exchanges (dispatch/ invitation) and joint research are planned.

Researcher	Theme						
Y. Umeno	Analysis on unstable deformation of solids by collective motion of atoms						
M. Tanaka	Establishment of Complex System Simulation for Fracture Behavior of Fiber Reinforced Composite						
	Materials						
I. Kannno	Manipulation of droplets for molecular tapestry						
M. Suzuki	Control of nano-morphology and mechanical properties of compound thin films using dynamic						
	oblique deposition						
K. Tanaka	Development of testing method for environmental mechanical properties of composite materials and						
	evaluation of the localized environmental effects						
M. Hasuo	Photo-induced changes of semiconductor thin films on TiO ₂						
F. Tsumori	Microstructure Design of Powder Particles under Magnetic Field with Discrete Element Method						
H. Hirakata	Strength of microstructured small components						
K. Nakamura	Analysis of Vibrational Behavior in Solid Materials by Perturbational Approach to Electronic Wave						
	Function						
K. Doi	Theoretical study on electronic states of bulk, surface, and interface under external fields in						
	electronic devices						
T. Hobbiebrunken	Mesoscopic Failure Prediction of Composite Materials A Multi-scale Analysis						
F. Shang	Molecular Dynamics study on the internal stress problem of piezoelectric thin films						
Y. Doi	The fracture of materials due to energy localization with lattice scale						
T. Tsuchiya	Development of high-cycle fatigue tester and mechanical properties database for MEMS/NEMS						
	materials						
T. Adachi	Multi-scale modeling and simulation of bone regeneration/functional adaptation as a complex						
	biological system						

Table 1.	Themes	in	frontier	research	project
----------	--------	----	----------	----------	---------

4 CONCLUSIONS

Mechanical engineering has a long history and as the field can be regarded as a mature, but "machines" are transforming themselves day by day. Currently, machines (systems) that by definition didn't exist yesterday are being continuously produced. Materials constituting machines form the foundation of the present time and it is indispensable for a deep understanding of the complicated internal structures (systems) that materials themselves have in order to correspond to functional demand. The first-stage objective of this program is to grasp the nature and properties of materials that have internal structures by clarifying elements and their dynamical interaction. The second stage to develop a comprehensive and systematic understanding of <u>"Mechanics of materials": Raw material => member => structure (physical properties -> function)</u> . One goal is to establish a common basis for dealing with "complexity" by reconsidering deformation/fracture and function from an atomic level and understanding the influence of inhomogeneity. The third stage is to develop fields in cooperation with other groups, while recognizing the internal structure of each field. We hope that this program will show a new direction for "Materials science in mechanical engineering".

Research Topics in Complex Mechanical Systems Engineering

Kazuo Tsuchiya

Project Leader of the COE Department of Aeronautics & Astronautics Graduate School of Engineering, Kyoto University

The purpose of mechanical engineering is the analysis and design of mechanical systems, but the systems of interest are becoming increasingly complex. The ability to generate long-term weather forecasts has many socially and economically important consequences, and, at its core, this problem is governed by complex hydrodynamic phenomena arising from the interaction of different elementary processes at the atmosphere-ocean interface. Likewise, the development of artificial bone, the major structural material in living system, is a fundamental problem of biomechanics. Bone is a complex living system that results from the interplay between the physiologic and structural properties of its constituent cells and minerals, and remodeling can occur in response to specific signals. Finally, the development of robots that behave autonomously in a changing environment will be of great importance to many fields. The interaction of robots with their surroundings is extremely complex and requires a mechanical systems engineering approach for its full understanding.

Complex systems are generally composed of a large number of components that are coupled by nonlinear interactions.

A key discovery of complex systems science is the description of complex systems, themselves. In particular, fractal systems exhibit regularity through self-similarity while chaotic systems are simply nonlinear. As a consequence, complex systems form an ordered structure through self-organization in response to the environment. A complex system also develops its functions through this ordered structure. For example, the adaptive function, a typical function of complex systems, arises when a pre-existing structure in the system is preferentially selected and modified in response to the environment.

We wish to use the concepts and methodologies of complex systems science as they apply to complex mechanical systems. The combination of these fields would constitute complex mechanical systems engineering. Our specific research interests are as follows:

1. The modeling and analysis of complex mechanical systems

(1) Derivation of a reduced order model of complex systems

(2) Analysis of the adaptive functions of complex systems

2.Control and design of complex mechanical systems

- (1) Stabilization control of the complex system based on the reduced order model
- (2) Development of autonomous robots
- (3) Development of a man-machine interface with adaptive functions

3. Study of the basic mathematics of the complex mechanical systems engineering

- (1) Development of new analytical methods based on stochastic calculus
- (2) Development of new model reduction methods
- (3) Study inverse problem analysis as the basic mathematics of design theories

Uncertainty is inherent in complex systems; their behavior is hard to predict or control. To accomplish this, however, a reduced order model of a system must be developed. Our first goal is to develop a reduced order model for a complex mechanical system. This requires modeling the elementary processes that influence the behavior of the complex system as determined by experimental data, and constructing a reduced order model that retains the global ordered structure.

We are constructing a precise model of the mechanism of heat and mass transfer at the atmosphere-ocean interface. A model of the basic elementary processes that govern the atmosphere-ocean system will greatly facilitate long-term weather forecasts. We are also investigating the global structure of turbulence. Once developed, a reduced order model of turbulence will work as the basic equations for the stabilization control of turbulence.

Complex systems typically exhibit adaptation by altering their internal structure in response to their environment. We wish to better understand the adaptive function of complex systems. We define the adaptive response mechanism of a complex system as follows:

- 1. The components of the complex system change their properties and interactions in response to the environment.
- 2. New structures are potentially formed within the system.
- 3. One of the structures is selected and expands in response to the environment.

We are studying adaptive structure formation of bones under a stressed environment. Our findings will facilitate the development of artificial bones.

Conventional stabilization control theories are difficult to apply to complex systems due to their large size and nonlinearity. We wish to better understand the stabilization control of a specific complex mechanical system through identifying unstable structures inherent in the complex system and constructing a reduced order model. We will then manipulate the reduced order model to achieve greater stabilization control.

A Couette flow is the turbulence generated in the flow between two moving planar plates which mutually have relative speed. It was recently discovered that the average behavior of a Couette flow is expressed as an unstable limit cycle. Thus, stabilizing the unstable limit cycle should allow for the stabilization control of a Couette flow. We are studying stabilization control based on the reduced order model of turbulence for relatively simple structures such as a Couette flow.

The development of mechanical systems with adaptive functions such as robots that behave autonomously in a changing environment is strongly desired. We wish to develop artificial complex systems with adaptive functions. The three design principles of artificial complex systems with adaptive functions are called "internal model principles." They are as follows:

- 1. Constructing an information processing system of the complex system with a dynamic system called an internal model.
- 2. Constructing attractors corresponding to respective adaptive responses within the internal model by learning.
- 3. One of the attractors is selected and amplified according to the environmental influence.

The locomotion patterns of ambulatory animals such as horses spontaneously changes from walking to trotting and galloping in accordance with increases in locomotion speed. We are studying walking robots with adaptive responses to such environmental changes. We are also

developing a man-machine interface system capable of adaptively changing its internal structures in response to the movements of the machine and the man who operates it.

The full development of complex mechanical systems engineering requires further mathematical studies of its basic theories in parallel with individual studies on the modeling, analysis, control and design of specific complex mechanical systems. Some of the phenomena related to complex systems cannot be analyzed by conventional methods. For example, thermal diffusion processes or wave propagation on fractal structures cannot be analyzed by conventional methods, and it is necessary to develop new analysis methods based on stochastic calculus. We are currently developing new methods such as fractal analysis to solve this problem. Once developed, these methods will function as the basic mathematics for the analysis of the mechanical properties of mechanical structural materials with complex internal structures.

To date, reduced order models have been derived individually for specific systems, but these models need to be reorganized from a comprehensive and uniform mathematical standpoint. We are studying a uniform model reduction method called dynamic model construction. We are using the Boltzmann equation to derive hydrodynamic equations as a model for the development of an asymptotic theory to derive a macro model from a micro model.

The basic mathematics for system control and design are inverse problem analysis and optimization. We are studying the basic mathematics of inverse problem analysis and developing algorithms based on our preliminary results. These achievements will work as the basic theories and calculation methods for the control and design of complex systems.

Some Factors Affecting the Air-Sea Gas Transfer

-Towards Modeling of Turbulent Transport Phenomena in Atmosphere-Ocean System-

Satoru Komori

Department of Mechanical Engineering and Advanced Institute of Fluid Science and Engineering, Kyoto University

Abstract

The effects of swell on the turbulence structure and mass transfer mechanism at the sheared wavy air-water interface are experimentally and numerically investigated. The frequency of the appearance of surface-renewal eddies that dominate mass transfer across the air-water interface is estimated from the velocity signal measured in wind-driven turbulence affected by swell. The results show that the surface-renewal frequency decreases in the presence of swell at wind speeds less than 10m/s, compared to the pure wind wave case. This means that swell acts to reduce the mass transfer across the air-sea interface. To give a physical reason why the surface-renewal frequency decreases in wind-driven turbulence affected by swell, direct numerical simulation is applied to the air boundary layer over wavy walls. The DNS predictions show that despite the increase of the total drag the friction drag decreases for a wavy wall with the shape similar to swell wind-waves, compared to a wavy wall with the shape similar to pure wind-waves. This suggests that the decrease in the friction drag results in a decrease in the surface-renewal frequency in wind-driven turbulence affected by swell. In addition, the effects of rain droplets on both mass transfer across the air-water interface and turbulence structure in the interfacial region were investigated through laboratory experiments in a turbulent open-channel flow. The CO_2 absorption rate due to rain droplets impinging on the free surface and turbulence quantities were measured. The results show that turbulent mixing in the free surface region is significantly promoted by rainfall and therefore the turbulent mixing enhances the CO₂ transfer across the airwater interface. The mass transfer velocity (mass transfer coefficient on the liquid side) is well correlated by the mean kinetic energy of rain droplets impinging on the unit area of the air-water interface. The mass transfer velocity corresponds to that obtained in wind-driven turbulence with wind speeds ranging from 4m/s to 12m/s. This suggests that it is of great importance to consider the effects of rainfall on the CO_2 exchange rate in a general circulation model for estimating global warming.

1 INTRODUCTION

Global warming owing to increasing release of carbon dioxide has been alarmingly predicted through numerical simulations based on the general circulation model (GCM). However, the GCM predictions on the mass exchange rate across the air-sea interface are so sensitive to the CO_2 transfer velocity (mass transfer coefficient on the liquid side) that poor estimation of the

transfer velocity leads to uncertainty in the GCM. The CO_2 transfer velocity has been assumed to be simply proportional to the wind speed in previous studies and a few empirical formulas (Liss and Merlivat, 1986; Wanninkhof, 1992) based on the proportional relation to the wind speed have been used in the GCM. On the other hand, recent laboratory measurements (Komori et al., 1999; Komori, et al., 1993; Komori et al., 2002) have shown that the transfer velocity strongly depends on both the frequency of the appearance of surface-renewal eddies and wave breaking. Furthermore, the mass transfer velocity has been estimated only for pure wind-waves in previous laboratory measurements, but few studies have discussed the mass transfer velocity for the windwaves superimposed on swell which is often observed in the actual ocean (hereafter we call these wind-waves as swell wind-waves). These results suggest that the mass transfer velocity should be more carefully estimated.

Another significant factor which has not been considered in the conventional GCM is the effect of rainfall on the CO_2 transfer across the air-sea interface. Generally, the effects of rainfall are expected to promote the mass transfer, since the air-water interface is broken and mixed by impinging rain droplets (Banks et al., 1977). Ho et al. (2000) carried out the gas transfer experiments in a closed chamber by using an open rain-generator and estimated the mass transfer velocity by measuring the rate of gas desorbed from a rain-receiver tank with saturated gas to the atmosphere. However, it is difficult to precisely estimate the mass transfer velocity in such a rain-receiver tank, since the gas concentration unsteadily changes with time and well-mixed condition used to estimate the adsorption rate is not easily realized in the tank. In order to demonstrate how the promotion effect of rainfall on the mass transfer velocity by performing gas absorption experiments and to compare the mass transfer velocity with that obtained in a wind-wave tank in which turbulence is driven by wind shear and mass transfer is controlled by surface-renewal eddies (Komori et al., 1993).

This report aims to introduce our current study on the effects of swell and rainfall on the turbulence structure and the mass transfer across the air-water interface. Swell was mechanically generated in a wind-wave tank by means of a wave-maker and wind-driven waves were superimposed on the swell. The frequency of the appearance of surface renewal eddies was conditionally estimated from streamwise velocity signals measured for both swell wind-waves and pure wind-waves. From the surface-renewal frequency, the effects of swell on the turbulence structure and mass transfer were discussed. Furthermore, in order to explain the swell effects, direct numerical simulation was applied to two wavy walls with similar shapes to swell wind-waves and pure wind-waves, and the shear stress and pressure acting on the wavy walls were estimated.

The rainfall experiments were conducted in a closed chamber contacted on the free surface in a developed turbulent open-channel flow. Rain droplets fell in the chamber filled with pure CO_2 and the CO_2 absorption rate due to the droplets impinging on the free surface was measured.

2 EXPERIMENTS

2.1 Swell experiments

The experimental apparatus used here is shown in Fig.1. The apparatus was a wind-wave tank, and it had a glass test section of 7m long, 0.3m wide and 0.8m high. The water depth in the tank was 0.5m and the vertical height of the air flow above the air-water interface was 0.3m. Pure wind-waves were driven in the wind-wave tank by winds with free-stream velocity of U_{∞} = 2~20m/s. Especially for high free-stream wind speeds of U_{∞} >10m/s, wind waves were intensively broken and many bubbles and spray droplets were entrained into water and air flows,
respectively. Swell was mechanically generated by a wave-maker and the wave-maker was oscillated up and down at a low frequency less than 1Hz. The mean wave height and period for pure swell free of wind shear were 1.97cm and 1.0s, respectively and the ratio of the wave height to the wave length was 0.02. The details of the wind-wave tank are described in Komori *et al.*(1999, 1993).

Instantaneous streamwise and vertical velocities were measured on the water side at x=5m from the entrance to the test section (x=0) by using a two-colour laser-Doppler velocimeter (LDV) with a forward scattering mode. The frequency of the appearance of surface-renewal eddies in the water flow, f_S , was estimated by applying a VITA technique to the instantaneous velocity signal processed by a digital high-pass filter (Komori et al., 1993). Instantaneous wave height was measured using a wave crest meter.



Figure 1. Schematic of a wind-wave tank.

2.2 Rainfall experiments

Figure 2 shows the experimental apparatus. The rain droplets were generated in a closed rain chamber by using 532 needles with the same diameter, located at about 1.5m elevation from the free surface in a developed turbulent open-channel flow and they impinged on the free surface. Seven diameters of the needles (d_n = 0.4, 045, 0.5, 0.55, 0.65, 0.7 and 0.8mm) were used here and the diameter of the generated droplets, d, ranged from 2mm to 2.8mm. The rainfall rate, R, was changed in the range of 13~511mm/h. Pure CO₂ was filled at the atmospheric pressure in a rain chamber and the bottom edge of the chamber was slightly contacted by using a surface tension on the free surface to prevent outward leak of CO₂. The absorption rate was measured using a soap-film meter. From the absorption rate the mass transfer velocity, k_L , was estimated. The motions of the droplets and breaking interface were visualized by means of a high-speed video system. The impinging velocity of a droplet, v_p , was measured by analyzing the video frames of a falling droplet and the diameter of a droplet, d, was estimated from the rain rate for 100 falling droplets by assuming a spherical shape. Turbulence quantities in an open-channel flow were measured by a laser Doppler velocimeter (LDV).



Figure 2. Schematic diagram of experimental apparatus.

3 DIRECT NUMERICAL SIMULATION

Direct numerical simulation (DNS) has often been applied to wind-driven turbulence with the free surface. However, the DNS is still limited to weakly sheared interfaces with low wind speeds less than 2-3m/s because of computer performance (Kunugi and Satake, 2002). Therefore, we applied the DNS to two wavy walls with similar shapes to swell wind-waves and pure wind-waves, and we estimated the wall shear stress and wall pressure from the DNS predictions.

Figure 3 shows a schematic diagram of the computational domain for two two-dimensional wavy walls. The computational domain was $0.06 \times 0.02 \times 0.03$ m in the streamwise (x), vertical (y) and spanwise (z) directions. The numbers of grid points used here were $151 \times 101 \times 61$ in the streamwise, vertical and spanwise directions. The grid spacing was equally distributed in the streamwise and spanwise directions but the vertical spacing was condensed in the vicinity of the wall. The free-stream wind speed over the wavy walls was set to 6m/s. The height and length of the pure wind-wave type of wall were 0.001m and 0.01m, respectively, and for the swell wind-wave type of wall they were 0.00165 and 0.03m. These values of the wave height and length corresponded to about 30 times smaller than the mean dimensions of swell wind-wave tank.





Figure 3. Schematic diagram of the computational domain for two wavy walls.

Periodic boundary conditions were imposed in the streamwise and spanwise directions, while in the vertical direction the slip and non-slip conditions were used at the top boundary and at the wavy wall, respectively.

The governing equations are the equation of continuity and the Navier-Stokes equation for an incompressible flow;

$$\frac{\partial U_i}{\partial x_i} = 0$$
(1)
$$\frac{\partial U_i}{\partial t} + \frac{\partial U_j U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j}$$
(2)

The advection terms in the above Navier-Stokes equations were discretized by a fifth-order upwind scheme and other spatial derivatives by a second-order central difference. The MAC method was used to solve the discretized governing equations. The time integration of the Navier-Stokes equations was carried out by a second-order Runge-Kutta method. The details of the DNS are described in Nagata and Komori (2001).

4 RESULTS AND DISCUSSION

4.1 Effects of swell

Figure 4 shows the frequency of the appearance of surface-renewal eddies, f_s , against the freestream wind speed, U_{∞} . As mentioned in the section 2, f_s was estimated by applying a VITA technique to the instantaneous velocity signal processed by a digital high-pass filter (Komori et al., 1993). In the high wind speed region of $U_{\infty}>10$ m/s with intensive wave-breaking, there is no big difference in f_s between pure wind-waves and swell wind-waves, whereas significant difference is observed in the low and middle speed region of $U_{\infty}<10$ m/s. For the swell windwaves, the surface-renewal frequency is damped, compared to the pure wind-waves. When the ratio of the square root of the surface-renewal frequency f_{S-SW} for the swell wind-waves to that of f_{S-W} for the pure wind-waves is plotted, the swell effects are more obvious as shown in Fig.5. These results show that the mass transfer across the air-water interface is reduced by swell in the wind-speed region of $U_{\infty}<10$ m/s, since the mass transfer velocity is proportional to the square root of the surface-renewal frequency f_s (Komori et al., 1993). In the high wind-speed region of $U\infty > 10$ m/s, intense breaking waves are predominant and therefore they counteract the swell effects.



Figure 4. Surface-renewal frequency versus free-stream wind speed; open square, for pure wind-waves; solid square, for swell wind-waves.

In order to discuss the above swell effects, the friction velocity defined at the interface on the air side was estimated by the DNS for two wavy walls. Figures 6 and 7 show the distributions of the mean wall pressure and horizontal component of the mean wall shear stress on the two wavy walls, respectively. Solid lines show the streamwise variations for the wavy wall with the shape similar to swell wind-waves and dotted lines for the wavy wall similar to pure wind-waves. The streamwise co-ordinate is normalized by the vertical height of the computational domain. For the swell wind-wave wall, the pressure is much larger than that for the pure wind-wave wall. This means that the pressure drag increases in front of the wave crest owing to the blocking effect of the swell wind-wave wall. However, the horizontal component of the shear stress on the swell wind-wave wall is rather smaller behind the wave crest than that on the pure wind-wave wall. Even in front of the crest the shear stress is not much larger than that on the pure wind-wave wall. The decrease of the wall shear stress behind the crest is caused by the flow separation. Taking the averaged values in the streamwise direction, we can estimate the pressure drag and friction drag. As listed in Table 1, the total drag increases due to remarkable increase of the pressure drag in the swell wind-wave case, whereas the friction drag decreases. These predictions suggest that the decrease in the surface-renewal frequency f_S is caused by the decrease in the friction drag for swell wind-waves. If we can accurately measure the friction drag for both swell and pure windwaves at the same wind speed, the relation between f_s and friction drag can be confirmed experimentally. However, we could not conclude whether the surface-renewal frequency is uniquely correlated with the friction velocity or not, since it was difficult to accurately measure the friction drag because of strong separation behind the wave crest.



Figure 5. The ratio of the square root of the surface-renewal frequency for swell wind-waves to that for pure wind-waves. The solid line shows a best-fitting curve.

