



## Report on EMMC international Workshop

Thursday 24 September 2015, 10:00 – 17:00h

COV2 building, room 15/SDR2, Brussels, BE

### Background

Materials modelling is a strong activity in Europe and Europe plays a recognised leading role in the world. Materials modelling will play a major part in the “4<sup>th</sup> generation industry”. The EU has supported this technology in the past with a total of more than €340 M€ to projects under the FP7 Framework Programme. The EU plans to continue this support in H2020 where materials modelling has obtained a prominent place in the Work Programmes.

The European Materials Modelling Council (EMMC) is a bottom-up group, not funded by the EU, which aims to gather the different stakeholders and exchange views on research and innovation policies in the field of materials modelling. The EMMC has the goal to connect all activities happening in the field of materials modelling. The EMMC has working groups on

- Business Decision Support System
- Translators
- Exploitation of academic software
- Data Repositories and the need for sharing across subdomains
- Modelling Market Place
- Model development (electronic, atomistic, mesoscopic, continuum, coupling & linking, open simulation platform, hpc)
- Validation and Characterisation
- Case studies for industry

The EMMC has had a very promising start and collected the needs of industry in a Research Road Map. This demonstrated the time is ripe for the introduction of materials modelling in industry. It also presented the need for a modelling market place where all stakeholders can be connected, exchange ideas, find tools and expertise and training.

This EC endorses the policy of Open Science and this involved enabling access to data, a topic high on the agenda of the EMMC where metadata and interoperability standards are under discussion to connect all aspects of the field.

The metadata under elaboration are based on the classification of models based the Review of Materials Modelling in 100 FP7 projects available on the EU-LEIT website.

These metadata will enable an overview of what models and data exists in the world. These metadata will enable searches in existing databases and will enable linking of models and data (the so-called interoperability).

The EC endorses the policy of Open to Innovation and introducing digital technologies into thematic policy areas like Energy, Environment, Transport are a must. This is thus high on the agenda in the EMMC in their translation and training activities.

The EC endorses the policy of Open to the World and we thus welcome participation of countries on other continents.

Joint Calls between EC-NMP and NSF (US) and DST (India) have taken place in the past. The reality was that the Europeans get funded by European funds, and the international partners by their authorities. The two self-contained projects were linked superficially and co-operation was not legally enforced. The cooperation was rather dependent on goodwill. The underlying philosophy for this meeting is that cooperation between parties with existing funding based on goodwill can also be started today without new Calls.

## **The meeting**

RTD.D3 and the European Materials Modelling Council (EMMC) have organised an International Workshop in order to explore the opportunities for International Cooperation between South Korea, Japan, USA and the EMMC.

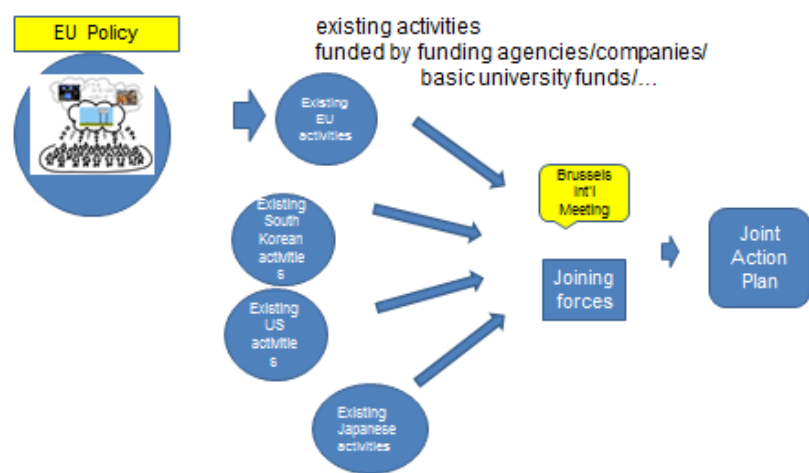
The goal of the meeting was to discuss and agree action plans for collaboration and to demonstrate that international collaboration can take off already today. Such demonstration will guide The EC when deciding where to invest in in the future in cross-ocean collaboration.

**The purpose was to elaborate action plans for the coming year that can start immediately on funding streams already allocated.**

*Please note that the meeting was not to discuss future Calls, but such proposals are of course harvested for later use.*

Slides depicting the workshop objectives:

 **The European Materials Modelling Council**  
**Linking of existing activities**



The existing activities in the EU were represented by the EMMC. The EMMC had proposed names of people abroad who present existing activities that could be linked and collaborate internationally.

