RESEARCH REPORT

Name: Frédéric PEYRANE
Affiliation (University): ICSN, Gif/Yvette, FRANCE

Research Advisor: Prof. Mitsuo SEKINE

Host Institution: Tokyo Institute of Technology

Research Subject:
Nucleoside and oligonucleotide chemistry

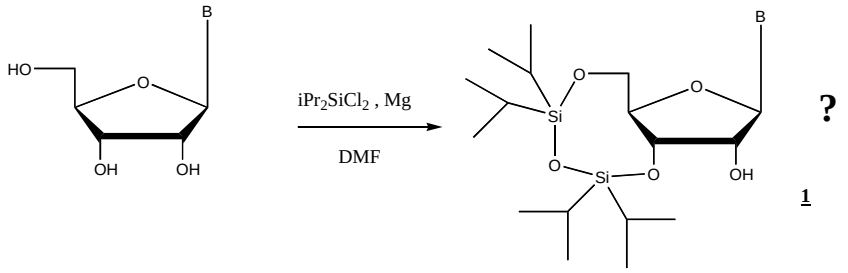
1. Research Description:

Since the discovery of DNA structure, a great deal of work has been accomplished to achieve the synthesis of oligonucleotides in an automated manner. Facile synthesis of sequence-defined oligonucleotides is the starting point of numerous biochemical and biological studies. It is also possible to incorporate in such structures, modified motifs to mimic DNA lesions. As a result, such a useful tool always needs to be improved.

In particular, the synthesis of oligoribonucleotides (small RNA), still suffers from some drawbacks in term of efficiency and cost; new hot topics, such as RNA interference, have engendered an increasing demand in oligoribonucleotide productivity.

2. Research Activities:

Recently, a new reaction has appeared in the field of silicon chemistry, involving the use of magnesium reagent. Under such conditions, the authors were able to synthesize cyclic siloxane derivatives from 1,2 diols. If such an inexpensive reaction could be applicable to ribonucleosides, it would be a major improvement in the synthesis of the building block of the oligoribonucleotides.



1

B= uracil, adenine, cytosine, guanine

My work this summer included the study of different sets of conditions to obtain the target compound **1**; attention has been paid on substrate, solvent and metal nature, order of additions…unfortunately, the products obtained were always different from the target compound, that could be obtained by classical (but expensive) methods.

3. Perspective of Research after this Program:

Some work needs to be done to gain further insight into this intriguing reaction, in order to determine what are the basic requirements for this cyclization to occur. For example, is the size of the siloxane ring a limiting condition? Or the nature of the substituents? Where does this extra oxygen atom come from?

4. Advisor's Remarks:

By using this summer program, I asked Mr. Peyrane to examine the possibility of application of a new fascinating finding recently reported by Prof. Nishiguchi to nucleic acid chemistry. This subject was a little bit risky but interesting in this field. He worked energetically and quickly responded to my long-standing question with a number of experiments he did. He discussed his experimental data with my young staff and students involving several doctor course students. Such an opportunity was really fruitful for him and us. He also contributed to our lab starting another project. I believe he could enjoy Japanese historical places using nonworking days as well as our beer parties so that he would serve as a friendly bridge between France and Japan through his wonderful experience here in Japan.

RESEARCH REPORT

Name: BESSON Eric Affiliation (University):University of Montpellier 2(France)	
Research Advisor: Pr. K.TAMAO Host Institution: Institute for chemical research, Kyoto university, Uji, Kyoto, 611-0011	
Research Subject: Stereoselective synthesis of oligosilanes based on configur ationally bicyclic disilane units	

1. Research Description:

In 1964, oligosilanes were found to absorb near ultra-violet light as a result of sigma delocalization of Si-Si bond. Afterwards soluble polysilanes were prepared and their UV absorption spectra showed thermochromism and related phenomena. This has introduced a concept of silicon backbone conformation dependence of sigma-delocalization. It has been widely accepted that the 'trans' conformation effectively extends sigma delocalization and 'gauche' does not. It has been shown, that a 'trans' conformer of a tetrasilane affords a first absorption maximum at longer wavelength and a 'gauche' conformer at shorter wavelengths. In another work in has been shown that :

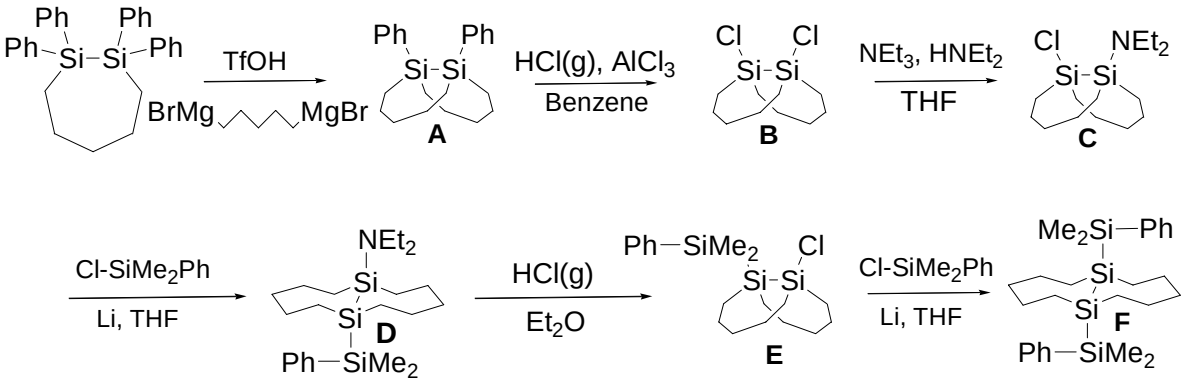
- there is an absorption maximum wavelength red shift as the 'trans'(or anti) segment is elongated
- for a anti-cisoid alternating oligosilane, the absorption maximum wavelength doesn't depend on the chain length

In addition, it is known that the Si-Si bond has an HOMO of energy comparable to the most HOMO's of π-systems. Consequently, there is a σ-π conjugation between a Si-Si system and a π system, and the σ-delocalization of an anti-disilane unit can be transmitted by a π system

2. Research Activities:

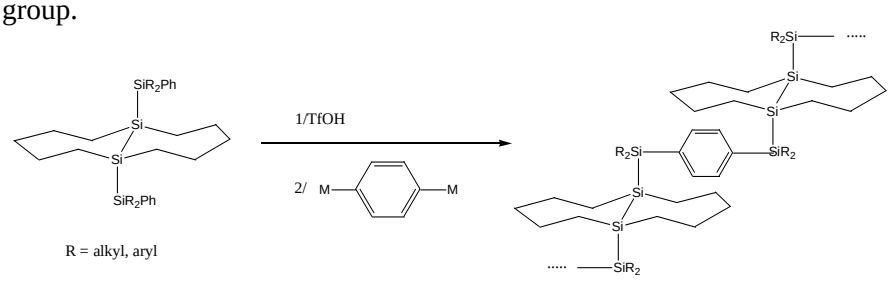
My work, during this training period, was to synthesize in a first part, a configurationally constrained bicyclic disilane unit, and in a second part to synthesize short oligomers of this unit separated by a phenylene spacer.

Then the first part was the syntheses of constrained disilane in the trans conformation. This is a 10 steps synthesis but I started at the fifth step and I followed this scheme:

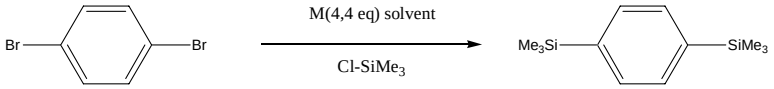


I obtained 70 mg of the desired product but this was sufficient to continue my work.

The second part was to find the conditions to prepare short oligomers of the unit F separated by phenylene group.

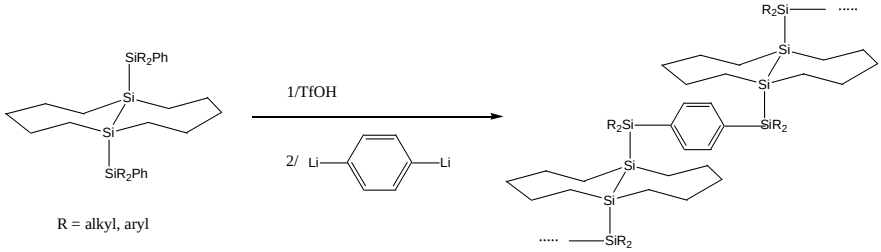


The best choice is the use of triflate group as leaving group. Then we must work with diethyl ether as solvant to avoid the cationic ring opening polymerization of cyclic ether like tetrahydrofuran. We tried to obtain the dimetallophenyl intermediate in ether in the following reaction.



Solvent	M	Temperature(°C)	Yield(%)
THF	tBuLi	-78	80
Ether	tBuLi	-78	45
Ether	Mg	Room temperature	No product

We tried to do the reaction between the dilithio reagent and the anti-disilane unit in order to prepare short oligomers with the following scheme:



The triflate reagent was prepared in benzene and the dilithio reagent was prepared in THF.

But after purification, we obtained a very low yield of short oligomers. It seems that the dilithio-reagent is to strong and that we need to use another organo-metallic reagent.

3. Perspective of research after this program

In a scientific point of view, my stay in the group of Pr. TAMAO has been very beneficial. I have learned a lot about silicon chemistry as main element. I mean that I did some organic reactions on silicon like on carbon, that I have never done.

