UK-Japan Workshop:

HIGH PERFORMANCE MODELLING OF MULTISCALE BIOMOLECULAR SYSTEMS

17-18 December 2012

sponsored by the British Embassy, Tokyo
with support from
RIKEN

Accommodation

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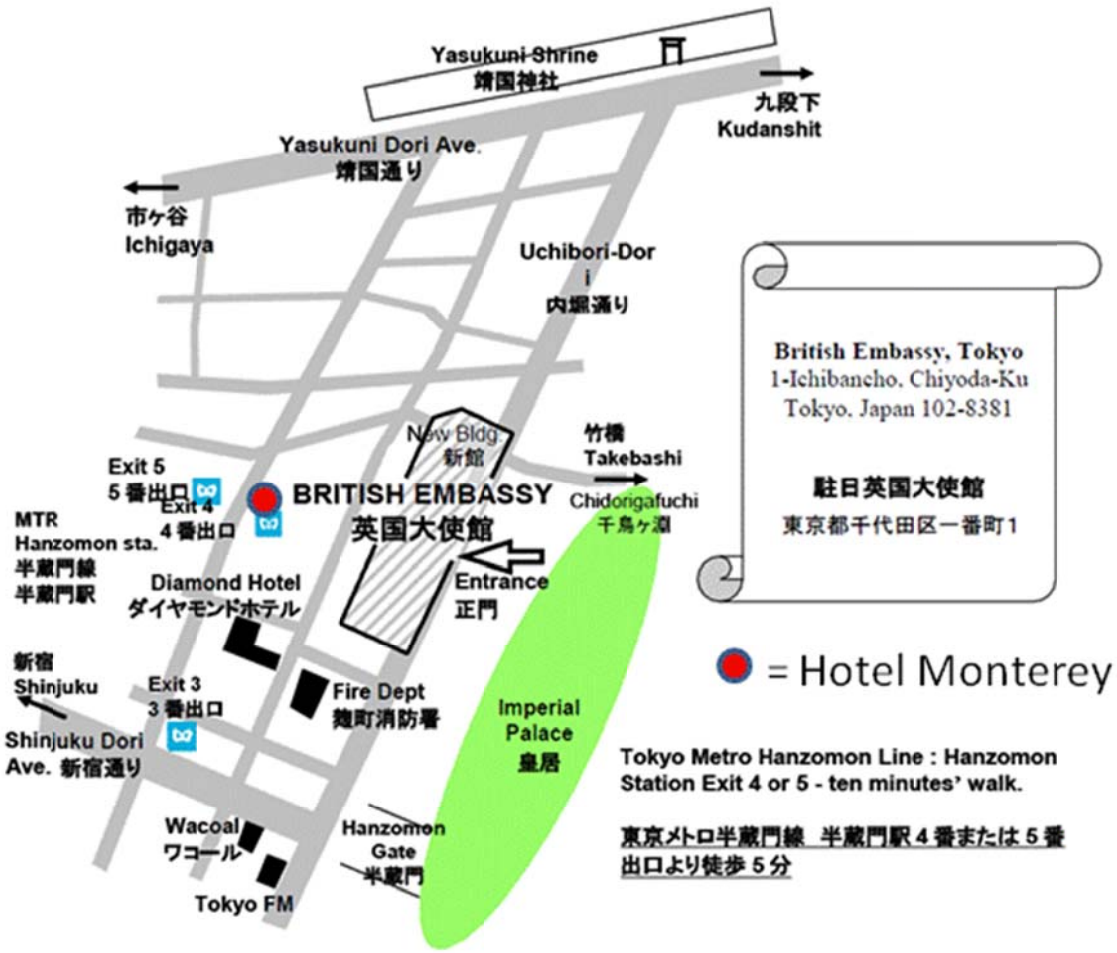

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Participant List

UK Speakers

	Name	Department	Affiliation	e-mail
1.	Dr Dmitry Nerukh	Department of Mathematics	Aston University	d.nerukh@aston.ac.uk
2.	Dr Sergey Karabasov	School of Engineering and Materials Science	Queen Mary University of London	s.karabasov@qmul.ac.uk
3.	Dr Anton Markesteijn	Department of Engineering	University of Cambridge	a.markesteijn@qmul.ac.uk
4.	Prof Peter Coveney	Department of Chemistry	University College London	p.v.coveney@ucl.ac.uk
5.	Dr Jochen Blumberger	Department of Physics and Astronomy	University College London	j.blumberger@ucl.ac.uk
6.	Dr Riam Kanso	Computational Life and Medical Sciences Network	University College London	riam.kanso@sjc.ox.ac.uk r.kanso@ucl.ac.uk

Japanese Speakers

	Name	Department	Affiliation	e-mail
1.	Dr Makoto Taiji	Quantitative Biology Center (QBiC)	RIKEN	taiji@riken.jp
2.	Dr Shu Takagi	Department of Mechanical Engineering, School of Engineering	University of Tokyo	takagish@riken.jp
3.	Dr Ryoichi Yamamoto	Department of Chemical Engineering	Kyoto University	ryoichi@cheme.kyoto-u.ac.jp
4.	Dr Akinori Kidera	International Graduate School of Arts and Sciences	Yokohama City University	kidera@tsurumi.yokohama-cu.ac.jp
5.	Dr Nobuyasu Ito	Graduate School of Engineering	University of Tokyo	ito@ap.t.u-tokyo.ac.jp

Observers

	Name	Department	Affiliation	e-mail	availability
1.	Dr Koji Kaya	Computational Science Research	RIKEN	Kaya@riken.jp	17
2.	Dr Ryutaro Himeno	Advanced Center for Computing and Communication	RIKEN	himeno@riken.jp	17 & Reception
3.	Dr Peter Karagiannis	Quantitative Biology Center (QBiC)	RIKEN	peter@riken.jp	17-18 & Reception
4.	Dr Eietsu Tamura	Computational Science Research Program	RIKEN	etamura@riken.jp	17-18 & Reception
5.	Dr Kazuyasu Sugiyama	Advanced Center for Computing and Communication	RIKEN	Kazuyasu.sugiyama@riken.jp	17 & Reception 18 am
6.	Dr Yoshinori Hirano	Laboratory for Computational	RIKEN	hirano@riken.jp	17-18 & Reception