The EU has invited seven people who have accepted (paid invitation)

Invited speakers list (cv's are attached in Annex ):

Last Name	First Name	Workplace
Itoh	Satoshi	RIKEN Advanced Institute for Computational Science, Kobe, Japan
Takemura	Masahiro	Japan Science and Technology Agency (JST)
Lee	Kwang-Ryeol	Korea Institute of Science and Technology (KIST)
Han	Seungwu	Seoul National University, South Korea
Warren	James	Material Genome Initiative; NIST, USA
Court	Christa	MRI Global, USA
Strachan	Alejandro	Purdue University, USA

EMMC participants:

Last Name	First Name	Workplace
Adamovic	Nadja	Vienna University of Technology, Austria
Asinari	Pietro	Politecnico di Torino, Italy
Goldbeck	Gerhard	Goldbeck Consulting LTD, UK

Hashibon	Adham	FRAUNHOFER IWM, Germany
Hermansson	Kersti	University of Uppsala, Sweden
Hristova-Bogaerds	Denka	Dutch Polymer Institute
Noro	Massimo	UNILEVER, UK
Schmitz	Georg J.	ACCESS E.V, Germany
Wimmer	Erich	MATERIALS DESIGN, France
Kremer	Kurt	Max-Planck G Mainz, Germany

European Commission participants:

<b>Last Name</b>	<b>First Name</b>	<b>Workplace</b>
de la Torre	Clara	European Commission - Director RTD.D
Tokamanis	Christos	European Commission - RTD.D.3
de Baas	Anne	European Commission - RTD.D.3
Rosso	Lula	European Commission - RTD.D.3
Martins	René	European Commission - RTD.D.3
Katalagarianakis	Georg	European Commission - RTD.D.3
Morrissey	Anne	European Commission - JRC.C.4 (responsible Japan)

Each invitee from Japan, SK or US has been allocated a contact person in the EMMC matching topics of interest. This EMMC contact person has held telephone conferences with the invitees to establish a non-paid action plan linking existing activities in advance of the meeting. Other WG leaders then talked to the invitees if relevant.

These action plans were presented on 24<sup>th</sup> September and discussed in the group on 25<sup>th</sup>. The meeting was concluded with concrete steps for the near future.

On 24<sup>th</sup> September the participants met with the EC being present, while on the 25<sup>th</sup> they refined their draft action plans.

The presentations on the first day had as objective to

- Inform:
  - Understand what efforts are in place at a high level that require materials modelling in the geographies
- Common ground:
  - Understand what areas will benefit from a global collaboration scheme
- Path forward:
  - Selected areas of interest with actionable co-operation plans funded by existing funding streams.



### AGENDA 24/9/2015

10:00 – 10:30	Registration and Coffee
10:30 – 10:45	Welcome by Clara de La Torre, Director of Directorate D – Key Enabling Technologies
10:45 – 11:00	Welcome by Christos Tokamanis, Head of Unit D3 –Advanced Materials and Nanotechnologies
11:00 – 12:00	Presentation of EMMC roadmap and working groups
12:00 – 13:00	Networking Lunch
13:00 -15:00	Proposals for cooperation, proposed steps and their timelines by USA
15:00 – 15:15	Coffee break
15:15 – 16:00	Proposals for cooperation, proposed steps and their timelines by South Korea
16:00 - 16:45	Proposals for cooperation, proposed steps and their timelines by Japan (2 invited experts 20 minutes each)
16:45 – 17:00	Open discussion
17:00 – 17:15	Closure of first Day by Commission

## Annex

### CV's International Participants

#### USA

#### Christa Court, MRI Global

Christa Court is from US MRI Global (private non profit organisation).

Dr. Christa Court has undergraduate degrees in Economics and Spanish from Middle Tennessee State University and a Master's degree and Ph.D. in Economics from West Virginia University. Currently, Christa is a Staff Scientist at MRIGlobal, an independent, not-for-profit research institute that specializes in innovation, technical excellence, and problem solving across the full spectrum of research and development. She also holds the position of Industry Liaison at West Virginia University's Regional Research Institute.

As a Staff Scientist for MRIGlobal, she primarily performs economic impact analyses for the U.S. Department of Energy's National Energy Technology Laboratory but has also worked on contracts involving the National Science Foundation, the U.S. Environmental Protection Agency, the U.S. Agency for International Development, and the Missouri Energy Initiative. She has been involved in numerous funded projects involving input-output analysis and economic impacts assessments over the last decade and has a growing list of related publications.

Christa is currently involved in an effort to evaluate the benefits of computational modelling efforts at the National Energy Technology Laboratory. The analysis estimates the economic, energy-related, and environmental impacts of potential design improvements through the use of these computational models on the existing U.S. coal-fired power fleet. Initial results indicate that there are not only substantial reductions in fuel use and CO<sub>2</sub> emissions but also in labour hours.

Christa Court works for a private not for profit research organization MRI Global who does subcontractor to the U.S. Government. She deals with development of a standard method to estimate the economic impacts of materials modelling. She will present her experience of measuring economic impact and your proposals for methods that could be used to estimate the economic impacts associated with materials modelling.

Christa Court presented a short report on the qualitative and some quantitative impacts that she estimated for 2 NETL efforts related to computational chemistry and multi-phase flow reactors.

## USA

### **Alejandro Strachan, Purdue University**

He represents nanoHUB a market place for modelling and training, see [www.nanohub.org](http://www.nanohub.org).

This HUB now serves over 280.000 users annually. NanoHUB is an organisation where users can run over 320 simulation tools in a web browser. The cyber infrastructure used is a scientific computing cloud that taps into Purdue University and national grid resources.