On the other hand, an empirical relation between mass transfer velocity and wind speed at the elevation of 10m from the sea surface has been usually used in GCM not only for pure wind-waves but for swell wind-waves. However, the wind speed at the 10m elevation does not always reflect the change of the friction drag due to swell wind-waves and this leads to uncertainty in the previous empirical relation of mass transfer velocity. This suggests that we have to develop a technique to precisely measure the friction velocity and from the precise measurements we have to establish the reliable empirical relation between mass transfer velocity and a unique parameter based on the friction velocity



Figure 6. Mean pressure on wavy walls; -----, pure wind-waves; _____, swell wind-waves.



Figure 7. Streamwise component of mean shear stress on wavy walls. Lines as in Fig. 6.

	Pure wind-waves	Swell wind-waves
Pressure drag [N]	1.97x10-4	4.44x10-4
Friction drag [N]	1.15x10-4	1.01x10-4
Total drag [N]	3.12x10-4	5.45x10-4

Table 1. Pressure and friction drags on the wavy walls.

4.2 Effects of rainfall

Figure 8 shows the vertical distributions of the mean velocity, turbulent intensities and Reynolds stress in an open-channel flow. It is found that the mean velocity field is not influenced by rain. On the other hand, the turbulence intensities increase in the free surface region of y/h>0.7. In particular, the vertical motion is significantly promoted. The Reynolds stress is suppressed in the free surface region of y/h>0.6 by rainfall. The facts show that turbulent mixing is promoted in the free surface region by the rain droplets impinging on the free surface.

Figure 9 shows the mass transfer velocity k_L against the rain rate R. The mass transfer velocity is well correlated with the rain rate. However, it is not reasonable to correlate k_L with R, since impinging velocities of rain droplets on the free surface are not reaching to their terminal velocities because of short height of the present rain chamber. To avoid this problem, we used mean kinetic energy flux of the rain droplets impinging on the unit area of the air-water interface per second, *KEF*. The *KEF* is defined by

$$KEF = \frac{1}{2}\rho R v_p^2$$
(3)

where vp is the mean impinging velocity of rain droplets.



Figure 8. Vertical distributions of (a) the mean streamwise velocity, (b) the turbulence intensities of streamwise (open triangle, solid triangle) and vertical (open circle, solid circle) velocity fluctuations *u* and *v*, (c) the Reynolds stress (open square, solid square) normalized by the friction velocity. The open symbols show no rain case of *R*=0mm/h and solid symbols show the rain case of *R*=110mm/h. The solid lines in (a) and (c) indicate the log-law and the equation of -uv/u * 2 = 1 - y/h, respectively.

Figure 10 shows the mass transfer velocity k_L against mean kinetic energy flux *KEF*. The mass transfer velocity k_L is well correlated with *KEF*. If *KEF* can be expressed by Eq.(3) in natural oceans, we can estimate k_L by using the database of the rain rate *R* and mean diameter of rain droplets, since vp is represented by the terminal velocity. The values of k_L in Fig.10 range from 8.9×10 -6m/s to 1.6×10 -4m/s. This range is indicated by two horizontal bars in Fig.11 showing the correlation between k_L and wind speed U_{∞} in wind-driven turbulence (Komori et al., 2002). It is found that the rainfall with *KEF*=1.5[J/m2s] has the same promotion effect on the mass transfer as in the wind-driven turbulence with wind speed of 14m/s. This suggests that it is of great importance to consider the rain effects on the air-sea mass transfer in a general circulation model.



Figure 9. Relationship between R and k_L ; solid square: no rain, open square: d_n =0.40mm, solid circle: d_n =0.45mm, open circle: d_n =0.50mm, solid triangle: d_n =0.55mm, open triangle: d_n =0.65mm, down pointing solid triangle: d_n =0.70mm, down pointing open triangle: d_n =0.80mm.



Figure 10. Relationship between *KEF* and k_L . Symbols as in Fig.9.



Figure 11. Comparison of k_L by rainfall with that by wind shear; open circle: in wind- driven turbulence (Komori et al., 2002).

5 CONCLUSIONS

We have investigated the effects of swell and rainfall on the turbulence structure and mass transfer across the air-water interface. The main results are summarized as follows:

(1) Swell acts to decrease the frequency of the appearance of surface-renewal eddies in winddriven turbulence, compared to pure wind-driven turbulence. The swell effects on the surfacerenewal frequency lead to the reduction of the mass transfer across the sheared air-water interface.

(2) The swell effects can be explained by the turbulence structure. Swell promotes the total drag over the air-water interface because of large wave amplitude, but the friction drag is decreased by the flow separation generated behind the wave crest. The reduction of the friction drag results in the decrease in the surface-renewal frequency.

(3) Turbulent mixing is significantly promoted in the free surface region by rainfall and therefore it enhances the CO2 transfer across the air-water interface.

(4) The mass transfer velocity is well correlated by the mean kinetic energy of rain droplets impinging on the unit area of the air-water interface. The values of the mass transfer velocity correspond to those measured in wind-driven turbulence with wind speeds ranging from 4m/s to 12m/s.

These results suggest that the effects of swell and rainfall on the CO2 exchange rate should be considered in a general circulation model for estimating global warming.

Acknowledgements

This work was supported by the Japanese Ministry of Education, Science and Culture through grants-in-aid (No.14102016) and the 21st Century Center of Excellence Program for Research

and Education on Complex Functional Mechanical Systems. The DNS was carried out by using a parallel super computer of the Center for Global Environment Research, National Institute for Environmental Studies, Environmental Ministry of Japan. The author would like to thank K. Tanno and N. Takagaki for their help.

References

Banks, R.B. & Herrera, F.F. (1977). Effect of wind and rain on surface reaeration. J. Environ. Eng. Div, ASCE, 103, 489 - 504.

Ho, D.T., Asher, W.E., Bliven, L.F., Schlosser, P. & Gordon, E.L. (2000). On mechanisms of raininduced air-water gas exchange, *J. Geophys. Res.*, 105, 24045 - 24057.

Komori, S., Nagaosa, R. & Murakami, Y. (1993). Turbulence Structure and Mass Transfer across a Sheared Air-Water Interface in Wind-Driven Turbulence, *J. Fluid Mech.*, 249, 161-183.

Komori, S., Shimada, T. & Misumi, R. (1999). Turbulence Structure and Mass Transfer at a Wind-Driven Air-Water Interface, in *Wind over Wave Couplings* (eds. S. G. Sajjadi, N. H. Thomas and J. C. R. Hunt), Oxford University Press, pp.273-285.

Komori, S. & Misumi, R.(2002). The Effects of Bubbles on Mass Transfer across the Breaking Air-Water Interface, in *Gas Transfer at Water Surfaces* (eds. E. S. Saltzman, M. Donelan, W. Drennan and R. Wanninkhof), AGU Monograph, pp.285-290.

Kunugi, T. & Satake, S. (2002) Direct Numerical Simulation of Turbulent Free Surface Flow with Carbon-Dioxide Gas Absorption, in *Gas Transfer at Water Surfaces* (eds. E. S. Saltzman, M. Donelan, W. Drennan and R. Wanninkhof), AGU Monograph, pp.77-82.

Liss, P. S. & Merlivat, L. (1986). Air-Sea Gas Exchange Rates: Introduction and Synthesis, in *The Role of Air-Sea Exchange in Geochemical Cycling* (ed. P. Buat-Menard), D. Reidel, pp.113-127.

Nagata, K. & Komori, S. (2001) The Difference in Turbulent Diffusion between Active and Passive Scalars in Stable Thermal Stratification, *J. Fluid Mech.*, 430, 361-380.

Tans, P.P., Fung, I.Y. & Takahashi, T. (1990). Observational constraints on the global atmospheric CO2 budget., *Science*, 247, 1431-1438.

Wanninkhof, R.(1992). Relationship between Wind Speed and Gas Exchange over the Ocean, J. *Geophys. Res.*, 97, 7373-7382.

Zhao, D., Toba, Y., Suzuki, Y. & Komori, S.(2003). Effect of wind waves on air-sea gas exchange: Proposal of an overall CO2 transfer velocity formula as a function of breaking-wave parameter. *Tellus*, 55B, 478-487.

Dynamical and Complex Behaviors in Control Systems and Human-Machine Co-Adaptive Systems

Tetsuo Sawaragi

Department of Precision Engineering Graduate School of Engineering, Kyoto University

Abstract

Human and computer subsystems should be structured and designed to work in mutually cooperating ways guaranteeing a user's usability. For this purpose, progressive system redesigns are needed with respect to human computer interactions to increase system reliability and transparency by increasing human-system interactions and especially a human user's proactive participation, rather than by eliminating the human out of the loop. Such a socially-centered view on the human-machine system design regards a human and an automated agent as equivalent partners, and through their mixed-initiative interactions some novel relations of mutual dependency and reciprocity would emerge as well as flexible changes of role-taking are expected. To realize such a kind of new style of human-machine relationships, we develop a new idea called co-adaptive design principle, which means that both a human user and a machine should be able to adapt to the other through experiencing the interactions occurring between them. We applied this idea to an artifacts design; interface agent of robot tele-operation and human-agent collaborative systems.

1 INTRODUCTION

The conventional division between human beings and machines should be modified in the context of thinking about evolutionary engineering processes. Human beings and the technologies including computers, communication devices, electronic networks, etc. should all be understood to be part of the system. Wherein, changes in the individual parts may take place through introducing alternate components, and all of these changes are part of the dynamics of the system. Sometimes such changes may be too complex for a designer to predict the behaviors emerging out of those.

Today's advanced automation might be indeed experts in solving/performing particular tasks, but have no means of relating to human users. Thomas Sheridan at MIT has called this "autistic automation"[3]; "autism" represents those humans who seem to have lost their skill of becoming engaged, being embedded in a situation, a sense of belonging to the world and to their partners. Actually, such an aspect is becoming an origin of a new type of human errors caused by some mismatch between a human and machine autonomy (e.g., a well-known *automation-induced surprise* in aviation [4]). As a concept of human-centred automation [5] reveals, automation needs to behave "socially"; automation should learn a variety of powerful social rules which

minimize interference and maximize group (i.e., human-automation) benefit and automation systems should be designed from the perspectives of "relations" and "processes" that may emerge out of the interactions between the automation and the human user.

In this paper, after surveying the problems incurred by the conventional technology-centered automation in a variety of fields, we put an emphasis on the fact that a concept of sociality is really needed to form the ideal relations of human-automation and to let them emerge out of intimate interactions. To realize such a kind of new style of human-machine relationships, we develop a new idea called *co-adaptive* design principle, which means that both a human user and a machine should be able to adapt to the other through experiencing the interactions occurring between them. We applied this idea to a variety of artifacts design of robot tele-operation and human-agent collaborative systems.

2 HUMAN-AUTOMATION DIS-COORDINATION

One of the domains in which the most advanced automation is prevailing is an aviation domain, but the interactions among the pilots, air traffic controller and many automated devices may cause a new type of incidents and/or accidents initiated by a human error triggered by an usage of automation devices. The following is an overview of the actual accident of "near-miss," that was caused by the dis-coordination among a human air traffic controller and a pilot as well as an automated device of TCAS (i.e., warning device for aircraft collision avoidance).

In January 31, 2001, Japanese Commercial Airlines, aircraft A and B (Boeing 747-400D and a McDonnell Douglas DC-10) came within 10m of a collision in a nearmiss incident in which the 747 crew ignored evasive action advice compounding suspected errors by air traffic control (ATC). On beginning a descent to 35,000 ft (10,675m) ordered by ATC, aircraft A's TCAS gave a serious 'RA' warning and the verbal order 'climb.' However the captain disregarded the advice and continued the descent. Meanwhile aircraft B's pilot was following descend advice from TCAS. But on seeing A's descending too, he started climbing back to 37,000ft. At some point during this maneuver both aircraft came within 10m as they crossed over. Air traffic controllers conducting training apparently gave confused instructions and repeatedly used the wrong flight numbers putting them on the same altitude and similar course.

The direct cause of the above accident is an air traffic controller's confused instructions, but this accident is revealing one aspect of limitation of current automation technologies. Human's judgment is "dynamic" in nature; his/her judgment is formed by a series of instructions by gathering cues to confirm his/her hypothesis under uncertainty. On the other hand, the judgment mechanism of the automation (such as a TCAS above) and its ways of conducting a human user is solely based upon a static status according to the predefined control logics, which may sometimes cause a conflict. This is illustrated in Fig.1.



Figure 1. Autistic automation.

Here, we think that progressive system redesigns are needed with respect to human-automation interactions to increase system reliability and transparency by increasing interactions and especially a human user's proactive participation, rather than by eliminating the human out of the loop. Such a *socially-centered* view on the human-machine system design regards a human and an automated agent as equivalent partners, and through their mixed-initiative interactions some novel relations of mutual dependency and reciprocity would emerge as well as flexible changes of role-taking are expected. Our idea of *co-adaptive* design principle is illustrated in Figure 2.



Figure 2. Co-adaptive system design principle (Modified from [8]).

3 HARNESSING: A NOVEL CONTROL AND DESIGN PRINCIPLE FOR COMPLEX SYSTEMS

In order to enrich the interactions between a human and machine autonomy and to let such a friendly and social relationships emerge through those interactions, we should abandon the conventional straightforward "control" doctrine and develop a novel principle for human-machine interactions. We think that a promising idea as an alternative to that is "harnessing", whose characteristics are described as follows.



Figure 3. Tele-operated mobile robot

- (1) External input only gives direction for the path and its strength is kept as small as possible.
- (2) Minimize the control input and let the system move by its own dynamics with reasonable resolution (i.e., not seeking for preciseness).

Machines to which this harnessing capability is embedded are assumed to generate a humanfriendly mechanical behavior and as well as to present biological significance. For this purpose, machines should be evolvable though experiencing the interactions with a human, who is allowed to interact with a machine demonstrating a human competency.

4 SHARED AUTONOMY BETWEEN HUMAN AND MACHINE

As a testbed for constructing a human-machine collaborative system, we deal with a teleoperation system for a mobile robot as shown in Fig.3. We characterize this system as a shared autonomy system, meaning both machine autonomy and human autonomy must be shared. A main focus of a conventional simple tele-operation system has been attended to design an interface so that it could transfer an operator's control intentions and commands to a robot exactly as well as it could show a robot's behavior to a human as transparent as possible. Wherein, an ideal interface is the one that can establish a *morphological* mapping between a human task and a robot's task.

On the other hand, in a shared autonomy system both a human and a machine have their own autonomies, whose intentions are sometimes competitive and conflictive at least at the initial time. Through experiencing those conflicts and introspecting those competitions, both a machine and a human should be able to mutually adjust their judgments with each other and to find their own "niche" to perform collaboratively.

5 A GENERIC MODEL FOR CO-ADAPTATION BETWEEN TWO HETEROGENEOUS AUTONOMOUS AGENTS

As a generic model for such a co-adaptive process emerging in collaboration by two autonomous entities, we construct a model shown in Fig.4 as a pair of autonomous entities, each of which is a self-organizing system consisting of hierarchical structures simultaneously undergoing a variety of distinguishable activities. Different sets of variables and parameters are appropriate to a state

space description pertaining to these activities taking place at the individual levels. Wherein, independence of descriptions of state spaces between the two entities is essential, and just a physical channel interconnecting them is shared. We do not assume that neither any "symbols" nor any "meanings" can be transferred on this channel, since symbols should be constructed and grounded by the autonomous entities by themselves in a self-enclosed way rather than by a system designer's ad hoc definition. We just assume that what can be shared between them should be restricted to information of an object level in terminologies of Pierce's classical idea of *semiosis*.

One of the key concepts of complex systems is a paradox that more than two competitive criteria may co-exist within a single entity as well as within an organization and/or team of them



Figure 4. Human-robot Co-adaptation

[1], [2]. This characteristic is making the behaviors generated both at a single agent level and at an organizational level dynamical and complex. That is, they cannot be implemented as a simple input-output function and is quite different from a classical stimulus-response model proposed in conventional behavioral psychology. Rather, a complex system behavior is characterized by the key properties of "open" systems, where flows of matter, energy and information can occur across their boundaries, and this makes them undergo spontaneous transformations of structure and functionality within and among entities. Successive instabilities occur each time that existing structure and organization fail to withstand the impact of some new circumstance or behavior. When this occurs, the system re-structures and becomes a different system, subjected in its turn to the disturbances from its own non-average individual entities and situations. It is this interaction between successive systems and their own inner richness that provides the capacity for continuous adaptation and changes.

For realizing such a dynamics between two heterogeneous autonomous agents (i.e., a human and a machine agent), a hierarchical structure consisting of two layers is essential. Lower layer deals with the basic competitive and cooperative dynamics, and upper layer called an internal model maintains macroscopic status of its internal states evolving at lower layer from meta-level perspectives. In each of the autonomous entities, this basic architecture enables a reciprocal and



Figure 5. Payoff table for dynamics

bidirectional interactions. In the bottom-up direction some kind of order parameter constructed from the lower level is viewed as a representation of the internal model at a higher level, related with some macroscopic behavior ranging between two extremes of "autistic" and "social". In the top-down direction, on the other hand, only a few instructions and/or simple parametric commands are sent to a lower level intermittently, and then ongoing non-equilibrium statistical mechanics at the lower level may be affected indirectly and another equilibrium phase transitions may occur. In a word, the upper level takes a role of "harnessing" a dynamic behavior at the basic level by just adjusting a single parameter governing the dynamics at the lower.

In our framework, dynamics at lower level is implemented as non-constant-sum, nonnegotiable "Paradoxical" games in order to implement an "Ego" drifting between "selfishness" and "altruism" [6]. This game is wellknown as a Prisoner's Dilemma (PD) game and Chicken game (CG). In this model, each of the two players (agent 1 and 2) takes either of cooperation (C) or defeat (D) on the partner, thus their state is one of the four possible states of CC, CD, DC, or DD. For each state, payoffs that each of the players can get are defined as illustrated in Fig.5. In CC (both players take a cooperation), both of them can get a payoff of 1.0, but when either of the player takes defeat and the other takes cooperation, the payoff of a defeating player is ξ , while the payoff of a defeated one is $-\xi$. If both of them take defeat, the payoffs of the both players are reduced to -1.0 and this paradoxical outcome leads to "behavioral paralysis". If the payoff for DD is increased from -1.0 to -2 ξ , then the state DC and CD become local equilibria since DD state is too expensive for the players to afford ("Chicken game").

By assuming the games are played in iteration, learning takes place, which means that the time evolution of the propensities is governed by a system of two first order non-linear differential equations; the time derivatives of the propensities are proportional to the gradient of the expected payoffs with respect to that propensity. This is illustrated in Fig.6, in which a parameter ξ is set to a particular value. This figure shows; when two agents start from particular initial values of the propensities to keep taking cooperation, they get to be converged into one of the four states through iterating the games. Thus, this illustrates the internal dynamics of a single autonomous agent, in which competition and cooperation with its partner coexist. This Markovian kinetics providing the basic dynamics at the lower level do not evolve under a fixed ξ (i.e., a game type), but the changeover between game types might be possible within each individual when the expected payoff with the previous game seems to be reaching local plateaus, and this changeover may be adjusted by changing a parameter ξ from the upper layer.

Then, how and when does this parameter of ξ should be adjusted from the upper level? It depends both on;

(1) Its own state: how consistent so far within itself (i.e., entropy of the state

occupancy) that drives transitions of states at the higher level towards autistic attitude.

(2) Its partner's state: how consistent so far with its partner's (i.e., cross-correlation with the partner's behaviors) that drives transitions of states at the higher level towards social attitude.



Figure 6. Evolution of transients of internal states along lerning.

Communication channel between the two autonomous agents is used for calculating the above cross-correlation. In other words, neither of any explicated intentions nor symbolic information is transmitted on it, but just cues that indirectly affect on both of the dynamics are transferred. Interpretation of those and how they are transformed into the adjustment of the parameter ξ are done in a self-enclosed way within the individual agents according to the above rules (1) and (2).



Figure 7. Complex System Model for Co-Adaptation

6 CONSTRUCTIVE APPROACH TO DESIGN AND CONTROL OF HUMAN-MACHINE CO-ADAPTIVE SYSTEMS

Based on the generic model for co-adaptation mentioned in the previous subsection, we are now taking a constructive approach to design and control of a variety of human-machine co-adaptive systems [7]. Constructing and simulating this model, we compare the model output with the reality. Based upon the above co-adaptation model, we are investigating into design of human-machine interface for tele-operated mobile robot and human-agent collaboration for a task of simulated boat rowing.

The former study aims at a new design framework for combining and capitalizing on both advantages of the human- and the mechanized automatic controls into their joint activity (i.e., shared control), wherein their well-coordinated collaboration is achieved through the interaction of dynamic and mutual shaping function allocations among them. Implementations of shared communicational modality between a human and a machine autonomy is realized by letting the interaction of the robot autonomy transfer onto the joystick using the feedback force and by letting the operator's and the autonomy's input actions be mutually restricted through that joystick. Through experiments of a navigating problem of a mobile robot in a simple corridor environment, we identify the difference of cue-utilization style between human operator and robot autonomy. Developing an algorithm of machine autonomy's adaptation, we verified that a human and a

machine get to find their own niche; they get to take different roles and to construct their own control policies through experiencing the interactions.



