



Franco–Scottish Science Seminar

Linear Algebra and Parallel Computing at the Heart of Scientific Computing

Workshop Programme

Wednesday 21 September 2016
at

The Royal Society of Edinburgh
22–26 George Street
EH2 2PQ

Participation in this seminar is by invitation only. To register your interest to attend please contact Rita Velaviciute, email: rvelaviciute@royalsoced.org.uk, tel: 0131 240 2782

Introduction

The Royal Society of Edinburgh (RSE) and the French Embassy in London are collaborating in a programme of science events designed to explore and publicly present areas of science where both Scotland and France have a powerful presence. These events are intended to stimulate Franco–Scottish collaboration in science, present new scientific ideas and their social and commercial implications to the public and increase awareness of French and Scottish science in each other's country. This year, the seminar, to be held at the Royal Society of Edinburgh, will focus on the topic of 'Linear Algebra and Parallel Computing at the heart of Scientific Computing'.

Most numerical computations and simulations have at their core the solution of systems of linear equations. As the computations increase in scale and the simulations become more detailed, the size of such system increases. This seminar is focused on recent research into improving the solution of such large systems and some novel applications which can now be addressed. Much of this research has involved direct collaboraton between Scotland and France.

Practitioners from all areas of science and engineering will be familiar with the need for the efficient solution of large linear systems and the seminar should appeal to researchers in numerical methods and scientists and engineers involved in numerical simulation related to innovation in aerospace, semiconductor design, the chemical and oil industry, transport, energy, telecommunications, medical imaging and diagnosis, non-destructive testing and financial mathematics.

The talks will include both theory and applications covering a diverse range of topics, including partitioning, combinatorial algorithms, randomization and an award - winning innovation in medical diagnosis.

Participation has been by invitation and limited to 40 people, in order to encourage an exchange of views and experiences, with everyone able to join the discussion.

The seminar day is divided into morning and afternoon sessions. In each, there will be presentations by academics from Scotland and from France.

The seminar programme is enclosed.

The seminar will be held at:

The Royal Society of Edinburgh
22–26 George Street
Edinburgh
EH2 2PQ

This event is supported by the Royal Society of Edinburgh and the French Embassy in London.

Workshop Programme

Wednesday 21 September 2016

- 09:00** **Registration**
- 09:30** **Welcome and Introductions**
- RSE representative**
 Dr William Duncan
 Chief Executive, The Royal Society of Edinburgh
- French Embassy representative**
 Dr Ludovic Drouin
 Science Attaché, French Embassy
- 09:40** **Introduction to Morning Session**
 Chairperson
 Professor Iain Duff FRSE
 Visiting Professor of Mathematics, University of Strathclyde
- 09:45** **A Theory for the P.L. Lions Algorithm in the Framework of Optimized Schwarz Methods**
 Dr Frédéric Nataf
 CNRS Senior Scientist, J.L. Lions Laboratory, Pierre et Marie Curie University
- 10:15** **Discussion Session**
- 10:35** **Uncovering Hidden Block Structure**
 Dr Philip Knight
 Lecturer in Mathematics, University of Strathclyde
- 11:05** **Discussion Session**
- 11:25** **Tea/Coffee break**
- 11:40** **Identifying Blocks in Matrices with Information from both Numerical Values and Sparsity Pattern**
 Dr Daniel Ruiz
 Lecturer in Applied Mathematics and Computer Science, ENSEEIHT
- 12:10** **Discussion Session**
- 12:30** **Lunch**

- 13:30** **Introduction to Afternoon Session**
Chairperson
Professor Iain Duff
Visiting Professor of Mathematics, University of Strathclyde
- 13:35** **Microwave Tomographic Imaging of Cerebrovascular Accidents
by Using High-Performance Computing**
Dr Victorita Dolean
Reader, Department of Mathematics and Statistics, University of Strathclyde
- 15:05** **Discussion Session**
- 15:25** **Tea/Coffee break**
- 15:40** **Bipartite Matchings in Solving Sparse Linear Systems**
Dr Bora Uçar
CNRS Scientist, ENS - Lyon
- 16:00** **Discussion Session**
- 16:20** **Randomized Iterative Methods for Solving Linear Systems**
Professor Peter Richtárik
Associate Professor, School of Mathematics, University of Edinburgh
- 16:50** **Discussion Session**
- 17:10** **Concluding Remarks**
- 17:30** **Close**

