Kobe Opportunities for EU-Japan Research Collaboration

Kobe University, RIKEN, and European Institutes

Tuesday 5th July 2022
L42 Business Center

SPEAKERS' BIOGRAPHIES
AND ABSTRACTS

Session 1: ***Kobe as a leading base for computational sciences*** 09:00-10:30

Speaker **Makoto Tsubokura**, Kobe University and RIKEN (Japan)
Mario Rüttgers, Jülich Supercomputing Centre (Germany)
Alfonso Valencia, Barcelona Supercomputing Center (BSC) (Spain)

Coffee break 10:30-11:00

Session 2: ***Place-based innovation through international cooperation*** 11:00-12:30

Speaker **Satoru Oishi**, Kobe University and RIKEN (Japan)
Elpida Kolokytha, Aristotle University, Thessaloniki (Greece)
Audrey Gailler, Commissariat à l'énergie atomique (CEA)-DAM/DIF (France)

Networking lunch 12:30-13:30

Digital Transformation of Droplet/Aerosol Infection Risk Assessment and Evaluation of Countermeasures Realized on the Supercomputer "Fugaku"

Makoto Tsubokura

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Virus droplet infection caused by sneezing, coughing, or talking is strongly influenced by the flow, temperature and humidity of the air around an infected person and potential victims. Especially in the case of COVID-19, possibility of aerosol infection by atomized droplets is suggested, in addition to the usual direct droplet infection. Because smaller aerosol particles drift in the air for a longer time, it is imperative for the precise infection risk assessment to predict their scattering route and to estimate how surrounding airflow affects the infection. This is also the case when proposing countermeasures to reduce the infection risk. The fastest supercomputer in 2020, "Fugaku", has not only achieved digital transformation of epidemiology in allowing end-to-end, detailed quantitative modeling of COVID-19 transmissions for the first time, but also transformed the behavior of the entire Japanese public through its detailed analysis of transmission risks in multitudes of societal situations entailing heavy risks. A novel aerosol simulation methodology was synthesized out of a combination of a new computational fluid dynamics methods meeting industrial demands, "CUBE", which not only allowed the simulations to scale massively with high resolution required for micrometer virus-containing aerosol particles, but also extremely rapid time-to-solution due to its ability to generate the digital twins representing multitudes of societal situations in minutes not week, attaining true overall application high performance; such simulations have been running for the past 2 years on "Fugaku", cumulatively consuming top supercomputer-class resources and the result communicated by the media as well as becoming official public policies. In this talk, the details of the digital transformation of virus droplet/aerosol infection risk assessment and countermeasure proposal realized by the collaboration of "Fugaku" and "CUBE" will be introduced.

Makoto Tsubokura has been the professor of computational fluid dynamics at the Graduate School of System Informatics, Kobe University since 2015, and the leader of Complex Unified Simulation Research Team at the Center of Computational Science, RIKEN since 2012. After earning a PhD from the University of Tokyo in 1997, he first became a lecturer at the Tokyo Institute of Technology in 1999, then associate professor at the University of Electro-Communications in 2003, then at Hokkaido University in 2007, and then obtaining current positions. He specializes in research and development of mathematical modeling and simulation algorithms for thermal fluids in turbulent state, and their expansion to massively parallel environment on high-end supercomputers. He is a fellow of the Japan Society of Mechanical Engineers, the Japan Society of Fluid Mechanics, and Society of Automotive Engineers of Japan. He has been a member of the Engineering Academy of Japan since 2020

Combining Flow Simulations and Machine Learning Techniques for Improved Diagnostics and Treatments in Rhinology

Mario Rüttgers

Institute of Aerodynamics and Chair of Fluid Mechanics, RWTH Aachen University,

Jülich Supercomputing Centre, Forschungszentrum Jülich, m.ruettgers[@]fz-juelich.de