Figure 8. Boat rowing simulator

The latter study deals with a micro world simulation testbed for human-agent collaboration as shown in Fig.8. Wherein, a human and an automated agent take parts of rowing individual oars to steer the boat to the destination. The difficulty in this collaborative task is that this task requires balanced rowing of both oars. Here, our interest lies in what kinds of information in the display of the simulator the human is using as cues needed for the collaboration with the automated agents that row the oar in three different autonomous ways. Wherein, a human and an automated agent are, at least initially, two independent judges making individual judgments within the common task ecology of the boat-rowing system. To see the effects of an agent's autonomy on a human, we design the cues available to an agent in three different ways. Moreover, in order to investigate into the relationships among the human-agent-environment we design a number of displays by changing the perspectives of the ongoing task within the virtual display of the simulator, and thus by changing available cues to a human rower. We change the parameters of the co-adaptation model and compare the results with the actual data obtained in the experiments using the boat-rowing simulator.

7 CONCLUSIONS

In this paper, we stressed an importance of automation's ability to form relations and to share a process with a human operator through intimate interactions. Proposing a novel design principle of co-adaptive systems, we analyzed a set of experimental results of human-machine collaboration and showed a way of constructive approach to the design of complex human-machine interactions. Preliminary experiments were performed and satisfactory results were obtained, that are to be presented at the final version of the manuscript. This work is attained under the 21st Century COE (Center of Excellence) Program of "Research and Education on

Complex Functional Mechanical Systems" that is ongoing at Kyoto University. For more detailed information, please refer to the following home page of our program; <u>http://www1.mech.kyoto-u.ac.jp/coe21/</u>.

References

- [1] Kaneko, K. and Tsuda, I.: Chaotic Scenario of Complex Systems, Springer-Verlag Berlin and Heidelberg GmbH & Co. K (2000)
- [2] Bar-Yam, Y.: Dynamics of Complex Systems: Studies in Nonlinearity, Perseus Books (2003)
- [3] Sheridan, T. B.: Humans and Automation: System Design and Research Issues, Wiley-Interscience (2002)
- [4] Bainbridge, L.: The Change in Concepts Needed to Account for Human Behavior in Complex Dynamic Tasks, Trans. of IEEE on SMC, 27-3, pp.351-359 (1997)
- [5] Billings, C.E.: Aviation Automation: The Search for a Human Centered Approach, Lawrence Erlbaum Ass. (1997)
- [6] Axelrod, R.: The Complexity of Cooperation: Agent-Based Models of Competition and Collaboration, Princeton Univ Pr (1997)
- [7] Sawaragi, T.: Human-Automation Coordination Mediated by Reciprocal Sociality, Preprints of IFAC 15th Triennial World Congress, CD-ROM (2002)
- [8] Dautenhahn, K.: I could be you: the Phenomenological Dimension of Social Understanding, Cybernetics and Systems, 25(8), pp.417-453 (1997)

Momentum and Heat Transport Mechanisms of Fluid Motion in a Rotating Annulus

Phan Vinh Long and Masato Nagata

Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University

Abstract

Fluid motions induced by thermal buoyancy in a rotating system and in the presence of a mean zonal shear have been of considerable interest to geophysical fluid dynamicists and astrophysicists. In this paper, we analyze the momentum and heat transport mechanisms due to the interaction between convection and the Taylor vortices between two coaxial differentially rotating cylinders fixed at different temperatures. We attempt to apply the results of our analysis to geophysical problems.

1 INTRODUCTION

Hydrodynamic instability of fluid motion in rotating spherical shells with spherically symmetric gravity and heat source distributions is one of the fundamental problems of geophysical fluid dynamics. The problem describes the dynamics of convection in the liquid outer core and in the deep atmospheres of the Earth. Furthermore, it is not unlikely that convection in the Earth's core is responsible for the generation of the Earth's magnetic field.

Fortunately, much can be learned about the problem in spherical shells from the simpler problems of convection in a layer with a vertical axis of rotation and in a layer with an axis of rotation at a right angle to gravity. For the latter case the problem can be realized in the form of a rotating cylindrical annulus in which the centrifugal force replaces gravity (Auer et al., 1996; Kropp et al., 1991). The annulus model has thus become the primary tool for the investigation of convection in the equatorial region of spherical shells. Besides their potential geophysical and astrophysical applications the flows observed in those configurations have received much attention on their own right because of their interesting dynamical properties. In this paper the problem of the instabilities of flow in a differentially heated rotating annulus is revisited and a new type of instability is pointed out which may be relevant for some of the laboratory experiments

2 ANALYSIS

We consider the motion of a viscous incompressible fluid between two concentric cylinders of infinite extent in the axial direction. The flow is induced by the differential rotation and the

differential heating of the two cylinders. The system is subject to the constant rotation about the common axis of the cylinders. Therefore, the centrifugal force replaces gravity. The Boussinesq approximation is used in which the buoyancy force due to the density variation in the radial direction is taken into account only through the gravity term in the governing equations.



2.1 Geometrical configuration

Figure 1. (a) The geometrical configuration. (b): The A-type and (c): the B-type.

The cylindrical coordinate system shown in Figure 1(a) is used in the analysis. The basic steady conductive state represented by the flow in the azimuthal direction and the temperature variation across the cylinders exists as the exact solution of the system of the relevant differential equations. Both the flow and the temperature variations are independent of the axial coordinate z and the azimuthal coordinate . We are interested in the development of the flow field bifurcating from this basic state as the parameters of the system are varied. Two typical non-linear states are shown schematically in Figures 1(b) and (c). The A-type is described by the transverse roll solution where the wavenumber in the azimuthal direction is non-zero with the vanishing in the axial direction while the B-type is characterized by the longitudinal roll wavenumber solution represented by the wavenumbers = 0 and 0. As described below three-dimensional 0) are also possible. states (0,

2.2 Controlling parameters

The dimensionless parameters which control the motion of the fluid flow of the system are the Reynolds number Re, which measures the differential rotation of the cylinders, Rayleigh number Ra, which describes the temperature difference of the cylinders, the system rotation number ., the radius ratio ______, of the two cylinders and the Prandtl number Pr, which characterises the material property of the working fluid.

2.3 Numerical methods

Discretisation of the system of the relevant partial differential equations must be made for numerical purposes. Here, we use the Chebyshev collocation method in the radial direction combined with Fourier series expansions in the axial and the azimuthal directions. For the stability of the flow field we carry out the normal mode analysis for a perturbation imposed on the undisturbed state. When the perturbation grows to a state where its magnitude cannot be neglected anymore the non-linear analysis must be required. For obtaining non-linear solutions we apply the bifurcation analysis to the corresponding non-linear dynamical system which is solved numerically by the Newton-Raphson iterative method.

3 RESULTS

Figure 2(a) shows the critical Rayleigh number in the *Re*- space for the case of a narrow gap =0.999 for air (*Pr*=0.7). The A-type or the B-type solution bifurcates supercritically above the critical Rayleigh number depending on the values of *Re* and . The heat transport of the bifurcating A-type is given in Figure 2(b) for *Re*=0 and =25. It is found that the momentum transport of the transverse roll solution is the same as the basic flow.





(a): The momentum transport. (b): The heat transport.

The momentum transport and the heat transports for the longitudinal roll solution are compared with those of the basic flow Re=20 and =17 in Figure 3. As we can see both the transverse roll and the longitudinal roll solutions enhance the heat transport drastically from the conducting state.



Figure 4. The critical Rayleigh number for =0.8 and Pr=7.

When water (*Pr*=7) is filled in a relatively wide gap between the cylinders three-dimensional flows (0, 0) may bifurcate above their critical Rayleigh numbers. Figure 4 indicates the critical Rayleigh number in the Re- space for the three-dimensional solutions as well as the A-type (0, = 0) and the B-type (= 0, 0) solutions for =0.8. Among the wide variety of combination of the controlling parameter values we concentrate on the following three cases.

3.1 Case I

No heating (Ra = 0) is imposed so that the flow properties are independent of the Prandtl number. Fluid is confined in the limit of narrow gap (=1) between the cylinders which rotate at almost equal angular speed (=<< Re). For this case the curvature effect is negligible and the differentially rotating cylinders can be regarded as parallel planes which move in the opposite directions with the same speed as shown in Figure 5(a). In the absence of the system rotation with the axis of rotation in the spanwise direction y, the problem is reduced to the well known plane Couette flow (see Figure 5(b)).



Figure 5. (a): Rotating plane Couette flow and (b): the (non-rotating) plane Couette flow.

Plane Couette flow with no inflection point in its basic velocity profile is the simplest form of shear flows. Yet, the problem of its non-linear stability has been the most difficult one in the fluid

mechanics for decades. The reason for this is that the flow had been proved to be stable for any finite Reynolds numbers and therefore no direct bifurcation from the basic state is possible, whereas experiments have observed various types of instabilities leading to turbulence.

In 1990 Nagata solved the problem finally by extending his non-linear analysis on Taylor-Couette flow in the limit of the narrow gap and almost co-rotating case (Nagata, 1986, 1988). Nagata discovered that the branch of three-dimensional tertiary flows bifurcating from the secondary flows in the form of the A-type still exists as the system rotation is reduced to zero for some wavenumbers (Nagata, 1990). Since the discovery of the non-linear state Nagata's solution is considered to be precursors of the turbulent dynamics and to assist in the process of transition from the laminar state.

3.2 Case II



Figure 6. The critical Rayleigh number for the case of Pr=0.7, Re=200 and =0.999.

Figure 6 shows the critical Rayleigh number for various types of solutions for Pr=0.7, Re=200 and = 0.999. It can be seen that for moderate rotation rates the longitudinal roll solutions are responsible for instability whereas instability takes a transverse roll pattern for high rotation rates. Three-dimensional flow may appear in the small neighbourhood where the A-type and the B-type become equally competitive. It is found that the three-dimensional flow manifests itself in the form of a spiral pattern.

3.3 Case III



Figure 7. The heat transport of the A-type for Re=0, =8, =0.8 and Pr=7.

The critical Rayleigh number for water in a wide gap annulus was given in Figure 4. Here, the case of the rigid rotation (Re=0) is of our interest. The heat transport for the transverse roll solutions for =8 is given in Figure 7.

It may be seen from Figure 4 that there is a region of low rotation rates (0 < < 2) on the line of Re = 0 where three-dimensional instabilities set in. The bifurcation is degenerate at their onset in the sense that developed flow patterns cannot be predicted by the linear analysis. In our case the non-linear analysis reveals that the bifurcating three-dimensional solutions are actually two-folded; two distinct forms of solutions, spirals and zigzags, are identified with different transport properties as shown in Figure 8.



Figure 8. (a):The momentum transport and (b): the heat transport for Re=0, =1, =0.8 and Pr=7.

4 SUMMARY

The bifurcation of flows in a differentially heated rotating annulus has been presented for three typical cases. The momentum transport and the heat transport depend upon the flow pattern of bifurcating solutions.

The analysis on our simple system should contribute towards the understanding of the basic mechanism of the complex heat and momentum transports in the Earth's global structure.

References

Auer, M., Busse, F. H. & Gangler, E. (1996) Instabilities of flows between differentially rotating coaxial vertical cylinders in the presence of a radial temperature gradient, *Eur. J. Mech., B/Fluids*, 15, No. 5, 605-618.

Kropp, M. & Busse, F. H. (1991) Thermal convection in differentially rotating systems, *Geophys. Astrophys. Fluid Dynamics*, 61, 127-148.

Nagata, M. (1986) Bifurcations in Couette flow between almost co-rotating cylinders, J. Fluid Mech., 169, 220-250.

Nagata, M. (1988) On wavy instabilities of the Taylor-vortex flow between co-rotating cylinders, *J. Fluid Mech.*, 188, 585-598.

Nagata, M. (1990) Three-dimensional finite-amplitude solutions in plane Couette flow: bifurcations from infinity, *J. Fluid Mech.*, 217, 519-527.

Bone Functional Adaptation by Remodeling through Hierarchical Mechanical Systems from Cell to Tissue

Taiji Adachi

Department of Mechanical Engineering, Graduate School of Engineering Kyoto University

Abstract

At the tissue level, living bone dynamically adapts its internal structure by remodeling to accomplish its mechanical function as a load bearing structure under the influence of mechanical environment. This functional adaptation by remodeling is accomplished by complex coupled osteoclastic resorption and osteoblastic formation at the cellular level. In this article, how mechanical viewpoints can approach to better understanding of the adaptive bone remodeling mechanism through the hierarchical mechanical function-structure relations from cell to tissue will be addressed, and computational simulations for trabecular surface remodeling in a proximal femur and for cancellous bone regeneration using a porous scaffold are presented.

1 INTRODUCTION

Living bone tissue has an ability to adapt its internal structure and outer shape to the mechanical environment through the processes of remodeling as well as regeneration (Martin et al., 1998); those are defined as the coupled formation and resorption by cellular activities (Parfitt, 1994). One of the important questions is how mechanical stimulus at the cellular level is integrated into the tissue level remodeling/regeneration, through the complex hierarchical systems (Fig.1), that construct trabecular bones with a mechanical integrity to match with their functional demands.



Figure 1: Hierarchy in bone mechanical system from tissue to cells and molecules.

The author have been conducted mathematical modeling and computational simulation of trabecular surface remodeling (Adachi et al. 1997; 2001a, Tsubota et al., 2002 2003, 2004) and in vitro experimental studies on osteoblastic responses to the mechanical stimulus (Adachi, et al., 2001b, 2003), in which how mechanical information transduced into the osteoblastic cells and how these information is integrated into the osteoblastic bone forming activities that construct well-organized macroscopic trabecular architecture. In this report, computational simulations for trabecular surface remodeling in a proximal femur and its application to the design of porous microstructure of the scaffold for bone regeneration will be discussed.

2 CANCELLOUS BONE ADAPTATION IN PROXIMAL FEMUR PREDICTED BY TRABECULAR SURFACE REMODELING SIMULATION

Trabecular structure in cancellous bone changes by surface remodeling due to cellular activities, where local mechanical stimulus plays an important role (Cowin et al., 1991). So far, bone remodeling simulation based on macroscopic continuum mechanics has been performed to investigate the relationships between bone structure and mechanical function at cancellous level (Huiskes et al., 1987, 2000; Jacobs et al., 1997). To understand the mechanism of functional adaptation in cancellous bone, adaptation process at microscopic level should be considered in the remodeling simulation. In this chapter, two-dimensional simulation of trabecular surface remodeling was conducted for a proximal femur to investigate the relationship between local adaptation process at trabecular level and functional adaptation phenomenon at cancellous level.

2.1 Simulation Methods for Trabecular Surface Remodeling

A computational model of a human proximal femur was created by using about 0.67 million twodimensional finite elements, as shown in Fig.2(a). Assuming an isotropic trabecular structure at the initial stage, the cancellous bone morphology was created by randomly pasting circular trabeculae, as shown in Fig.2(b), whose external and internal diameters were 1680 μ m and 1120 μ m, respectively. The principal values of the fabric ellipse of the cancellous bone, H_i (i = 1, 2, H₁ > H₂), were H₁ = 714 μ m, and H₂ = 713 μ m. The bone was assumed to be a homogeneous and isotropic material with Young's modulus E = 20 GPa and Poisson's ratio $\nu = 0.3$.

As a daily loading condition, multiple-loading condition was assumed, which consists of three loading cases, (i) a one-legged stance (6000 cycles/day), (ii) extreme ranges of motion of abduction (2000 cycles/day), and (iii) adduction (2000 cycles/day) (Beaupré et al., 1990). These external loadings were applied as distributed forces generated by using a sine function to the joint surface and the greater trochanter. The lower boundary that corresponds to the diaphysis was fixed. To neglect the effect of the fixed boundary condition on the results, only the proximal region of the model above the line A-A' shown in Fig.2(a) was discussed. The two-dimensional stress analysis was performed under the plane strain condition with a 10mm thickness.

In the remodeling simulation, the local stress nonuniformity on a trabecular surface was evaluated by $\Gamma = \ln(\sigma_c/\sigma_d)$ where Γ_c denotes the stress at point x_c on the trabecular surface and δ_d denotes the representative stress within sensing distance l_L . By regarding local stress nonuniformity Γ as the driving force of the trabecular surface remodeling, a rate of surface movement \dot{M} at the point xc was determined by Γ as $\dot{M} > 0$ ($\Gamma > 0$) and $\dot{M} < 0$ ($\Gamma < 0$) to seek a local uniform stress state (Adachi et al., 1997; 2001). Model parameters introduced in the

remodeling rate equation were set as sensing distance $l_L = 1.0$ mm, and threshold values $\Gamma_u = 1.0$ and $\Gamma_l = 2.0$.



(a) Large scale pixel-based FE model (b) Initial morphology of cancellous bone Figure 2: Computational model of human proximal femur.

2.2 Results and Discussion

A trabecular surface remodeling simulation was conducted for cancellous bone in the human proximal femur under multiple loadings for 12 steps. Nonuniform stress on the trabecular surface induced bone resorption and formation, which resulted in the change of trabecular architecture from the random one at the initial stage, as shown in Fig.2(a), to the anisotropic one at the 12th step, as shown in Fig.3. In the femoral head (region 1), trabeculae were aligned along the direction of the compressive joint reaction force. In the greater trochanter, the trabeculae were aligned along the tensile abductor force direction. On the other hand, in the lower region of the femoral neck (region 2), compressive trabeculae formed from the medial to the lateral near the greater trochanter, and tensile trabeculae formed from the lateral to the neck of the femoral head, forming the orthogonal trabecular pattern.





To investigate the functional adaptation phenomenon at cancellous level, the apparent principal stress in the regions 1 and 2 at the initial stage and the 12th step was calculated by averaging stress components over the each cancellous area. The stress components were averaged with the weight depending on the loading frequency. The principal stress is defined as $|c_1| > |c_2|$. At the initial stage, the ratio of the magnitude of two principal stresses was large in the regions 1 ($|c_1|/|c_2|=12.6$), where a unidirectional trabecular pattern formed. Therefore, the mechanical environment was a uniaxial compressive state in the region 1 and a uniaxial tensile state in the trochanter region. Although the trabecular structure changed by remodeling, the two principal stresses, $|c_1|$ and $|c_2|$, and direction Θ_{δ} at the 12th step did not change much from the values at the initial stage. In the region 2, where the orthogonal trabecular pattern emerged, the ratio $|c_1|/|c_2|$ was relatively close to unity ($|c_1|/|c_2|=1.4$). This result indicates that the mechanical environment was a bi-axial compressive-tensile state.

An anisotropic structure of trabecular bone was obtained according to the mechanical environment in the proximal femur by trabecular surface remodeling to seek a local uniform stress state. The trabecular orientation predicted in the simulation was similar to that observed in the actual proximal femur. The principal direction of the fabric ellipse approximately agreed with that of the principal stress, and the degree of anisotropy of the trabecular structure corresponded to the ratio of magnitude of the two principal stresses. These results indicate that the local regulation process at trabecular level causes cancellous-level functional adaptation to the mechanical environment. It is also shown that the proposed simulation method is capable to provide insight into the micro- to macro- hierarchical mechanism of trabecular surface remodeling.

3 MICROSTRUCTURAL DESIGN OF POROUS SCAFFOLD USING COMPUTATIONAL SIMULATION FOR BONE REGENERATION

Microstructure of porous scaffold (Taboas et al., 2003) affects bone regeneration in which new bone formation and scaffold degradation occurs in the same time frame. Thus, geometry and size of the microstructure are important factors to control the regenerated bone properties as well as regeneration process. The purposes of this chapter are to propose an optimum design method of porous scaffold using a computational simulation for bone regeneration, and to investigate the effect of the porous scaffold design parameters, such as pore size, on regenerated trabecular bone structure using a computational simulation of bone regeneration.

3.1 Simulation Methods for Bone Regeneration Using a Porous Scaffold

Both scaffold degradation and new bone formation were computed to simulate the bone regeneration process. Scaffold degradation rate due to hydrolysis, decrease in polymer molecular weight, was simply assumed to be determined by water content diffused from the surface into a polymer material governed by the diffusion equation. A rate equation of trabecular surface remodeling (Adachi, 2001a) was used for new bone formation, in which new bone forms on bone and scaffold surfaces. In this model, local stress nonuniformity on the bone and scaffold surfaces is assumed as a driving force of new bone formation.

Scaffold and bone were modeled as isotropic elastic materials with Young's modulus Es and Eb, respectively, where Es decreases proportionally to a decrease in the molecular weight of the

scaffold. Stress was analyzed by a finite element method, and the water diffusion in the scaffold material was solved by a finite difference method.

Bone regeneration was simulated for simple porous scaffolds with lattice-type and sphere-type cavities under uniaxial compressive stress, $\delta = 2.0$ MPa. Assuming a periodic scaffold structure, a unit cell model with edge length of 2.4 mm was discretized with 0.1 mm voxel finite elements. Design valuables were lattice interval and sphere diameter. Materials properties were set as Young's modulus $E_s = 20$ GPa and Poisson's ratio $v_s = 0.3$ for scaffold, and $E_b = 20$ GPa, $v_b = 0.3$ for bone, respectively.