Principal Organiser

Professor Iain Duff FRSE



Iain S. Duff is an STFC Senior Fellow in the Scientific Computing Department at the STFC Rutherford Appleton Laboratory in Oxfordshire, England. He is also the Scientific Advisor for the Parallel Algorithms Group at CERFACS in Toulouse and is a Visiting Professor of Mathematics at the University of Strathclyde.

After completing his D Phil at Oxford, he was a Harkness Fellow in the United States, visiting Stony Brook and Stanford. He then spent two years lecturing at the University of Newcastle upon Tyne, before joining the Harwell Laboratory, where he became Group Leader of Numerical Analysis in 1986.

In 1990, the Group moved to the Atlas Centre at the Rutherford Appleton Laboratory. He has had several extended visits to Argonne National Laboratory, the Australian National University, the University of Colorado at Boulder, DTU in Lyngby Denmark, the University of Newcastle in NSW, Stanford University, and the University of Umeå.

He is a life Fellow of the Institute of Mathematics and its Applications and a member of LMS (UK), SIAM (USA), and SMAI (France). He is an IMA representative on the ICIAM Board and is chairman of the IMA Journals Board of Management. He was Chairman of the SIAM Board of Trustees for seven years until December 2011 and was on the Applied Mathematics panel for RAE 2008. He was elected as a Fellow of the Royal Society of Edinburgh in 2006 and was selected as a SIAM Fellow in 2010.

His current research interests include numerical linear algebra, sparse matrices, parallel computing, scientific computation and mathematical software. He has written several books and over 200 papers in these areas, more than half of which have appeared in refereed journals. He is recognized by ISI Thomson as a Highly Cited Researcher.

Speakers

Dr Victorita Dolean

Reader, Mathematics and
Statistics, University of Strathclyde



Biography Victorita Dolean is currently a Reader in the Department of Mathematics and Statistics, University of Strathclyde, Glasgow, United Kingdom. She has been a research assistant at the CMAP (Center of Applied Mathematics) at the École Polytechnique in Paris, assistant professor at the University of Evry and at the University of Nice, and visiting professor at the University of Geneva. Her research has been oriented toward practical and modern applications of scientific computing by developing interactions between academic and industrial partners through interdisciplinary projects and, more precisely, the design of numerical models applied to electromagnetic wave propagation problems. She has co-authored around 50 research papers and conference proceedings and has been part of the team that obtained the Bull-Joseph Fourier Prize 2015, awarded yearly in France for important algorithmic advances in high-performance computing.

Talk Title *Microwave Tomographic Imaging of Cerebrovascular Accidents by Using High-Performance Computing*

Abstract The motivation of this work is the detection of cerebrovascular accidents by microwave tomographic imaging. This requires the solution of an inverse problem relying on a minimization algorithm (for example, gradient-based), where successive iterations consist in repeated solutions of a direct problem. The reconstruction algorithm is extremely computationally intensive and makes use of efficient parallel algorithms and high-performance computing. The feasibility of this type of imaging is conditioned on one hand by an accurate reconstruction of the material properties of the propagation medium and on the other hand by a considerable reduction in simulation time. Fulfilling these two requirements will enable a very rapid and accurate diagnosis. From the mathematical and numerical point of view, this means solving Maxwell's equations in time-harmonic regime by appropriate domain decomposition methods, which are naturally adapted to parallel architectures.

Speakers

Dr Philip Knight

Lecturer, Mathematics and
Statistics, University of Strathclyde



Biography Philip Knight is a Lecturer in Mathematics at the University of Strathclyde, UK. He obtained his PhD in Mathematics from the University of Manchester in 1993 and has spent most of his career carrying out research into matrix algebra. His interest in applications drew him inexorably towards network theory, and his research interests now centre on the algebraic structure of networks, and in particular the use of tools from linear algebra to reveal relevant structure in real world networks.