7.	Dr Motoi Okuda	Technical Computing Solutions Unit	Fujitsu Ltd.	m.okuda@jp.fujitsu.com	17 pm & Reception
8.	Dr Koichi Takahashi	RIKEN Quantitative Biology Center	RIKEN	ktakahashi@riken.jp	17 & Reception
9.	Dr Adnan Hamid	Department of Chemical Engineering	Kyoto University	hamid@cheme.kyoto-u.ac.jp	17-18 & Reception
10.	Dr Antti Lamberg	Department of Chemical Engineering	Kyoto University	antti@cheme.tokyo-u.ac.jp	17-18 & Reception
11.	Dr Teruhisa Komatsu	Department of Applied Physics	University of Tokyo	komatsu@serow.t.u-tokyo.ac.jp	17-18 & Reception
12.	Dr Yousuke Ohno	QBiC	RIKEN	ohno@riken.jp	17-18 & Reception
13.	Dr Satoshi Hashimoto	Department for Administration of Research Promotion	JST	s2hashimoto@jst.go.jp	17-18 & Reception
14.	Dr Kenji Yamamoto	Research Institute	National Center for Global Health and Medicine	backen@ri.ncgm.go.jp	17 pm & 18 pm
15.	Dr Mikiko Azuma	Department of Innovation Research	JST	mazuma@jst.go.jp	17-18 & Reception
16.	Dr Mitsunori Ikeguchi	Graduate School of Nanobioscience	Yokohama City University	ike@tsurumi.yokohama-cu.ac.jp	17& Reception
17.	Dr Hiroshi Watanabe	Institute for Solid State Physics	University of Tokyo	hwatanabe@issp.u-tokyo.ac.jp	17-18 & Reception
18.	Ms Hiroko Kondo	Department of Computational Biology	University of Tokyo/RIKEN	h_kondo@gsc.riken.jp	17-18 & Reception
19.	Dr Ayako Maesawa	Biomedical Innovation Cluster Headquarters	Kobe City	Ayako_maesawa@office.city.kobe.lg.jp	17 am & Reception
20.	Dr Gentaro Morimoto	Laboratory for Computational Molecular Design	RIKEN	gentaro.morimoto@riken.jp	17-18 & Reception

Workshop Programme

Monday 17 December

Time	Activity
0930 - 1000	**Briefing for UK delegate from British Embassy (BE)** Attendees: UK and Japanese speakers and Embassy staffs
1000 - 1015	**Registration + Coffee**
1015 - 1020	**Opening remarks by Kevin Knappett (BE)**
1020 - 1030	Self-introduction of all speakers
1030 - 1035	Objectives of the workshop (Dr Taiji & Dr Nerukh)
1035 - 1215	**Session 1:** (30 min and 35 min presentations) Chair: Dr Nerukh
1035-1105	"UK Government Policy and Plans for High Performance Computing and E-Infrastructure" (30 min) by **Peter Coveney** (University College London)
1105-1140	"High-resolution algorithms for multiscale modelling in continuum fluid mechanics: from computational aeronautics and geophysics to fluctuating hydrodynamics of nano-scale flows" (35 min) by **Sergey Karabasov** (Queen Mary University of London)
1140-1215	"Multi-scale simulation studies on protein structural changes upon ligand binding" (35 min) by **Akinori Kidera** (Yokohama City University)
1215 - 1235	Discussion (Q&A)
1235 - 1330	Lunch
1330 – 1440	**Session 2:** (35 min X 2) Chair: Dr Taiji
1330-1405	"Multiscale biological and materials modelling: from quantum to continuum level" (35 min) by **Peter Coveney** (University College London)
1405-1440	"Multiscale Modeling for Fluid-Structure Interaction Problems with its Applications to the Initial Stage of Thrombosis" (35 min) by **Shu Takagi** (University of Tokyo)
1440 - 1510	Discussion (Q&A)
1510 - 1530	Coffee Break
1530 – 1640	**Session 3:** (35 min X 2) Chair: Dr Karabasov
1530-1605	"Small ligand diffusion in proteins: bridging the nano and millisecond time scales" (35 min) by **Jochen Blumberger** (University College London)
1605-1640	"From molecule to flow, and beyond" (35 min) by **Nobuyasu Ito** (University of Tokyo)

1640 - 1700	Discussion
1700 - 1730	Wrap-up for the first day
1730 - 1900	Reception

Tuesday 18 December

Time	Activity
0845 - 0900	Registration & coffee
0900 - 1010 0900-0935 0935-1010	**Session 4:** (35 min X 2) Chair: xxxx "Multiscale dynamics of biomolecular systems" (35 min) by **Dmitry Nerukh** (Aston University) "Simulations of colloids and self-propelled particles with fully resolved hydrodynamics" (35 min) by **Ryoichi Yamamoto** (Kyoto University)
1010 – 1025	Discussion (Q& A)
1025 – 1040	Coffee Break
1040 – 1055	"RIKEN Quantitative Biology Center (QBiC)" (15 min) by **Peter Karagiannis** (RIKEN)
1055 – 1240 1055-1130 1130-1205 1205-1240	**Session 5:** (35 min X 3) Chair: xxxx "Connecting Molecular Dynamics, Computational Fluid Dynamics, and Fluctuating Hydrodynamics" (35 min) by **Anton Markesteijn** (University of Cambridge) "MDGRAPE-4: a special-purpose computer for molecular dynamics simulations" (35 min) by **Makoto Taiji** (RIKEN) "Open Science, Open Data" (35 min) by **Riam Kanso** (University College London)
1240 - 1255	Discussion (Q&A)
1255 - 1325	Final wrap-up
1325 -	Lunch
1600	Depart the Embassy for Haneda Airport by car (UK speakers)
1755	Depart Haneda for Kobe (SKY113)
1910	Arrive at Kobe Airport
	Dinner
	Overnight in Kobe (Kobe Portopia Hotel)

Wednesday 19 December

Time	Activity
0945	Meet up at Lobby of Kobe Portpia Hotel
1000- 1145	Tour of Center for Molecular Imaging Science (CMIS) and Center for Developmental Biology (CDB)
1145-1300	Lunch at Kachoen
1300-1430	Tour of K computer
1430-1530	Research Interaction and Discussion with Dr. Takahashi