The integration of numerical flow simulations into daily clinical practice represents a key aspect for the improvement of diagnostics and treatments in rhinology. Such an integration is, however, only feasible if the involved numerical methods provide accurate results, are fast, and fully automated. This presentation describes how highly-resolved and parallelized lattice-Boltzmann simulations are combined with machine-learning-based techniques to automatize workflows for analyzing respiratory flows. Two types of applications are presented. The first application demonstrates how the complete process from medical imaging to the visualization of simulation results can be automatized[1]. An automated pipeline is presented that has already been used for multiple studies that require many nasal respiration simulations[2,3]. This pipeline circumvents the otherwise highly time-consuming semi-manual extraction of the geometry, which is obviously impractical for clinical use. The second application is a virtual surgery that helps surgeons in their decision-making process. Three different approaches for virtual surgeries are presented and evaluated, i.e., (i) an approach based on 3D-prints, (ii) one that computes fluid mechanical properties for all states between pre- and post-surgical geometries[4], and (iii) a reinforcement-learning-based approach that optimizes a shape with respect to fluid mechanical parameters[5].

References:

[1] M. Rüttgers, M. Waldmann, W. Schröder, and A. Lintermann, "A machine-learning-based method for automatizing lattice-boltzmann simulations of respiratory flows," Applied Intelligence, 2022.

[2] H. Aljawad, M. Rüttgers, A. Lintermann, W. Schröder, and K. C. Lee, "Effects of the nasal cavity complexity on the pharyngeal airway fluid mechanics: A computational study," Journal of Digital Imaging, vol. 34, pp. 1120 – 1133, 2021.

[3] H. Aljawad, M. Rüttgers, W. Schröder, A. Lintermann, and K. C. Lee, "Long-term evaluation of the upper airway following mandibular setback surgery in class iii patients using computational fluid dynamics," submitted to American Journal of Orthodontics & Dentofacial Orthopedics, 2022.

[4] M. Waldmann, M. Rüttgers, A. Lintermann, and W. Schröder, "Virtual surgeries of nasal cavities using a coupled lattice-boltzmann-levelset approach," Journal of Engineering and Science in Medical Diagnostics and Therapy, vol. 5, no. 3, 2022.

[5] M. Rüttgers, M. Waldmann, W. Schröder, and A. Lintermann, "Machine-learning-based control of perturbed and heated channel flows," in High Performance Computing: ISC High Performance Digital 2021 International Workshops, Frankfurt Am Main, Germany, June 24 -July 2, 2021.

Mario Rüttgers received the B.S. degree in mechanical engineering from RWTH Aachen University in 2015. He attended full-time Korean language courses at Chonnam National University (CNU) in Gwangju, South Korea, from 2015 to 2017 and received the M.S. degree in mechanical engineering from Pohang University of Science and Technology (POSTECH) in 2019. Since 2019, he has been working as a researcher at the Institute of Aerodynamics and Chair of Fluid Mechanics at RWTH Aachen University, and at the Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich. At the same time, he is a PhD student at RWTH Aachen University and associated with the Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE). His research focuses on combining CFD and machine learning.

High performance computing in biomedicine. The BSC perspective.

Alfonso Valencia
ICREA Research Professor
Life Sciences Dept. Director, Barcelona Supercomputing Center (BSC)
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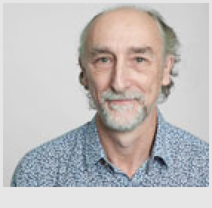
The new generation of High Performance Computing systems – the exascale generation- open interesting challenges and possibilities for the applications in biomedicine. At the technical level, the general challenges include the heterogenous nature of the new systems and processors, as well as the complexity of the operations with large quantities of personal and confidential data.
Beyond the data access and handling issues, the new infrastructures are essential for three of the application areas in which BSC is interested:

- Natural Language Processing for the extraction of information from medical documents. In our, experience the development of BERT-like approaches in specific areas, e.g., a COVID-19 requires substantial investment in terms of corpus collection, expert labelling, computing time for training and depuration.
- Artificial Intelligence and Machine Learning applications, for the prediction of the consequences of mutations, disease classification, and the prediction of disease trajectories based on the combination of medical and molecular data.
- The simulation of biomedical systems from the organs to the cell level- the Human Digital Twin. The European HPC/Exascale Centre of Excellence for Personalised Medicine (PerMedCoE https://www.hpccoe.eu/permedcoe/) coordinated by BSC, aims to set the basis for the simulations of complex systems, e.g., tumours or organoids, embedding intracellular level (metabolic, signalling and regulatory networks) into inter-cellular environments, i.e., agent based simulations accounting for cell-cell and cell-environment interactions.