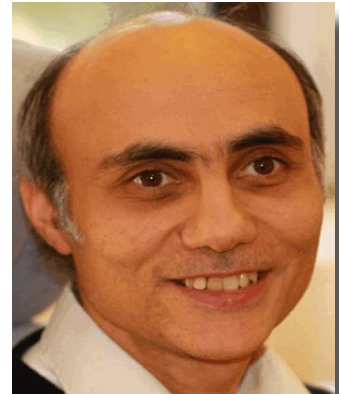
Talk Title *Uncovering Hidden Block Structure*

Abstract We can apply a two-sided diagonal scaling to a nonnegative matrix to render it into doubly stochastic form if, and only if, the matrix is fully indecomposable. The scaling often reveals key structural properties of the matrix as the effects of element size and connectivity are balanced. Exploiting key spectral properties of doubly stochastic matrices, we will show how to use the scaling to reveal hidden block structure in matrices without any prior knowledge.

Speakers

Dr Frédéric Nataf

CNRS Senior Scientist; J.L. Lions
Laboratory, Pierre et Marie Curie
University



Biography Frédéric Nataf is senior scientist at CNRS in laboratory J.L. Lions at university Pierre and Marie Curie, France. His field of expertise is in high performance scientific computing (domain decomposition methods/approximate factorizations), absorbing/PML boundary conditions and inverse problems. He has co-authored nearly one hundred papers and has given several invited plenary talks on these subjects. He developed the theory of optimized Schwarz methods and, very recently, the GENE0 coarse space. This last method enables the solving of very large highly heterogeneous problems on large-scale computers.

Talk Title *A Theory for the P.L. Lions Algorithm in the Framework of Optimized Schwarz Methods*

Abstract The Schwarz algorithm is the basis of many parallel algorithms used in modern computers. Its mathematical theory is well established thanks, to the works of the domain decomposition method community. We developed recently such a theory for the more recent and more efficient P.L. Lions algorithm. We also present numerical results on saddle point problems.

Speakers

Professor Peter Richtárik

Associate Professor, School of
Mathematics, University of Edinburgh



Biography Peter Richtárik is a Reader in the School of Mathematics, University of Edinburgh. He obtained his PhD from Cornell University in 2007, after which he spent two years as a postdoctoral fellow at Université Catholique de Louvain. Recently, he has been a visiting researcher at the Simons Institute at UC Berkeley. He is a Faculty Fellow at the Alan Turing Institute – the UK national research centre for data science. Prof Richtárik has made fundamental contributions to “big data optimization”, which is an emerging field at the intersection of mathematical optimization, convex analysis, probability theory, computer science, machine learning and high-performance computing. He is the recipient of an EPSRC Fellowship in the Mathematical Sciences, which allows him to focus on further developing this line of work.

Talk Title *Randomized Iterative Methods for Solving Linear Systems*

Abstract We develop a novel, fundamental and surprisingly simple randomized iterative method for solving consistent linear systems. Our method has six different but equivalent interpretations: sketch-and-project, constrain-and-approximate, random intersect, random linear solve, random update and random fixed point; and admits a fundamental dual interpretation. By varying its two parameters – a positive definite matrix (defining geometry), and a random matrix (sampled in an independently and identically distributed fashion in each iteration) – we recover a comprehensive array of well-known algorithms as special cases, including the randomized Kaczmarz method, the randomized Newton method, the randomized coordinate descent method and the random Gaussian pursuit. We naturally also obtain variants of all these methods using blocks and importance sampling. However, our method allows for a much wider selection of these two parameters, which leads to a number of new specific methods. We prove exponential convergence of the expected norm of the error in a single theorem, from which existing complexity results for known variants can be obtained. However, we also give an exact formula for the evolution of the expected iterates, which allows us to give lower bounds on the convergence rate.