On a more personal point of view, my stay in Japan has been very enriching. I have discovered very kind people, have had some insights into its culture and way of living. This short experience gave me the opportunity to visit this beautiful country but I didn't have enough time to visit all places I wanted in two months. But perhaps it will be possible in a next stay in Japan. In conclusion, thank you very much for this great summer.

4. Advisor's Remarks:

It was pleasure for us to have Mr. Eric Besson from Prof. Corriu's group, Monpellier, France, as a short-term research student under the MEXT program. He has a high-sense in chemistry and has a good personality, We asked him to take part in our new research project on the conformation dependence of the sigma-pi conjugated systems consisting of a configuration-restricted oligosilane unit and a phenylene unit. I was occasionally impressed by the fact that he was always enjoying the laboratory experiments of this rather difficult research project. He obtained a strong clue for the synthesis of the final target molecules. I am sure that he has obtained a lot of new experiences and new techniques through his short stay in our laboratory, as well as a variety of Japanese cultures. I really hope that this visit to our group in Kyoto, Japan, is useful for his researches in France.

With best wishes for his good success. Kohei Tamao

RESEARCH REPORT

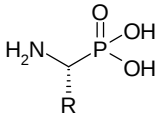
Name:	Affiliation (University):
Nicolas Boutard	University of Montpellier II
Research Advisor:	**Host Institution:**
Pr. Masato Kitamura	Research Center for Material Science University of Nagoya

Research Subject:

Synthesis of Enantiomerically Pure α-Amino Phosphonic Acid Monomers for the Solid Phase Synthesis of Related Phosphonopeptides

1. Research Description:

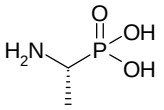
α-Amino Phosphonic acids **1** are significant elements in peptide science and future biochemical technology. They are analogues of α-amino acids in which a carboxylic group is replaced by a phosphonic function.



1

The tetrahedral arrangement of the sp^3 hybridized phosphorus atom and the dibasic acid properties modify the size and shape of the three dimensional structures as well as the isoelectronic point of the parent α-amino acid, which possess a smaller, flat monobasic function. These differences influence their chemical and biological characteristics. Incorporation of such unusual amino acids in peptides and proteins brings about interesting pharmacological properties like protease inhibition due to their analogy with tetrahedral proteolysis transition state. Their unusual binding features affords in some cases useful agonist and antagonists. This confers them a wide range of activities such as antibacterial activity, antiviral activity, neuroactive, hypotensive, analgesic or pesticide properties. In addition, many α-amino phosphonate-based haptens have been designes to generate catalytic antibodies.

Our goal was to synthesize enantiomerically pure alanine type **2** and phenylalanine type **3** α-amino phosphonic acids on a several grams scale. The preparation of their suitably protected derivatives would lead to useful building blocks for the solid phase synthesis of oligo-aminophosphonic acids.



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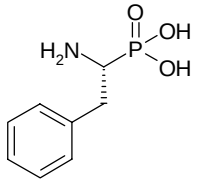

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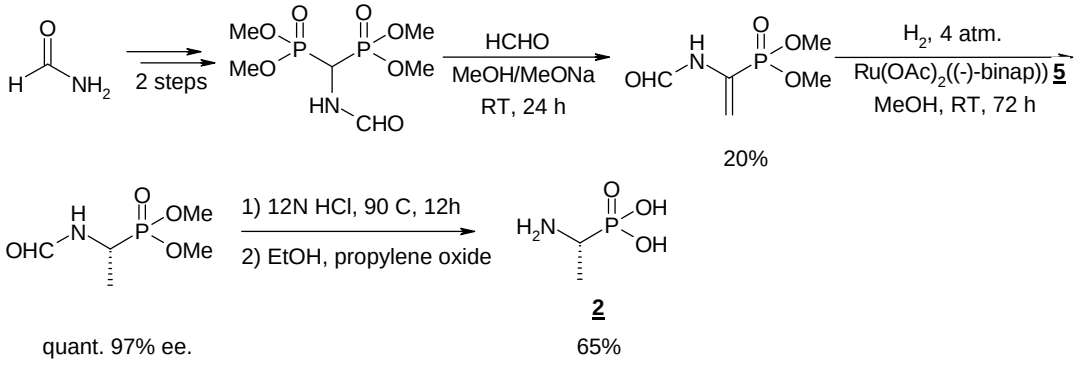
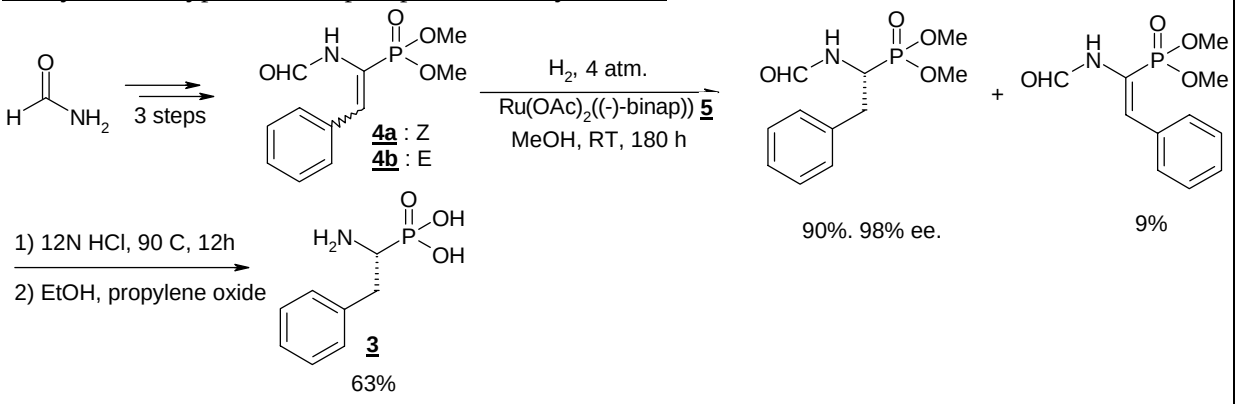
2. Research Activities:

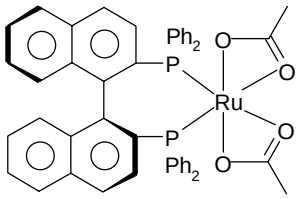
Alanine-type α-amino phosphonic acid synthesis :



Phenylalanine-type α-amino phosphonic acid synthesis :



The key steps of these two syntheses is the Noyori enamide hydrogenation reaction developed in this laboratory. The catalyst **5** used is based on ruthenium and the chiral ligand is (-)-S-Binap.

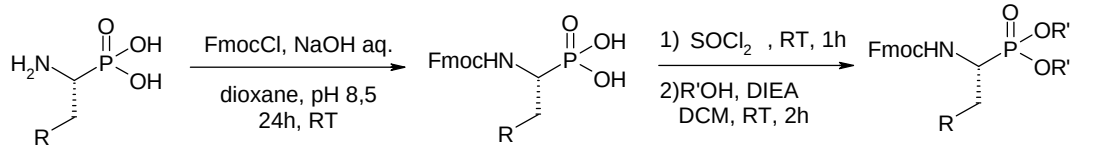


5

The reaction proceeds with a quantitative yield and an excellent enantiomeric excess. The substrate/catalyst ratio is 1/200. It is interesting to note that the Z isomer **4b** is practically inert under those hydrogenation conditions and can be recovered as an inchanged starting material in 9% yield.

Protected derivatives synthesis :

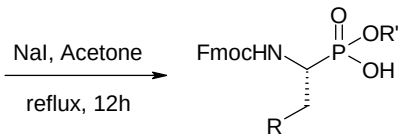
The protected derivatives suitable for Fmoc solid phase synthesis were synthesized according to conventional procedures.



2 : R=H
3 : R=Ph

6 : R=H
7 : R=Ph quant.

8a : R=H, R'=All 81%
8b : R=H, R'=Me 77%



9a : R=H, R'=All 75%
9b : R=H, R'=Me 94%

3. Perspective of Research after this Program:

Synthesis of enantiomerically pure alanine type **2** and phenylalanine type **3** α-amino phosphonic acids has been accomplished, using an highly efficient hydrogenation reaction as the key step. Their conversion into protected derivatives **9** provided multigram quantities of building blocks available for solid phase synthesis of phosphonopeptides.

My stay in Professor Kitamura laboratory has been very beneficial. I could learn new techniques and improve my manipulation skills especially for handling very air- and moisture-sensitive material. I could work on an organic chemistry field I had never seen before. I could also attend to very high quality seminars and I was impressed by the excellence of Japanese students and researchers.

On a personal point of view, my stay in Japan was a very enriching experience. I have had the opportunity of visiting some very interesting and culturally rich places. Moreover, I met some very nice people I wish to keep in touch with as long as possible.

4. Advisor's Remarks:

Mr. Nicolas Boutard has been involved in one of my main projects, Solid-phase Synthesis of Unnatural Peptides, in collaboration with a M2 student, Mr. Yoshitaka Ishibashi. His role has been establishment of the synthetic procedure for optically pure alpha-amino phosphonic acids having methyl or benzyl group at alpha carbon on the basis of our asymmetric hydrogenation methodology. Irrespective of his very short stay here and of his first experience for manipulation of highly air- and water-sensitive organometallics, he has not only successfully synthesized the key monomers for the solid-phase synthesis but also supplied the precursors in a large scale. The result will certainly make the project close to the goal. The success is apparently due to his diligent, critical, and constructive attitude toward the given project, that has made me feel intuitively his highly promising future as a world-standard scientist. More important is that he has an excellent sense of association with his colleagues. Mr. Boutard has made a significant influence to many Japanese, Indian, and Chinese researchers in my group. All of them have enjoyed learning both of French Culture and French Chemistry from him. I am sure that such a human relationship he has established in Japan is extremely important for both countries to develop new chemistry in this century. We all hope that his experience in Nagoya will be certainly valuable for his future research and social activities in the world, realizing international collaboration between Japan and France.