These and other areas of Biomedicine posse significant challenges that will be better addressed by collaboration, like for example the possible collaboration with R-CCS at RIKEN at Kobe city/region.



Prof. Alfonso Valencia is ICREA Research Professor and Director of the Life Sciences Department at the Barcelona Supercomputing Centre (BSC), Director of the Spanish National Bioinformatics Institute (INB) and head of the Spanish Node of the European Bioinformatics Infrastructure ELIXIR. He is a member of the European Molecular Biology Organisation (EMBO), and former President of the International Society for Computational Biology (ISCB). He has served in numerous Scientific Advisory Boards, including the Innovative Medicines Initiative (IMI), of which he is currently Vice Chair, EMBL, the Swiss Institute for Bioinformatics, among others. He is Co-Executive Editor of journal Bioinformatics and he has published more than 450 articles with an h-index of 97 (Scopus profile).

Breaking walls to make a safe and secured society based on simulation

Satoru Oishi

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Many natural disasters and anthropogenic hazards surround us. For example, Japan has earthquakes, tsunamis, volcanic eruptions, typhoons, long-lasting rainfalls, and mudslides. Some parts of the world may have frequent and more devastating fires when it becomes dryer, or some parts may have an incredible amount of rain in the future. The recent and upcoming climate will change the types of natural hazards. Our society should adapt to the change to decrease damage.

In order to adapt to the change or in order to prepare for less frequent hazards, we use physics-based simulation. Physics-based simulation gives detailed information about damage when something happens, even though it is difficult to predict when it will happen. Moreover, physics-based simulation counts the relationship among stakeholders having the same driving force, for example, water resource shortage and frequent fire, sea-level increase and increased risk of high tide.

However, making comprehensive physics-based simulation is not easy; even one-way information paths like weather information from meteorological simulation to high tide simulation because information formats between them are not uniform. Technology progression and legacy constructions exist at the same time. It prevents easier data exchange. We developed a "Data Processing Platform (DPP)" to transform data with less effort for developing software. The DPP will automatically connect user-defined libraries and third-party libraries to transform data from one source of information to a format required by the other software.

We archived to make a three-dimensional (3D) model of concrete bridges from their two-dimensional (2D) CAD data by using DPP. Moreover, DPP has created input data for FEM of the bridges from the same 2D CAD by adding a library. The library has a function to transform the format and create files for input files of FEM simulation. It decreased the time to make another application that reads 2D CAD, and extracts required information. The talk will explain the basic concept, case studies, and benefits.

Satoru Oishi obtained a Dr. of Engineering from Kyoto University in 1998. He was a research associate of Disaster Prevention Research Institute, Kyoto University (1993-2000), conducting the fundamental mechanism of cumulus cloud generation and development by using numerical simulation of the cloud-resolving model. He was an associate professor at the University of Yamanashi (2000-2009), conducting river engineering and Sabo engineering. He also conducted many field studies abroad. He has been a professor at Kobe University (2009-present). He mainly focuses on the application of remote sensing techniques to disaster prevention. As a team leader of RIKEN R-CCS (2017-present), he is working to promote high-performance computing simulation of disasters, including earthquakes, tsunamis, and weather-related disasters.

Integrated Approach to Urban Water Management and Safe Cities

Elpida Kolokytha

Department of Civil Engineering, Division of Hydraulics, Aristotle University of Thessalo niki

In our complex, interdependent, and rapidly changing world which faces multiple crises, new strategies and new paradigms are needed to deal with both the global environmental changes due to resources limited supply factors (water, land, air) and also the anthropogenic changes of overpopulation, mega-urbanization and severe climate change. More than half of the world’s population live in cities. Water is central in both sustainable and safe cities. In this sense, a new understanding of “security” in an interrelated context of social-economic-political-environmental conditions, closely associated to the emerging new paradigm of green development is gaining increasing attention. Integrated urban water management with emphasis to resiliency, efficiency and water quality underline our approach. Water-related disaster risks, water scarcity, water availability, flood risk are of major importance for resiliency. Ageing infrastructure, leakages, metering, water charges, water reuse form critical components of efficiency whereas water quality is related to health, sanitation, drinking water and pollution, all in all are part of the integrated water management and planning. Cities need to start investing in adaptation measures based on long-term visions and strategies, and in sharing best practices.