NanoHUB has assembled course materials on many aspects of nanotechnology with materials modelling as subpart. KanoHUB publishes research with the developed tools and data in a form that others can immediately use. Simulation tool authors can host only their executable on nanoHUB, or they can release the code as open source. For "and more" content authors, we suggest publishing using the Creative Commons license.

#### Funding:

nanoHUB is operated by the Network for Computational Nanotechnology (NCN), whose mission is to enable the use of modelling and simulation in the advancement of nanoscience and nanotechnology. Most of the tools on nanoHUB are derived from NCN's contributions to research in the nano-areas of electronics, mechanics, bio, photonics, and materials, primarily through leveraged funding.

## USA

### **James Warren, NIST**

The National Institute of Standards and Technology (NIST, [www.nist.gov/](http://www.nist.gov/)) is the US federal technology agency that works with industry to develop and apply technology, measurements, and standards.

James Warren deals with databases for Materials Genome Initiative, standardisation and interoperability. He was also in the EU-NSF-DOE workshop in San Francisco, April 2014.

The following thoughts on opportunities for collaboration: The MGI and the EMMC do not represent official NIST policy, although it could eventually serve as the basis for any number of memoranda of understanding.

The strategic plan of the Materials Genome Initiative includes four goals in support of its overall goal of accelerating the discovery, design, development, and deployment of new materials:

- Facilitating a paradigm shift in the culture of how materials science is done,
- Deepening the integration of materials modelling and simulation with experimental effects



- Facilitating the sharing of materials data and models,
- Training the next generation of scientists and engineers to use MGI approaches.

Not surprisingly, these goals are similar in character to related efforts in Europe. In particular, Europe with its H2020 program shares the same overarching goal as the MGI of accelerating product and new material design and towards high technology readiness levels. Multiple Agencies of the US Government are supporting the MGI, including the NSF, DOE, DOD, NASA, and NIST, with each agency framing the goals of the MGI within the context of their mission. NIST, in particular, with its long history in the provisioning of high quality data, had developed own goals in support of the MGI, specifically,

- Enabling the improved exchange of materials data and models,
- Ensuring the quality of materials data and models,
- Developing new methods and metrologies on leveraging the evolving MGI infrastructure.

## **South Korea**

### **Seungwu Han, Seoul National University**

Seoul National University, Korea, B.S. Physics, Spring 1993

Seoul National University, Korea, M.S. Physics, Spring 1995

Seoul National University, Korea, Ph.D. Physics, Summer 2000

Postdoctor, Center for Strongly Correlated Materials Research, Seoul Nat. Univ. 2000-2001

Postdoctor, Princeton Materials Institute, Princeton University, 2001-2003

Full-time lecturer, Dept. of Physics, Ewha Womans University, 2003-2004

Assistant Professor, Dept. of Physics, Ewha Womans University, 2004-2008

Associate Professor, Dept. of Physics, Ewha Womans University, 2008-2009

Associate Professor, Dept. of Materials Science and Engineering, Seoul Nat Un, 2009-2013

Prof, Dept. of Materials Science and Engineering, Seoul National University, 2013-15.9.2015.

Seungwu Han is Professor at the Materials Theory and Computation Group, Department of Materials Science and Engineering at Seoul National University (<http://mtcg.snu.ac.kr>). Seungwu Han is doing atomistic simulations and is interested in automatization. Scientifically he is interested on phase change models for electronic memory and in breakdown of organic polymers for lifetime prediction of OLEDs.

## **South Korea**

### **Kwang-Ryeol Lee, Korea Institute of Science and Technology (KIST)**

Kwang-Ryeol Lee is Principal Research Scientist at the Center for Computational Science, Korea Institute of Science and Technology, Seoul, KOREA (<http://diamond.kist.re.kr/DLC> and <http://cscweb.kist.re.kr>). He received Ph.D degree in 1988 from KAIST in Materials

Science Discipline. After postdoctoral research at Harvard University, he joined KIST in 1991 and has been studying both fundamental aspects and industrial application of the diamond-like carbon (DLC) coating technology. From 2001, his research was extended to the computational nano-science to understand atomistic or sub-atomistic behaviour of materials. He is now developing the web-based multiscale materials design platforms, which would reduce the entrance barrier to the computational nano-science. As of May 2015, he published 199 SCI papers and has total citation about 3,200 (H-index 30 by [www.researcherid.com](http://www.researcherid.com)). He also filed more than 60 patents (both domestic and international). He received 4 times the Best Research Award of KIST and the Commendation of the Prime Minister of Korea in 2005.

Kwang-Ryeol Lee presented the status of web-based multiscale materials design platform for specific applications. Kwang-Ryeol Lee plans to build a number of materials design platform as one of the core infrastructures for nanotechnology. Specific applications are nano-devices, virtual fab for Li-ion battery materials, virtual fab for nano catalyst, etc. <http://vfab.org>.

In the virtual fab, they are integrating various models and methods ranging from electronics, atomic to microscopic ones (mainly sequential modelling). The range of the used models is dependent on the specific application. Common philosophy is to minimize the entrance barrier for the researchers to do the computational research. These fabs are thus designed according to the needs from experimental researchers. Every fab has thus the unique structure depending on the application area.