Masato Kitamura
Professor

RESEARCH REPORT

Name:	Affiliation (University):
CHAMBON JP.	Université Montpellier II
Research Advisor:	**Host Institution:**
Pr. SATOH N.	University of Kyoto
Research Subject:	
Caspases expression in *Ciona intestinalis* swimming larvae	

1. Research Description:

The ascidian *Ciona intestinalis*, an invertebrate member of the Chordate phylum, presents a spectacular metamorphosis. The swimming planctonic larval stage (tadpole) exhibits a remarkable chordate body plan, characterized by a dorsal neural tube and a typical notochord. Metamorphosis into a sessile filter feeder invertebrate involves an extensive reorganization of the body plan and most notably the regression of the tail.

Previously of my stay in Japan, we show that programmed cell death controls tail regression at metamorphosis, occurs through a polarized wave originating from tail extremity, and is caspase dependent. In silico analysis of Ciona genome pointed to 15 caspases with high homology with humans. Recently, this result was supported by the complete *Ciona intestinalis* genome sequencing. We think that *Ciona* provides an exquisite model to study developmentally regulated apoptosis in the context of an organism that is equipped with the similar caspase complexity of a higher vertebrate. Ciona has the genomic capacity of controlling cell death with comparable caspase equipment as mammalian.

Programmed cell death is one of the central cellular processes involved in development, aging, disease or stress response in metazoans. Comparative analyses of the components of the apoptotic machinery have shown that many of the proteins that play a crucial role in this process were already present in Porifera and Cnidaria. Indeed, from hydra to man, the activation of caspases, a family of aspartic acid-directed proteases, is a conserved feature of cells undergoing apoptosis. Almost of the study on caspases, were done on cell culture model with great understanding of their biochemistry. However, very few are known about the expression of caspases in vivo, except the very variable level of transcript of one given caspase in regard of the mammalian tissue observed. This last result permit to hypothesize that transcriptional regulation may exist for caspases, and could be a first level of apoptosis regulation.

One of my research interests is the pattern expression (where and when) of *Ciona* caspases in tail before the metamorphosis. In order, to make a spatio-temporal map of caspase expression and then study further the transcriptional regulation of caspases genes.

2. Research Activities:

First of all, Seven weeks in biology is a very short time to expect strong result, with the different experimental troubles that you could have.

The objective of my stay in Pr. Satoh lab was to observe the expression of the different caspases in the tail of the larvae.

I spend three days at Maizuru, Marine Biology center, to collect ands fix embryo to make *in situ* hybridization in the lab at Kyoto university.

Then using techniques familiar in the lab, I have investigated the expression of 8 potential caspases in the tail of larvae. These techniques include: Plasmid purification, sequencing, labeling RNA probes, *in situ* hybridization.

3. Perspective of Research after this Program:

After the program, I will return to the University of Montpellier II for further investigation of caspases expression. I will continue this work using molecular tools that I make here in Japan.

The following work will be to disturb expression of caspases, to further investigate the pathway of apoptosis during metamorphosis associated with tail regression.

I plan to investigate this work in collaboration with the laboratory of Pr. Satoh which develops morpholino anti-sense for gene expression disturbing.

4. Advisor's Remarks:

Apoptosis or programmed cell death is one the major research subjects in the field of molecular and cellular biology. Recent studies have disclosed many genes and molecules that are involved in apoptosis. Ascidians are primitive chordates which share many features with vertebrates, and their embryogenesis from fertilized eggs through swimming larvae to sessile adults has been well described. In addition, recently, the draft genome of the ascidian *Ciona intestinalis* has been sequenced to reveal all of the molecular staffs for apoptosis in this animal. Therefore, *Ciona* may provide a good model for future investigation of apoptosis *in vivo*. JP Chambon (Phil) visited my lab with an interest to determine the expression profiles of genes for caspases. Phil first visited Maizuru Fisheries Station of our University to collect samples of embryos and larvae for *in situ* hybridization. Then, after selecting several genes for caspases, he attempted to determine the expression pattern of these genes. Although, due to so short time period of staying here, he is on the middle of the way of research, he really worked hard. I do hope it was great fun of him. Simultaneously, all of graduate students and postdoc in my lab have enjoyed his staying here with discussion of various ideas for future studies. It was really good time for both Phil and my lab.

RESEARCH REPORT

Name:	**Affiliation (University):**
Sandrine ALINAT	CIRAD Montpellier Université III

Research Advisor: Dr. SAITO Kaoru
Host Institution: Laboratory of Biosphere Information Science, Tokyo University

Research Subject:
" Development a new digital cartography technique with movie and sound data in fore st environment"

1. Research Description:

The aim of this collaboration with the laboratory is to discover, to optmize new tools for landscape modelization. This simulating tools are innovating because they are crossing in same time cartographic representation by G.I.S. (Geographical Information System) and multimedia. They allow to simulate lansdcape evolution along the seasons and the years, and distinguished real items with virtual items.

The aim of the collaboration is to get a photorealistic forest landscape simulation technique with GIS forest type map data and plant modeling (AMAP), GIS-AMAP method he called. In the GIS-AMAP simulation, there were seasonal changing one. It is not easy to simulate a seasonal changing, to setting on the method and applicated it. That is why this laboratory started recording the real forest view monitoring in Chichibu University forest in 1995, which it is the starting point of the cyberforest research project.
Some traditional GIS digital data in field are DEM, remote sensing data, meteorological data and fieldwork data. The laboratory wants to add some movies and soundtrack to those GIS data, and found a good adequation for treatment beetween the both datas. GIS are new type of map, and allow to develop a kind of deal with digital data. Sounds, photographs, movie are already digitalized in this IT ages.
There are forest management GIS data, DEM, individual tree data, data all available for my PhD thematic (territorial planning, GIS, cartography in three dimension, landscape).
The purpose is to develop a new cartography technical using movie and sound data from 2000 to 2002 in the Tokyo University forest applying GIS ans AMAP method.

2. Research Activities:

- I gave 2 presentations of my thesis in my laboratory "Laboratory of Biosphere Information Science", with Dr. Saito, University of Tokyo.
- I gave one presentation about AMAP Software and how to use it.
- Members of my laboratories presented me what they do.
- We could talk together about the discordance between Europe and Japan, around the concepts "Landscape, Environment, GIS tools".
- We talked how to realize the scientist project of this summer program.
- After visiting the Chichibu forest and discoverd their studies, their data I suggest a concrete schedule to associate multmedia data and GIS on Chichibu forest.

- I visited with the laboratory, twice (1 day + 1 day) the field of their study, Chichibu forest
- I made a movie of 10min, with a Sony camera, and on Imac software called Imovie. The video should present their work in Chichibu forest, in french.
- I visited always with members of my laboratory (4 days trip) :
  - the Forestry and Forest Products Research Institute, Kansai resaerch Center in Kyoto
  - the Himeji Institute of Technology, Awaji Landscape Planning and Horticulture Academy

I could met some scientist staff.

- I collaborate one week, with the departement of "landscape" with Dr. Tsuyoshi HONJO and one PH Candidate, in Faculty of Horticulture, Chiba University. I gave one presentation of my work, and they present to me also what they do.

3. Perspective of Research after this Program:

This collaboration allow to the french partner to keep in touch with japonese laboratories, and exchange their work, exchange others students or researchers.

In France, the laboratory of CIRAD - UMR AMAP develop this software, and this collaboration with japan allow UMR AMAP to modelling new plants, and work on new field of study.

The other side, with the laboratory CNRS - UMR ESPACE, the reflexion about the association between GIS and multimedia dat for a new kind of cartography, called “Interactive cartography” is develop.

An other reflexion is also develop with laboratory CIRAD –TERA is about the modelling tools used for a territorial planification, mainly landscape managment.

Today, the possibility to apply for a post-doc in Japan can be possible, it should be an other rich experience.

4. Advisor's Remarks:

Miss Sandrine ALINAT has done good research work on “Developing a new digital cartography technique using movie and sound data in forest environment.” She already has obtained the necessary technique to get, analysis and evaluate the digital movie and sound data in the natural forest. She has got a new idea for developing a new digital cartography technique in this collaboration with our laboratory.

On the other hand, our laboratory and my students could have latest knowledge about AMAP (Plant modeling technique) from her.

I found her industrious and dedicated to her research. Her overall performance is satisfactory.

RESEARCH REPORT

Name: **Marche Hélène**	**Affiliation (University):** **Université de Toulouse le Mirail**
Research Advisor: **Dr. Yamazaki Yoshihiko**	**Host Institution** **University of Tokyo, Hongo**
Research Subject: **Social construction of the quality of life of cancer patients**	

1. Research Description:

My research interests in the general framework of politics of care given to persons striken of cancer in a context of transformation of medical institutions and medical techniques. Improving the quality of the life of patients became a public health issue since the beginning of the 70's. Curative logics aiming to restore or to maintain biological functions has been supersede by the global management of the patient as a "subject". Althougt the notion of quality of life directs the practices of cure and care aimed at populations with cancer, it runs against the economic, cultural and social complex of the organisation of the health care system.In Japan as most of the industriallized countries, improving the quality of life and the quality of the end of life of cancer patients is a claim done by medical institutions as well by civil society. This ethical concern aims at taking into account subjective experience of patients in the activities of care, promoting their autonomy and favoring their participation. In the field of research, evaluation of quality of life have taken more and more importance since the last decade in clinical and social science.