Safe cities require a strategy that combines "envisioning", "empowerment", "enactment". To achieve these, international cooperation, technology transfer and synergies are important. Moreover, it requires “a journey of transformation” based on the re-definition of the city’s infrastructure and services. Water acts as the connector incorporating the nexus between energy, food, waste, transport and other parts of the built environment. New adaptive governance is required to new conditions, residents should be actively engaged to decision making, technology and “big data” work as a “smart” tool in order the cities to become safe, sustainable and resilient living environments.

Elpida Kolokytha obtained a Ph.D. at Aristotle University of Thessaloniki (AUTh) in 1999 and she is Professor in Water Resources Management and Engineering in AUTh. Good communication skills gained as teacher, Director of water Center, scientific project responsible, expert, EU evaluator grants. She has served as Head of Div. of Hydraulics & Environmental Engineering, Dept. of Civil Engineering, AUTh (2019-2021), Head of AUTh Water Center (2011-2016), Director of AUTH UNESCO C2C Center for Integrated Water Resources Management (2016 -today), Chair of IAHR WRM TC Group (2019-today), General Secretary of the Administrative Board of the Science Center and Technology Museum “NOESIS” (2010-2014) https://www.noesis.edu.gr/. Coordinator of (6) IMOU in AUTh with Universities in Cyprus, Italy, Japan, Israel, Kazakhstan, USA.

The challenge of real-time forecasting of coastal tsunami impact within the French tsunami warning center (CENALT)

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For tsunami warning centers, obtaining real-time coastal inundation prediction maps in near-field or regional context appears as a major challenge, increasingly discussed within the European and international community. Currently, tsunami warning systems are mainly focused on the first parameters of the earthquake and the tsunami models provided only give information at the scale of the corresponding hazard basin. No values of water heights at the coast are calculated, because unlike in the deep ocean, the full simulation of tsunami propagation at the coast requires a nonlinear model with fine resolution bathymetry/topography to cope with the complex coastal morphology. Therefore, it imposes, despite a parallelization of the codes and the power of the computers used, a considerable computation time (> 45 min) which may not be suitable for real-time tsunami forecasting in the near field or regional. In this context, the rapid determination of water heights at the coast, and even the estimation of run-ups, are among the objectives of the CENALT to improve the level of expertise and information that can be provided his correspondents.

To overcome the problem of the race against time for the determination of the water level at the coast, warning centers are developing tools for rapid prediction of the amplitude of coastal tsunamis, calculated from empirical laws. This type of linear approximation provides tsunami heights along the coastline very quickly, with error bars on the calculated values of a factor of 2 at best. Such approaches are suitable for the near-field context, but flooding estimation is lacking.

Applications of deep learning methods for geosciences are newly being adapted in an innovative way for near-field tsunami forecasting, and would allow adding complexity to the predicted models (run-up, local effects, currents) compared to amplification law approaches that do not capture these three aspects. The objective is to develop a tool to quickly transform a deep ocean tsunami simulation result into a coastal inundation model and associated velocity field. Several learning methods (MLP, CNN) are being explored using dedicated libraries and toolboxes, with first encouraging results.

Audrey Gailler obtained a PhD in marine geophysics at the University of Nice in 2005. She has specialized in wide-angle seismic data acquisition, processing and numerical modeling, and held postdoc positions at IPGP (2006), University of Birmingham (2007) and Ifremer (2008-09). Since 2010, she is geophysicist at CEA and tsunami expert since 2021. Her expertise at CEA belongs to tsunami simulation with respect to Early Warning and Hazard Assessment, and to the modeling of historical tsunami triggered by earthquakes and/or landslides. She takes an active part in the implementation of simulation systems for tsunami forecasting within the French tsunami warning center (CENALT). She collaborates in several European and international projects dedicated to tsunami research, and co-chairs the Working Group I of the ICG/NEAMTWS since 2018.