CV & Abstracts

Professor Peter Coveney

"UK Government Policy and Plans for High Performance Computing and E-Infrastructure"

In October 2011, the UK Government announced the allocation of £165M for High Performance Computing and E-Infrastructure, aimed at bringing UK back to a leading international level after some years of underspending. These capital funds were committed across the whole research computing ecosystem and various new systems were put in place by end of March 2012. David Willetts MP, the UK Science and Universities Minister, also established an E-Infrastructure Leadership Council (http://www.bis.gov.uk/policies/science/science-funding/elc) which is now working on recommendations for a five year business plan in this domain, designed to cover not only hardware and software but also education and training of the personnel required to exploit these new technologies. One of the principal reasons for Government support for this area is to promote uptake of these new capabilities, within academia, private and public sectors, in support of a forward-looking economic growth agenda according to which information technology is to be viewed on a par with other infrastructures such as roads, railways, electricity, water and other utilities.

"Multiscale biological and materials modelling: from quantum to continuum level"

Living systems are complex, more so than most materials. Both, however, include complex interactions at multiple spatial, temporal, and organizational levels. Understanding this complexity requires that existing and future models are used and interpreted within a framework that incorporates knowledge derived from investigations at multiple levels of physical and biological function. The challenge of such multidisciplinary research is to integrate the knowledge of all different components into robust and reliable computer models. Great progress has been made in multiscale modelling and simulation, which involves crossing the boarders of different disciplines such as information technology, computer and computational science, mathematics, biology, and medicine (basic and clinical). Examples are given in this talk of how multiscale models are developed and applied for better understanding of complex nanomaterials as well as major diseases such as HIV and cancer, and their growing impact on the development and testing of new therapies in healthcare.

Biography

Professor Peter Coveney holds a Chair in Physical Chemistry and is Director of the Centre for Computational Science (http://ccs.chem.ucl.ac.uk/), an Honorary Professor in Computer Science and a member of CoMPLEX at UCL. He is also Professor Adjunct within the Yale School of Medicine at Yale University, and Director of the UCL Computational Life & Medical Sciences Network (http://www.clms.ucl.ac.uk/). Coveney is active in a broad area of interdisciplinary theoretical research including condensed matter physics and chemistry, materials science, life and medical sciences including collaborations with clinicians. Coveney is PI of the Virtual Physiological Human (VPH) Network of Excellence; inter alia he is also a co-PI on the new EPSRC Cross-Disciplinary Landscape Award on a New Approach to Science at the Life-Science Interface. He has held and holds a large number of EPSRC and EU grants, including that as PI of the RealityGrid e-Science project and its extension as a

Platform Grant; he also led the GENIUS project, which applies lattice-Boltzmann fluid simulation techniques to model patient-specific brain blood flow in support of clinical decision making. In 2010, Coveney was awarded funding for the EU FP7 p-medicine project which aims to develop a distributed data warehouse to store and exchange clinical data in heterogeneous formats, as well as the VPH-Share project which seeks to develop lightweight middleware that will simplify access to high performance computing resources for data-intensive and data-driven projects. In addition to major participation in the EU FP7 MAPPER project on multiscale modelling on EU infrastructures, he is also active in the new EU FP7 EUDAT and CRESTA projects, which aim respectively to build a persistent European data infrastructure and to evolve petascale codes to the exascale. Coveney has been the recipient of several major US NSF and DoE funded supercomputing grants, and similar ones in Europe on DEISA and PRACE. He also received an HPC Challenge Award (Supercomputing 2003), an HPC Analytics Challenge Award (SC05), and International Supercomputing Conference Awards (2004 and 2006). He is a founding editor of the Journal of Computational Science and to date has published more than 280 scientific papers, edited 20 books and coauthored two best-selling popular science books (The Arrow of Time and Frontiers of Complexity, both with Roger Highfield).

Dr Sergey Karabasov

"High-resolution algorithms for multiscale modelling in continuum fluid mechanics: from computational aeronautics and geophysics to fluctuating hydrodynamics of nano-scale flows"

Multiscale problems are encountered in many areas of unsteady fluid dynamics modelling. For their solution, one typically requires a model which has two key components. One component is a high-resolution computational algorithm for accurately solving unsteady flow equations with a limited number of degrees of freedom. One of such algorithms, the CABARET scheme developed by authors, will be considered, examples of its applications for direct simulation of aeronautical and geophysical flows will be discussed, and the authors' experience of implementing these algorithms within a supercomputing framework will be shared. The other important component is a technique for consistently coupling coarse-scales with fine-scales in space and time that differ by many orders of magnitudes within the same computational framework. For this talk, two topical fluid dynamics applications that require multiscale coupling schemes will be considered. One is the modelling of sound generated by turbulent jet flows in aerospace engineering. The other example is micro/nano-scale flow modelling using Landau-Lifshitz Fluctuating Hydrodynamics equations which describe thermal fluid fluctuations at nano-scale, and which are computed with a variable space-time-scale approach.

Biography

Sergey Karabasov is Senior Lecturer in Modelling and Simulation in the School of Engineering and Materials Science and Royal Society University Research Fellow in Queen Mary College University of London (QMUL). Before joining QMUL, he spent 12 years in the Whittle Laboratory, University of Cambridge, working on aeroacoustic projects supported by the leading UK industry such as Rolls-Royce, GKN Westland Helicopters and Thales Underwater Systems. Currently, Sergey is involved in 2 aeronautics research projects supported by the UK Engineering and Physical Sciences Research Council. The projects combine mathematical modelling and high-performance computations with the aim to capture multiscale temperature, propagation and airframe-coupled effects as related to turbulent jet noise. Another field of Sergey's interests is high-resolution modelling in

computational geophysics. At present, he is involved in the Turbulent Oscillator project with Imperial College London which is supported by the UK Natural Environment Research Council and devoted to eddy-resolving modelling of oceanic flows.