2. Research Activities:

- Bibliographical research at the University of Tokyo at the main library and at the medical library : experience of health and illness, announcement of cancer by doctors, palliative care in Japan, home-care, self-care.
- Participation in laboratory activities : seminars, discussions around scientific articles.
- Observations at the National Cancer Center at Chiba and the Peace House Hospice in Kanagawa prefecture.
- Interviews with doctors, nurces, psychologists, psycho-oncologists.
- Discussions and exchanges with sociologists and cultural-anthropologists from the university of Tokyo and Okayama.

3. Perspective of Research after this Program:

This program anable me to come into contact with japanese researchers from social sciences and humanities. Fieldwork partly analyzed permits me to observe some aspects of the care done by medical institutions to cancer patients in Japan : social conditions of the announcement, changes of terminal care (hospice, palliative care), social management of emotions (psycho-oncology, emotional work of medical staff), cooperation between professionals and volontaries. By the future, I would like to increase exchanges with japanese sociologists and anthropologists This experience gave me an opportunity to underline the value of international view on quality of life as a social construction. It also confirms the interest of qualitative researches on this field. I would like to make a post-doctoral research in Japan to explore these points.

4. Advisor's Remarks:

Ms. Helene Marche concentrated on her researches during her short stay in Japan and achieved the expected results, though I wish I could have spared more time to help her as Japanese advisor. During substantially only a month, she started library research to learn the illness experience of cancer patients and the provided care in Japan and engaged in fieldwork by observing several Japanese medical institutions for cancer and interviewing with many experts in cancer patients care. Besides she was enthusiastic about modern Japanese culture and society. I am sure she learned a lot about them. I admire her as a promising young health sociologist. I expect that she will complete her doctoral dissertation making full use of this research and come back to Japan to conduct further research in near future.

RESEARCH REPORT

Name: Renouf Mathieu	**Affiliation (University):** Laboratoire de Mécanique et de Génie Civil - Université Montpellier 2, France.
Research Advisor: Pr. Yuji Kishino	**Host Institution:** Mechanics of Materials, Dep. of Civil Engineering, Tohoku University, Sendai
Research Subject:	Comparison of the Granular Element Method and the Non Smooth Contact Dynamics method.

Research Description:

Please see the attached report.

Research Activities:

Please see the attached report.

Perspective of Research after this Program:

Please see the attached report.

Advisor's Remarks:

He has been staying for the programmed period as a co-worker rather than a student. As is stated in the report, he has worked on diverse aspects of the mechanics of granular media. One of his major research backgrounds is in the computation, and his suggestions for my simulation code are very precious. At the same time the discussion between us, I believe, will be a big help for his future research. This opportunity will be the starting point of our collaboration. Finally, I would like to thank him for visiting me.

A short comparison between the Granular Element Method and the Non Smooth Contact Dynamics method.

Mathieu Renouf,
LMGC - Université de Montpellier, Montpellier, France
Yuji Kishino,
Department of Civil Engineering, Tohoku University, Sendai, Japan

August 19, 2003

1 Introduction

In recent years, the interest for granular materials has been increasing. This may be due to the fact that a liquid, a solid or a gas can be microscopically looked upon as a kind of granular materials. In complement of experiments to clarify their mechanicals behaviours, some numerical tools have been developed. Among these numerical tools, we find a pionneering method of Cundall, which is called *the Distinct Element Method* (*DEM*) [3]. By modeling each particles as distinct elements with suitable contact interactions, we consider a material like a collection of particles instead of a continuum. The DEM is not the only method to deal with granular materials. *The Molecular Dynamics Method* (*MD*) [5], *the Granular Element Method* (*GEM*) [11] and *the Non Smooth Contact Dynamics* (*NSCD*) method [8, 16] have been also developped for the same purpose.
Among these, *GEM* and the *NSCD* are the methods used by the authors. The *GEM* have been developped by Y. Kishino [11] and the *NSCD* method by M. Jean and J.-J. Moreau [9]. These two methods are different on numerous points, and it is interesting to detect differences as well as common points between the two methods. We have been collaborating in this respect and we hope that this short report enables us to find the axe in getting improved codes.

2 GEM and NSCD

2.1 About the formulation

The *GEM* uses the bases of the *DEM* as explained in [4, 1, 10]. These bases stay on five points. Particles are circles or spheres and treated like rigid bodies. Each

contact point between particles occur through a small surface. A slight penetration is allowed between particles. The contact force is a linear function of this penetration and friction law is given by the Mohr Coulomb-Law. For *NSCD*, the penetration is prohibited, so the contact between particles occur at one point (for circular particles) and so the contact force can't be a linear function of the penetration.
For the two methods, when two particles P and P' are in contact, we define a local frame at the contact point I, $(\mathbf{t}, \mathbf{n})$, where $\mathbf{n}$ is the unit normal vector of contact and $\mathbf{t}$ the tangential one (see figure 1). We note $\mathbf{q}$ the configuration parameter,

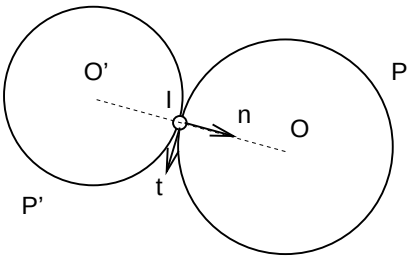


Figure 1: Local frame between two particles for *NSCD*. For *GEM*, $\mathbf{n}$ take the opposite sense.

$\dot{\mathbf{q}}$ and $\ddot{\mathbf{q}}$ the first and the second time derivatives. For the interval $[t^i, t^{i+1}]$, we note $\mathbf{q}(\mathbf{i+1}) = \mathbf{q}(\mathbf{t^{i+1}})$. The starting point of the two methods are the dynamical equation,

$$\mathbb{M}\ddot{\mathbf{q}} = F(\mathbf{q}, \dot{\mathbf{q}}, t) + \mathbf{r}, \tag{1}$$

where $\mathbb{M}$ is the mass matrix, and F the internal and external forces and $\mathbf{r}$ the contact forces. Classicaly, the *DEM* writes F using the viscosity and stiffness matrix, $\mathbb{C}$ and $\mathbb{K}$,

$$F(\mathbf{q}, \dot{\mathbf{q}}, t) = -\mathbb{C}\dot{\mathbf{q}} - \mathbb{K}\mathbf{q}, \tag{2}$$

but for the *NSCD*, F represents only external forces like gravity. The two methods use different approaches to solve equation (1). These approaches lead to analysis with different unknowns. Details on the time discretization are in [8] and [1]. The *DEM* uses an explicit scheme where the unknown is the incremental displacement $\Delta\mathbf{q} = \mathbf{q}(i+1) - \mathbf{q}(i)$ and *NSCD* an implicit one where unknown is the couple $(\dot{\mathbf{q}}(i+1), \mathbf{r}(i+1))$. For granular assemblies, the formulation consits of two level: the level of bodies (global) and the level of contacts (local). While the *DEM* deals with the global level, the *NSCD* method deals with the local one. The couple $(\dot{\mathbf{q}}(i+1), \mathbf{r}(i+1))$ is converted into the couple $(\mathbf{U}(i+1), \mathbf{R}(i+1))$ by using linear mappings, $\mathbb{H}$ and $\mathbb{H}^*$, to pass from the local level to the global one:

$$\mathbf{r}(i+1) = \mathbb{H}\mathbf{R}(i+1) \text{ and } \mathbf{U}(i+1) = \mathbb{H}^*\dot{\mathbf{q}}(i+1),$$

$\mathbf{U}(i+1)$ represents the relative velocity at the contact point between particles and $\mathbf{R}(i+1)$ the local contact impulsion. For contact law, the Velocity Signorini Condition, we use the normal component of $\mathbf{U}(i+1)$ and $\mathbf{R}(i+1)$,

$$U_N(i+1) \geq 0,\ R_N(i+1) \geq 0 \text{ and } U_N(i+1)R_N(i+1) = 0, \tag{3}$$

The *GEM* differs from the *DEM* by the calculation algorithm. The former one uses *stiffness method* [10]. The principle of the stiffness method is to express the incremental contact reaction in terms of the product of a stiffness matrix and the incremental displacement. The stiffness matrix is composed of primary and subordinate element matrices determined by a combination of the normal and tangential stiffnesses, k_n and k_t. So the incremental displacement is obtained by inversion of the stiffness matrix and an iterative process. The linear mapping $\mathbb{H}$ and $\mathbb{H}^*$ used in the *NSCD* method can be applied to compute primary and subordinate element matrices appearing in the stiffness method.