Speakers

Dr Daniel Ruiz

Lecturer, Applied Mathematics
and Computer Science, ENSEEIHT



Biography Daniel Ruiz is “Maître de Conférences” (Lecturer) at the Applied Mathematics and Computer Science Department of the School of Engineering ENSEEIHT in Toulouse, France. He did his PhD from 1987 to 1991 at CERFACS (European Center for Research and Advanced Training in Scientific Computation) in France, under the supervision of Iain Duff, Mario Arioli and Joseph Noailles. Since 1992, he has been employed by the Polytechnical National Institute (INPT), member of the University of Toulouse, as Lecturer at ENSEEIHT, and also belongs to the Computer Science Research Institute of Toulouse (IRIT-CNRS), as a researcher in the Parallel Algorithms and Optimisation research team. His research interests are in linear algebra, optimisation and machine learning; including, in particular, sparse hybrid solvers, Krylov methods, preprocessing and scaling of sparse matrices, numerical simulation, parallel computing and spectral clustering.

Talk Title *Identifying Blocks in Matrices with Information from both Numerical Values and Sparsity Pattern*

Abstract Considering any square fully indecomposable matrix A , we can apply a two-sided diagonal scaling to $|A|$ to render it into doubly stochastic form. The Perron-Frobenius theorem is a key tool to exploit and we aim to use spectral properties of doubly stochastic matrices to reveal hidden block structure in matrices. We also combine this with classical graph analysis techniques to design partitioning algorithms for large sparse matrices, based on both numerical values and pattern information.

Speakers

Dr Bora Uçar

CNRS Scientist, ENS - LYON



Biography Bora Uçar has been a CNRS research scientist at LIP, ENS-LYON since 2009. He received his PhD degrees (2005) in Computer Engineering from Bilkent University, Ankara, Turkey. Afterwards he worked as a post-doc research associate at Emory University, Atlanta, USA and at CERFACS, Toulouse, France. His research interests are combinatorial scientific computing and high performance computing.

Talk Title *Bipartite Matchings in Solving Sparse Linear Systems*

Abstract This talk will cover the use of weighted matching algorithms for bipartite graphs in solving sparse linear systems with direct methods and also with iterative methods. On the direct methods side we will see how such matchings can be used for effective pivoting and reduced space and time requirements. On the iterative methods side, we will see how such matchings can be used to construct effective preconditioners.

Additional Information

About the Royal Society of Edinburgh (RSE)

We are an educational charity, registered in Scotland, operating on a wholly independent and non-party-political basis and providing public benefit throughout Scotland. We were established in 1783 and since then have drawn upon the considerable strengths and varied expertise of our Fellows, of which there are currently more than 1600, who are based in Scotland, the rest of the UK and beyond.

Unlike similar organisations in the rest of the UK, our Fellowship includes people from a wide range of disciplines - science & technology, arts, humanities, social science, business and public service. This breadth of expertise makes us unique in the UK. The time that our Fellows spend in supporting and enabling the delivery of our activities is an exceptional free resource, the annual public value of which is in excess of £0.7 million.

Our current strategic aspirations, objectives, and the impact we aim to make, are set out in our Strategic Framework: <https://www.royalsoced.org.uk/cms/files/aboutus/framework.pdf> and on the RSE web site: <https://www.royalsoced.org.uk/>

About the French Embassy in London

The Science and Technology department has three main missions, detailed as follows:

1. It keeps abreast of UK national and regional policies, public and institutional strategies, as well as scientific and technological activities taking place in the research, development and innovation sectors. It produces notes and documents intended for the French stakeholders concerned;
2. It promotes bilateral scientific cooperation and collaborations within the context of the European Research Area, via specific calls for proposals, organisation of workshops and symposia in priority topics for both our countries, and long-term agreements in strategic areas;
3. It promotes French scientific and technological achievements via the co-organisation or the partnerships with British research institutions of seminars and events targeting non-specialist audiences.

To find out more, please visit www.ambascience.co.uk or contact the team at: info@ambascience.co.uk

Notes

Notes



THE ROYAL
SOCIETY
OF EDINBURGH

The Royal Society of Edinburgh
22–26 George Street
EDINBURGH
EH2 2PQ

T. 0131 240 5000
F. 01312405024
E. info@royalsoced.org.uk
www.royalsoced.org.uk

The Royal Society of Edinburgh, Scotland's National Academy, is Scottish Charity No. SC000470