3.2 Results and Discussion

Morphological change in bone-scaffold system in the bone regeneration process simulated by proposed method is shown in Fig.4. At the initial stage, new bone formation occurred on pore surfaces. Gradually the scaffold degraded and disconnected each other, loosing its mechanical function. Subsequently, newly formed trabeculae connected with each other, and finally, the scaffold was replaced by new trabecular structure.

From a mechanical viewpoint, stiffness as a bone-scaffold system is required to keep at the desired level during and after the process. To evaluate mechanical function in the process, change in strain energy of the bone-scaffold system was calculated, as plotted in Fig.5(a), showing that functional transition between two materials as a load-bearing component was accomplished. The regeneration process and the regenerated bone structure changed much depending on the initial scaffold pore size. Thus, the design problem was formulated to find an optimal initial scaffold pore size that minimizes the evaluation (objective) function.

$$\boldsymbol{\Phi}(r) = \int_{0}^{T} |U(t) - U_{h}| dt$$

(1)

where r represents the initial pore size, U_b is strain energy for an ideal bone, and T is the completion time of bone regeneration.





Figure 5(b) illustrates the dependence of cavity volume fraction on the evaluation function Φ for both lattice and spherical cavity scaffolds. In this case study, the optimum solutions were determined at the minimum point with $V_c = 0.62$ for the lattice-type scaffold and $V_c = 0.59$ for the spherical-type scaffold.

These simulation results demonstrated that potential of the proposed design method to determine the scaffold microstructure. For further application to design actual three-dimensional scaffold microstructure, quantitative characteristics of scaffold degradation and new bone formation have to be clarified experimentally those enable us to obtain appropriate rate equations.

The author would thank Dr. Ken-ichi Tsubota at Tohoku University and Prof. Masaki Hojo at Kyoto University for their valuable comments and discussions.

References

Adachi, T., Tomita, Y., Sakaue, H., and Tanaka, M. (1997), Simulation of trabecular surface remodeling based on local stress nonuniformity," *JSME Int. J.*, 40C-4: 782-792.

Adachi, T., Tsubota, K., Tomita, Y., and Hollister, S. J. (2001a), Trabecular surface remodeling simulation for cancellous bone using microstructural voxel finite element models, Trans ASME, *J. Biomech. Eng*, 123-5: 403-409.

Adachi, T., Murai, T., Hoshiai, S., and Tomita, Y. (2001b), Effect of actin filament on deformation-induced Ca2+ response in osteoblast-like cells, *JSME Int. J.*, 44C-4: 914-919.

Adachi, T., Sato, K., and Tomita, Y. (2003), Directional dependence of osteoblastic calcium signaling response to mechanical stimulus, *Biomech. & Model. Mechanobiol.*, 2-2: 73-82.

Beaupré, G. S., Orr, T. E., and Carter, D. R. (1990), An approach for time-dependent bone modeling and remodeling - Application: A preliminary remodeling simulation, *J. Orthop. Res.*, 8: 662-670.

Cowin, S. C., Moss-Salentijn, L., and Moss, M. L. (1991), Candidates for the mechanosensory system in bone, Trans. *ASME*, *J. Biomech. Eng.*, 113-2: 191-197.

Huiskes, R., Weinans, H., Grootenboer, H. J., Dalstra, M., Fudala, B., and Slooff, T. J. (1987), Adaptive bone-remodeling theory applied to prosthetic-design analysis, *J. Biomech.*, 20-11/12: 1135-1150.

Huiskes, R., Ruimerman, R., van Lenthe, G. H., and Janssen, J. D. (2000), Effects of mechanical forces on maintenance and adaptation of form in trabecular bone, *Nature*, 405-6787: 704-706.

Jacobs, C. R., Simo, J. C., Beaupré, G. S., and Carter, D. R. (1997), Adaptive bone remodeling incorporating simultaneous density and anisotropy considerations, *J. Biomech.*, 30-6: 603-613.

Martin, R. B., Burr, D. B., and Sharkey, N. A. (1998), Skeletal Tissue Mechanics, Springer-Verlag.

Parfitt, A. M. (1994), Osteonal and hemi-osteonal remodeling: The spatial and temporal framework for signal traffic in adult human bone, *J. Cell. Biochem.*, 55: 273-286.

Taboas, J. M., Maddox, R. D., Krebsbach, P. H., and Hollister, S. J. (2003), Indirect solid free form fabrication of local and global porous, biomimetic and composite 3D polymer-ceramic scaffolds, *Biomat.*, 24-1: 181-194.

Tsubota, K., Adachi, T., and Tomita, Y. (2002), Functional adaptation of cancellous bone in human proximal femur predicted by trabecular surface remodeling simulation toward uniform stress state, *J. Biomech.*, 35-12: 1541-1551.

Tsubota, K., Adachi, T., and Tomita, Y. (2003), Effects of a fixation screw on trabecular structural changes in a vertebral body predicted by remodeling simulation of trabecular surface remodeling, *Ann. Biomed. Eng.*, 31-6: 733-740.

Tsubota, K. and Adachi, T. (2004), Changes of fabric and compliance tensors of cancellous bone due to trabecular surface remodeling predicted by digital-image based model, *Comp. Meth. Biomech. & Bioeng.*, 7-4: 187-192.

From "Function Designing" to "Bio-Environment Designing"

Naohide Tomita

International Innovation Center Kyoto University

Abstract

As living tissue maintains its shape and function by adaptive self-remodeling, it is difficult to design an artificial shape and a function in the body. Our theme is the "in-vivo environment designing" which is the key factor for successful tissue-engineering treatment. Several biological, clinical and mathematical approaches to the "in-vivo environment designing" was introduced in the presentation to discuss how to design the proper environments and how to control the shape and the function of living tissues. Following issues were the examples;

1. Effect of environment on differentiation of stem cells

2. Total Joint Regeneration system as an environment-designing treatment.

1 "SELECTION FOR FUNCTION" AND "SELECTION OF EFFICIENCY"

The word "Function" has its origin in living thing. And Darwinistic consideration teach us that the function of the living thing have its origin in "selection". However, it is difficult to simulate the process of the "selection for function", because it should have a process to produce "aim" of the function. It is impossible to prove by simulation methods that some function is produced without any intention.

My opinion is that the "selection" should be divided into two categories; "Selection for function" and "Selection of efficiency". It would be possible that adaptive function would be produced by selection from diversity as shown in Fig. 1 (a). Each diverse shape is not a function, but become a adaptive function when it is selected in certain environment. This "selection for function" have high adaptability to the environment change. However, this selection process require relatively long time and high energy. "Feed back system"(which is a short-term memory system) can be produced by "selection of efficiency" as shown in Fig. 1(b). This system have higher efficiency in function generation. However, the adaptability is lower than (a). This system thought to have advantage in relatively stable environment. Some kind of "program" such as genome, may be produced as a result of the "selection of efficient and strong adaptation to the environment change. This kind of "program" might be too complicated to be produced by selection. However, no matter how low the possibility may be, only one accidental production of the reproducible program may enough to make the growing system. As the "program" such as

genome have efficient and strong adaptations to the environment, the "program" may have selected to spread on the earth.

These considerations (that the function is not designed but selected), give us some hint to reach an another understanding of biological function. For example, some diseases would be defined as malfunctions of the feed back system. And, some "selection" process could be assume to explain the differentiation of cell. Our approach is to explain some biological phenomenon by the "selection", and to argue that biological function should not be designed. Not the "Function Designing" but the "Bio-Environment Designing" thought to be the reasonable approach to the living function.



Fig. 1 Adaptative function would be produced by selection from diversity as shown in (a). The "selection for function" have high adaptability to the environment change. However, this selection process waste time and energy. "Feed back system" (which is a short-term memory system) can be produced by "selection of efficiency" as shown in (b). This system have higher efficiency in function generation. However, the adaptability is lower than (a). Some kind of "program" such as genome, may be produced as a result of the "selection of efficiency" as shown in (c). The "program" is a long-term memory system which shows efficient and strong adaptation to the envilonment.
2 EFFECT OF ENVIRONMENT ON DIFFERENTIATION OF STEM CELLS

12-week-old SD rats (Charles River Japan Inc., Yokohama, Japan) were used in this study. ES cells (CCE ES-cells) were transplanted subcutaneusly, or injected in knee joint of the rats. For other rats, full-thickness osteochondral defects were created in the articular cartilage on the patella groove, and the ES-cells were transplanted into the defects embedded in collagen gel. The animals were sacrificed 1,4, and 8 weeks after surgery, and the knee joints were evaluated histologically.



Fig. 2 Summary of the results for embryonic stem-cell differentiation. ES cells transplanted subcutaneusly or injected in knee joint formed teratomas(1) a,b). Whereas, ES cells transplanted in osteochondral defect, form cartilage tissue (2)c).

Fig. 2 shows summary of the results, where ES cells transplanted subcutaneusly or injected in knee joint formed teratomas (1)Fig. 2a,b). Whereas, ES cells transplanted in osteochondral defect, form cartilage tissue(2)Fig. 2c).

It was suggested that some kind of interaction between ES cell and surrounded tissue affects the differentiation. The interaction thought to be categorized into two factors; One is bio-

chemical and the other is bio-mechanical interactions. It is well-known that stem cells tend to form the some tissue as surrounds. McDonald et al. and Wichterle et al. reported that ES cells could differentiate into neural cells in vivo when transplanted into the spinal cord 3, 4).

Several reports have suggested that the bio-mechanical interaction is also an important factor. Salter et al 5). reported that the metaplasia of the healing tissue within the cartilage defects from undifferentiated mesenchymal tissue to hyaline articular cartilage, was affected by slow joint motion. Our previous study 6) reported the response of mesenchymal tissue to mechanically controlled motion in vivo, where middle portion of the coccygeal vertebra of rats was osteotomized, and continuous bending motion was applied for 4 weeks. Hyaline cartilage tissue was generated at the osteotomized ends, and joint-like functional structure was seen when sliding motion was added to the bending motion. Whereas sliding motion without bending formed imperfect structure without layer formation. (6)Fig.3)



Fig. 3 Responses of mesenchymal tissue to mechanically controlled motion in vivo. The middle portion of the coccygeal vertebra of rats was osteotomized, and continuous bending motion was applied for 4 weeks. Hyaline cartilage tissue was generated at the osteotomized ends, and joint-like functional structure was seen when sliding motion was added to the bending motion. Whereas sliding motion without bending formed imperfect structure without layer formation. (6)

As shown in Fig.1, all the ES-cell transplanted in the joint cartilage formed hyaline-like cartilage having a smooth surface and was elevated with the cells resembling well-differentiated chondrocytes surrounded by a metachromatic matrix. Our recent result also showed that when the joints were immobilized, teratomatous tissue was formed in the ES-cell transplanted knee joint. These results suggests that the bio-mechanical interactions are the dominant for the ES cell differentiation into chondrocyte

In this study, I adopted following hypothesis to explain our results. It could be "tissue selection" due to a severe mechanical environment. Articular cartilage is exposed to repetitive pressure and shear stress. The ES-cells transplanted into the osteochondral defect were likely to be exposed to severe mechanical stress, where the chondrocyte phenotype might be selected by

the joint movement and/or loading. In other words, other phenotypes may undergo apoptosis and/or necrosis in such a severe mechanical environment.

Fig. 4 shows the result of computer simulation for tissue-regeneration model using cellular automaton. Selection by durability to mechanical environment was adopted in this model, where shear-strain tolerant, compressive-strain tolerant, and tensile-strain tolerant tissues were defined resembling cartilage, bone, and fibrous tissue respectively 7). This is just the start of the simulation where several feed back system was tried to fit the in vivo results. The purpose of this simulation is not to demonstrate the "Selection for function", but is to demonstrate the "Selection for function", but is to demonstrate the "Selection for function", because It is impossible to prove by simulation methods that some functional structure are produced without any intention. Trial-and-error methods may reveal some feed back system which explain the in-vivo results.



Fig. 4 Result of computer simulation for tissue-regeneration model using cellular automaton. Selection by durability to mechanical environment was adopted in this model, where shear-strain tolerant, compressive-strain tolerant, and tensile-strain tolerant tissues were defined resembling cartilage, bone, and fibrous tissue respectively 7).

3 CLINICAL RELEVANCE OF THIS STUDY

The bio-environment designing is the fundamental concept to apply to living thing. Several biological phenomenon, such as adaptation (as shown in Figs.2,3,4), tissue regeneration, and ethiology of diseases, may be explained by the "Selection for function" or the "Selection of efficiency". For example, some diseases would be defined as malfunctions of the feed-back system produced in the "Selection of efficiency", and the selection process could be assume to explain the differentiation of cell as shown in Fig. 4.

Direct clinical relevance of this concept is also proposed, where the bio-environment designing is applied to the treatment of joint diseases. "Total Joint Regeneration system(TJR)" has been proposed to control the mechanical environment of joint(7,8,9).Fig. 5). Tissue engineering seems to be one of the most promising methods for treatment of joint disease.

However, current techniques for treatment of osteoarthritis or rheumatoid arthritis require a long period of recovery before the patient is able to walk with full weight bearing. The TJR devices support a part of weight in order to allow patients to maintain a normal life during treatment. Three types of device for our TJR System were proposed, as shown in Fig.5

The first type of TJR device is the external type, which fundamentally is an external fixation or brace with hinge joints to enable knee flexion and to enable load-bearing walking. Load applied to the joint surface can be controlled by springs. This type of device can be used not only for osteoarthritis or rheumatoid arthritis, but also for cases of intra-articular fracture. The second type of TJR device is the internal type. The whole device is implantable like an artificial joint. The original joint surface is not sacrificed. Load applied to the joint is supported by the middle or peripheral part of the femoral condyle. The third type of TJR device is the "magnet type", where an implantable magnet is fixed to the joint surfaces and the body weight is supported by the mutual repulsion of the magnets. These devices are now at the trial and error stage of development.



Fig. 5 "Total Joint Regeneration system" as an environment-designing treatment for joint desease 8,9,10). a: external type. b: internal type. c: magnet type.

REFERENCES

- 1. Wakitani, S., Takaoka, K., Hattori, T., Miyazawa, N., Iwanaga, T., Takeda, S., Watanabe, T.K., and Tanigami, A. Embryonic stem cells injected into the mouse knee joint form teratomas and subsequently destroy the joint. Rheumatology (Oxford) 42, 162, 2003.
- 2. Wakitani S, Aoki H, Harada Y, Sonobe M, Morita Y, Mu Y, Tomita N, Nakamura Y, Takeda S, Watanabe TK, Tanigami A. Embryonic stem cells form articular cartilage, not teratomas, in osteochondral defects of rat joints. Cell Transplant. 2004;13(4):331-6.
- 3. McDonald, J.W., Liu, X.Z., Qu, Y., Liu, S., Mickey, S.K., Turetsky, D., Gottlieb, D.I., and Choi, D.W. Transplanted embryonic stem cells survive, differentiate and promote recovery in injured rat spinal cord. Nat. Med. 5, 1410, 1999.

- 4. Wichterle, H., Lieberam, I., Porter, J.A. and Jessell, T.M. Directed differentiation of embryonic stem cells into motor neurons. Cell 110, 385, 2002.
- 5. Salter, R.B., Simmonds, D.F., Malcolm, B.W., Rumble, E.J., MacMichael, D., and Clements, N.D. The biological effect of continuous passive motion on the healing of full-thickness defects in articular cartilage. An experimental investigation in the rabbit. J. Bone Joint Surg. Am. 62, 1232, 1980.
- 6. Harada, Y., Tomita, N., Wakitani, S., Mii, Y., Oka, M., and Tsutsumi, S. Use of Controlled Mechanical Stimulation in Vivo to Induce Cartilage Layer Formation on the Surface of Osteotomized Bone. Tissue Eng. 8, 969, 2002.
- Koji Yamamoto, Yasuji Harada, Masaaki Nakajima, Shigeyuki Wakitani and Nohide Tomita : Cellular Automaton Model for Bio-environment Designing, MECJ-04, O, A-B, 2004
- 8. Tomita, N., Aoki, H., Harada, Y., Ikeuchi, K., Wakitani, S., Hattori, K., and Suguro, T. Reconstruction of the knee joint using the total joint regeneration system. Tissue Engineering for Therapeutic Use 6, 41, 2002.
- 9. Hideyuki Aoki, Naohide Tomita, Yusuke Morita, Koji Hattori, Yasuji Harada, Masato Sonobe, Shigeyuki Wakitani and Yasushi Tamada, Culture of chondrocytes in fibroinhydrogel sponge, Bio-Medical Materials and Engineering, 13(4) (2003), 309-316
- 10. Hideyuki Aoki, Naohide Tomita, Yasuji Harada, Koji Hattori, Masato Sonobe and Toru Suguro, The report of the cartilage regeneration using Total Joint Regeneration System(Internal-fixator type), Bio-Medical Materials and Engineering, 13(4) (2003), 411-417

Structural Topology Optimization for the Design of Novel Mechanical Structures

Shinji Nishiwaki

Department of Precision Engineering, Kyoto University

Abstract

In general mechanical designs, the stiffest structures or the structures having the highest eigenfrequencies have been considered optimal. However, if we can provide appropriate flexibility or appropriate eigen-frequencies and eigen-modes, additional kinematic functions and dynamic functions can be implemented in the mechanical structures. In this paper, a structural topology optimization methodology for the design of mechanical structures having new types of functions such as kinematic functions and dynamic functions is developed. This methodology is applied to various designs such as compliant mechanisms and mechanical resonators.

1 INTRODUCTION

In general mechanical designs, the stiffest structures or the structures having the highest eigenfrequencies have been considered optimal. However, if we can provide appropriate flexibility or appropriate eigen-frequencies and eigen-modes, additional kinematic functions and dynamic functions can be implemented in the mechanical structures.

A typical example of a mechanical structure incorporating the kinematic function is a compliant mechanism. It is designed to be flexible in order to achieve a specified motion as a mechanism (e.g., (Frecker et al., 1997), (Howell & Midha, 1994)). On the other hand, a typical example using the dynamic function is a mechanical resonator, which is used as sensors (Howe & Bose, 1996), filters (Lin & Howe, 1998), and actuators (Seeman, 1996). They are of great interest in the field of micro-electro-mechanical systems (MEMS). Other application areas include oscillators such as micro-vibromotors that translate mechanical vibration to linear (Saitou et al., 2000) or rotary motion (Lee & Pisano, 1992). Despite such broad application areas using kinematic and dynamic functions, general methods for integrating optimal compliant mechanisms and resonator structures and support systems have not been established. In this paper, a structural topology optimization methodology for the design of mechanical structures having new types of functions such as kinematic functions and dynamic functions is developed. This methodology is applied to various designs such as compliant mechanisms and mechanical resonators.

2 DESIGN DOMAIN SETTINGS AND RELAXATION OF DESIGN DOMAIN

Here, we briefly discuss a new type of Homogenization Design Method (HDM) in which continuous material distributions are assumed, using a continuous interpolation function at each node. Consider the design problem of determining the boundary of the design domain Ω_d by minimizing or maximizing objective functions. The key idea of the topology optimizations

method is the introduction of a fixed, extended design domain D, that includes the original design domain Ω_d , *a priori*, and the utilization of the following characteristic function.

$$\chi_{\Omega}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega_d \\ 0 & \text{if } \mathbf{x} \in D \setminus \Omega_d \end{cases}$$
(1)

where x denotes a position in the extended design domain D. Using this function, the original structural design problem is replaced with a material distribution problem incorporating an elasticity tensor and mass density, $\chi_{\Omega} E$ and $\chi_{\Omega} \rho$, respectively, in the extended design domain D, where E and ρ are the elasticity tensor and mass density, respectively, in the original design domain Ω_d . Since this characteristic function can be very discontinuous, i.e., resides in $L^{\infty}(D)$. some regularization or smoothing technique should be introduced for the numerical treatment. The homogenization method is used to perform the relaxation of the solution space with the introduction of microstructures standing for the composite materials (Bendsøe & Kikuchi, 1988). In two scale modelling, which is based on the homogenization method, microstructures are continuously distributed almost everywhere in the extended design domain D, and this status must hold even after the finite element discretization. The design variables, however, are approximated by piecewise constants in the finite element implementation in both the original HDM method (Suzuki & Kikuchi, 1991), and the SIMP method (Bendsøe & Sigmund, 1999) that directly assumes that the material density is a continuous function. Thus, we conjecture that there is inconsistency in the procedures, i.e. the assumption of continuous material distributions and the piecewise distribution of design variables, and that the approximation based on a piecewise constant in each element is the cause of checkerboard patterns.