2.2 Example

The fact that the *GEM* allows penetration between particles while the *NSCD* method doesn't is a very important point. This penetration causes differences between simulated results by the two methods. To illustrate this, we have treated a one-dimensional example (figure 2). The ball is constrained to move between two

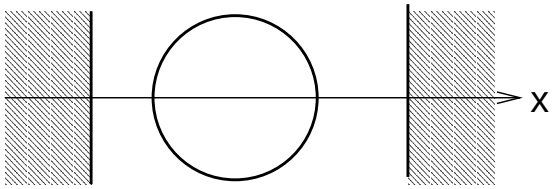


Figure 2: Example of a ball confine between two walls.

walls. The *GEM* treats contact properties between ball and walls with a classical spring-dashpot model where the stiffness and the viscosity are represented as k_n and c. The *NSCD* method uses a restitution contact law where the coefficient of restitution is represented as ρ_n. For weak values of k_n, the penetration is significant, and we can't fit the two curves of particle displacement obtained by the two methods (see figure 3 a)). But for strong stiffnesses, we got similar results (see figure 3 b)). For the last fitting, the restitution property is very important. In the *GEM*,

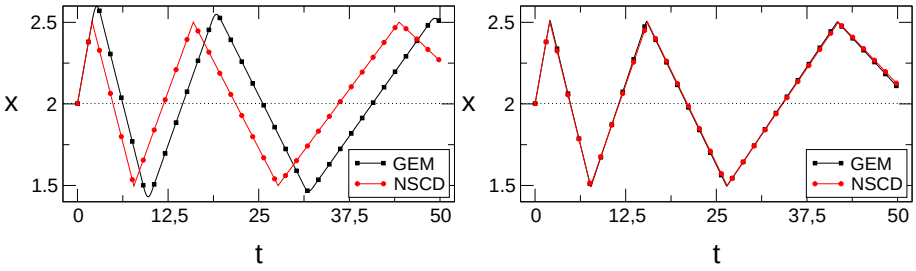


Figure 3: (left-a) $k_n = 2.10^4$ (right-b) $k_n = 2.10^6$

the restitution depends strongly on the viscosity coefficient c, while in the *NSCD*

method it is only characterized by the restitution coefficient ρ_n. The good fitting was obtained with $c = 2.10^4$ and $\rho_n = 0.715$. For strong stiffnesses, curves fit very well because the impenetrability of the *NSCD* method can be looked upon as having infinite normal stiffness. So for future comparisons between the two methods, such a basic fitting seems to be very important and necessary before starting further comparisons.

3 Code Implementation

The NSCD algorithm have implemented in the *LMGC90* software [6] and have been applied to the studies of different kind of problems [14]. Many results have also been obtained with *GEM* [13], an example of the latter is the study of triaxial test (figure 4) to investigate the different types of deformation modes in plasticity. The initial version of *GEM*, proposed for quasi-static analyses, has been recently extended to a dynamic version [12].

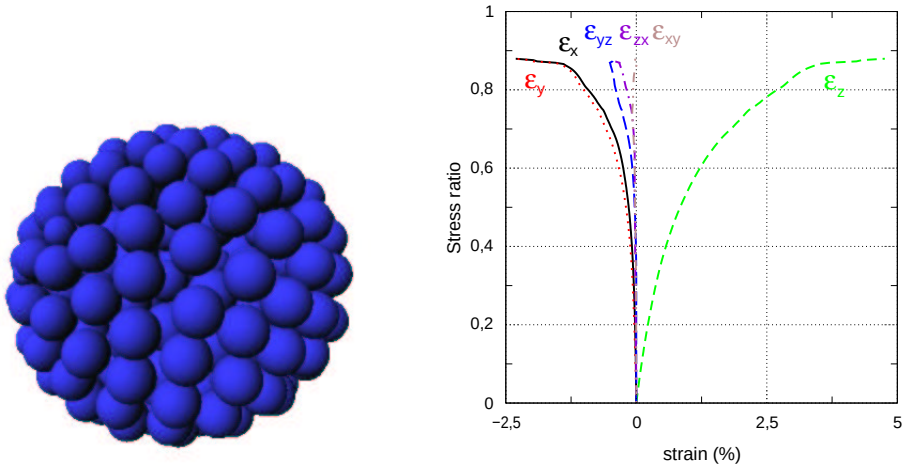


Figure 4: Stress-strain relationship in triaxial compression test: stress ratio = absolute value of stress deviator / mean stress

3.1 Multithreading

The standard version of the static *GEM* code version is written in fortran 77. This classical programming language doesn't allow wide extension. For this reason, the code script for multithreading has been written in fortran 90. Whith this transition from fortran 77 to fortran 90, we could take advantage of fortran 90 specificities and easily extend to the multithreading. We have performed a CPU time analysis on different simulations. All simulations are triaxial tests. The first case S1 are the simulations where the maximum number of loading step was reached. The second case S2 are simulations where the calculations were stopped because the maximum number of iterations was reached. In two cases, even though percentages

are different, it appears that the main part of CPU time (see table 1) is taken by two subroutines. The first one (*cont*) is the subroutine to revise contact forces and get

	cont	stress	unbl	gmove
S1	50%	2%	10%	35%
S2	20%	1%	4%	75%

Table 1: Repartition of elapsed time taken by subroutine (%).

true contact matrix. The second one (*gmove*) is the subroutine to translate particles and revise tangential forces. Note that the latter subroutine contains detection and revision of contacts. The CPU time taken by one of the other subroutine (*stress*) is less than 3%. But the subroutine *unbl* to check convergence takes, in the S2 case, 10% of the CPU time. A preliminary analysis has been achieved by developping a *MPI-GEM* version. The conclusion was that the iterative process in the stiffness method don't fit very well with *MPI* directives [2]. Indeed we need at each iteration to exchange a large flow of data between processors. So the time required for the communication between processors is long and the elapsed CPU time of the code is deteriorated. As a consequence of preliminary analysis, we decided to use OpenMP directives. With these directives, we can perform the same kind of multithreading as in [17]. The fact that the architecture of the code is suited very well for OpenMp directives [7] is also a beneficial point for us. The only limitation is that we need to work on shared memory computer and not on distributed memory computer. As a consequence of the time analysis, we have performed a parallel treatment on three of the fourth subroutines: *cont, unbl* and *gmove*. We need now to perform numerical tests on shared memory computers to check the efficiency of this multithreading.

3.2 Visualisation

For numerical method, which deals with granular materials, getting an efficient visualisation tool for observing results at each time step is very important. Right now, the *LMGC90* code uses *General Mesh Viewer* [15] for visualisation. This free software has many functions which are very interesting but files become very heavy for 3D simulation. The *GEM* uses a basic version of Strata 3D. Files can be lighter but this tool doesn't have all the functions of *GMV*. The VRML language may offer an alternative procedure in 3D simulation. We have developped a preliminary tool of post-treatment for the *GEM* code. It is less complete than the GMV viewer. However, files are light and the post processing can be easily performed. With this tool, we could visualize particles as well as the contact networks. The contact networks were splitted into two parts: the strong and weak networks. The figure 5 represents the initial and final states of our sample for a triaxial test.

This kind of language may be take an important role in future development, and the improvement in this respect is one of the important element in coding.

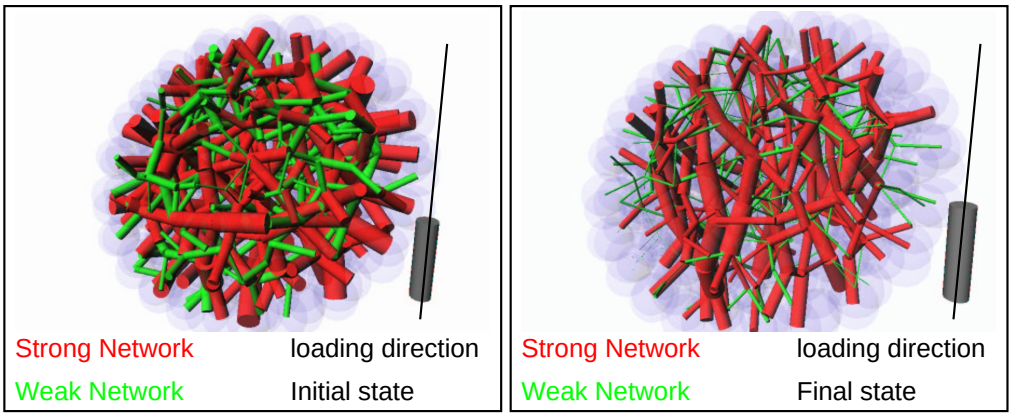


Figure 5: Initial and final state of a triaxial test.

3.3 Few words about the contact detection

To keep a short elapsed CPU time, the contact detection is one of key issues. The contact detection methods in the two codes are different from each other. The method used by *LMGC90* is the Manhattan Box method. It consists in decomposing granular domain in small boxes and detecting contacts between particles only in neighbouring boxes. This method is convenient to apply but its performance may not be the best. The *GEM* code uses a look-up table method that consists in checking neighboring particles when some amount of movement occur to each particle. This method may be not so expensive in CPU time for small samples, but it can take a big part of CPU time for large samples. We should find in the litterature different kind of more efficient methods (for example dynamic graphs), and a good choice of contact detection method may lead to efficient algorithm for the two code.

4 Conclusion

It is well known that *DEM* (and consequently *GEM*), and *NSCD* are methods with a lot of differences. But the computation algorithm used in *GEM* (the "stiffness method") appears to have some common points with *NSCD*. On these points the more intense study should be performed. Especially, the future development of visualisation and contact detection techniques which are important both in the two methods can be lead in common.

References

[1] J.-P. Bardet and R. F. Scott. Seismic stability of fractured rock masses with the distinct element method. In *26th US Symposium on Rock mechanics*, pages 139–149, 1985.