## **Japan**

### **Satoshi Itoh, RIKEN Advanced Institute for Computational Science**

Born in 1956, he graduated School of Engineering, University of Tsukuba, Dr. Eng.

Nationality: Japanese

#### Professional Experience

2015- Japan Science and Technology Collaboration (JST), Program Manager

2011- RIKEN Advanced Institute for Computational Science, Coordinator

1985-2011 TOSHIBA Corporation

Dr Satoshi Itoh works at RIKEN Advanced Institute for Computational Science, Kobe, Japan. He presented two national projects in Japan nl the "Kei" supercomputer project and the "Materials research by Information Integration" Initiative (MI2I). This project just started.

He introduced two topics on materials modelling in Japan:

- the high-end supercomputer development project and its application,
- new national project of materials informatics.

The problem to be solved in advancing such projects is a lack of human resources. The materials modelling and materials informatics are emerging and interdisciplinary academic fields, so that RIKEN Advanced Institute for Computational Science has to develop human resources urgently, in particular young talents. On this subject, Dr Satoshi Itoh thinks that it is necessary to approach to human resource development through international cooperation, like an international school.

## **Japan**

### **Masahiro Takemura, Japan Science and Technology Agency (JST)**

Mr. Masahiro Takemura received B.Eng. and M.Eng. in Aeronautics from the University of Tokyo, Japan, in 1985 and 1987, respectively. He also received M.Sci. in Metallurgy from the University of Illinois at Chicago, the US, in 1995. He entered NKK Corporation in 1987, mainly in charge of R&D of heat resistant and corrosion resistant steels and alloys. In 2003, he moved to the National Institute for Materials Science, Japan, to be Senior Researcher of the Nanotechnology Researchers Network Center and Office Chief of International Affairs Office and Research and Analysis Office. In April, 2014, he moved to the Japan Science and Technology Agency, and since then he has been Research Manager of Project “Structural Materials for Innovation” of the Cross-ministerial Strategic Innovation Promotion Program of the Cabinet Office of the Government of Japan.

Masahiro Takemura works for the Department of Innovation Platform, Japan Science and Technology (JST). He presented, at a high level, the Cross-ministerial Strategic Innovation Promotion Program on Structural Materials (SM4I) he chairs. This project is focussing on strong, light, and heat-resistant materials for the application in transportation industry, especially aircraft engines and airframes, and energy industry. The materials dealt with are (A) polymers and FRP, (B) heat resistant alloys and intermetallic compounds, (C) ceramics coatings, and (D) materials integration. The goals are i) to predict the performance (life-time) of structural components depending on materials, manufacturing processes and service conditions, ii) to integrate theories, experimental knowledge, computation, measurement, database, etc., and iii) to realize innovatively efficient materials designing, reducing costs and saving time for development. Materials informatics is included as a tool for the integration.

In SIP, industry-academia-government collaborate on fundamental scientific research and applied technology development.

Concrete projects undertaken are

- development of system for materials microstructure (ex. simulation of casting of metallic materials by phase field method)
- development of system for materials performance (ex. life-time prediction, fatigue and creep) by using empirical rules and database)
- development of system for data assimilation

- development of integrated system
- development of molecular dynamics and first principle calculation
- development of software platforms.

## **Members of EMMC**

### **Nadja Adamovic, Vienna University of Technology, Austria**

Dr. Nadja Adamovic MSc in Electrical Engineering (1993), PhD in MicroSystemTechnologies at the TU Vienna (in 1996), employed on TU Vienna since 1994, Certificated Project Manager since 2005 and manager of EU- and national projects, senior researcher on Institute of Sensor and Actuator Systems, having 20years experience in micro- and nanotechnologies and numerical modelling, participant in more than 20 EU- and national projects (as coordinator, manager and senior researcher). In last 8 years, she researched in the field of renewable energies. She is external expert for evaluation of HORIZON2020 projects and Review Panel Member for COST Actions. Since April 2014, Dr. Adamovic is chairing the European Materials Modelling Council (EMMC). She is a member of the Austrian Photovoltaic Technology Platform, a member of the Council of the Faculty of Electrical Engineering and Information Technology and a member of the Working Group for the Equal Opportunity and Gender programmes at TU Vienna.

### **Pietro Asinari, Politecnico di Torino, Italy**

Pietro Asinari received his B.S. and M.S. (summa cum laude) in Mechanical Engineering in 2001 and his Ph.D. in Energetics in 2005 from Politecnico di Torino. In 2005, he won the ENI Award. He is the Director of the Multi-Scale Modelling Laboratory - SMaLL - ([www.polito.it/small](http://www.polito.it/small)) and Associate Professor of Applied Physics. He is member of the operational management board of the European Materials Modelling Council - EMMC - (<http://emmc.info>) and operational team manager of the working group on discrete modelling of materials. He is member of the International Scientific Committee of the International Conference for Mesoscopic Methods in Engineering and Science (ICMMES) and member of the Editorial Board of the international journal Computation. He is the Principal Investigator of many projects on materials modeling (including THERMALSKIN and NANOBRIDGE). Since 2002, he has (co-) authored over 70 publications (54 peer-reviewed articles, 34 as senior author) about multi-scale modelling in nanotechnology and biotechnology.