In application to biological flows, Sergey is very keen to extend the hybrid modelling approaches he used in other areas to multi-scale phenomena at small scale. Currently, in collaboration with his colleagues from Aston University, UK, Riken Institute, Japan and a few other research institutions in Japan and Russia he is involved in a multi-lateral G8 INGENEOUS project. Under this project Sergey is contracted to numerically couple continuum fluid dynamics equations with molecular dynamics in the framework of a novel multi-space-time method.

Sergey holds PhD in mathematical modelling from Moscow State University (1999) and Full Doctorate of Science from Moscow Keldysh Institute for Applied Mathematics (2010). He is a Senior Member of American Institute of Astronautics and Aeronautics, a Member of the Aeroacoustic Section of the Physical Acoustics Panel of Russian Academy of Science, and a Member of the Royal Society's Grant Panel and Newton International Fellowship Board (Physical Sciences).

Dr Akinori Kidera

"Multi-scale simulation studies on protein structural changes upon ligand binding"

Large-scale structural changes in biomolecules involve barrier-crossing transitions on the rugged free energy surfaces of high-dimensional space. Such rare events cannot be efficiently captured by conventional molecular dynamics simulations. To solve this problem in the biomolecular simulations, we have developed multi-scale simulation methods, which combine the all-atom model with explicit solvents (MM) and a coarse-grained model (CG). The configurational sampling of the MM model is enhanced by coupling the accelerated dynamics of the CG model. In the talk, I will introduce two methods and their applications.

1. Path search by the on-the-fly string method: Large scale structural change in adenylate kinase upon ligand binding
The influence of ligand binding on the pathways of dynamical motions from the open form to the closed form was characterized in terms of domain motions of adenylate kinase.

2. Multiscale enhanced sampling simulation (MSES): Disorder to order transition of the ligand binding loop in sortase

Sortase has an intrinsically disordered region undergoing a disordered-to-ordered transition upon binding of a signal peptide and a calcium ion. Using MSES, we examined how the binding of the peptide and/or calcium influences the conformational ensembles.

Biography

Professional experiences
1982 Ph.D. Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University
1982 Posdoc assoc. Department of Chemistry, Cornell University, USA
1986 Research associate, Department of Chemistry, Kyoto Institute of Technology
1988 Senior research scientist, Protein Engineering Research Institute.
1996 Associate Professor, Graduate School of Science, Kyoto University

2001 Professor, Graduate School of Integrated Sciences, Yokohama City University
2006 Team Leader, Computational Science Research Program, RIKEN (concurrent)
2011 Deputy Program Director, HPCI Program for Computational Life Science, Riken (concurrent)

Dr Shu Takagi

"Multiscale Modeling for Fluid-Structure Interaction Problems with its Applications to the Initial Stage of Thrombosis"

We have been working on the software development of multiscale human body simulator. A novel simulation method for solving fluid-structure coupling problems suitable for the massively parallel computing has been developed [1]. All the basic equations in continuum scales are numerically solved on a fixed Cartesian grid with finite difference discretization. An incompressible fluid flow solver is extended to the incompressible fluid-structure system. A volume-of-fluid approach, which has been developed for computing multiphase flows, is applied to describing the multi-component geometry. So, the present method treats non-linear deformation of hyperelastic materials in fully Eulerian way on a fixed grid without generating the boundary-fitted meshes. The simulator is developed for the massively parallel computation and the excellent scalability of the computation will be also presented.

The method has been further developed for fluid-membrane interaction problems [2] and applied to the blood flows containing Red Blood Cells and platelets. Then the method has been extended to multiscale thrombosis simulation. Thrombosis is very important circulatory disease which causes the myocardial infarction and stroke. In the present simulation, the molecular scale protein-protein interactions are solved using Monte-Carlo method [3] coupling with continuum scale simulations. The results show that the continuum scale flows affects the platelet adhesion on the vessel walls where the adhesion force itself is given by the molecular scale binding between GP1b□ proteins on the platelet and vWF proteins on the injured vessel wall.

References
[1] Sugiyama, K. et al., *J. Comput. Phys.*, **230** (2011), pp. 596-627.
[2] Ii, S., et al., *Commun. Comput. Phys.*, **12** (2012), pp. 544-676.
[3] Shiozaki, S. et al., *J. Biomech. Sci. Eng.*, **7** (2012) pp.275-283.

Biography

Education:
1995: Doctor of Engineering, Department of Mechanical Engineering, The University of Tokyo

Professional Position:
1995.4-1996.10: Research Associate, Department of Mechanical Engineering, The University of Tokyo
1996.10-1998.3: Research Associate, Department of Mechano-Aerospace Engineering, Tokyo Institute of Technology
1998.4-2002.1: Lecturer, Department of Mechanical Engineering, The University of Tokyo
2002.1-2010.3: Associate Professor, Department of Mechanical Engineering, The University

of Tokyo
2007.4- current: Team Leader, Organ and Body scale Team, CSRP, RIKEN
2010.4-current: Professor, Department of Mechanical Engineering, The University of Tokyo

Dr Jochen Blumberger

"Small ligand diffusion in proteins: bridging the nano and millisecond time scales"

In this talk I will describe a general microscopic model that we have developed for the calculation of diffusion rates of small ligands (e.g. gas molecules) in proteins[1,2]. The diffusive hopping of the ligand within the protein, which occurs over a range of time scales, is coarse grained using a master equation approach. The transition rates between the coarse states (protein cavities) is estimated from equilibrium and non-equilibrium pulling MD simulations. The master equation is propagated to obtain the ligand population of the active site as a function of time. A fit of the time-dependent populations to a phenomenological rate law gives the phenomenological diffusion rate constants that can be compared to experimental measurements. I will report on the application of this methodology to a number of enzymes that have recently attracted much interest for biotechnological applications such as H_2 oxidation and production in biofuel cells ([NiFe]-hydrogenase)[1,2,3] as well as CO_2 reduction and production of biomass (Carbon-monoxide dehydrogenase/acetyl co-enzyme A synthase (CODH/ACS))[4]. Experimentally determined diffusion rates of inhibitors in wild-type[1,2] and mutant[3] hydrogenases could be well reproduced with our method. Moreover, our simulations could explain how mutations impact on inhibitor diffusion[3]. I will show that the method developed can give unprecedented insight into the structural features that are built into enzymes to guide the directed flow of ligands into and between active sites. I will also demonstrate that incorporation of protein dynamical effects is crucial for a more complete understanding of small ligand transport within and between proteins.