[2] J. Chergui, I Dupays, D. Girou, and S. Requena. *Message Passing Interface - 1.* IDRIS, Fvrier 2003.

[3] P. A. Cundall. A computer model for simulating progressive large scale movements of blocky rock systems. In *Proceedings of the symposium of the international society of rock mechanics*, volume 1, pages 132–150, 1971.

[4] P. A. Cundall and O. D. L. Strack. A discrete numerical model for granular assemblies. *Géotechnique*, 29(1):47–65, 1979.

[5] T.-J. Drake and O.-R. Walton. Comparison of experimental and simulated grain flows. *J. Appl. Mech.*, 62:131–135, 1995.

[6] F. Dubois and M. Jean. Lmgc90 une plateforme de développement dédiée à la modélisation des problèmes d'interaction. In *Actes du sixième colloque national en calcul des structures*, volume 1, pages 111–118. CSMA-AFM-LMS, 2003.

[7] E. Gondet and P.-F. Lavallee. *Cours OpenMP.* IDRIS, septembre 2000.

[8] M. Jean. The non-smooth contact dynamics method. *Comp. Meth. Appl. Mech. Engrg*, 177:235–257, 1999.

[9] M. Jean and J.J. Moreau. Unilaterality and dry friction in the dynamics of rigid bodies collection. In A. Curnier, editor, *Contact Mechanics International Symposium*, pages 31–48. Presses Polytechniques et Universitaires Romanes, 1992.

[10] Y. Kishino. *Mechanics of Granular materials: an introduction*, chapter 3, pages 147–159. Balkema.

[11] Y. Kishino. Disk model analysis of granular media. *Michromecanics of Granular Materials*, pages 143–152, 1988. (eds. M. Satake and J.T. Jenkins),Elsevier.

[12] Y. Kishino. Granular flow simulation by granular element method. In *Slow Dynamics in Complex Systems*, November 2003. Sendai, Japan.

[13] Y. Kishino, H. Akaizawa, and K. Kaneko. On the plastic flow of granular materials. In Y. Kishino, editor, *Powder and grains*, pages 199–202, 2001.

[14] J. Lanier and M. Jean. Experiments and numerical simulations with 2d disks assembly. *Powd. Tech.*, 109:206–221, 2000.

[15] Los Alamos, http://www-xdiv.lanl.gov/XCM/gmv/GMVHome.html. *General Mesh Viewer.*

[16] J-J. Moreau. New computation methods in granular dynamics. In Thornton, editor, *Powder & Grains*, pages 227–232. Balkema Press, 1993.

[17] M. Renouf, Dubois F., and P. Alart. A parallel version of the non smooth contact dynamics algorithm applied to the simulation of granular media. *Comput. Appl. Math.* submit nov. 2002.

RESEARCH REPORT

Name: BREMAUD Iris
Affiliation (University):
Montpellier II University, Montpellier, FRANCE
Laboratory of Mechanics and Civil Engineering, CNRS UMR 5508,
Wood and Tree Mechanics Team

Research Advisor: Professor Shigeru YOSHIKAWA
Host Institution: Kyushu Institute of Design,
Department of Acoustical Design
Other Host Professors and Institutions:
*Professor Kiyoko MOTEGI,
Joetsu University of Education, Music Studies
*Professor Kazuya MINATO,
Kyoto Prefectural University, Graduate School of Agriculture

Research Subject:
Diversity of Woods in Musical Instruments:
Acoustical and Musical Functions, and related Material Properties

1. Research Description:

My PhD research is focused on the diversity of timber species used – or usable – in musical instruments making. If the different parts and types of instruments are considered, very different material properties are involved, from acoustical/mechanical to physical. Also, numerous timber species are considered, and this especially if we look towards instruments from different cultures. In this respect, Japanese tradition of Musical instruments making is very interesting to get a different point of view than the usual violin quartet focus, because it is both very highly skilled, and very different from Western Music standards in terms of expected musical result.

Characterization of the role of the wood-material in finished instruments involves studies about the material selection and the making process -through concertation with skilled instrument makers; acoustical tests and understanding the expected musical/aesthetical result; and characterization of wood material properties. Also, some of the traditionally preferred woods –especially tropical ones- exhibit very peculiar physical/mechanical behaviour, like very low vibration damping or very high dimensional stability, which cannot always be explained by the "standard" polymeric composition of wood. Origin to these behaviours -which are of special interest for musical instruments making- can then be searched for in the content and composition in "extractives", secondary metabolites of smaller size and great diversity.

2. Research Activities:

Due to the interdisciplinary nature of such a research, my study stay in Japan this summer has been divided between three institutions, in order to try to cover the different aspects involved –at least as an "initiation".

During the first stay, in KID (Fukuoka) in Yoshikawa Sensei laboratory, I did some acoustical experiments on classical guitar top plate response. Two guitars of different building qualities were compared, together with a folk guitar as reference to very different sound and making. First I played and recorded individual notes (open strings and fretted strings), which were later –after Fourier Transform - to be compared by means of their waveform and sonogram representations. Special focus has been on the often problematic ranges: Bass E string (sometimes too loud), G string (often "dull"), high e string up to e4 (high notes are sometimes weak). Then we used an impact method to record a frequency response of the top itself, with back and ribs damped in sand. The impact is a hammer choc on the bass side of the bridge, whose force is recorded by a mounted accelerometer. Response is recorded by another accelerometer fixed on vibrating part of the top. Short "Matlab" programs were used to calculate and draw the response curves. These response curves were compared for the different guitars, and for response sensed on basses', or trebbles', side of the top. The results of the comparisons indicate some clear differences between the two classical guitars top responses; though, these are not easy to find again in played notes characteristics. This may be due to the hand plucking – not standardized- during

recording, and/or to the combination with the other guitar parts'responses. These experimental results have been further exploited afterwards in the laboratory, and published, as states Pr. Yoshikawa in his remarqs. During this stay I was also lucky enough –thanks to Pr. Yoshikawa- to visit a manufacture of guitar making, and a luthier/repairer of Japanese Biwa.

Then I spent one week in Naoetsu, under the direction of Pr. Motegi, to discover some first aspects of Japanese traditional musics and instruments. Though short, this stay has been extremely rich of learning for me. I could participate to Koto and Shamisen playing lessons, make observations on the instruments of the very big collection of Motegi Sensei, assist to Japanese music performances, and talk with the performers. I also could interview a Koto and Shamisen maker – with kind help for Japanese translation, and "craftsmen solidarity". After leaving Naoetsu I could also assist with Motegi Sensei to a bunraku performance in Osaka, and visit the backstages, and talk about the instruments with the performers.

The third part of this research stay is concerned with characterization of vibrational properties of woods, and study of the effect of extractives on these properties, in Kyoto, under the direction of Minato Sensei. This stay is to be continued until beginning of September, and hence is in progress for the moment. The sampling material comes from France. It has been selected according to three aims:

*one set is to study relationship between vibrationnal properties (specific Young's modulus, tan δ) and extractives content on *Pterocarpus* species from Africa (*P. soyauxii* and *P.erinaceus*), which both exhibit very high dimensional stability, peculiar extractives contents, and are used in traditional African musical instruments. First measurements show that these species' timbers have very low damping as compared to some species of same elastic modulus and density. These samples are currently being extracted, and their tan δ are to be measured again after extraction and stabilization to search for some extractives effect on this low damping. This sampling covers several different location within tree (sapwood, and heartwood at different distances from transition zone). The first results show a clear increase in tan δ (mean increase 35%) after extraction (and re-stabilization in the same humidity and temperature conditions).

*Another set consist of several lesser known species, mainly from French Guyana, wich exhibited very low shrinkage/swelling and potential interest for instrument making. No data exist about vibrational properties for these species. Some exhibit damping values that are in the lowest range known for wood ($\approx 4.10^{-3}$).

*Third set of sample have been collected from French makers, together with their appreciations of these woods qualities when used. The first results on these species seem very interesting: Firstly, grading after empiric appreciation is very closely related to low damping for some uses; Secondly, some of these species exhibit extremely low tan δ, amongst the lowest values that have been found for wood up to now.

3. Perspective of Research after this Program:

Though each individual research stay during this summer has been quite short, I think it gives a good introduction to some methods or thematics.

The acoustical methods used in Pr. Yoshikawa Laboratory may have several applications for my PhD research:

*investigations on the effect of humidity changes on the instruments, through dimensional and acoustical changes of wood components (tuning, damping, playability…);

*responses on blank wood plates for instruments, with adding rigidity and/or mass and/or damping; *(relative effect of different material properties, and ofinstruments' structure);*

*validations of psychosensitive trials with instrument makers/musicians' judgement of woods: comparison of recorded characteristics and objective appreciation;

*acoustical characterization of some traditional instruments from different cultures, using different woods and building techniques, and with different expected sound types.

This first introduction I had –thanks to Motegi Sensei- to Japanese traditional musics and musical instruments was extremely interesting. It may be an excellent reference to serve as counterpart to classical Western music and its instrumentarium, (*which is up to now the main "sampling" for research*

of wood in musical instrument, but limitates very much the analysis), due to the high skill of Japanese makers and performers, and the very different musical culture. I hope to learn more about this musical culture, and maybe to try to have other opportunities to debate about sound specificities, instruments' use, etc. Also and in a different field, I would love to make some exchanges between French and/or Southern Europe traditional musics and Japanese music, though I don't know yet in which way.