### **Adham Hashibon, Fraunhofer Institute for Mechanics of Materials, Germany**

PhD in Physics (2002). Since 2002, he is a senior scientist and project manager at the Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany. His main research interests are integrated platforms for multiscale simulations of nano-scale phenomena, solid-liquid interfaces, flow in nano confined geometries and complex fluids. His expertise includes modelling materials using electronic DFT, atomistic molecular dynamics, discrete mesoscopic

and continuum modelling approaches. He is the coordinator of the FP7 SimPhoNy project and a member of the Management Board of the European Material Modelling Council EMMC. He also acts as Operational Team Manager (OTM) of two EMMC working groups: Material Market Place and Interoperability.

### **Gerhard Goldbeck, GOLDBECK CONSULTING LTD, UK**

Dr. Gerhard Goldbeck is an experienced materials modelling software professional. He received his Diplom in Physics from RWTH Aachen University in 1986 and a PhD in Polymer Physics from Bristol University in 1992. His career so far encompassed academic research at Forschungszentrum Jülich (Dendritic Growth), H.H. Wills Physics Laboratory (Polymer Crystallisation) and Cambridge University Department of Materials Science and Metallurgy (Liquid Crystal Polymers), and software development, product management and marketing in industry (Molecular Simulations, Accelrys). In 2011 he formed Goldbeck Consulting Ltd, a company that aims to bridge gaps in the materials modelling value chain from science to engineering and academia to industry. Gerhard has published more than 60 papers and articles in the scientific literature and authored reports on the industrial impact of modelling as well as on academia-industry collaborations. He assists the European Commission in running and monitoring Research Projects as well as the European Materials Modelling Council.

### **Kersti Hermansson, University of Uppsala, Sweden**

Kersti Hermansson is strongly involved in e-science modelling for materials chemistry, especially the development of multiscale methods to bring chemical modelling closer to the complex dynamical systems of the real world, using various types of electronic structure and force-field simulations. Her current applications focus on chemistry on metal oxide surfaces and nanoparticles, and molecular dynamics in aqueous media, including computational vibrational spectroscopy and hydrogen bonding. She is a Professor of Inorganic Chemistry at the Ångström Laboratory of Uppsala University and a member of the Royal Swedish Academy of Sciences. She is a member of the operational Management Board of the European Materials Modelling Council (EMMC), Webpage: [www.teoroo.kemi.uu.se](http://www.teoroo.kemi.uu.se).

### **Denka Hristova-Bogaerds DPI Stichting Dutch Polymer Institute, The Netherlands**

Denka Hristova-Bogaerds was born in Bulgaria in 1973, where she finished her PhD in Polymer Physics (2002). Same year she moved to The Netherlands for a PostDoc position at Eindhoven University of Technology (TU/e) on the topic of rheology and flow induced crystallization of polymers, experimental and modelling analysis. In 2005 she joined for one

year a spin-off company of TU/e. One year later she became Assistant Professor at TU/e in the field of structure-properties relationship for bio-based plastics and composites. In 2012 she joined the Dutch Polymer Institute (DPI) as coordinator of the European project COMPANOCOMP dealing with computational analysis of nanocomposites. Currently she is a Program Area Coordinator of the DPI technology area Performance Polymers and initiator of research activities between industry and academia in the field of polymers. She is involved in evaluation of H2020 proposals and in monitoring of running EU projects. In 2015 she joined EMMC and recently she took the role of a group leader of the Translators working group within EMMC.

### **Georg J. Schmitz, ACCESS E.V, Germany**

Dr.rer.nat. Georg J. Schmitz earned his PhD in Materials Science in 1991 from RWTH Aachen University in the area of microstructure control in high temperature superconductors. At present he is senior scientist at ACCESS e.V., a private, non-profit research centre at the RWTH Aachen University. His research interests comprise microstructure formation in multicomponent alloys, modelling of solidification phenomena, phase-field models and thermodynamics. He is the official agent for Thermo-Calc Software AB in Germany and provides global support for MICRESS®. Dr. Schmitz is the coordinator of the European “Integrated Computational Materials Engineering expert group - ICMEg”. He has been appointed as expert by several institutions and is active member of the TMS committee on Integrated Computational Materials Engineering “ICME” and of the European Materials Modelling Council EMMC. He is editor and reviewer for a number of journals and has published more than 150 scientific articles and a recent book on a platform concept for ICME.