References
[1] P. Wang, R. B. Best, J. Blumberger *J. Am. Chem. Soc.* **133**, 3548 (2011).
[2] P. Wang, R. B. Best, J. Blumberger *Phys. Chem. Chem. Phys.* **13**, 7708 (2011).
[3] P. Wang, J. Blumberger, *Proc. Natl. Acad. Sci. USA* , **109**, 6399 (2012).
[4] P. Wang, M. Bruschi, L. De Gioia, J. Blumberger, manuscript in preparation.

Biography

Jochen Blumberger obtained his PhD in 2004 from Cambridge University, UK, where he helped develop ab-initio molecular dynamics methods for the simulation of redox reactions under the supervision of Prof. M. Sprik. He then spent two years of post-doctoral research with Prof. M. Klein's group at the University of Pennsylvania, USA, and returned to Cambridge in 2006 on a Royal Society University Research Fellowship to start his independent research group. He is currently a lecturer at University College London (since 2009). His research is focused on the development and application of computer simulation methods for the microscopic description of charge transport, ligand transport and chemical transformations in materials and proteins that are of particular relevance to energy generation and conversion. Methods being developed and used range from electronic structure calculations on the density functional theory level to quantum/mechanical molecular mechanical calculations to classical molecular dynamics.

Dr Peter Karagiannis

"RIKEN Quantitative Biology Center (QBiC)"

Because RIKEN Quantitative Biology Center (QBiC) was only founded in the spring of 2011, it has yet to establish a profile domestically, let alone internationally. This brief talk will give an overview of QBiC's research aims, which can be decomposed into three categories – measurement technologies, modeling techniques, and design innovations – and discuss some of its challenges regarding recruitment and research output.

Biography

Peter Karagiannis is responsible for international communications at QBiC. He did his Ph.D. on muscle research at Case Western Reserve University (Cleveland, Ohio). Upon graduating in 2004, he joined the laboratory of Toshio Yanagida at the Graduate School of Frontier Biosciences (FBS), Osaka University, (Osaka, Japan) as a JSPS post-doctoral fellow to study single molecule imaging techniques. In 2006 he joined Agnes Wong's group at Toronto Western Hospital (Toronto, Canada) to model neural palsies, but returned to the FBS in 2007 in an administrative role. He joined QBiC in 2012.

Dr Dmitry Nerukh

"Multiscale dynamics of biomolecular systems"

The dynamics of biomolecular systems, from small peptides to large multidomain complexes, takes place, both in space and time, at scales that are larger than atomistic but usually smaller than continuum macroscopic. For example, the dynamics of protein conformations constituting protein folding phenomenon is known to include not only the protein's atoms but also a significant part of water molecules surrounding the protein. Temporally this dynamics happens at the nanoseconds to seconds scales. Therefore, understanding how the small scale atomistic motion results in complicated behaviour at larger scales is necessary for uncovering the mechanisms of biomolecular motions. Conceptually, the transformation between the scales for liquid state of matter is only explained for the extremes of the scales: for example, macroscopic properties of the system as a whole are obtained by averaging the atomistic details. The picture is much less clear when the physics at the intermediate scales are considered. Thorough investigation of concepts such as fluctuating hydrodynamics (the fluctuations at the continuum fluid dynamics level are hypothesised to be random processes resulted from the averages over not large enough number of atoms) is only recently started. But this is exactly the time and space scales at which the most important biomolecular motions happen! Are the fluctuations near the protein the same as in pure water? How far from the protein should you take water to have statistically the same fluctuations? Are they random fluctuations at all or something fundamentally different? From this point of view high performance computer simulation is currently reaching the time and space scales at which direct "experimental" verification of

these interscale phenomena becomes possible. At the talk I will illustrate such across-the-scales phenomena by examples of small peptides in water.

Biography

Career:

2010 – : Lecturer at Department of Mathematics, Aston University, UK.
2005 – 2009: Senior Research Associate at Department of Chemistry, Cambridge University, UK.
2000 – 2005: Research Associate at newly opened Unilever Centre for Molecular Sciences Informatics, Department of Chemistry, Cambridge University, UK.
1998 – 2000: Research Associate at the University of Nevada, Department of Chemistry, Reno, USA.
1997 – 1998: Royal Society - NATO Postdoctoral Fellowship at the University of Leeds, School of Chemistry, UK.

Education:

1993 – 1996: PhD training at the Department of Inorganic Chemistry, Kharkov State University
1986 – 1993: MSc training at Kharkov State University, School of Chemistry (dates include 2 years of army service)

Research: **Complex quantum and classical dynamics of molecular systems**

Kinetics of ligand binding. Obtaining the rates of binding of small molecules to proteins from realistic full-atom molecular dynamics simulations. Developing approaches for calculating correct bio-molecular transformation rates, taking into account non-Markvoian behaviour of states. **Hybrid hydrodynamics – molecular dynamics simulation**. Modelling bio-molecular systems where fully atomistic and purely hydrodynamic representations coexist and smoothly transform into each other at different spatial locations. **Complexity of dynamical systems**. Quantitative approaches to computing the complexity of physical systems. Informational contents of classical dynamics of molecular systems. Molecules as non-linear dynamical systems. **Protein folding**. Molecular Dynamics simulation of protein folding. Complexity of the dynamics of folding. "Controlled MD" – a correct methods for accelerated folding simulations. **Bohmian quantum dynamics**. Application of Bohmian mechanics to realistic molecular systems. Developing methods for effective propagation of Bohmian quantum trajectories for multidimensional systems.