The first meetings with instruments makers have been very interesting. I would love to be able to follow this discussion with Japanese makers, especially if I can get to speak a bit of Japanese in the following years. The same kind of enquiries with makers is a part of my research in France, and I would like to extend it to other musical instruments making cultures also.

Concerning the current stay, in Kyoto, it is closer to my main research activities in France. It is a great chance for me to be able to work with Pr. Minato, who has published some of the reference works about the subject.

One of the very first future applications of what I learn here will be to reproduce in France an equipment for making precise and reliable damping measurements, such as the one in use in Pr. Minato Laboratory. The sample preparation methods also seem to be very good.

From the first results here, some species are very interesting. I will collect larger samplings (different trees, location within trees, empiric grading) and study further the vibrational and phytochemical properties of these species.

After finishing the work planned in here, I shall bring back to France the wood samples and the obtained extracts. For those species for which a clear effect of extractives would have been observed, some first chemical analysis shall be run, in order to get a first idea of the different chemical families involved. Some histochemical observations on the extracted and unextracted specimens are to be made, knowing that chemicals do not have the same effects depending on their location within wood structure. Also, new serie of extraction, with solvents of different polarities, would be interesting for the species were first results are positive.

Last, a wider collecting of wood samples from many French, and hopefully foreign, instrument makers, has to be run, accompagnied by enquiries about the observed qualities in used.

I hope I can stay in contact and exchange scientific information with the researchers I met in Japan, and that these first aspects can be further developed, despite of distance.

4. Advisor's Remarks:

In my eyes she (Iris Bremaud) is very flexible and open-minded. She exhibited her sincere interest in acoustical measurement at my lab in Kyushu Institute of Design in collaboration with my graduate students and developed her own insight to the acoustics of guitars. Also, I believe that she absorbed many things and matters concerning Japanese traditions in music and musical instruments (in Joetsu University of Education) and wood science for the application to conventional and future musical instruments (in Kyoto Prefectural University). Since musical instruments consist of their music, physics, and culture, her attitude with wide viewpoints toward musical instruments will create favorable opportunities for her PhD research.

A part of her research carried out during her stay in KID is supposed to be published at the Technical Committee Meeting of Musical Acoustics (September 5-7, 2003) under the title of "Vibrational response characteristics of guitar top plates and the effects of signal processing".

RESEARCH REPORT

Name:	**Affiliation (University):**
Deroin Bertrand	Ecole Normale Supérieure Lyon
Research Advisor:	**Host Institution:**
Takashi Tsuboi	Tokyo University
Research Subject:	
Foliation theory, Complex geometry	

1. Research Description:

I'm interested in the study of qualitative behaviour of holomorphic singular foliations over projective manifolds. For instance a differential equation $\frac{dy}{dx} = \frac{P(x, y)}{Q(x, y)}$ (1)

when P, Q an polynomials on the complex variables x, y, defines a singular holomorphic foliation of $\mathbb{C}^2$ that can be extended to $\mathbb{C}P^2$. Even the basic property like: "Is a solution of (1) accumulating to a singularity" are not yet know!

2. Research Activities:

I participate to Takashi Tsuboi's seminar at the beginning of July, and give there a talk "Non Rigidity of Riemann surface lamination." I participate also to the so-called "Saturday seminar" at TIT on foliation theory and gave there a talk "Holomorphic embedding of laminations by complex manifolds on projective spaces." Professor Takeo Ohsawa invited me in Nagoya University to give a talk on my results on the rigidity of Levi-flat hypersurface immersed into a complex surface of positive curvature.

3. Perspective of Research after this Program:

I have discovered some transversely holomorphic foliation with singularities which carry the same dynamic as the one of a rational endomorphism of $\mathbb{C}P^2$, or more generally of a correspondence. The leaves of these foliation are of dimension 2. I want to know if these foliation can be realized a holomorphic one on a complex surface.

4. Advisor's Remarks:

Dr. Deroin came and participate in our seminar and gave several number of talks on his recent research. It was really stimulating and me appreciate this JSPS program very much for enabling us to discuss on the future researches.

RESEARCH REPORT

Name:	Affiliation (University):
Nadine RICHARD	ENST, Paris (France)
Research Advisor:	**Host Institution:**
Pr. Haruki UENO	National Institute of Informatics, Tokyo
Research Subject:	
Human-robot interaction	

1. **Research Description:**

My main research topic addresses the problem of explicit description of autonomous agents (virtual agents and real robots). I am now focusing on the different kinds of possible interactions between a human being and an autonomous agent, especially in the case of a physical robot. For this reason, I visited two research teams at NII:

- Pr. Haruki UENO, leader of the Symbiotic Robotics Group, which develops service robots for aged or disabled people (using a frame-based reasoning system).
- Pr. Seiji YAMADA and Dr. Daisuke KATAGAMI, who study situations where a user needs to teach behaviours to a robot (using classifier systems for on-line learning).

2. **Research Activities:**

I gave several talks to explain my previous results and start collaborations with both research teams. For Pr. Ueno's team, I implemented a demonstration, where a user can control an AIBO robot using my multi-agent platform. This example includes a connection with a specific application for human face detection. I observed problems for developing a more complex AIBO controller, and then proposed solutions and perspectives.

3. **Perspective of Research after this Program:**

I hope that the demonstration I developed will be useful for the research of Pr. Ueno's team. It proved that the model and platform I proposed is suitable for various kinds of human-robot interactions. With Pr. Yamada and Dr. Katagami, we plan to collaborate later in order to mix our approaches in a common platform. This fruitful experience will enable me to pursue my research in the domain of human-robot interaction.

4. **Advisor's Remarks:**

Dr. Richard's stay at our laboratory on Symbiotic Systems Research of National Institute of Informatics, also Department of Informatics of The Graduate University of Advanced Studies (SOKENDAI) was definitely fruitful both for us and for her. She has exchanged ideas for further research on Symbiotic Robot through discussions with my Ph.D. students as well as faculties. This visit was an important event for establishing future collaborations.

RESEARCH REPORT

Name: Caroline Levy
Affiliation (University): Institut Européen des Membranes
Université Montpellier II

Research Advisor: Dr Toshinori Tsuru
Host Institution: Department of Chemical Engineering
Hiroshima University

Research Subject: Catalytic membrane reaction for methylation of toluene using MFI zeolite membrane

1. Research Description:

Various types of zeolite membranes have been used for their excellent gas separation properties, due to their specific pore size and morphology. The gas permeation mechanism through the porous membranes is classified into Knudsen diffusion, surface diffusion and molecular sieving. On the other hand, little attention has been given on the use of zeolite membranes as membrane reactors, in comparison with separation applications.

The purpose of this research is to study the catalytic potential of the MFI zeolite membrane for the methylation of toluene using methanol.

2. Research Activities:

The MFI zeolite membrane was synthesized by hydrothermal synthesis using distilled water, tetrapropylammonium bromide (TPABr), sodium hydroxide and TEOS in a molar composition of $TPABr/SiO_2/H_2O/NaOH$ at 0.1/1/80/0.1. Cylindrical α-alumina microfiltration membranes were used as substrates for the zeolite membranes. After the ion-exchange of MFI zeolite membranes from the Na-type to the H-type, the alkylation of toluene with methanol was carried out. A p-xylene selectivity of 80% were attained using H-MFI zeolite membranes at 450-500°C, confirming the possible application of a MFI zeolite membrane for use in a catalytic membrane reactor.

3. Perspective of Research after this Program:

The composition and the component of the solution will be modified ($SiO_2/H_2O/NaOH/NaAlO_3$) to prepare a MFI zeolite membrane containing Aluminum. In this case, we hope to enhance the p-xylene selectivity after methylation of toluene with methanol.

4. Advisor's Remarks:

Ms. Levy stayed in our laboratory for 7 weeks under the JSPS Summer Program. During her stay, she was involved in catalytic membrane reactors, one of the most promising research field of membrane separation. In addition, she visited several laboratories to extend her experiences for her future research activities.

I believe this stay, in spite of the short period, would be fruitful for her to enhance the understanding about the research as well as Japanese culture.

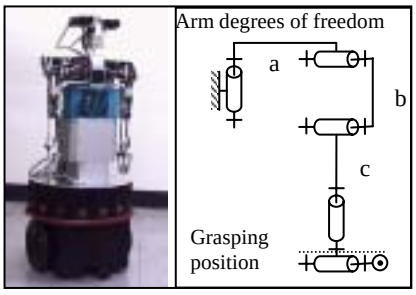
RESEARCH REPORT

Name:	Affiliation (University):
Fabien Gravot	University of Toulouse III
Research Advisor:	**Host Institution:**
Hirochika Inoue	University of Tokyo
Research Subject:	
Motion and manipulation planning for robot with two arms	

1. Research Description:

In the past few years the humanoid robot field has grown intensively in Japan. Those robots are able to walk but also to do manipulation task with both arms. Some of those robots are already able to do simple manipulation tasks, but they are not able to choose a grasping position to pick an object or to manipulate objects with both arms when regrasping position are needed.
On the other hand my PhD. Research involves the manipulation planning techniques than enable to choose grasping position in a continuous or discrete space definition. The methods are based on the Probabilistic Roadmap Methods and use heuristic search space with motion that are not feasible but that can be transformed into a succession of valid transit and transfer motions. We succeed to find very complex solutions when one arm has to extract an object in a complex environment and needs several regrasping positions.
The goal of my research is to use similar planning method to deal with two arms manipulation and implement an example on real robot. This time the object is not placed on the ground when the arm want to change its grasping position, but it is hold by the other arm and can also move. One of the most challenging issues is to deal with arm that have only 4 degrees of freedom and then cannot catch an object in any positions and orientations.