### **Kurt Kremer, Max-Planck Institute for Polymer Research, Germany**

Joined the Max-Planck Society in September of 1995 as the sixth director of the Max-Planck Institute for Polymer Research, heading the newly established theory group. After studying physics he received his PhD in 1983 from the University of Cologne under the supervision of Prof. Binder, working at the National Research Center KFA Jülich. He performed computer simulations for dynamic and static properties of polymers in bulk and near surfaces. After spending another year at Jülich he moved for a post-doctoral stay to Exxon Research and Engineering Corporation, Annandale, New Jersey, USA, working on polymers and on charge stabilized colloids in collaboration with Drs. Grest, Pincus, and others. In 1988 he obtained his Habilitation at the University of Mainz and returned to the KFA Jülich as senior scientific staff. He spent several extended visits as guest professor/scientist at Exxon Research (Dr. Grest), UC Santa Barbara (Materials Dept., Prof. Pincus), and University of Minnesota (Dept. Chem. Engineering and Materials Science, Profs. Davis, Bates, Tirell,...). After a short stay at Bayer AG, Leverkusen, he moved to the Max Planck Institute for Polymer Research. Kurt

Kremer received several awards and recognitions and is member of the German National Academy of Science, Leopoldina.

**Massimo Noro, UNILEVER, UK**

Massimo Noro is a Science Leader at Unilever R&D Port Sunlight (UK), the largest global research laboratory of the company. Unilever is a large multinational and a market leader in the fast moving consumer goods business, with well-known products in home care, personal care, refreshments and foods. He received his undergraduate education at University of Padova (IT), with a degree in Chemistry (Laurea, Magna-Cum-Laude), and completed a PhD in Physical Chemistry at the University of California, Los Angeles (USA). He received a Marie Curie EU Fellowship for post-doctoral work at FOM-AMOLF, in Amsterdam (NL). Massimo joined Unilever in 2000 and since then he assumed a variety of roles and responsibilities, ranging from Project Leader, Modelling Group leader and Operations Manager for the Director of the Laboratory. He is the director of the Unilever strategic partnership with STFC Daresbury on high performance computing. STFC Daresbury is a Tier-1 National computing facility in the UK of strategic importance for the development of the UK eScience infrastructure. He leads the High Performance Computing team.



## **Annex II**

### **Topics for international collaboration proposed in agreed action plans**

- Materials Modelling Market Place
- Interoperability
- Open Simulation Platform
- Translators
- Model development
- Business Decision Support System
- Software Owner

## **Materials Modelling Market Place**

### *Contributions proposed by*

Adham Hashibon, FRAUNHOFER IWM, Germany  
Kwang-Ryeol Lee, Korea Institute of Science and Technology (KIST), South Korea  
Alejandro Strachan, Purdue University, USA  
James Warren, Material Genome Initiative, NIST, USA

### *Supporting partners (willing to participate actively)*

Masahiro Takemura, Japan Science and Technology Agency (JST), Japan  
Satoshi Itoh, RIKEN Advanced Institute for Computational Science, Kobe, Japan

### *Collaboration Topics*

- Create an EMMC-nanoHUB (similar initiatives are welcome to join) coordination group (as part of the International Materials Modelling Board)
  - Coordinate development of novel online dissemination activities
  - Make sure that tags of publications and simulations on potential market place and nanoHUB should be compatible
  - nanoHUB could/should be linked to a potential Marketplace and provide the facility to run simulations.
  - Material Marketplace can provide access to Translator activities in linking end user question to simulation methodology and/or already existing answers.
  - Make use of nanoHUB UQ capabilities
  - Need to identify partner(s) for integration and interesting problems
  - Use data from existing EMMC (Marketplace) resources as input to nanoHUB tools
  - Need to identify database (e.g. pseudopotentials for DFT, discrete model databases, experiments and validation)
- Boost efforts and collaboration to build the Foundation of Materials Informatics
- Build a usable big data on a global scale:
  - Combine efforts to boost activities on repositories.
  - Discuss and set plans to increase material data flow from all models

- Plan joint actions (workshops) with industry

#### *Activities and dates*

- Oct 2015: Create an EMMC-nanoHUB coordination group, as part of the planned International Material Modelling Board (IM2B). The goal is to coordinate information between the EMMC (in particular the Marketplace, OSP and IntOP) to nanoHUB. Similar actions from Japan and Korea can also join the coordination actions.
- Nov 2015: Agree on workshop/meeting plans, including if possible those that host industry participation
- Jan 2016: Start exchange and dissemination of case studies
- Mar-Jun 2016: Identify, assess and tag simulation tools of interest in a similar unified manner, based on agreed metadata schema.
- 3-4Q 2016, jointly with the discrete EMMC WG, gathers requirements for databases beyond electronic (DFT) modelling. What is needed for mesoscopic discrete models?

## Interoperability

### *Contributions proposed by*

Adham Hashibon, FRAUNHOFER IWM, Germany  
Kwang-Ryeol Lee, Korea Institute of Science and Technology (KIST), South Korea  
Alejandro Strachan, Purdue University, USA  
James Warren, Material Genome Initiative, NIST, USA

Supporting partners (willing to participate actively):  
Masahiro Takemura, Japan Science and Technology Agency (JST), Japan  
Satoshi Itoh, RIKEN Advanced Institute for Computational Science, Kobe, Japan

### *Activities and dates*

- 2Q 2016: EMMC provides a first draft of metadata keyword proposal to nanoHUB. NanoHUB to identify and assess the use of tags that reflect the terminology of models and metadata on materials modelling as elaborated by the EMMC.
- 1Q 2016: Standard data approaches: Collect current activities that aim to establish standard data specifications including metadata of models.
- 3Q 2016: Determine joint strategies for common standard modelling data, (a joint position document or the like)
- 4Q2016: Database activities: Discuss and establish requirements for databases beyond electronic (DFT) modelling. What is needed for mesoscopic discrete models?.
- 2Q 2016: Keywords to be used for tags agreed.