To overcome the above problems, and to maintain procedural consistency, we approximate the design variable $r(\mathbf{x})$ as,

$$r(\boldsymbol{x}) \approx r^{h}(\boldsymbol{x}) = \boldsymbol{N}^{r}(\boldsymbol{x})\boldsymbol{R} = \sum_{i=1}^{n} N_{i}^{r}(\boldsymbol{x})\boldsymbol{R}_{i}$$
(1)

where h stands for the discretized quantity using FEM, N^r is a vector whose components are $N_i^r(\mathbf{x})(i=1,...,n)$, \mathbf{R} a vector of nodal (discrete) design variables $R_i(i=1,...,n)$, and n is the total number of nodes and also design variables. Using the above approximation, the design variables can hold the C0-continuity over the domain due to the partition-of-unity of $N_i^r(\mathbf{x})$, and are continuously distributed in and through an element. The bi-linear interpolation function is used as $N_i^r(\mathbf{x})$ in the case of four-node quadrilateral elements for its simplicity in this research, and because it preserves the C0-continuity. Note that $N_i^r(\mathbf{x})(i=1,...,n)$ are selected and evaluated independently of the shape functions for displacement fields.

Figure 1 shows the microstructure used for the relaxation of the design domain in the two-dimensional problem. As shown in this figure, its shape is hexagonal where the design variable is a geometrical parameter r. In order to for a unit cell to be void, r must be 1, and for it to be solid material, r must be 0. This microstructure has an isotropic response.



Figure 1. A microstructure for the relaxation of design domain

3 FORMULATIONS OF OPTIMIZATION PROBLEMS

3.1 Design of Compliant Mechanisms

Consider that an elastic structure occupying a two-dimensional design domain $\Omega_{d.}$ is fixed at boundary Γ_{u} . Body forces applied to this elastic body are ignored for the simplicity of the formulation. Now, we intend to design a compliant mechanism that starts to deform in the specified direction t^2 at boundary Γ_{t^2} in order to perform certain operations when the traction t^1 is applied at boundary Γ_{t^1} . To implement this function, we must take into account the kinematic and structural requirements. For the kinematic requirement, the compliant mechanism must have sufficient flexibility, which provides sufficient deformation in the specified direction t^2 at boundary Γ_{t^2} when the traction t^1 is applied at boundary Γ_{t^1} . It is obtained by the maximization of the mutual mean compliance. The objective function is formulated as, maximize $l^2(u^1) = \int_{\Gamma_{t^2}} t^2 \cdot u^1 d\Gamma$ (2)

where t^1 is the displacement field of the elastic structure when the traction t^1 is applied at boundary Γ_{t^1} .

For the structural requirement, the compliant mechanism must have two sufficient stiffnesses at two different boundaries. One is the stiffness at boundary Γ_{t^1} when the traction t^1 is applied, in order to maintain the shape of the structure against excessive deformation due to the traction t^1 . This stiffness is obtained by minimizing the mean compliance at boundary Γ_{t^1} imposed by the traction t^1 while boundary Γ_{t^2} is fixed. The objective function is formulated as,

minimize
$$l^1(\boldsymbol{u}^3) = \int_{\Gamma_1} \boldsymbol{t}^1 \cdot \boldsymbol{u}^3 d\Gamma$$

where u^3 is the displacement field of the elastic structure when the traction t^1 is applied at

boundary Γ_{t^1} while boundary Γ_{t^2} is fixed.

The other is the stiffness at boundary Γ_{t^2} when the reaction force is imposed by a workpiece, in order to maintain the shape of the structure against excessive deformation due to the reaction force. Here, the direction of the reaction force is assumed to be that of the traction t^2 . Therefore, this stiffness is obtained by minimizing the mean compliance at boundary Γ_{t^2} imposed by the traction $-t^2$ while boundary Γ_{t^1} is fixed. The objective function is formulated as, minimize $l^4(\mathbf{u}^4) = \int_{\Gamma_{t^2}} t^4 \cdot \mathbf{u}^4 \, d\Gamma$ (4)

where $t^4 = -t^2$, and u^4 is the displacement field of the elastic structure when the traction t^4 is applied at boundary Γ_{t^1} while boundary Γ_{t^2} is fixed.

As we explained above, the three objective functions must be taken into account for the design of the compliant mechanism. Here, the following multi-objective function is proposed in order to solve the optimization problem.

maximize
$$f_1 = \frac{l^2(u^1)}{w_3 l^1(u^3) + w_4 l^4(u^4)}$$
 (5)

where W_3 and W_4 are weighting coefficients.

3.2 Design of Mechanical Resonators

Consider that an elastic and vibrating structure occupying a two-dimensional design domain Ω_d is fixed at boundary Γ_u . Body forces applied to this elastic body and damping effects are ignored for the simplicity of the formulation. Here, we intend to maximize the vibrating deformation of the j-th excitation frequency (j=1,..., m_s) along the direction of a unit load vector t_j^{Outmax} at boundary Γ_{ij}^{Outmax} , and minimize the vibrating deformation of the j-th excitation frequency (j=1,..., m_s) along the direction of the j-th excitation frequency (j=1,..., m_s) along the direction of the j-th excitation frequency (j=1,..., m_s) along the direction of a unit load vector t_j^{Outmax} at boundary Γ_{ij}^{Outmin} at boundary Γ_{ij}^{Outmin} when a harmonic exciting traction t_j^{In} is applied at boundary Γ_{ij}^{In} in order to specify the desired vibration mode , where the j-th excitation frequency is assumed to be ω_j^{In} . Instead of directly maximizing the specified dynamic deformation, we use the structure's resonance, which results in sufficient deformation in the desired direction.

Suppose that the *j*-th eigen-frequency and its corresponding eigen-mode of the vibrating structure are u_j and ϕ_j , respectively. To satisfy the above specification, first, one of the eigen-frequencies must match the excitation frequency ω_j^{\ln} . Here, we intend to match the *j*-th eigen-frequency u_j with the *j*-th excitation frequency ω_j^{\ln} (j=1,..., m_s). With respect to the practical design of vibrating structures, only a few eigen-frequencies starting with the lowest one (usually only the lowest one, and at most three) need to be specified, because the lower eigen-frequencies are usually easily handled in the mechanical design, and the higher ones are not practical due to their complex eigen-mode shapes. However, other eigen-frequencies and eigen-modes are dealt with during the optimization process. In cases where such reordering must be avoided, an appropriate number, m ($m > m_s$), of eigen-frequencies, $\omega_{m_s+1}^{\ln}$, $\omega_{m_s+2}^{\ln}$,..., ω_m^{\ln} , must be given fictitious and sufficiently large values. Therefore, the objective function concerning the eigen-frequencies can be formulated as:

$$\underset{r}{\text{minimize}} \quad f^{V} = \sum_{j=1}^{m} w_{j}^{V} \left(\frac{\lambda_{j}\left(r\right) - \lambda_{j}^{\ln}}{\lambda_{j}^{\ln}} \right)^{2}$$
(6)

where r is a design variable, $\lambda_j(r)$ is the *j*-th eigen-value, and w_j^{V} is the weighting coefficient for the *j*-th eigen-frequency matching.

In order to satisfy the design requirements, the shape of the eigen-modes must also be controlled. However, determining the entire outline shape of a selected eigen-mode that must satisfy orthogonal conditions is elusive. Furthermore, such details are not usually required for the design. The important design specifications are to determine the portions of the eigen-mode shape where the desired dynamic response is maximized, and other portions where undesirable dynamic response is minimized (leaving an unspecified remaining portion). Using this specification method, sufficient eigen-mode control can then be achieved for the design of vibrating structures and mechanical resonators. Thus, the following objective functions are formulated to satisfy the above specifications:

$$\underset{r}{\text{maximize}} \quad f^{M} = \sum_{j=1}^{m_{s}} \left\{ w_{j}^{M, \text{In}} \left(\boldsymbol{t}_{j}^{\text{In}^{T}} \boldsymbol{\phi}_{j}(r) \right)^{2} + w_{j}^{M, \text{Outmax}} \left(\boldsymbol{t}_{j}^{\text{Outmax}^{T}} \boldsymbol{\phi}_{j}(r) \right)^{2} - w_{j}^{M, \text{Outmin}} \left(\boldsymbol{t}_{j}^{\text{Outmin}^{T}} \boldsymbol{\phi}_{j}(r) \right)^{2} \right\}$$

$$\underset{M, \text{In}}{M, \text{Outmax}} \quad M, \text{Outmin}$$

$$(7)$$

where $w_j^{w_j^{m,m}}$, $w_j^{w_j^{m,outmax}}$, and $w_j^{w_j^{m,outmax}}$ are the weighting coefficients for the maximization of the j-th eigen-mode in the direction of , the maximization of the j-th eigen-mode in the direction of , and the minimization of the j-th eigen-mode in the direction of , respectively.

Let us consider that the vibrating structure is subjected to the dynamic traction t_j^{out} at boundary Γ_{ij}^{\ln} in order to vibrate the structure, and is also subjected to the reaction traction t_j^{out} imposed by an object such as a workpiece at boundary Γ_{ij}^{out} . For the design specification concerning stiffness, two types of stiffness must be considered. One is the stiffness that maintains the structural shape when the dynamic traction t_j^{in} is applied at boundary Γ_{ij}^{in} while boundary Γ_{ij}^{out} is fixed in the direction of t_j^{out} , and the other is the stiffness that resists reaction traction t_j^{out} at boundary Γ_{ij}^{out} is a unit vector in the engineering sense. The objective function for the above stiffnesses is formulated as follows:

$$\underset{r}{\text{minimize}} \quad f^{S} = \sum_{j=1}^{m} w_{j}^{S,\text{In}} \left(\int_{\Gamma_{t_{j}}^{\text{In}}} \boldsymbol{T}_{j}^{\text{In}} \cdot \boldsymbol{U}_{j}^{\text{In}} d\Gamma \right)^{2} + w_{j}^{S,\text{Out}} \left(\int_{\Gamma_{t_{j}}^{\text{Out}}} \boldsymbol{T}_{j}^{\text{Out}} \cdot \boldsymbol{U}_{j}^{\text{Out}} d\Gamma \right)^{2}$$

$$(8)$$

where T_j^{In} and T_j^{Out} are the amplitudes of t_j^{In} and t_j^{Out} , respectively. U_j^{In} is the amplitude of the displacement field u_j^{In} when t_j^{In} is applied, and U_j^{Out} is the amplitude of the displacement field u_j^{Out} when t_j^{Out} is applied. $w_j^{S,\text{Out}}$ are the weighting coefficients for the stiffness

As we explained above, the three objective functions must be taken into account for the design of the mechanical resonator. Here, the following multi-objective function is proposed in order to solve the optimization problem.

$$\underset{r}{\text{minimize } f = (1 + w^V f^V) f^S - w^M f^M$$
(9)

where w^{V} and w^{M} are weighting coefficients

4 NUMERICAL EXAMPLES

Two numerical examples are presented in order to confirm the utility of the proposed method. The isotropic materials have a Young's modulus=200, Poisson's Ratio=0.3, and mass density = 7.8×10 -6. The magnitude of amplitude of an applied force is assumed to be a unit load. The weighting coefficients in the objective functions are set to 1.0 except for the coefficients specified in the following examples.

4.1 Design of Compliant gripper

Figure 2 shows a half view of the design domain where boundary conditions and specifications are indicated. As shown in this figure, the upper-left side boundary of the design domain is fixed to support the compliant gripper, and the symmetry condition is posed at the bottom boundary. The function of the compliant gripper is to (1) deform in the direction of dummy load F^2 in order to grasp a workpiece at point P_2 when the external force F^I is applied at point P_1 for the kinematic requirement, and (2) hold the workpiece while the external force F^I is continuously applied for the structural requirement. The mutual mean compliance defined by F^2 when F^I is applied, is to

be maximized, while the two mean compliances defined by F^1 at point P_1 and F^2 at point P_2 are to be minimized. The weighting coefficients, W_3 and W_4 , in Eq. (5) are set to 1.0 and 1.0, respectively, and the total volume constraint is set 20% of the entire design domain in the optimization.

Figure 3 shows the optimal configuration. As shown in this figure, the clear optimal structure without checkerboard patterns is obtained by the proposed method.



compliant gripper

configuration of compliant

4.2 Design of Mechanical Resonator

Figure 4 shows the design domain. As shown in this figure, the second eigen-mode along the direction f_2^{Outmax} at point P_2^{Outmax} , along the direction $f_{2,1}^{\ln}$ at point $P_{2,1}^{\ln}$, and along the direction $f_{2,2}^{\ln}$ at point $P_{2,2}^{\ln}$ is to be maximized, and the second eigen-mode along the direction f_2^{Outmin} at point is to be minimized, according to the eigen-mode specification shown in Figure 4 (a), while the lowest and second eigen-frequencies are required to conform to target values, 350Hz,and 500Hz, respectively, according to the eigen-frequency specification. Further, the static stiffness along the direction of $f_{2,1}^{\ln}$ at point $P_{2,1}^{\ln}$ and along the direction $f_{2,2}^{\ln}$ at point $P_{2,2}^{\ln}$ is to be maximized to resist the applied force as shown in Figure 4 (b), and the static stiffness along the direction of f_2^{Out} at point P_2^{Out} is to be maximized while point $P_{2,1}^{\ln}$ is fixed along the direction of $f_{2,1}^{\ln}$, and point $P_{2,2}^{\ln}$ is fixed along the direction of $f_{2,2}^{\ln}$ to resist the reaction force imposed by a workpiece, as shown in Figure 4 (c). The weighting coefficients, w^{V} and w^{M} , in Eq. (9) are set to 5.0 and 0.1, respectively, and the total volume constraint s is set to 20% of the volume of the whole design domain in the optimization.

Figure 5 (a) shows the optimal configuration, and Figure 5 (b) shows the eigen-mode shape corresponding to the second eigen-frequency. As shown in this figure, the optimal configuration is also clear, and does not have checkerboard patterns. Further, it is observed that this satisfies the eigen-mode specification.



Figure 4. Design domain for mechanical resonator



(a) Lowest and second target frequencies = 350Hz and 500Hz



(b) Second eigen-mode shape

Figure 5. Optimal configuration of mechanical resonator

5 CONCLUSION

In this paper, a structural topology optimization methodology for the design of mechanical structures having new types of functions such as kinematic functions and dynamic functions was developed. Two examples were provided in order to examine the characteristics of the resulting optimal configurations. It was confirmed that the proposed method provides checkerboard-free optimal configurations without any artificial elimination schemes. It was also confirmed that the proposed method can produce compliant mechanisms and mechanical resonators.

References

- 1. Bendsøe M. P. & Kikuchi N. (1988). Generating optimal topologies in structural design using a homogenization method. *Computer Methods in Applied Mechanics and Engineering*, 71, 197-224.
- 2. Bendsøe M. P. & Sigmund O. (1999). Material interpolation schemes in topology optimization. Archive of Applied Mechanics, 69, 635-654.
- Frecker, M. I., Annathasuresh, G. K., Nishiwaki, S., Kikuchi, N., & Kota, S. (1997). Topological synthesis of compliant mechanisms using multi-criteria optimization. J. of Mechanical Design, *ASME*, 119, 238-245.
- 4. Howe R. T. & Boser B. E. (1996). Surface micromachined accelerometers. *IEEE Journal of Solid-State Circuit; 31,366-375*.
- 5. Howell, L. L. & Midha A. (1994). A method for the design of compliant mechanisms with small-length flexural pivots. J. of Mechanical Design, *ASME*, 116, 280-289.
- 6. Lin L. & Howe R. T. (1998). Microelectromechanical filters for signal processing. *Journal of Microelectromechanical Systems*, 7, 286-294.
- 7. Lee A. P. & Pisano A. P. (1992). Polysilicon angular microvibromotors. *Journal of Microelectromechanical Systems*, 1, 621-629.
- Saitou K., Wang D-A., & Wou S. J. (2000). Externally resonated linear microvibromotor for microassmbly. *Journal of Microelectromechanical Systems*, 9, 336-346.
- 9. Seeman W. (1996). Ultrasonic traveling wave linear motor. *Smart Structures and Integrated Systems, Seminar Proceedings of the International Society for Optical Engineering SPIE*; 2717, 554-564.
- Suzuki K. & Kikuchi N. (1991). A homogenization method for shape and topology optimization. *Computer Methods in Applied Mechanics and Engineering*, 93, 291-318.

Design of an Adaptive Control System by Modular Learning: Flight Control of an Autonomous Unmanned Helicopter

Hiroaki Nakanishi

Department of Aeronautics & Astronautics Graduate School of Engineering, Kyoto University

Abstract

Designing control system for complicated mechanical systems by training of intelligent system is developed. We propose a method to design robust control systems against stochastic uncertainties by use of off-line training of neural networks. On-line training is also important for control system because it enables to compensate undesirable effects which are not modeled or sudden changes of the controlled object and the environment. Therefore, a method to design an adaptive control system by modular learning is developed. Numerical simulations and experimental results of flight control of an autonomous unmanned helicopter demonstrate the effectiveness of proposed methods.

1 INTRODUCTION

Flight control of unmanned aerial vehicle (UAV) has been paid much attention recently. UAV is smaller, lighter and cheaper than manned vehicles so that UAV is very useful in many applications, such as disaster prevention and observation activities at dangerous area. The dynamics of UAV isn't linear, especially the dynamics of rotorcraft UAV is nonlinear, and so it was difficult to design flight controllers for UAV by use of linear control design methods. Calise et al proposed nonlinear adaptive flight control of UAV by use of neural network (Calise, 1996). Neural network is effective in designing controller for nonlinear plant. There are many uncertainties in the flight. Among of them, we must take into account the effect of wind in designing flight control systems, because the wind significantly influences the flying aircraft. Wind is usually treated as a disturbance in designing flight controllers. It is difficult to predict wind speed and direction because they vary stochastically. The wind speed is usually modelled as a colored noise. Dryden wind model, which is a stochastic model of the wind, is widely used to

evaluate the performance or stability of the flight control system. The margin of the thrust of UAV isn't enough generally, so influence of the wind is critical in UAV flight control. Therefore methods to design nonlinear robust flight controllers are required in designing UAV flight control system. In this paper, we propose methods to design robust controllers for a nonlinear system in which



80

Figure 1 Autonomous Unmanned Helicopter

stochastic disturbance exist. Training neural networks is important role of proposed methods and nonlinear robust controllers whose robustness is quantified can be easily designed. But it is wellknown that fixed robust controllers suffer from conservativeness, and they are very sensitive to perturbations that are not considered in designing. Adaptive methods to compensate for various environmental changes are also required, and a method to design an adaptive control system by modular learning is developed.

2 AUTONOMOUS UNMANNED HELICOPTER

YAMAHA RMAX, which is used in our study, is a very small helicopter whose main rotor's diameter is 3.115m and the maximum payload is 30kg, so that it can perform many activities. The specification of RMAX can be found in the web pages(http://www.yamaha-motor.co.jp). We are now developing autonomous unmanned helicopter for disaster prevention and disaster response based on RMAX, and its picture is shown in Figure 1. The helicopter equips an attitude sensor and a GPS sensor. The attitude sensor consists of a geomagnetic azimuth sensor, 3 gyros and accelerometers. To ensure the accuracy of measurement of position and velocity, a kinematics D-GPS is used. To improve the performance and reliability of autonomous flight controllers, it is necessary to use more accurate states of the helicopter, such as the position, velocities, and the attitude. Therefore GPS-INS integrated navigation system using the extended Kalman Filter is developed. The integrated navigation system is designed to cancel the offset of gyros and accelerometers and the effect of the distance from the GPS antenna to the center of gravity. Moreover, it is also able to compensate time delay in GPS measurement and data transmission. Real time processing is required in the computation, so that RT-Linux and note PC, which is light but has enough computational capability, are used for flight control system. Figure 1 is a picture of the unmanned helicopter used in our experiments.

3 DESIGN OF ROBUST CONTROL SYSTEM BY TRAINING NEURAL NETWORK

3.1 Formulation

Consider a nonlinear system described as x(t+1) = f(x(t), u(t), w(t))

where x(t) is a state vector and u(t) is the control vector. w(t) is a stochastic disturbance vector. It is assumed that x(t) is measurable. If a noise exists in the measurement, then measured state y(t) is described as y(t)=x(t)+v(t) (2)

(1)

where v(t) is noise vector. Measurement noise is also classified as stochastic uncertainties. z(t) is a reference output vector of the system described as z(t)=h(x(t),u(t))(3)

The purpose of this paper is to build methods to design feedback controllers described as u(t)=g(x(t)) (4)

which can reduce the influence of the stochastic uncertainties. If the varying of stochastic uncertainties is enough slow to assume to be constant parameters, then the system is identical the

one which include only time-invariant structured uncertainties, so that the method proposed in 1998) (Nakanishi. is enough to design control systems. Therefore the time varying stochastic uncertainties should be taken



Figure 2 Block Diagram of a Control System

into account. It is assumed that averages of stochastic uncertainties are equal to 0, that is, E[w(x)] = 0, E[w(x)] = 0

E[w(t)] = 0, E[v(t)] = 0

(5)

It may seem that this assumption is hypothetical, because deviation often exists. If this assumption isn't satisfied and use the state feedback controller, the performance may not be enough because the steady error may exist. But controllers including an integral operator can easily remove the effect of the deviation of disturbance and we can easily extend proposed methods to design dynamic controllers.

A multi-layered neural network can be used as a feedback controller and the block diagram of the control system is described in Figure 2. In this paper, three layered neural networks are used to train because it can emulate any continuous functions to any desired accuracy. Training methods are explained in the next section. A training algorithm based on Powell's conjugated direction algorithm (Powell, 1964) (Nakanishi, 1997) is suitable to design robust control systems against stochastic uncertainties. In the training algorithm, it doesn't need to calculate any derivative, so that non-differentiable index can be used.