Most important publications:

- D Nerukh, N Okimoto, A Suenaga, and M Taiji, accepted for publication in *J. Phys. Chem. Lett.*;
- D Nerukh, C H Jensen, and R C Glen, *J. Chem. Phys.*, **132**, 084104 (2010);
- D Nerukh, V Ryabov, and M Taiji, *Physica A*, **388** (22), 4719 (2009);
- D Nerukh, *J. Mol. Liq*., **145**(3), 139-144 (2009);
- D Nerukh, *Chem. Phys. Lett*., **457**(4-6), 439 (2008);
- D Nerukh, V Ryabov, and R C. Glen, *Phys. Rev. E*., **77**, 036225 (2008);
- D Nerukh, G Karvounis, and R C. Glen, *J. Chem. Phys.*, **117**(21), 9618-9622 (2002);
- D Nerukh and JH Frederick, *Chem. Phys. Lett.*, **332**(1-2), 145-153 (2000);

Dr Ryoichi Yamamoto

"Simulations of colloids and self-propelled particles with fully resolved hydrodynamics"

Using the smoothed profile method (SPM) method [1,2] developed for direct numerical simulations (DNS) of colloidal dispersions, we studied several dynamical problems of particle dispersions, including their rheological behaviours under steady and oscillatory shear flows. Recently, the SPM is extended for dispersions of self-propelled particles by replacing the non-slip boundary condition (usual for colloids) with an actively slip boundary condition (to model microorganisms, see Fig.1 below) at the fluid/particle interface. Several dynamical behaviours of the hydrodynamically interacting self-propelled particles will be discussed [4].

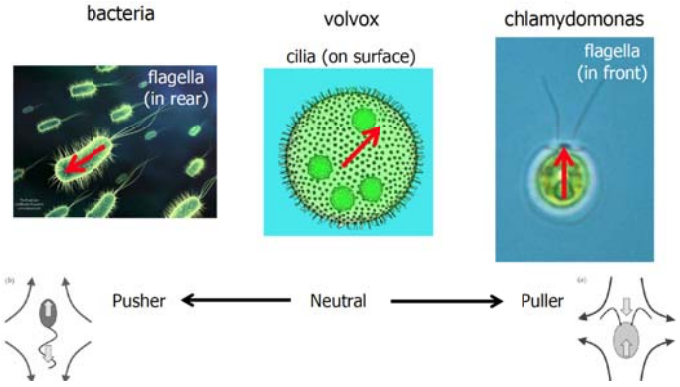

Fig.1 Examples of self-propelled (swiming) microorganisms. Pushers: microorganisms having locomotory appendages behind the cell body, relative to the swimming direction. Pullers: microorganisms having locomotory appendages in front of the cell body, relative to the swimming direction. Pushers and pullers create different flow profiles around them (see illustrations).

References

[1] Y. Nakayama, K. Kim and RY, EPJE, 26, 361-368 (2008)
[2] KAPSEL website, http://www-tph.cheme.kyoto-u.ac.jp/kapsel/
[3] R. Tatsumi and RY, PRE, 85, 066704 (2012).
[4] J. Molina, Y. Nakayama, and RY, preprint.

Biography

Degrees:

1996/03	Ph. D. in Molecular Engineering, Kyoto University, Japan
1992/03	M.En. in Chemical Engineering, Kobe University, Japan
1988/03	B. En. in Chemical Engineering, Kobe University, Japan

Interests:
Computer simulations of soft matters (complex fluids, glasses, polymers, and colloids) and biological materials (microorganisms, soft tissues).

Professional Experience:

2008/10-Present	Professor, Department of Chemical Engineering, Kyoto University.
2004/10-2008/09	Associate Professor, Department of Chemical Engineering, Kyoto University.
2000/01-2004/09	Lecturer, Department of Physics, Kyoto University.
1996/03-1999/12	Research Associate, Department of Physics, Kyoto University.
1994/09-1996/02	Research Associate, Graduate School of Science and Technology, Kobe University.
1988/04-1989/06	Honda Motor Company

Visiting Experience:

2000/09-2001/08	Visiting Scientist, Chemistry Department, University of Cambridge, UK (also Research Associate of Corpus Christy College)
1993/10-1994/03	Visiting Student, Max-Planck Institute for Chemistry, Mainz, Germany.

Dr Anton Markesteijn

"Connecting Molecular Dynamics, Computational Fluid Dynamics, and Fluctuating Hydrodynamics"

On the molecular scale, Molecular Dynamics (MD) provides a powerful tool to simulate the dynamics of individual atoms up to very complex molecules. However, because of the computational constraints, MD can only be applied to relatively small systems and short time scales. In this case, solving continuum equations, i.e. solving the average (bulk) behaviour of a very large number of atoms, is much more efficient while providing satisfactory results. Nevertheless, in the micrometer and nanometer scale, both the bulk and atomistic behaviour is important. It is at this scale, where the thermal fluctuations are noticeable, while the system is too large to solve with MD. Furthermore, conventional continuum methods do not take these important fluctuations into account.

One possible solution to this problem is to use both methods at the same time and only apply it to the region where the specific method is most suitable. However, in order for this to work, these methods should communicate with each other, i.e. the need to be coupled. This will be the subject of the first part of the presentation.

Another interesting framework to connect the macroscopic scales and molecular scales is Fluctuating Hydrodynamics (FH). In this case the continuum equations are supplemented by random forces that mimic the thermal fluctuations. The correct thermodynamic state is obtained by using the fluctuation-dissipation theorem, while the equations that need to be solved become stochastic equations. The second part of the presentation will concentrate on fluctuating hydrodynamics. It will be shown how it can be used to study polymer flow, e.g. translocation through a nanopore. The last part of the presentation shows a recently developed multi space/multi time algorithm using fluctuating hydrodynamics, with the aim to accurately and efficiently simulate water salvation and the dynamics of large biomolecular systems.

Keywords of Research Interest
Fluid Dynamics, Non-Equilibrium Molecular Dynamics, Fluctuating Hydrodynamics for Nano-Scale Flows, Microfluidic Devices, Electrokinetic Flows, Multiscale Methods, Biophysical Systems and Simulations, Soft Matter

Biography

Education and Academic Qualifications
2011-Present University of Cambridge / Queen Mary, University of London
Post Doctoral Research Associate. Bridging computational fluid dynamics and fluctuating hydrodynamics with fully atomistic molecular dynamics simulations.
2004-2011 Delft University of Technology, The Netherlands
PhD research at the Laboratory for Aero & Hydrodynamics. PhD project:
"Connecting Molecular Dynamics and Computational Fluid Dynamics".
2008 University of Oxford, Rudolf Peierls Centre for Theoretical Physics

Visiting Researcher. "Research into computational method for simulation of flow injection of polymers into nanopores"
2002-2004 Delft University of Technology, The Netherlands
Master of Science with Honours 'Mechanical Engineering - Solid and Fluid Mechanics', specialisations 'Engineering Dynamics' and 'Fluid Mechanics'. Research on fluid dynamics and droplet formation inside a printhead nozzle.