### *Long term goals and actions:*

- Demonstrate interoperability between cyberinfrastructures
- Integrate EMMC market place and NanoHub

### *Means (Activities):*

- Monthly telephone conference starting from 10.2016 to coordinate
- Joint workshops in international conferences

**In Japan, Materials Informatics project just started. The discussed hits will be taken into account. The initiative on structured materials in Japan will keep contact and participate to the meetings. MGI will proceed in synergy with EMMC. Maybe there is a need for International Committee about Materials Informatics.**

## **Open Simulation Platforms**

### *Contributions proposed by*

Georg J. Schmitz, ACCESS E.V, Germany

Kwang-Ryeol Lee, Korea Institute of Science and Technology (KIST), South Korea

Alejandro Strachan, Purdue University, USA

Adham Hashibon, FRAUNHOFER IWM, Germany

Masahiro Takemura, Japan Science and Technology Agency (JST), Japan

Satoshi Itoh, RIKEN Advanced Institute for Computational Science, Kobe, Japan

Christa Court, MRI Global, USA

### *Collaboration Topics*

#### Generate Review Paper on Simulation Platforms by mid of 2016 (lead t.b.d)

- Establish common understanding of the term “platform” and its functionality and scopes (e.g. coupling of codes instead of linking)
- Compare different platform approaches

#### Study of OSP as a means to reduce costs of modelling (lead Christa Court)

- Study of OSP as a means to improve value/benefit to production
- Exchange case study information
- Exchange info about proven commercial benefits

### *Means (Activities) and due dates*

- Teleconferences, e-mail correspondence
- Mutual participation in Conferences and Workshops :  
(2<sup>nd</sup> International Workshop on Software Solutions in ICME Barcelona, April 2016, and 2<sup>nd</sup> International Symp. on SM4I Tokyo March 2016)

## Translators

### *Contributions proposed by*

Gerhard Goldbeck, Goldbeck Consulting LTD, UK  
Denka Hristova-Bogaerds, Dutch Polymer Institute, The Netherlands  
Alejandro Strachan, Purdue University, USA  
Kwang-Ryeol Lee, Korea Institute of Science and Technology (KIST), South Korea  
Masahiro Takemura, Japan Science and Technology Agency (JST), Japan

### *Collaboration Topics*

- Share experience about use of modelling and “translation”  
Adoption of modelling in industry across continents (frequency of use, types of models, benefits experienced)
- Share case studies
- Course deployment of edX MOOC (by NCN), <https://www.edx.org>
- Metadata from the end user point of view
- Impact tracking by model usage, model publication stats etc.

### *Means (Activities) and due dates*

- Organise joined activities (workshops etc.)
- November 2015: exchange of two show case with best/worst practises, translation approach, bottlenecks, common targets
- Early 2016: kick-off conference call of international translator group to outline common translation approach, training activities and plans
- 2016: Joint draft paper digesting best practice
- 2016: Joint training proposal covering different industries
- 2016: Joint draft paper on adoption.
- April 2016: Joint session at Barcelona ICMEg workshop

## Economic impact

### *Contributions proposed by*

Gerhard Goldbeck, Goldbeck Consulting LTD, UK  
Alejandro Strachan, Purdue University, USA  
Christa Court, MRI Global, USA  
Erich Wimmer, MATERIALS DESIGN, France  
Masahiro Takemura, Japan Science and Technology Agency (JST), Japan

### *Collaboration Topics*

- A set of standards to follow when performing economic impact assessments of materials models and the resulting materials
- A mini-knowledge base of information related to the set of standards
- Add-on to a meta-data library of data and information top allow within economic impact assessments
- Develop common methodologies to measure economic impacts (see actions and dates below)
- Develop common methodologies for cost benefit analysis of modelling technologies (software including specific models, codes and platforms)
- Model impact tracking usage, model publication stats etc. (NanoHUB)
- Stimulate the view to consider software as an industry itself in impact assessment
- Exchange case study information
- Check about any other impact assessment

### *Means (Activities) and due date*

- **Recurring:**  
Monthly update call between EMMC Economic Impact Representatives, Christa Court from US and potentially a representative from Japan (Takemura Masahiro)

- **December 2015** Joint EU-US report on economic impact assessments. This will be a report on the Economic Impact survey findings with an introduction to economic impact assessment by Christa Court.
- **May 2016:** U.S. visit by EMMC Economic Impact Working Group Representative (subject to funding being available within existing activities).
- **Autumn 2016:** Complete joint White Paper on methodologies to measure economic impacts related to materials modelling.
- **2016 – 2017:**
  - Complete joint White Paper on software impact and cost-benefit analysis
  - Joint Economic Impact Workshop
- **2016** (date subject to approvals process of US DOE): Qualitative and quantitative assessments of two open source models related to multi-phase flow modelling and computational chemistry. Final report by Christa Court at approval stage with U.S. DOE.