3.2 Design of Robust Control Systems against Stochastic Uncertainties

Because of stochastic uncertainties, the response of the systems is disturbed, so that a performance index J described as (6) becomes also stochastic.

$$J = \sum_{t=0}^{T} z^{2}(t)$$
(6)

Training using a particular time series of uncertainties isn't enough because the trained controller can't have proper robustness. Therefore a statistical value of the stochastic process is suitable for the performance index to learn robust control systems.

For training robust control systems, we propose to use a performance index J_{γ} described as $J_{\gamma} = \frac{1}{2\gamma} \log(E[\exp(2\gamma \cdot J)])$ (7)

where γ is a scalar parameter. If the performance index (7) can be expanded about γ , we can obtain an approximated index described as

$$J_{\gamma} = E[J] + \gamma \cdot Var[J]$$

The approximated index(7) shows that training can be classified into three cases by γ .

 $\gamma = 0$ In this case, $\gamma_{\gamma \text{ is }} E[J]$, and is the same as the classic performance stochastic optimal control.

 $\gamma < 0$ Training makes the variance of the sampled index big.

 $\gamma > 0$ Training makes the variance of the sampled index small.

The variance means the degree of influence of the stochastic uncertainties. The smaller the variance becomes, the smaller the influence of the uncertainties becomes. Therefore non-negative γ is used in training robust control systems and is quantified robustness of the trained controller.

3.3 Numerical and Experimental Results

To confirm the effectiveness of proposed methods, flight controllers for an autonomous unmanned helicopter are designed by use of a flight simulator. It is assumed that only vertical wind exits and horizontal wind doesn't exist in all simulations. Altitude controllers of the autonomous unmanned helicopter, which are nonlinear state feedback controllers, are designed by use of neural networks.

The sampled index J described as (8) is used in training, where d is the desired altitude, and

z is the altitude, and V_z is the vertical velocity.

$$J = \sum_{t=0}^{40 \text{sec}} \left((z(t) - d(t))^2 + v_z^2(t) \right)$$
(8)

Average and variance of the sampled index J are shown in Figure 3. Both average and variance of a neural network, which is trained without considering any winds, are big, therefore the network fails in reducing the influence of the wind, and the performances is not good enough. But both average and variance of neural networks trained by the proposed method are small, so that this figure shows that neural networks trained by the proposed method have excellent robustness and performance. Moreover, this figure shows a designer can perform the trade-off between robustness and performance by choosing γ .

To confirm that neural networks trained by the proposed method can work actually, flight control expements by use of the trained neural network were carried out. In these experiments, the helicopter was controlled to hover at a certain point, and to keep its altitude constant. The result is shown in Figure 4. For comparison, the result of a conventional linear controller,



Figure 3 Average and Variance of Sampled Index J



Figure 4 Results of Flight Experiments

which is a PD controller, is also shown in this figure. Gains of the conventional controller were determined to be optimal for the same performance index used in training neural networks, but no wind was considered in designing. Because it was very windy day, the altitude of the helicopter controlled by PD controller was fluctuated. But a neural network trained by the proposed method were much superior to the PD controller, Figure 4 shows that trained neural network can reduce the undesirable effect of the wind, and is much robust against the wind.

4 DESIGN OF CONTROL SYSTEM BY MODULAR LEARNING

Design of robust controllers is powerful tool for system with uncertainties or uncertain environment. But increasing makes the controller's robustness performance worse. Moreover designed controllers are robust against uncertainties or perturbations which is design to handle, but they are highly sensitive to perturbations which aren't considered in designing. To compensate for unexpected uncertainties or environmental changes, the adaptation is important. In this section, design of adaptive controllers is discussed.

Figure 5 shows the structure of the MMRL architecture. It is composed of n modules, each of which consists of a state prediction model and a reinforcement learning controller. The action output of



Figure 5 Block Diagram of Control System using Modular Learning

(8)

(9)

reinforcement learning controllers as well as the learning rates of both the predictors and the controllers are weighted by the "responsibility signal", which is a Gaussian softmax function of errors in output of the prediction models. In the following, we describe a specific algorithm of modular learning (Doya, 2001). A nonlinear system is considered $\dot{x}(t) = f(x(t), u(t))$

where x(t) is a state variable and u(t) is a control input. The goal of reinforcement learning is to find the policy that can maximize the cumulative future reward (Sutton, 1996). The task for the prediction model in each module is to predict the state derivative $\dot{x}(t)$. Output of the i-th module is denoted as $\dot{x}(t)$ and the prediction error as $\tau \dot{E}_i = -E_i + (\dot{x} - \dot{x}_i)^2$

The responsibility signal λ_i for the i-th module is then given by the softmax function of prediction errors

$$\lambda_{i}(t) = e^{-\frac{1}{2\sigma^{2}} \left\| \hat{x}_{i}(t) - \dot{x}(t) \right\|^{2}} / \sum_{j=1}^{n} e^{-\frac{1}{2\sigma^{2}} \left\| \hat{x}_{j}(t) - \dot{x}(t) \right\|^{2}}$$
(10)

where c is a parameter that controls the sharpness of module selection. Each module with a dynamic model is provided. Output of the i-th module

$$\dot{x}_i(t) = f_i(x(t), u(t))$$

(11)

is compared with the observed state dynamics \dot{x} to calculate the responsibility signal according to equation (10). Output of the prediction model of the i-th module is linearly weighted by the responsibility signal to make a prediction of the next state

$$\hat{\dot{x}}(t) = \hat{f}(x(t), u(t)) = \sum_{j} \lambda_{j} f_{j}(x(t), u(t))$$
(12)

 λ_i is then used for weighting the update of prediction models. Outputs of reinforcement learning controllers are linearly weighted by λ_i to make the action output to the environment. The parameters of the local linear model of the i-th module A_i , B_i are updated by the weighted prediction errors $\lambda_i(\hat{x}_i(t) - \dot{x}(t))$, respectively. However, there are obstacles to applying MMRL to practical problems where it is difficult to measure derivatives of state variables. Furthermore, steepest descent method is used in MMRL, the learning is generally slow and convergence cannot be guaranteed. In our approach, a Lyapunov function is used to formulate a learning rule using signals which are available to a reinforcement learning agent in a real environment. We assume that a local linearization of the controlled object (8) is described as

$$\dot{x}(t) = A(x_k, u_k)x(t) + B(x_k, u_k)u(t)$$
(13)

where x_k^{k} , u_k^{k} are a reference point and a prediction model $\hat{x}_k(t) = \hat{A}_k x(t) + \hat{B}_k u(t) + v_k$

$$A_i(t) - A_i \lambda(t) + D_i u(t) + v_i$$
(14)

for each module, where v is a pseudo control input which is introduced in order to guarantee stability. The error dynamics of the overall system can be expressed as

$$\dot{e}_{i}(t) = A_{i}x(t) + B_{i}u(t) - v_{i}$$
(15)

where
$$\dot{e}_i, \tilde{A}_i, \tilde{B}_i$$
 are $\dot{e}_i = \dot{x} - \dot{\hat{x}}_i, \tilde{A}_i = A - \hat{A}_i$ and $\tilde{B}_i = B - \hat{B}_i$. To derive the stable learning rules, we choose the following as a candidate of Lyapunov function

$$V_{i} = \frac{1}{2} e_{i}^{T} P e_{i} + tr(\widetilde{A}_{i}^{T} \Gamma_{A} \widetilde{A}_{i} + \widetilde{B}_{i}^{T} \Gamma_{B} \widetilde{B}_{i})$$
(16)

where P is a symmetric positive definite matrix and Γ_A , Γ_B are weight matrix and are positive defined. The derivative of the Lyapunov function is given by

$$\dot{V}_{i} = tr[\widetilde{A}_{i}^{T}(Pe_{i}x^{T} + \Gamma_{A}\widetilde{A}_{i}) + \widetilde{B}_{i}^{T}(Pe_{i}u^{T} + \Gamma_{B}\widetilde{B}_{i})] - v_{i}^{T}Pe_{i}$$

$$(17)$$

Therefore, let \hat{A} , \hat{B} , v be expressed as

$$\hat{A}_i = -\Gamma_A^{-1} P e_i x^T, \quad \hat{B}_i = -\Gamma_A^{-1} P e_i x^T, \quad v_i = e_i$$
(18)

Then (17) becomes

$$\dot{V}_i = -e_i^{\ I} P e_i \tag{19}$$

From (19), it is guaranteed that V is a decreasing function while P is positive definite matrix and the uniform ultimate boundedness of the error signal is achieved, then (15) is stable in the sense of Lyapunov stability.

Then, we apply the proposed method to design a flight control system for the autonomous unmanned helicopter to confirm that the proposed method is applicable to practical problems.

We used two modules, each of which had a linear dynamic model and a quadratic reward model. E_i can be implemented by using a short-term average of the prediction error instead of

model. ²⁷ can be implemented by using a short-term average of the prediction error instead of the instantaneous prediction error to prevent chattering.

$$\tau \dot{E}_i = -E_i + (x - \hat{x}_i)^2 \tag{20}$$

We set $\tau = 0.01$, c = 0.5 and initial value of parameters are obtained in advance using a flight simulator which can emulate flight state of the unmanned helicopter with

sufficient accuracy.

We test the performance of our proposed method and it turns out that the autonomous unmanned helicopter follows the desired output and our learning rules (18) works. Figure 6 show the relation between modules in phase plane. As shown in Figure 6, one module was specialized in negative accelerating dynamics and the other module took charge of all other domain in phase plane. The result shows that multiple prediction models are successfully trained and specialized for different domains in the state space.



Figure 6 Relation between Two Modules in the Phase Plane

5 CONCLUSIONS

In this paper, a method to design robust control systems by use of a neural network against stochastic uncertainties and to design adaptive control systems by modular learning are proposed.

Numerical and experimental results of flight control of an autonomous unmanned helicopter show that proposed methods are effective and practical. Proposed methods can improve the reliability of the autonomous flight of the unmanned helicopter because they can compensate for the undesirable environmental changes. Moreover proposed methods are general so that they can be applied to various problems.

Acknowledgement

The author would like to thank Miss Mai Bando, who is a graduate student and contributes a research on designing control system by modular learning.

References

B.S. Kim and A.J. Calise. (1996). Nonlinear Flight Control Using Neural Networks. Journal of Guidance, Control and Dynamics, Vol. 20, No.1, 26-33

H. Nakanishi and K. Inoue. (1998). Design Methods of Robust Feedback Controller by Use of Neural Networks, Proc. of the International ICSC/IFAC Symposium on Neural Computation, 731-736

M.J.D.Powell. (1964). An Efficient Method for Finding the Minimum of a Function of Several Variables Without Calculating Derivatives. Computer Journal, Vol. 7, 155-162

H. Nakanishi, T. Kohda and K.Inoue. (1997). A Design Method of Optimal Control System by Use of Neural Network. Proc. of the 1997 International Conference on Neural Network, vol. 2, 871-875

Doya, K., Samejima, K., Katagiri, K. & Kawato, M. (2002). Multiple model-based reinforcement learning, Neural Computation, vol. 14, 1347-1369.

Sutton, R.S. & Barto, A.G. (1998). Reinforcement Learning, Cambridge, MA, USA: MIT Press.

An Overview of the Structured Modeling Technology

Marek Makowski

International Institute for Applied Systems Analysis, Laxenburg, A-2361 Austria http://www.iiasa.ac.at/~marek e-mail:marek@iiasa.ac.at

Abstract

Making rational policy decisions for complex environmental problems typically requires comprehensive analyses of relations between decisions and various measures of the consequences resulting from their implementations. Such relations can be represented by various mathematical models, each having an infinite number of solutions of the decision problem. An efficient model-based decision-making support needs an appropriate modeling technology. This paper first summarizes the characteristics of model-based policy-making support, and uses as a concrete example a complex modeling application developed for supporting international negotiations, which requires various types of analyses of a complex model, as well as interaction with its users. Then it outlines the SMT (Structured Modeling Technology), which has been developed for model-based decision-making support for such problems.

Keywords: structured modeling, decision support systems, modeling systems and languages, model management, simulation, large scale optimization, data-base management systems, object-oriented programming, internet, environment.

1 Introduction

Rational solving of complex problems is based on a combination of knowledge, preferences, and intuition. Some of the knowledge pertinent to making correct decisions can be represented by mathematical models; these not only help to analyze the relations between the decisions and the resulting outcomes, but also facilitate identification of those decisions that correspond best to the preferences of the *Decision Maker* (DM).

However, decision making is becoming more and more difficult because decision problems are no longer well-structured problems that are easy to solve by intuition or experience supported by relatively simple calculations. Many decision problems are now more complex because of the globalization of the economy, and a much greater awareness of its linkages with various environmental, social, and political issues. A part of knowledge pertinent to making correct decisions can be represented by mathematical models, which help to analyze the relations between the decisions and the resulting outcomes, and facilitate identification of decisions that correspond best to the preferences of the *Decision Maker(s)* (DM). The preferences are implicitly defined by diversified (typically conflicting) goals; thus usually there is only partial ordering of an infinite (or at least large) number of possible solutions to a given decision problem.

The main purpose of this paper is to address the basic problems faced by modelers, which can be summarized by a single question: how can the modeling legacy be exploited to provide the best possible model-based decision-making support within time and budget constraints? The second purpose is to outline a new structured modeling technology which supports the development and use of models for complex problems for which the standard, general purpose modeling tools do not provide adequate support.

There are countless publications that document successful modeling stories, and also many publications presenting various modeling paradigms, techniques, and tools. Much less attention is paid to modeling failures and limitations of widely used modeling paradigms. The paper outlines a new modeling technology, which needed to be developed to adequately address the needs of modeling a complex problem. In other words, the requirements of an actual application have been driving the developments to be reported. Actually, many of these requirements have been formulated already by Geoffrion (1987), who also proposed a rigid methodology called Structured Modeling (SM). Over the last two decades several hundreds of papers presenting various elements of SM methodology, prototypes of software tools, and of SM applications have documented the developments of this methodology. Unfortunately, there have never been enough resources to unify the results of many diversified (not only related to the SM) modeling activities in order to develop a modeling environment that meets the requirements formulated in (Geoffrion, 1987), and accepted by most modeling practitioners. However, the results of various modeling activities have provided a good basis for the development of the Structured Modeling Technology (SMT) outlined in this paper, and presented by the author in more detail in (Makowski, 2005).

2 Models for decision-making support

Models for supporting decision-making represent and help to analyze those aspects of knowledge relevant to a decision-making process that can be used more efficiently in a computerized form than in any other way. A mathematical model describes the modeled problem by means of variables that are abstract representations of those elements of the problem that need to be considered in order to evaluate the consequences of the implementation of a decision (typically represented by a vector composed of many variables). More precisely, such a model is typically developed using the following concepts:

- Decisions (inputs) *x*, which are controlled by the user;
- External decisions (inputs) *z*, which are not controlled by the user;
- Outcomes (outputs) y, used for measuring the consequences of the implementation of inputs;

- Auxiliary variables introduced for various reasons (e.g., to simplify model specification, or to allow for easier computational tasks);¹ and
- Relations between decisions x and z, and outcomes y; such relations are typically presented in the form: y = F(x, z), where $F(\cdot)$ is a vector of functions.



Figure 1: Structure of the use of a mathematical model for decision-making support.

A structure of the use of a model for decision-making support is illustrated in Fig. 1. The basic function of a model-based *Decision Support System* (DSS) is to support the user in finding values for his/her decision variables x that will result in a solution of the problem that best fits the preferences of the user. More specifically, a DSS supports various analyses of the decision problem aimed at:

- suggesting decisions for reaching specified goals;
- analyses of trade-offs between conflicting goals; and
- evaluations of consequences of decisions specified by the user.

A typical decision problem has an infinite number of solutions. Thus, users are interested in those that correspond best to their preferences represented here by a *preferential* structure P(x, y) of the user. A preferential structure typically induces partial ordering of solutions obtained for different combinations of values of inputs; in a well-organized modeling process it is not included in the model but is defined during the model analysis phase, when typically users substantially modify their preferences provided this is made easily available. In fact, a well-organized model analysis phase is composed of several stages, see e.g., (Makowski and Wierzbicki, 2003), each serving different needs; thus, typically, not only are different forms of $P(\cdot)$ used for the same problem but also different instances of each of these forms are defined upon analyses of previously obtained solutions.

A more detailed discussion of various modeling paradigms, and an updated overview of the modeling state-of-the-art are presented by Makowski (2005).

3 RAINS models

The complexity of problems, and the role of corresponding models in decision support are the two main factors that determine requirements for the type of modeling technology that differs substantially from the technologies successfully applied for modeling well-

¹Although such variables typically constitute a large part of all variables (often a vast majority) for the sake of brevity we do not discuss them here.

structured and relatively simple problems. In most publications that deal with modeling, small problems are used as an illustration of the modeling methods and tools presented. Often, these can also be applied to large problems. However, the complexity is characterized not primarily by the size, but rather by the structure of the problem and by the requirements for the corresponding modeling process.

RAINS provides a consistent framework for the analysis of cost-effective emission reduction strategies, and is being used for supporting international negotiations aimed at improving European air quality² is a perfect example justifying the needs for new modeling technology. The quality of air is assessed by several indicators computed at a few hundred grids, their values depending on the locations and the amounts of emissions of various pollutants. Hence, the decision (input) variables are emissions, and output variables (used for assessing consequences of decisions) are composed of the costs for reducing emissions and of a set of various air-quality indicators; each indicator is composed of vectors of the values of the indicator at each of the grids into which Europe is divided for the purpose of air-quality assessment.



Figure 2: RAINS model structure.

The ever-growing needs of RAINS users require more detailed analyses of emission control options, and of more types of pollution. To address these needs, a new version of

²RAINS models are described in more detail by Amann and Makowski (2000).

RAINS is being developed. Its structure is outlined in Figure 2. RAINS comprises now modules for emission generation (with databases on current and future economic activities, energy consumption levels, fuel characteristics, etc.), for emission control options and costs, for atmospheric dispersion of pollutants, and for environmental sensitivities (i.e., databases on critical loads).

The new version of the RAINS model is a perfect example justifying the needs for new modeling technology:

- It is a large model (the currently developed version will have several millions variables) with a complex structure (Makowski, 2005);
- It is developed by interdisciplinary teams resident at distant locations;
- The amount of data (used for the model specification, and for various types of analyses) is huge (more than 10⁸ non-zero elements); various parts of the data are developed (typically by specific analyses of other models and by various data mining techniques) by diversified interdisciplinary teams;
- Various groups of users (also situated at distant locations) desire to use various types of model analysis, which in turn requires support for controlled modifications of parts of data;
- The whole modeling process (especially model specification, data collection and verification, specification of model instances, definitions of preferences, and the corresponding results of the model analysis) needs to be automatically documented;
- Solving the resulting optimization problems will require solvers that exploit the structure of the problem, and can be run on a computational grid.

Due to the space limitation we cannot provide details of the RAINS models here. However, even this short summary clearly shows that no general purpose modeling environment can be used for the development and exploitation of RAINS. A more detailed discussion of various aspects related to the development of RAINS models and their use for supporting international negotiations can be found in (Makowski, 2001), and (Makowski, 2005).

4 Structured Modeling Technology

Modeling technology is a craft of a systematic treatment of modeling tasks using a combination of pertinent elements of applied science, experience, intuition, and modeling resources, the latter being composed of knowledge encoded in models, data, and modeling tools. Thus the key to a successful modeling undertaking is defined by the appropriate choice of "*a combination of pertinent elements*".

The *Structured Modeling Technology* (SMT) outlined here is based on two successful paradigms: the Structured Modeling paradigm, which provides a proven methodological background, and the *Object-Oriented Programming* (OOP) paradigm which, combined with DBMS, XML, and the Web technologies, provides an efficient and robust implementation framework. Moreover, the development of SMT has not only been driven by the actual needs of modeling a complex problem, but it has also been tested by complex applications. With this foundation, SMT is applicable to a wide range of complex algebraic models.

The *divide and conquer* tactic combined with an integrating framework for the conquered elements is a natural way of dealing with the modeling of complex problems. Thus, we start the presentation of SMT with summarizing the basic elements of the modeling process.

4.1 Modeling process

Modeling is a network of activities, often referred to as a *modeling cycle*, or a *modeling process*, or a *modeling lifecycle*. Geoffrion (1989) provides a detailed specification of a modeling cycle, together with references to earlier works on this topic. Here, we discuss the modeling cycle composed of more aggregated elements which correspond to the elements of SMT presented below:

- Analysis of the problem, including the role of a model in the corresponding decisionmaking process; and the development of the corresponding *model specification*.
- Collection and verification of *the data* to be used for the calculation of the model parameters.
- Definition of various *model instances* (composed of a model specification, and a selection of data defining its parameters).
- Diversified analyses of the instances.
- Documentation of the whole modeling process.

Below we outline basic features of SMT that correspond to these elements of the modeling process.