Selected Scientific Publications

2012 A.P. Markesteijn, R.M. Hartkamp, S. Luding, and J. Westerweel, "A comparison of the value of viscosity for several water models using Poiseuille flow in a nano channel", J. Chem. Physics, 136, 134104 (2012)
2010, L.C. Jellema, A.P. Markesteijn, J. Westerweel and E. Verpoorte, "Tunable Hydrodynamic Chromatography of Microparticles Localized in Short Microchannels", Anal. Chem., 2010, 82 (10), pp 4027–4035
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2008, G.O.F. Parikesit, A.P. Markesteijn, O.M. Piciu, A. Bossche, J. Westerweel, I.T. Young, Y. Garini, "Size-dependent trajectories of DNA macromolecules due to insulative dielectrophoresis in submicrometer-deep fluidic channels", Biomicrofluidics, 2008, Volume 2, Issue 2, paper 024103
2005, G.O.F. Parikesit, A.P. Markesteijn, V.G. Kutchoukov, O.M. Piciu, A. Bossche, J. Westerweel, Y. Garini, I.T. Young, "Electroosmotic flow analysis of a branched U-turn nanofluidic device", Lab on a Chip, 2005, Volume 5, Issue 10, pages 1067-1074

Dr Makoto Taiji

"MDGRAPE-4: a special-purpose computer for molecular dynamics simulations"

Recent efforts in both algorithmic, software and hardware developments enhance the application fields of the Molecular Dynamics (MD) simulations for life sciences. The most important bottleneck lies in a large gap between the timescales of atomic motion of femtosecond and that of biological functions of millisecond or more. To accelerate MD simulations we have developed several special-purpose computer systems for particle simulations called "GRAPE (GRAvity PipE)". The GRAPE systems are dedicated or quasi-general-purpose accelerators attached to host computers. The efficient parallelization in GRAPE systems provided us high-performance at low cost and low energy. However, as the performance increases, it requires a more powerful host machine, which becomes the new bottleneck in performance. To solve the problem, we are currently developing the "MDGRAPE-4", the special-purpose computer system for MD simulations. The MDGRAPE-4 has similar structure with Anton by D. E. Shaw Research. It consists of System-on-Chip LSIs with general-purpose cores, dedicated pipelines, network interfaces, and memory units. By the integration of these elements we aim to achieve a simulation speed of a few ten microsecond per step by its low latency memory access and networking. In the talk we will introduce hardware of the MDGRAPE-4 system and discuss future high-end computing for molecular simulations.

Biography

Makoto Taiji is a Director of Computational Biology Research Core, RIKEN Quantitative Biology Center founded in 2011. He also has the other posts as Team Leader of High-

Performance Computing Team, RIKEN Computational Science Research Program, and Team Leader of Processor Research Team, RIKEN Advanced Institute for Computational Sciences.
His research interests cover computer science and computational science, especially computational biology. He developed several special-purpose computers for scientific simulations. In 2006 he developed “MDGRAPE-3”, a special-purpose computer for molecular dynamics simulation with world-top-class performance. He was awarded three Gordon Bell Prizes in 1995, 2006 and 2009. Currently he is developing the next-generation special-purpose computer “MDGRAPE-4”. He also applies molecular simulations using the K computer and his machine to molecular biophysics including drug discovery research.
Dr. Taiji was born in Tokyo in 1964. He was educated in University Tokyo and received a PhD in physics there. He was an Assistant Professor of University of Tokyo from 1992 and was an Associate Professor of Institute of Statistical Mathematics from 1997, before joining RIKEN in 2002.

Dr Riam Kanso

“Open Science, Open Data”

Open science policies have a crucial impact on the progress of research collaboration at the international level. Recently, a global Research Data Alliance (RDA) has been formed, which is concerned with accelerating international data-driven innovation and discovery. RDA aims to promote data sharing and exchange, through the development and adoption of common standards, infrastructure and policy issues associated with electronic data and its management. The data in question ranges from journals and their contents to raw data obtained in the course of research. Of particular importance to us here is the data derived from computer simulations, be they performed on desktops or the largest international supercomputers. We discuss UK and EU funded projects which are addressing these issues, including EUDAT (http://www.eudat.eu/) For the purpose of Japan-UK collaboration in the domain of research into multi-scale modeling and simulation on high performance computers, it is important that open standards are agreed and utilized to foster growth of the field. Verification and validation of such complex models necessitates access to data derived from these simulations, which may be run on multiple resources including those distributed geographically between both countries. These data should in general be made available to the scientific community. Awareness of and close involvement in the RDA initiative should serve accelerate these efforts.

Biography

Riam Kanso has completed her DPhil research in Neuroscience at the University of Oxford in brain imaging and electrophysiology. She is now actively involved in several science policy initiatives within UCL, at national and at international levels. She has worked at the Royal Society of London on projects that involve the use of neuroscience data for the benefit of society, with a focus on security and legal matters. She is currently working as a policy advisor and analyst within UCL’s Computational Life and Medical Sciences (CLMS) Network, where she is involved in diverse initiatives which concern the application of multiscale biological modelling and simulation data for the benefit of healthcare. She has been involved in drafting high performance computing strategies for forthcoming UK research institutes and in promoting open science and open data policies within several UK/EU funded projects.

USEFUL TELEPHONE NUMBERS

Japan is nine hours ahead of GMT, eight hours ahead of BST

Dialling codes: Japan-UK: From Embassy use FTN*
Japan-UK: (9)-0061-010-44- (using IDC*)

UK-Tokyo: 0081-3-xxxx-xxxx

Use the initial 9 when calling from an Embassy phone

*If calling from the Embassy it is far cheaper to use FTN, at least to the UK (calls to the GTN in the UK are free). To call a non-GTN UK number please dials in the form (using London as an example) 89-020-1111-1111. To call a GTN number refers to the handbook in the Embassy. Outside the Embassy, there are several long distance/international telephone carriers. The telephone subscriber needs to be registered with a carrier to use it. 0061 is the prefix for IDC Cable & Wireless, used by the Embassy before FTN came still in and still valid, and this prefix should work from any Embassy telephone if FTN is not working. If it doesn't, try 9-010-44- instead.