### **Business Decision Support System**

#### *Contributions proposed by*

Rudy Koopmans, DOW Europe, Switzerland

Massimo Noro, UNILEVER, UK

Alejandro Strachan, Purdue University, USA

Masahiro Takemura, Japan Science and Technology Agency (JST), Japan

#### *Collaboration Topics*

- Exchange results of US findings/methodology
- Define/exchange concepts pathways for integrating big data with ab initio materials modelling
- Identify people/institutes and organizations for driving the methodologies development
- Code of practice for decision support developments
- Summit organization
- Define pathways for establishing the MMP
- For economics Integrating UQ into nanoHUB and the Rappture toolkit=????
- Collaboration on decision support approaches

#### *Means (Activities) and due dates*



- **Oct 2015:** Establish International BDSS Interest Group of representatives and kick-off monthly update call. There is definitely interest from Takemura (JST).
- **Dec 2015:** Common slide set to be used in conference and meeting presentations.
- **Dec 2015:** Joint list of meetings and conferences where these slides are (to be) used. Establish feedback mechanism.
- **Feb 2016:** Establish a joint Code of practice for decision support developments
- **Spring 2016:** Joint paper on “Key elements of a BDSS and current status of capabilities” (e.g. Design-driven, Risk management, Validated models, known errors and UQ=???, Multi-objective optimisation, Data integration etc).
- **Summer 2016:** Joint paper/presentation on BDSS concept applied to specific industry (e.g. electronics, using vfab.org, nanoHub.org etc).
- **Date tbd:** Grand challenge summit with industry and academic stakeholders

## Model development

### *Contributions proposed by*

Kersti Hermansson, University of Uppsala, Sweden  
 Pietro Asinari, Politecnico di Torino, Italy  
 Kwang-Ryeol Lee, Korea Institute of Science and Technology (KIST)  
 Han Seungwu, Seoul National University, South Korea  
 James Warren, Material Genome Initiative; NIST, USA  
 Erich Wimmer, MATERIALS DESIGN, France

### *Collaboration Topics*

- Identification of which models are the worst or most lacking, and what broad application areas are the most needing (Nov2015)
- Identification of existing reports (in the US and elsewhere) containing analyses and inventories of "model gaps" (Dec2015)
- Collect international input into the next Roadmap on model development (Q4 2015)
- A survey of existing resources/repositories of force-fields (Mar2016)
- Reaching an international consensus (may be included in a white paper) concerning the following key topics (others to be added):

- Where should we set the target for model accuracy? Does accuracy exclude generality?
- Best practices how to reach an acceptance from industrial stakeholders of the long-term aspect *and*
- long-term benefit of model/method development.

### *Means (Activities) and due date*

- Regular telephone meetings monthly (starting with Nov 2015).
- Prepare a permanent mailing list (of the International Materials Modelling Board).
- Undertake tasks/commitment among the group members to move forward the topic/issues listed above, between the meetings.
- Involve the sub-groups of the EMMC Discrete models WG as well as other groupings who share our objectives and can participate in our efforts.
- Set up dedicated workshops/satellite meetings. Invite each other to key modelling meetings. *Example:* next multi-scale modelling meeting, Uppsala, June 2016.
- Plan a joint international white/review paper on state-of-the-art. *Example:* "state-of-the-art of advanced force-fields for complex (industrial) applications".
- Explore opportunities for joint international proposals on strategic developments towards more advanced industrial models and modelling practices.

### **Software Owners**

#### *Contributions proposed by*

Erich Wimmer, MATERIALS DESIGN, France  
 Anders Blom, QuantumWise, Denmark  
 Alejandro Strachan, Purdue University, USA

*Further invitations for contributions have been sent to*  
 James Warren, Material Genome Initiative; NIST, USA  
 Satoshi Itoh, RIKEN Advanced Institute for Computational Science, Kobe, Japan  
 Masahiro Takemura, Japan Science and Technology Agency (JST)  
 Kwang-Ryeol Lee, Korea Institute of Science and Technology (KIST)

*Collaboration Topics*

- Create a clearer picture of all major SWO's and their current software capabilities and activities (December 2015)
- Demonstrate the connection of discrete models – thermodynamic models – and phase field models for a specific case, thus setting the stage for better interoperability and data standards (April 2016)
- Share industrial success stories (Jan 2016)
- Identify areas related important to software owners of intrinsic international character (June 2016)

*Means (Activities) and due date*

- Jan 2016: Review existing compilations of available capabilities (e.g. “Integrative Computational Materials Engineering: Concepts and Applications of a Modular Simulation Platform” G. J. Schmitz and U. Prahl, editors) – coordinate with activities of Materials Modelling Market Place
- Work with international partners in the US, Japan and Korea to identify recent additions and new activities (ongoing)
- April 2016: Contribute to paper outlined by G. Schmitz in cooperation with Interoperability working group
- Jan 2016: Collect success stories in collaboration with international partners and provide information to the EMMC in coordination with Translators working group