2. Research Activities:



My work can be divided into three parts:
- The first part is about modelling the robot and its environment. This implies the direct and the inverse geometry. But to compute the inverse kinematic I need 6 degrees of freedom for each arm. To do this I use two of the three degrees of freedom of the grasping position. Those degrees of freedom cannot be controlled by the robot, but they can be used to compute a possible grasping position.
- The second part is the planner issue. As said before I use a heuristic search space where the grasping position can move. In this search space it is very easy to find a path between two robot and object positions. In reality, when a robot picks an object it does a transfer motion and the grasping position does not change. So I have to transform a path found in the heuristic search space into a succession of transfer motions. Here again, due to the lack of degrees of freedom of the arm, I had to build new methods based on depth search and backtracks to add dynamically intermediate goal positions.
- The last part is related to the real robot. The main work was to build an interface between the robot, the planner software and the user. This part takes into account local modifications on the robot itself and the implementation of new embedded controllers.

The result of this work is a new planning technique that enables to find solution of problems than need several regrasping positions for both arms of a robot. This method has been used to find a succession of transfer motions that is able to lift up a Japanese flag. This has been successfully implemented on the robot “H3” of the University of Tokyo.

3. Perspective of Research after this Program:

My collaboration with Professor Inoue at Tokyo University was very productive. The experiences of this laboratory in robotic field are simply amazing. My laboratory does not have robots that can carry out two arms manipulation problem. This research allowed attempting new problems by combining the specialities of two laboratories from different countries. I was able to learn many things both on robotic field and Japanese culture. After finishing my PhD, I would like to apply for post-doctoral funding to continue in this field of research.

4. Advisor's Remarks:

He has shown amazing results through applying his powerful robot planner to our laboratory robots in this short stay. The planner is design and implemented by him in his research. His idea for the motion and manipulation planning successfully proved its broad capability in a variety of complex situations where multiple robots are expected to perform complexes task executions. Additionally, he attended several research meetings of our laboratory, and discussed some matters of research with many students. I think this stay in Japan was very productive and significant for him.

RESEARCH REPORT

Name:	**Affiliation (University):**
Franck MARTIN	University of Montpellier II, France
Research Advisor:	**Host Institution:**
Pr. Yoshinobu BABA	Faculty of Pharmaceutical Sciences, Tokushima University
Research Subject: Synthesis and grafting of functionalized coupling agents on model silica surfaces for the bio-microsystems field.	

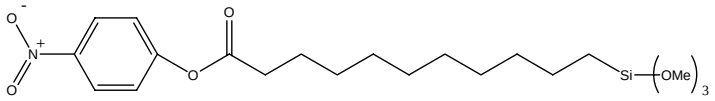
1. Research Description:

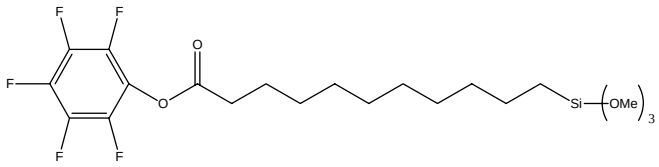
Chemical modification of metal oxide surfaces using coupling agents is an area of extensive research, in particular the grafting of organosilanes on silica surfaces, and these modified surfaces have a wide range of applications, especially biology and biosensors. The general formula of the used organosilanes is Z-R-$SiMe_{3-n}X_n$ with n = 1 to 3, and Z is a functional group which is extremely important for the different application domains (Z = -NH_2 for the interaction with DNA molecules, -OH and -CHO for oligonucleotide coupling, -SH for protein deposit…), R an organic spacer and X a hydrolysable function, usually a chloro, alkoxy or dimethylamino group. The silylation reactions of oxidized silicon wafers with some synthesized organotrialkoxysilanes Z-R-$Si(OMe)_3$ (Z = -NH_2, -OH, -CHO, -SH and –Br) were performed to make some novel and original modified silica surfaces applicable to the bio-microsystems domain. Because the research field to conjugate biotechnology with ordered molecular assembling is becoming more and more important to resolve a surface reproducibility problem and a control of the terminal function Z accessibility, which are crucial for the performance of these bio-microsystems, it is more convenient to deposit coupling agents as a monolayer than as a multilayer. The organization of the grafting organic monolayer will be favored by use of flat silica surface like oxidized silicon wafer because of the low surface roughness (0.1-0.2 nm).

2. Research Activities:

My research project can be divided in two parts.

The first one has consisted to synthesize two novel coupling agents:





And about the other one, with some used adequate reaction conditions (for example $C_mH_{2m+1}SiCl_3$ with m superior to 8 in dried solvent at room temperature), the functionalized organosilane self-assembled monolayer grafting on silica surface were performed, and these modified surfaces were characterized by ellipsometry, AFM and FTIR-ATR.

3. Perspective of Research after this Program:

In the next future, with a joint-research program between the Professor Baba's laboratory and my laboratory in France, it would be interesting to effect some experimentation concerning the interactions of several types of biomolecules with these original bio-microsystems and to compare the analysis results obtained with these obtained with some commercial chips.

4. Advisor's Remarks:

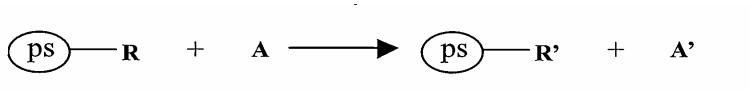
Nano-biodevice project, which is led by myself, is one of the most important national project in the field of the fusion of nanotechnology and biotechnology. In the nano-space on the nano-biodevice, so many different types of unique reactions occur and it is very difficult to control these reactions, including adsorption of protein on the surface of nano-space, enzymatic reactions near on the inner surface of nano-biodevice, and interaction between protein and the inner surface of nano-device. One of the most effective and smart solution of these problems must be surface treatment by self-assembled molecule. Research by Mr. Franck MARTIN is focused on the development of novel coupling agents and optimum reaction conditions for intelligent surface treatment. This research project will play a key role in the nano-biodevice project. For example, in the Point-of-Care technology project, his research result should be highly required for the pretreatment of protein samples from human cells. In conclusion, his research effort in this program has done significant contribution to my research project. I can easily expect that our future collaboration will produce high-efficient nano-biodevice system and should be world-leading research project in the field of nano-biodevice for genomics, proteomics and cellomics.

RESEARCH REPORT

Name: THIBAUD Sandrine **Affiliation (University):** Bordeaux I, France.	
Research Advisor: Pr. Isao ANDO **Host Institution:** Tokyo Institute of Technology.	
Research Subject: Study of soluble polymer supports by NMR spectroscopy.	

1. Research Description:

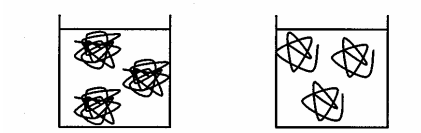
In the actual context of the green chemistry, the catalysts and reactants supported on polymer used in organic synthesis is efficient tool to recoverable them easily.



Most of the studies are about insoluble supports, which are separated from the reaction mixture by simple filtration. But the heterogeneous character of them leads to drawbacks. One alternative is the use of soluble polymer supports. In this way, we adjust new soluble polymer supports based on PS. The reactivity of supported functions is tested using a test reaction. In order to correlate the obtained results with the structure of support (Mn), these are analyzed with Nuclear Magnetic Resonance spectroscopy.

2. Research Activities:

In order to understand much better the dynamic behavior of polymer support in solution, ^{13}C spin lattice relaxation time (T1) and diffusion coefficients were determinate by NMR spectroscopy. Supports with various molecular weight (Mn) were analyzed (5000, 10000 and 20000 g/mol). At the concentration used for the study, the values of diffusion coefficient are not correlated with the molecular weight of the polymer and intermolecular aggregations were not observed. In the other side, T1 study has showed that the conformation of chain polymer support is correlated with the molecular weight. Higher values of T1 (for the side chain) were observed with the lower molecular weight polymer, meaning a higher mobility for these polymers.



Mn = 20 000 g/mol Mn = 5 000 g/mol

3. Perspective of Research:

In the future, this study will complete by analyzing another architecture of polymer to compare with his counterpart linear polymer. We will be able to conclude which structure (Mn, architecture…) of soluble polymer support is the more appropriate in our case of study.

4. Advisor's Remarks:

Sandrine Thibaud has been hardly working her research program on structural and dynamic characterization of soluble polymer supports by solution ^{13}C NMR spectroscopy and field gradient ^{1}H NMR spectroscopy, and has obtained fruitful experimental results. The solution 13C NMR spectroscopy has provide ^{13}C spin-lattice relaxation time (T_1) and dynamic information on the main chain and side chain carbons, and field gradient ^{1}H NMR spectroscopy has provided the self-diffusion coefficient of the polymer support in solution. She has successfully measured ^{13}C T_1 values of the individual carbons of the main chain and side chains and the diffusion coefficient. On the basis of these experimental results, she has successfully clarified the potential possibility for developing her designed soluble polymer supports as the catalysts and reactant supported on polymers in organic synthesis. She will be able to complete PhD thesis by adding these new experimental results to her previous experimental results. Her stay has greatly influenced on graduate students in my lab with different research style from her. I must greatly appreciate her for such a situation.