4.2 Model specification

Model specification is a symbolic definition of the model composed of variables and algebraic relations between them. In other words, model specification provides parametric definitions of all variables and constraints. In order to efficiently handle large and complex models the specification exploits the power of OOP combined with core concepts of the Structured Modeling, such as sets, ordered pairs, relations, classification, grouping, hierarchy, primitive and compound entities, various types of elements (such as attribute, function, test), and collections. Primitive entities have attributes and functions common for the derived types, namely parameters, variables, and constraints (representing parametric relations between variables), each possessing additional attributes specific for each of them. Compound elements of the specification are composed of sets of primitive entities.

In other words, model specification provides parametric definitions of all variables and constraints, and is equivalent to a commonly used symbolic definition of a problem by a specification of variables and constraints in which all distinct collections of variables and constraints are declared. The sets of indices needed for the instantiation of collections are only declared (they are defined later during instantiations of a model).

Symbolic model specification has a number of advantages, including:

• It is complete, i.e., properties of all entities of the model are defined.

- It is compact, e.g., the specification of the RAINS model presented in (Makowski, 2000) is composed of 21 variables and 25 constraints (both compound), while instances of this model have typically over 30,000 of each of the variables and the constraints.
- It presents the relations between the variables in the form of algebraic expressions, which is a commonly used (both by modelers, and users with different backgrounds) model representation.
- It makes it easy to verify (and also to use for various purposes, e.g., to provide relevant information to solvers) the structure of the model.
- Units of all entities are defined. This allows for a diagnostic not only of the syntax but also of the semantic correctness of the symbolic specification. Moreover, during the model instantiation, units of actual data are checked for consistency with the model specification.
- It makes it technically easy to combine specifications of two or more models.
- It makes it easy to extract part of a model, e.g., for either more detailed analysis or for use as a part of another model.
- It makes it easy to experiment with various modifications of the model specification.
- One source of model specification is used for the whole modeling cycle.
- A version control system makes it easy to document the history of modification and to retrieve various versions of a model.

Model specification, although technically made easy with SMT, still remains a challenging task that requires team work by people who can contribute various elements of the needed knowledge. Experienced modelers are aware of the fact that modeling skills are composed of knowledge, experience, art, and craft (Paczyński, Makowski and Wierzbicki, 2000) aimed at exploiting modeling legacy developed for various modeling paradigms (Makowski and Wierzbicki, 2003). An overview of various modeling paradigms can be found in (Makowski, 2005).

4.3 Data

Data for large models comes from different sources (also as results from analyses of various models), and larger subsets of data are maintained by teams. Fortunately, there is a natural division of data into subsets, which are maintained by individual persons or small teams. Persons working with well-defined subsets of data are experienced in collecting, cleansing, verifying, and maintaining the data they are responsible for. Therefore the "only" problem is how to structure the process of aggregating the subsets of data maintained by various teams into a data collection that can be used for model instantiation and analysis. To achieve this, a structured approach based on DBMSs is a must.

DBMSs have recently been used more often by various modeling systems for handling data. SMT, however, is most probably the first to use DBMS to handle all the persistent elements of the modeling process. Moreover, SMT exploits the concept of *Data Warehouse* (DW) for supporting persistency and efficiency of data handling. The latter is achieved by defining a base dataset, and supporting its incremental modifications (which allows for avoiding duplications of large amounts of data needed in more traditional approaches requiring the storage of complete datasets even when only a small fraction of the data is

modified).

The data structures of a DW are generated automatically from the model specification. This not only assures consistency between the declarations of the parameters in the model specification and the data used for instantiations of these parameters but also saves substantial resources that would otherwise have been needed for preparing and maintaining data structures for any complex model. Moreover, SMT supports import of data from DBs, and from files having a simple, self-documenting format.

Although SMT uses XML for data, it does so in a way that is different from that used in commonly known XML-based applications, which typically document each data item separately. SMT uses XML only for meta data, which contains all the necessary information about the data structure (including types and units of each data element) and documentation; sparse or dense data structures are used depending on the sparsity characteristics of the corresponding data items. Therefore, the actual data is stored without any redundant information.

Finally, we mention that various collections of data registered in SMT resources have different statuses that also determine access to each of them. A set of data is first accessible only to a person who collects and cleans the data; it is then made readable for a small team that may verify the data before it is made readable for a defined group of users. Write permissions (which imply persistent modification of the data) are typically restricted to a small group of developers. However, users with the read-only access to the data may have a possibility of modifying a copy of selected elements of data, and storing the modified data as a new resource.

4.4 Model instance

Model instance is defined by a selection of definitions of two objects: a model specification, and a set of data to be used later for defining all the sets of the compound variables, and values of all the parameters in the constraints, as well as for the Jacobian and Hessian, if the latter are used. During this procedure, the user can optionally select a data update that redefines the values of selected parameters (such as lower and/or upper bounds, tolerances, subsets of parameters, etc). A defined model instance is added to SMT resources. This is archived by a two-step procedure. First, the model specification and all used data items are assured to be persistent (i.e., the objects that are not yet in the corresponding DW are stored there). In this way it is always possible to generate an equivalent model instance without the need to keep multiple copies of persistent objects. Second, the instance is stored in the resources DB. The stored version contains automatically generated documentation about the definition of the instances, and mappings of the persistent objects needed for generation of an equivalent instance.

4.5 Instance analyses

Model analysis is probably the least-discussed element of the modeling process. This results from the focus that each modeling paradigm has on a specific type of analysis. However,

the essence of model-based decision-making support is precisely the opposite; namely, to support various ways of model analysis, and to provide efficient tools for comparisons of various solutions.

The instance analysis is composed of a sequence of steps, each of which consists of:

- 1. Selection of the type of analysis, which includes simulation, single-criterion optimization, soft simulation, multicriteria model analysis.
- 2. Definition of the corresponding preferential structure, which takes different forms for different methods of model analysis, e.g., for:
 - Classical simulation, it is composed of given values of input variables;
 - Soft simulation, it is defined by desired values of decisions and by a measure of the distance between the actual and desired values of decisions;
 - Single criterion optimization, it is defined by a selected goal function and by optional additional constraints for the other (than that selected as the goal function) outcome variables;
 - Multicriteria model analysis, it is defined by an achievement scalarizing function, which represents the trade-offs between the criteria used for the evaluation of solutions.
- 3. Selection of a suitable solver, and specification of parameters that will be passed to a solver.
- 4. Generation of a computational task representing a mathematical programming problem the solution of which best fits the user preferences.
- 5. Monitoring the progress of the computational task, especially if it requires a substantial amount of computing resources.
- 6. Translation of the results to a form that can be presented to the user.
- 7. Documenting and filing the results, and optional comments of the user.

More detailed discussions of various methods of model analysis and their implementation in SMT are provided in (Makowski and Wierzbicki, 2003) and (Chudzian, 2004), respectively.

4.6 Documentation

For any large modeling activity it is essential to provide automatic generation of a humanreadable documentation of the whole modeling process, including different model representations, history of changes, data used, various views on results, and other functions desired for a comprehensive and well-documented model analysis that allows auditing.

SMT exploits the XML capabilities for handling the documentation. XML is a data format for storing structured and semi-structured text, originally designed for publications on a variety of media. However, it can be also used for self-documenting various types of information that is exchanged between applications. A number of XML-based modeling approaches has been developed recently, see e.g., (Fourer, Lopes and Martin, 2004). For the efficient handling of large and complex models, however, a new approach to using XML capabilities is necessary. Such an approach for handling data is summarized above. Here, we outline the applicability of XML to a model specification.

An XML document type is defined for describing mathematics as a basis for computerto-computer communication. XML thus enables a single-source model symbolic specification that can be used for:

- High-quality documentation of the model specification that also conforms to strict rules regarding the mathematical notation and even the layout of equations or formulas;
- Definition of the model instances;
- Definition of various forms of preferential structures;
- Generation of the corresponding computational tasks;
- Processing solutions of computational tasks.

Using one source of a model specification for the whole modeling process is obviously critically important to assure consistency between the model specification, its documentation, and implementation.

The documentation of other elements of the modeling process is done on different levels of detail. The basic information (such as date, user name, options requested for each object to be used) is automatically stored in the DW by each SMT application. Additionally, a user accessing a DB with privileges for data creation or modification is asked to write comments, which are logged. A more advanced documentation (e.g., automatic logging of changes in a way that allows for documenting the complete history of modifications, and optional undoing of the changes) can be included in applications that manipulate data.

4.7 Integrating framework

After outlining the selected SMT elements we now summarize their integration into a modeling environment. SMT is used through the Web interface, and all persistent elements of the modeling process are maintained by a DBMS. Thus the Web and a DBMS provide an integrating framework for collaborative work of interdisciplinary teams that use SMT applications for various elements of the modeling process.

Each model developed with SMT has its own Data Warehouse. The DW handles not only data used for the computation of values of model parameters, but also all other persistent elements of the whole modeling process, including:

- Administrative data (about users, developers, administrators, access rights, etc.);
- A tree structure of updates defining various modifications of data;
- The specifications of elements of the modeling process, such as model specification, a selection of data (defined by a selection of updates), definitions of model instances;
- Results of various analyses of model instances.
- The documentation of the modeling process.

The functionality of SMT is provided by a suite of applications that currently run on IIASA's network of Sun workstations. However, they can be adapted to run on heterogeneous hardware available at distant locations, if needed. SMT is being implemented for two widely used DBMSs, namely Oracle and PostgreSQL.

SMT is designed to be used by any authorized person having access to the Web. Groups of users (in the sense of groups used by the Unix OS) are defined with different authorizations to perform certain modeling tasks for selected models. Such an approach supports

collaborative work of teams working at distant locations.

5 Conclusions

The modeling technology outlined here fulfills the requirements for model-based support for solving complex problems, where complexity is characterized by the features of:

- the modeled problem;
- the size of the data;
- the interdisciplinary teams developing the model; and
- the way the model is used.

SMT handles the components of a modeling process in a structured way exploiting the advantages of DBMS, XML, and OOP technologies. In particular, SMT has the following key advantages:

- 1. It supports basic modeling activities (and their documentation) through the full model life cycle.
- 2. It promotes quality (e.g., by assuring consistency throughout the whole modeling process, and using commercial DBMSs), and facilitates separation of data, model specification, model instantiation, and model analysis. Consistency is assured by using appropriate attributes of all model entities that allow for the semantic check of model specification, and also of actual data maintained by the automatically generated Data Warehouse.
- 3. It is efficient; in particular its implementation conforms to the three basic requirements for applications suitable for large models:
 - Each type of object is handled efficiently, i.e. without overhead caused by functionality needed for other types of objects;
 - Common (for more than one type of object) functionality is provided without reimplementations; and
 - The modeling process is integrated with modern DBMS technology, thus providing a natural way to use proven (and familiar to many practitioners) technology for management of all persistent elements of the whole modeling process.
- 4. It improves the reuse and sharing of existing modeling resources (composed of models, data, and modeling tools), making them available also to a broader audience.

While some features of SMT are already present in various modeling systems, SMT is probably the only modeling system that is fully integrated with DBMSs, and can actually be used for collaborative development and for the distributed use of models that are as complex as RAINS.

Thus, SMT effectively supports collaborative modeling (both model development and exploitation) by interdisciplinary teams working at distant locations. In particular, SMT supports the development of models with complex structures and huge amounts of data, and diversified analyses of such models; moreover, it provides automatic documentation of the whole modeling process. Thus, SMT promotes modeling quality and transparency, which are critically important for model-based support of decision-making, especially in environmental policy.

6 Acknowledgments

Several ideas exploited in SMT have resulted from many discussions and joint activities of the author with A. Geoffrion, J. Granat, and A.P. Wierzbicki. This paper is to a large extend based on (Makowski, 2004). The author gratefully acknowledges all these contributions, but he assumes the sole responsibility for the content of this paper.

References

- Amann, A. and Makowski, M.: 2000, Effect-focused air quality management, *in* Wierzbicki, Makowski and Wessels (2000), pp. 367–398. ISBN 0-7923-6327-2.
- Chudzian, C.: 2004, Support of model analysis within structured modeling technology, *Interim Report IR-04-051*, International Institute for Applied Systems Analysis, Laxenburg, Austria.
- Fourer, R., Lopes, L. and Martin, K.: 2004, LPFML a W3C XML schema for linear programming, *Technical report*, Department of Industrial Engineering and Management Sciences, Northwestern University, Chicago, Illinois.
- Geoffrion, A.: 1987, An introduction to structured modeling, Management Science 33(5), 547-588.
- Geoffrion, A.: 1989, Integrated modeling systems, Computer Science in Economics and Management 2, 3–15.
- Makowski, M.: 2000, Modeling paradigms applied to the analysis of European air quality, *European J. Oper. Res.* **122**(2), 219–241. available also as IIASA's RR-00-06.
- Makowski, M.: 2001, Modeling techniques for complex environmental problems, in M. Makowski and H. Nakayama (eds), Natural Environment Management and Applied Systems Analysis, International Institute for Applied Systems Analysis, Laxenburg, Austria, pp. 41–77. ISBN 3-7045-0140-9, available from http://www.iiasa.ac.at/~marek/pubs/prepub. html.
- Makowski, M.: 2004, Lessons from applications of structured modeling to solving complex policymaking problems, *Proceedings of the SICE Annual Conference 2004*, Society of Instrument of Control Engineers (SICE), Tokyo, pp. 2724–2729. ISBN 4-907764-22-7; CD edition of the Proceedings available from SICE.
- Makowski, M.: 2005, A structured modeling technology, *European J. Oper. Res.* (in press), draft version available from http://www.iiasa.ac.at/~marek/pubs/prepub.html.
- Makowski, M. and Wierzbicki, A.: 2003, Modeling knowledge: Model-based decision support and soft computations, in X. Yu and J. Kacprzyk (eds), Applied Decision Support with Soft Computing, Vol. 124 of Series: Studies in Fuzziness and Soft Computing, Springer-Verlag, Berlin, New York, pp. 3-60. ISBN 3-540-02491-3, draft version available from http://www.iiasa.ac.at/~marek/pubs/prepub.html.
- Paczyński, J., Makowski, M. and Wierzbicki, A.: 2000, Modeling tools, *in* Wierzbicki et al. (2000), pp. 125–165. ISBN 0-7923-6327-2.
- Wierzbicki, A., Makowski, M. and Wessels, J. (eds): 2000, Model-Based Decision Support Methodology with Environmental Applications, Series: Mathematical Modeling and Applications, Kluwer Academic Publishers, Dordrecht. ISBN 0-7923-6327-2.

A Robust Stabilization Technique for Uncertain Models of Global Carbon Cycle

Arkady Kryazhimskiy* and Nikolai Melnikov International Institute for Applied Systems Analysis, Laxenburg, A-2361 Austria

Abstract

The extreme complexity of large-scale environmental systems is often reflected in strong uncertainties in the corresponding models. This motivates the need for the elaboration of adequate control-theoretic methods. In this paper we present a robust technique for stabilization of an uncertain two-compartment model of the global carbon cycle dynamics.

Keywords: robust stabilization, nonlinear dynamical systems, stabilization of atmospheric carbon concentration.

The issue of controlling the global carbon cycle through the regulation of anthropogenic emissions is widely discussed in the context of global warming (see, e.g., Nordhous, 1980; Wigley, 2004). The tolerable windows approach (see, e.g., WBGU, 1995) suggests that, in order to prevent the harmful impact of global warming, the annual temperature should be kept within certain limits. The latter requirement implies that the concentration of carbon in the atmosphere should be stabilized within certain pre-set bounds. One of the ways to achieve this goal is to guide the atmospheric carbon concentration to a prescribed *target level* lying within these bounds. In this paper, we present an approach to solving this problem using a technique of stabilization of an uncertain dynamical system. For the sake of brievity, we omit mathematical details (for details, see Kryazhimskiy and Maksimov, 2003; 2004).

Within the highly complex global carbon cycle process, the ranges of the parameters and functional relationships between them are not clear enough. Therefore, it appears reasonable to assume that instead of the single "real" model of the process, we deal with a *set of admissible models*. Assuming this, we arrive at the problem of stabilizing a dynamical

^{*}Supported in part by the RFBR (project #03-01-00737) and by the Program on Basic Research of the Russian Acad. Sci., "Changes of Natural Terrestrial Objects in Russia in Zones of Intense Technogenic Influence" (project # 3 10002-251/II-13/196-018/300503-340).

system described by an ODE whose right-hand side is not specified. Taking a simplified carbon cycle model (Svirezhev, et al, 1999) for a basis, we arrive – after some generalizations – at the 2-dimensional dynamical system of the form

$$\dot{x}(t) = \varphi(t) + u(t) + g(x(t), y(t)), \dot{y}(t) = -g(x(t), y(t)).$$
(1)

Here t is time; x(t) and y(t) are the deviations of the total masses of carbon in the atmosphere and in the ocean, from their pre-industrial levels, respetively; $\varphi(t)$ is the basic scenario for the anthropogenic emissions of carbon into the atmosphere; and u(t) is an emission correction input. The function g = g(x, y) is decreasing in x and increasing in y.

The key point is that the function g is uncertain. Namely, we suppose that a class of *admissible* functions g is given, and each of these functions can correspond to the "real" carbon cycle dynamics. In other words, not knowing the "real" carbon cycle model, we are given a set of admissible models of form (1), which (we know this) contains the "real" one. The initial state,

$$x(0) = x^0, \quad y(0) = y^0,$$
 (2)

is also given inaccurately; some sets of *admissible* values for x^0 and y^0 are fixed. Taking that into account, we understand an *admissible model* as a triple including one of the admissible ODE's of form (1) and a pair of admissible values for x^0 and y^0 .

Let an appropriate limit value \hat{x} for the atmospheric carbon concentration be fixed. The stabilization problem we deal with consists in finding a strategy for forming emission corrections inputs u(t) which guide the "real" atmospheric carbon concentration x(t) to \hat{x} as time increases infinitely:

$$\lim_{t \to \infty} x(t) = \hat{x}.$$
(3)

The values u(t) are updated using the observations of the current atmospheric carbon concentrations, x(t).

As soon as every admissible model can be the "real" one, we understand the stabilization problem as that of *model-robust* stabilization: a sought strategy for updating u(t) should guarantee (3) for *every* admissible model chosen beforehand. In the sequel, we outline an approach to solving the model-robust stabilization problem.

For any admissible model (1), (2) we have

$$x(t) + y(t) = x^{0} + y^{0} + w(t) + \Phi(t)$$
(4)

where

$$\Phi(t) = \int_0^t \varphi(\tau) d\tau$$

and

$$w(t) = \int_0^t u(\tau) d\tau \tag{5}$$

are the accumulated basic emission and accumulated correction emission respectively. It is reasonable to assume

$$\lim_{t \to \infty} \Phi(t) = \bar{\Phi}, \quad \lim_{t \to \infty} w(t) = \bar{w};$$

note that $\overline{\Phi}$ is fixed, and \overline{w} is variable. Now (4) and (1), (2) imply

$$\lim_{t \to \infty} x(t) = \bar{x} \tag{6}$$

where \bar{x} depends on the saturation level of the accumulated correction emission, \bar{w} (not depending on the "transition path" w(t)). Hence, given an admissible model (1), (2), one can construct an input-output map M that associates every admissible emission correction saturation level \bar{w} to a limit value in the atmospheric carbon concentration, \bar{x} (Figure 1). It can be stated that M is monotonically increasing (see Kryazhimskiy and Maksimov, 2003). Therefore, there exists the unique *target* saturation level $\bar{w} = \hat{w}$ corresponding to the target carbon concentration level \hat{x} , i.e., such that $M(\hat{w}) = \hat{x}$. If the model is "real", any accumulated emission correction path w(t) which saturates at \hat{w} ensures the validity of the desired limit relation (3).

However, instead of the "real" model we are given the set of admissible models (which includes the "real" one), and each admissible model is associated with a particular target saturation level \hat{x} . The set of the target saturation levels \hat{x} corresponding to all admissible models covers a solid interval $[w^-, w^+]$; we call it the *uncertainty interval* (Figure 1). The identification of the "real" target saturation level \hat{x} , which corresponds to the "real" model, is obviously a key task in the design of the desired robust stabilization process.

The proposed robust stabilization strategy identifies the "real" saturation level \hat{x} through an infinite sequence of observation and emission correction periods, each of which results in a considerable reduction of the length of the current uncertainty interval. In what follows, for brevity, we call the current emission correction inputs u(t) the *correction inputs* and the accumulated emission correction curves w(t) (5) the *correction paths*. The stabilization process consists in sequential replanning the future correction inputs $u_0(t), u_1(t), \ldots$ and the corresponding correction paths $w_0(t), w_1(t), \ldots$,

$$w_0(t) = \int_0^t u_0(\tau) d\tau, \quad w_1(t) = \int_0^t u_0(\tau) d\tau, \dots,$$
(7)

at "switching" times $t_0 = 0, t_1, \ldots$



Figure 1: The input-output map.