British Embassy (03) 5211-1100 (Embassy Switchboard)
(03) 3262 9644 (Duty Officer out of hours)
090 8515 8314 (Duty Officer mobile)
(03) 5275 3164 (Fax)
(03) 5211-1344 (Chancery Fax)
(03) 5211-1114 (Residence Staff)
(03) 5276-0580 (Residence Fax)
(03) 5211-1290 (Embassy Main Gate – usually only Japanese spoken)

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Emergency

Tokyo Medical & Surgical Clinic Tel (03) 3436 3028
Police 110 / Fire and Ambulance 119
Kojimachi Police Station Tel (03) 3234 0110 (Close to the Embassy)

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Tokyo British Clinic (24 hours) (03) 5458-6099
Tokyo Medical & Surgical Clinic (24 hours) (03) 3436-3028

Empire Dental Clinic	(03)	3356-2910

Hospitals

St Luke's International Hospital 9-1 Akashi-cho, Chuo-ku	(03) 3541-5151
Nippon Medical School Hospital 1-1-5 Sendagi, Bunkyo-ku	(03) 3822-2131

Emergency Services

Police	110
Fire/Ambulance	119
Kojimachi Police Station (close to Embassy)	(03) 3234-0110

Airlines

Narita Airport Flight Information	(0476) 348 000
Narita Airport Customs	(0476) 322 802
British Airways (Narita)	(0476) 327 222
British Airways (Tokyo)	(03) 3593-8811
JAL (Narita)	(0120) 255 931
Lufthansa (Narita)	(0476) 348 130
Singapore Airlines	(03)32133431Ext2
Virgin Atlantic (Narita)	(0476) 303 611
Virgin Atlantic (Tokyo)	(03) 3499-8811
United Airlines (Tokyo)	(03) 3817-4411
Quantas (Narita)	(0476) 348 285
Quantas (Tokyo)	(03) 3593-7700
Haneda Airport Information	(03) 5757-8111
Kansai International Airport Information	(0724) 552-500

Earthquake Preparedness

Japan lies in a major earthquake zone. The country is subject to frequent tremors of varying intensity, the vast majority of which will not cause any damage or injury. There is, however, always the possibility of a strong earthquake occurring, and despite much research and speculation, it is very difficult to predict if and when such a quake might strike.

During An Earthquake

First, stay calm. Do not rush out of doors. Open a door to secure a way out. Get under a table to protect yourself from falling furniture and objects.
If you are outside, there is great danger from falling window glass, signs and from cement block walls. Take refuge in a sturdy, modern building if you can, but at the very least protect your head with your hands or bag.
If you are in a department store, cinema or underground shopping centre, follow the

instructions given by the staff and do not panic. Even if you cannot understand the instructions given follow the example of the Japanese around you. According to the Tokyo Metropolitan Government, underground malls are considered comparatively safe during an earthquake.

If you are in a lift, press all the buttons on the panel and get off as soon as the lift stops. If you get trapped, call for help on the interphone. Do not use lifts during earthquakes or fires.
If you are on a train, hold on to something secure and follow the instructions broadcast in the train. In a subway station, follow the same advice and avoid rushing to the exit as this causes dangerous panic.

Japanese names

In Japan the first name follows the family name. The Japanese commonly address each other by their family name. Only close friends and children are usually addressed by their first name. So it is best to make sure you know the family name and then address the person as Mr Tanaka or Ms Sato, unless they invite you to use their first names.

You may hear people say “Tanaka-san”, “Ishigaki-sama” or “Sato-sensei” when addressing others. The suffix “san” and the very polite “sama” are used for both genders and denote respect. You should never use “san” or “sama” to refer to your own colleagues or with your own name. The suffix “sensei” is for MPs, professors, doctors etc. Within organisations, people are known by the name and their job title, e.g. “Tanaka-bucho” for Mr Tanaka, the Department Head.

Doing Business

Punctuality is important. Try to arrive at least 10 minutes early for any meeting or social occasion. The Japanese tend to arrive early.

Addresses can be hard to find as the Japanese don’t always use street names, so it is a very good idea to have a Japanese map of the meeting location as even taxi drivers will need this.

The giving of gifts is important in Japan. But gifts are not usually given when meeting officials. Depending on the circumstances of your trip, it might be useful to take gifts and the Embassy can offer advice on this. Gifts should be neatly wrapped. If you receive a gift, do not unwrap it immediately without asking the host’s permission. If you do unwrap it, try to take the paper off neatly.

Business entertaining tends to be formal and takes place in hotels and restaurants. The seating arrangement is likely to be determined by seniority, so wait to be shown where to sit.

Business Card Etiquette

Always bring sufficient business cards. Business cards are always exchanged formally, often standing up, when meeting for the first time.

When exchanging, try to offer your card with both hands, or just the right hand. When accepting, use two hands as this shows deference.

The card is seen to represent the individual, so should be treated with respect. Do not play with the card or stuff it in your pocket. Do not write on it in the other person’s presence. If you are meeting more than one person you can lay their cards out neatly in front of you.

Communication

Problems sometimes arise as to whether to bow or shake hands when first meeting. As a Westerner you are not expected to bow. When meeting someone for the first time, Japanese people tend to stand at a respectful distance.

Use less eye contact than you would normally.

Personal posture is important. Do not slump; maintain a fairly formal style.

When speaking in English, be clear and concise. Speak more slowly than usual, keep sentence structures simple and try to avoid double negatives and colloquialisms. Be prepared to repeat what you have said in a different way to ensure you have been understood.

Do not take nods or repeated “yes” (“hai” in Japanese) to mean agreement. This merely indicates that they are hearing and noting what you are saying, not necessarily agreeing with it. Direct negative expressions such as “No” are rarely used. For a Japanese to say something is “difficult” is tantamount to a negative reply.

Silence is considered a virtue. If things go quiet during a meeting then do not panic. Silence gives the Japanese time to collect their thoughts.