At the initial time $t_0 = 0$ the controller sets $u_0(t) = 0$, implying that $w_0(t) = 0$ and $\bar{w}_0 = 0$. The motion of the real system goes along a trajectory $x_0(t)$. At each time $t \ge 0$
the controller observes $x_0(t)$ and decides if $u_0(t)$ must be switched to $u_1(t)$. The decision on a switch is made upon the receipt of the *inconsistency signal* at time $t_0^* > 0$. At $t = t_0^*$ the inconsistency signal is received if $x_0(t)$ hits the boundary of the *calibration funnel*

$$\hat{x} - \nu(t) \le x \le \hat{x} - \nu(t);$$

here $\nu(t)$ is the positive *calibration radius* satisfying

$$\lim_{t \to \infty} \nu(t) = 0$$

 $\nu(t)$ is chosen beforehand. If the upper boundary of the calibration funnel is hit (Figure 2, left), i.e., $x_0(t_0^*) = \hat{x} - \nu(t_0^*)$, the controller learns that the correction input $u_0(t) = 0$ is too high. Consequently, all the admissible saturation levels \bar{w} that are not smaller than $\bar{w}_0 = 0$ are too high too. As a result, the initial uncertainty interval $[w^-, w^+]$ is shortened to $[w_0^-, w_0^+] = [w_0^-, \bar{w}_0] = [w^-, 0]$ (we assume that $w^- < 0 < w^+$).

If the lower boundary of the calibration funnel is hit (Figure 2, right), i.e., $x_0(t_0^*) = \hat{x} + \nu(t_0^*)$, the controller learns that all the admissible saturation levels $\bar{w} \leq \bar{w}_0$ are too low. The initial uncertainty interval $[w^-, w^+]$ is shortened to $[w_0^-, w_0^+] = [\bar{w}_0, w^+] = [0, w^+]$.

The next planned saturation level \bar{w}_1 is set to be the middle point of the new uncertainty interval $[w_0^-, w_1^+]$:

$$\bar{w}_1 = \frac{1}{2}(w_0^- + w_0^+).$$

The controller fixes some delay $\delta(t_0^*)$ for the switch to the new correction input $u_1(t)$.

At time $t_1 = t_0^* + \delta(t_0^*)$ the controller switches to

$$u_1(t) = \begin{cases} \gamma(t_1) \text{ or } -\gamma(t_1) & \text{if } t \le \tau_1, \\ 0 & \text{if } t > \tau_1. \end{cases}$$

Here $\gamma(t_1)$ is a prescribed positive value; the *acting time horizon* τ_1 for the correction input $u_1(t)$ is determined from the requirement that the new correction path $w_1(t)$ (see (7)) is saturated at \bar{w}_1 :

$$\lim_{t \to \infty} w_1(t) = w_1(\tau_1) = \bar{w}_1.$$

The motion of the real system switches to a trajectory $x_1(t)$. At $t = t_1^* > t_1$ the controller receives the inconsistency signal if $x_1(t)$ hits the boundary of the new calibration funnel (see Figure 2),

$$\hat{x} - \nu(t - t_1) \le x \le \hat{x} - \nu(t - t_1).$$

If the upper boundary of the calibration funnel is hit, i.e., $x_0(t_1^*) = \hat{x} - \nu(t_0^*)$, the controller learns that the admissible saturation levels $\bar{w} \ge \bar{w}_1$ are too high. As a result the uncertainty interval $[w_0^-, w_0^+]$ is shortened to $[w_1^-, w_1^+] = [w_0^-, \bar{w}_1]$, and the controller sets

$$\bar{w}_2 = \frac{w_1^- + w_1^+}{2}$$



Figure 2: Identification of an inconsistency moment.

The controller fixes a delay $\delta(t_1^*)$ for the switch to the new correction input $u_2(t)$. For technical reasons, the switch to $u_2(t)$ is performed at $t_2 = \max\{t_1^* + \delta(t_1^*), \tau_1\}$.

The described decisionmaking procedure repeated step by step infinitely many times produces the entire trajectory x(t) of the real system: $x(t) = x_k(t)$ ($t \in [t_k, t_{k+1})$, k = 0, 1, ...). Note that the procedure involves 3 key functional parameters: the calibration radius $\nu(t)$, the size of the correction input $\gamma(t)$, and the delay $\delta(t)$. The major analytic task is to establish the existence of $\nu(t)$, $\gamma(t)$ and $\delta(t)$ such that the associated decisionamaking procedure guides the trajectory x(t) to the target value \hat{x} (i.e., ensures (3)) irrespective of the choice of the admissible model acting as the real system. If the latter takes place, we call the suggested decisionmaking procedure the *robust stabilization strategy*.

The major result (see Kryazhimskiy and Maksimov, 2003) states the existence of functional parameters $\nu(t)$, $\gamma(t)$ and $\delta(t)$ of a robust stabilization strategy. Moreover, it is stated that one can take any $\gamma(t)$ such that $\lim_{t\to\infty} \gamma(t) = 0$ and any $\delta(t)$ such that $\lim_{t\to\infty} \delta(t) = \infty$; having $\gamma(t)$ and $\delta(t)$) one can provide a formula for $\nu(t)$.

Kryazhimskiy, et al, 2004, and Melnikov, 2004 present some results of the implementation of a robust stabilization strategy for sets of linear admissible global carbon cycle models (1), (2) (in which g(x, y) is linear).

References

- 1. Nordhaus, W.D., 1980, Thinking about carbon dioxide: theoretical and empirical aspects of optimal control strategies, Cowels foundation discussion paper No. 565, Yale Univ., New Haven.
- 2. Wigley, T.M.L., 2004, Modelling climate change under no-policy and policy emissions pathways, in Benefits of Climate Policies: Improving Information for Policymakers, OECD, Paris (in press).
- WBGU German Advisory Council on the Global Change, 1995, Scenario for the Deviation of Global Reduction Targets and Implementation Strategies, AWI, Bremerhaven.
- Kryazhimskiy, A., and Maksimov, V., 2003, On the exact stabilization of an uncertain dynamics, Interim Report IR-03-067, IIASA, Laxenburg (available from www.iiasa.ac.at).

- 5. Kryazhimskiy, A., and Maksimov, V., 2004, On exact stabilization of uncertain dynamical systems, J. Inv. Ill-Posed Problems (to appear).
- 6. Svirezhev, Yu., Brovkin, V., von Bloch, W., Schellnhuber, H.J., and Petschel-Held, G., 1999, Optimization of reduction of global *CO*₂ emissions based on a simple model of the carbon cycle, Environmental Modelling and Assessment, 4, 23–33.
- 7. Kryazhimskiy, A., Maksimov, V., and Korobochkina, S., 2004, On the design of robust emission strategies to stabilize the concentration of carbon in the atmosphere, in: Pahl, C., Schmidt, S. and Jakeman, T. (eds) iEMSs 2004 International Congress: "Complexity and Integrated Resources Management", International Environmental Modelling and Software Society, Osnabrueck, Germany, June 2004.
- 8. Melnikov, N., 2004, Robust stabilization of atmospheric carbon within a family of uncertain carbon cycle dynamics, Interim Report IR-04-053, IIASA, Laxenburg (available from www.iiasa.ac.at).

Report on

IIASA – Kyoto University

First Joint International Seminar on Applied Analysis and Synthesis of Complex Systems

Gunnar Johannsen

Professor of Systems Engineering and Human-Machine Systems Institute for Measurement and Automation Department of Mechanical Engineering University of Kassel Germany

1 INTRODUCTION

The "First Joint International Seminar on Applied Analysis and Synthesis of Complex Systems" of IIASA and Kyoto University was held on June 28-29, 2004 at the International Institute for Applied Systems Analysis (IIASA) in Laxenburg, Austria.

The seminar was a joint initiative of Kyoto University and IIASA with the main objectives of introducing a new COE project at Kyoto University to IIASA, as well as exchanging ideas and discussing about methodologies for analysis and modeling of complex systems. The COE project "Center of Excellence for Research and Education on Complex Functional Mechanical Systems" at Kyoto University belongs to the COE (Center of Excellence) Program of the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT). The COE Leader is Kazuo Tsuchiya of Kyoto University, the Seminar Organizers have been Marek Makowski of IIASA and Tetsuo Sawaragi of Kyoto University.

2 PRESENTATIONS AT THE SEMINAR

The seminar was opened by the IIASA Director Leen Hordijk. He gave a wide ranging informative overview of the history and the research of IIASA. Particularly, he pointed out that IIASA has been an important multinational research bridge and interlink between different countries, societies, and disciplines in East, West, North, and South over several decades.

The Project Leader of the COE, Kazuo Tsuchiya, presented an overview of the COE program indicating the mission and scope of the program and briefly highlighted the aims of the three research groups of the COE project – (1) Complex Fluid Mechanics Group, (2) Complex System Control and Design Group, and (3) Materials Group.

The Leader of the Complex Fluid Mechanics Group, Satoru Komori, explained modeling approaches for turbulent transport phenomena in atmosphere-ocean systems. The wind-wave tank and other experimental setups were also introduced. The discussion showed that IIASA values the importance of uncertainty in atmosphere-ocean systems differently and focuses their research on more global and multi-dimensional aspects whereas Kyoto University investigates the transfer processes in more detail from the view-points of fluid mechanics and thermal engineering. In a further presentation, Masato Nagata dealt with momentum and heat transport mechanisms of fluid motion in a rotating system. IIASA contributed with a paper on the exact stabilization of uncertain dynamics, authored by Arkady Kryazhimskiy and Vyacheslav Maksimov and presented by Nikolau Melnikov.

The Leader of the Complex System Control and Design Group, Tetsuo Sawaragi, talked about dynamical and complex behaviors in control systems and human-machine co-adaptive systems. Collective behaviors of complex functional mechanical systems, such as self-organization, pattern formation, evolutionary and adaptive dynamics, learning, etc., have been assumed to emerge out of interactions among individual subsystems or agents. The design and analysis of novel control mechanisms for autonomous robots and human-in-the-loop systems were presented. Further presentations discussed the structural topology optimization for the design of novel mechanical structures, by Shinji Nishiwaki, and the design of an adaptive control system by modular learning, exemplified with the flight control of an autonomous unmanned helicopter, by Hiroaki Nakanishi. The contribution from IIASA dealt with a structured modeling technology. This talk presented by Marek Makowski outlined the methodological background and implementation of a structured modeling environment developed to meet the requirements of modeling activities undertaken to support inter-governmental negotiations aimed at improving European air quality. The main part of the paper presented the structured modeling technology which was developed to support the implementation of the structured modeling principles for modeling complex problems.

The two invited keynote speeches also mainly covered aspects and approaches of the methodologically most central perspective for this COE project, namely the issues of the Complex System Control and Design Group. The keynote speech by Gunnar Johannsen from the University of Kassel in Germany dealt with the analysis and design of, and displays for, complex human-machine interactions. The structures and functionalities of human-machine systems and interactions were explained, referring to various levels of responsibility, flexibility, and autonomy. Functional and cognitive task analyses as well as various modeling techniques have been used as means for understanding complex interactions and for designing appropriate information displays. A human-centered design technique was introduced based on a systems engineering life-cycle methodology, including prototyping and evaluation. The design was exemplified with auditory displays for mobile service robots and with visual/graphical displays for a chemical process.

The second keynote speech by Martin Buss from the Technical University of Munich in Germany presented haptics and control in human interactive telepresence systems. It was explained that multi-modal telepresence systems enable human operators to become present and active in remote or inaccessible environments, with multi-modality including visual, auditory, and haptic channels. Haptics (force and tactile feedback) was described as an energy exchange between the telerobot/environment and the human operator/human system interface. The presentation was focused on key issues in haptic telepresence and teleaction systems from a control point of view. The major challenges of time-delay (latency) in the communication network and transparency issues as well as mechatronic solutions to haptic interfaces and telerobots were discussed.

The Materials Group was represented by its Leader, Takayuki Kitamura. From his part in the distributed overview paper and from discussions during breaks, the full range of material research issues from the atomic level through the lattice and cell levels to the macroscopic structure level

became visible. In the seminar, the presentation by Taiji Adachi exemplified the cell level with a paper on bone functional adaptation by remodeling through hierarchical mechanical systems from cell to tissue. It was discussed how mechanical viewpoints can contribute to a better understanding of the adaptive bone remodeling mechanism through hierarchical mechanical function-structure relations from cell to tissue. A related paper by Naohide Tomita on tissue-engineering discussed the design process from "Function Designing" to "Bio-Environment Designing". Several biological, clinical and mathematical approaches to the "in-vivo environment designing" were introduced.

3 EVALUATION OF THE SEMINAR

The scientific quality of the seminar was of highest caliber compared with strong international standards. Almost all presentations were excellent in contents and style. The preparations and efforts of the Japanese colleagues were admirable. The discussions were very cooperative, open-minded, and fruitful.

The scientific approaches and the application domains of the COE Project of the Kyoto University and those of IIASA are different but, in many ways, complementary. Thus, it was extremely valuable to contrast the differences in order to learn from each other. This is particularly important for the COE Project itself within which other kinds of differences also exist. These are quite natural with the wide scope of the COE Project and its early state.

Under these circumstances, it was very important for the participating members of the COE Project that they forced themselves with this seminar to understand each other's approaches and to discuss in an international environment, without distractions from their normal work environment, about the truly existing common aspects of the subprojects as well as of their approaches and methodologies.

Common grounds for the whole COE Project can mainly be found on the methodological levels and the higher levels of structural and functional abstraction. This is in full agreement with the overall objective of the COE Project to advance research in "modeling, analysis, and control of phenomena and design theory geared specifically for complex mechanical systems" towards a novel field of "Complex Systems Mechanical Engineering".

Comments on the 21st Century COE Program

COE for Research and Education on Complex Functional Mechanical Systems

(Kyoto University)

First Joint International Seminar on Applied Analysis and Synthesis of Complex Systems

IIASA, Vienna – Kyoto University

Martin Buss

Professor, Chair and Director Institute of Automatic Control Engineering, <u>M.Buss@ieee.org</u> Faculty of Electrical Engineering and Information Technology Technische Universität München, Munich, Germany

1 INTRODUCTION

On 28/29 June 2004 the above mentioned 1st joint International Seminar was held in Laxenburg, Austria, jointly organized by the COE (Kyoto Univ.) and the International Institute for Applied Systems Analysis (IIASA). The seminar agenda and scheduling is available at

http://www1.mech.kyoto-u.ac.jp/coe21/seminar/20040628/agenda.html

The presentations during the seminar were of world-leading quality, in particular the presentations by COE members of Kyoto University and the plenary talk by Prof. G. Johannsen were extremely inspiring because of their high scientific quality. Some of the presentations by people from IIASA were not a good balance in terms of quality. After all presentations by COE members there was a lively and fruitful discussion generating new ideas with all participants of the seminar. The athmosphere during these discussions and the seminar overall was very fruitful.

With the external influence by IIASA and the plenary talks it was nice to see that the COE members stood together behind their topic of complex systems and really conveyed a unified picture of a well established cooperation within the COE. It is conjectured that the COE was also strengthened in its research line and focus by the external influences in Laxenburg, also because the members were away from their usual businesses and could therewith freely discuss visionary research ideas.

Mild criticism is in order because of the weak IIASA commitment to the joint seminar. Apparently, the institution IIASA seems to be moving with too much political inertia and therefore may not be the best sparring partner for visionary scientific discussions with COE members. If one imagines a group of scientists in Europe with vividness and positive spirit like the COE members from Kyoto University, a joint seminar with such a group could have been even more productive.

The joint seminar is to be considered a very important milestone and without hesitation a very successful one for the COE in that members found together even more closely and that by external influences a fruitful scientific discussion took place.

It is my pleasure to congratulate the COE leaders to this success and wish the whole research team all the best for their future research agenda. With confidence I am looking forward to hearing more news about this COE pushing new boundaries for science and engineering in complex mechanical systems.

APPENDIX

Seminar Program

IIASA – Kyoto University

The First Joint International Seminar on Applied Analysis and Synthesis of Complex Systems

The 21st Century COE Program for Research and Education on Complex Functional Mechanical Systems, Kyoto University

> June 28-29, 2004. International Institute for Applied Systems Analysis Laxenburg, Austria

28 June, Wodak Room			
SESSION 1:			
9:30 - 10:00	An Overview of IIASA's Research,		
	Leen Hordijk, IIASA Director		
10:00 -10:30	An Overview of the COE Program,		
	Kazuo Tsuchiya, COE Leader (Kyoto University, Jp.)		
10:30 - 11:00	Coffee break		
11:00 – 12:00	Some Factors Affecting the Air-Sea Gas Transfer -Towards Modeling of Turbulent Transport Phenomena in Atmosphere-Ocean System, Satoru Komori (Kyoto University, Jp.)		
12:00 - 13:45	Lunch		
SESSION 2:			
13:45 - 14:30	Dynamical and Complex Behaviors in Control Systems and Human-		
	Machine Co-Adaptive Systems,		
	Tetsuo Sawaragi (Kyoto University, Jp.)		
14:30 - 15:15	Coffee break		
SESSION 3: Invited Keynote Speech Session			

15:15 - 16:15	Analysis and Design of, and Displays for, Complex Human-Machine			
	Gunnar Johannsen (University of Kassel, Germany)			
16:30 - 17:30	Haptics and Control in Human Interactive Telepresence Systems,			
	Martin Buss (Technische Universität München, Germany)			
18:00	Social event			
29 June, Wodak Room				
SESSION 4: Global Modeling of Environmental Issues				
9:30 - 10:00	Momentum and Heat Transport Mechanisms of Fluid Motion in a Rotating Annulus,			
10.00 10.20	Masato Nagata (Kyoto University, Jp.)			
10:00 - 10:30	Arkady Kryazhimskiy and Vyacheslav Maksimov (IIASA), presented by Nikolau Melnikov (IIASA)			
10:30 - 10:45	Coffee break			
SESSION 5: Adaptation in Biomechanics				
10:45 - 11:15	Bone Functional Adaptation by Remodeling through Hierarchical Mechanical Systems from Cell to Tissue, Taiji Adachi (Kyoto University, Jp.)			
11:15 - 11:45	From "Function Designing" to "Bio-Environment Designing", Naohide Tomita (Kyoto University, Jp.)			
11:45 - 14:00	Lunch			
SESSION 6: Introduction of Research from IIASA				
14:00 - 14:45	A Structured Modeling Technology, Marek Makowski (IIASA)			
14:45 - 15:15	Coffee break			
SESSION 7: Design and Control of Complex Mechanical Systems				
15:15 - 15:45	Structural Topology Optimization for the Design of Novel Mechanical Structures, Shinji Nishiwaki (Kyoto University, Jp.)			

15:45 – 16:15	Design of an Adaptive Control System by Modular Learning: Flight Control of an Autonomous Unmanned Helicopter, Hiroaki Nakanishi (Kyoto University, Jp.)		
SESSION 8: Closing Session			
16:15 - 16:45	From Seminar Organizer,		
	Marek Makowski (IIASA) and Tetsuo Sawaragi (Kyoto University, Jp.)		
16:45 - 17:00	Concluding Remarks,		
	Kazuo Tsuchiya (Kyoto University, Jp.)		

List of Participants

Organizers	E-mail address	Institution
Marek Makowski	marek@iiasa.ac.at	IIASA (RMS)
Tetsuo Sawaragi	sawaragi@prec.kyoto-u.ac.jp	Kyoto University, Dept. of
		Precision Engineering

Participants	E-mail address	Institution
Leen Hordijk	hordijk@iiasa.ac.at	IIASA, Director
Kazuo Tsuchiya	tsuchiya@kuaero.kyoto-u.ac.jp	Kyoto University, Dept. of
		Aeronautics & Astronautics
Satoru Komori	komori@mech.kyoto-u.ac.jp	Kyoto University, Dept. of
		Mechanical Engineering
Takayuki Kitamura	kitamura@kues.kyoto-u.ac.jp	Kyoto University, Dept. of
		Engineering Physics &
		Mechanics
Naohide Tomita	ntomita@mech.kyoto-u.ac.jp	Kyoto University,
		International Innovation Center
Masato Nagata	nagata@kuaero.kyoto-u.ac.jp	Kyoto University, Dept. of
		Aeronautics & Astronautics
Shinji Nishiwaki	shinji@prec.kyoto-u.ac.jp	Kyoto University, Dept. of
		Precision Engineering
Taiji Adachi	adachi@mech.kyoto-u.ac.jp	Kyoto University, Dept. of
		Mechanical Engineering
Hiroaki Nakanishi	hiroaki@kuaero.kyoto-u.ac.jp	Kyoto University, Dept. of
		Aeronautics & Astronautics
Gunnar Johannsen	g.johannsen@uni-kassel.de	University of Kassel, Dept.
		of Mechanical Engineering
Martin Buss	Martin.Buss@ei.tum.de	Technische Universitaet
		Muenchen, Institute of
		Automatic Control Engineering
		(LSR)
Nikolai Melnikov	melnikov@iiasa.ac.at	IIASA
Brian Fath	tath@iiasa.ac.at	IIASA
Yuri Ermoliev	ermoliev@iiasa.ac.at	IIASA
Sergey Aseev	aseev@iiasa.ac.at	IIASA