Institution: University of Greenwich

Unit of Assessment: (UoA 10) - Mathematical Sciences

Title of case study: Decomposition, defect correction, and related numerical methods

1. Summary of the impact

Spatial decomposition methods have been extended to apply to spatial, scale, and temporal domains as a result of work at the Numerical and Applied Mathematics Research Unit (NAMU) at the University of Greenwich. This work has led to a numerical framework for tackling many nonlinear problems which have been key bottlenecks in software design and scientific computing. The work has benefitted the welding industry in the UK because these concepts are now embedded, with parallel computing, in the industry's modern welding design process software.

2. Underpinning research

Spatially motivated decomposition (1997-2011)

Key outcomes from the research were formulation and solution of the problem using a defect correction equation which produced an iterative sequence of corrections. The concept of coupling was encapsulated in a simple formulation, thereby giving convergence of the approximate solutions sequence to the defect correction equation. This structure forms the defect correction framework, which we initially applied to homogeneous mathematical problems defined in different subdomains. The importance of this framework is the extension to multi-mathematical models and multi-scale problems, described later. The work was rated as internationally leading by peers, and led to a TSB project [3a] where Greenwich is a partner in a consortium led by TWI Ltd which has demonstrated the convergence result of the method when applied to industrial problems [3.1].

Key UoG personnel involved: M. Cross, Director of Centre for Numerical Modelling and Process Analysis, left to Swansea in 2004; C.-H. Lai, Senior Lecturer and later Professor of Numerical Mathematics; K. Pericleous, Professor of CFD; A.L. Siahaan, researcher, joined in 2006 and left to Cambridge in 2011.

Projects:

1) EPSRC GR/50600 (1997) – Domain Decomposition Methods for Partial Differential Equations;
2) British Council UK-Dutch Joint Scientific Research Grant JRP433-AMS/884/4 (1997) – Coupling mathematical models.

Scale motivated decomposition (1999-2012)

The defect correction concept was used in the derivation of multi-mathematical models with disparate scales for application to aeroacoustic problems. An EPSRC grant (GR/M60804) entitled 'Computational Aeroacoustics' was obtained for the work. At the continuum level the formalism follows perturbation methods. At the discretised level the defect correction method [3.2] offers a robust way of handling high order schemes, large eddy simulations, and turbulence sub-grid modelling using existing CFD software. A suitably constructed residual defect correction term is obtained from existing CFD software output [3.3]. Further theory appeared in the PhD thesis by L. Lai in June 2013.

Key UoG personnel involved: G.S. Djambazov, researcher and later senior research fellow; C.-H. Lai, Senior Lecturer and later Professor of Numerical Mathematics; L. Lai, researcher, (2004 – 2007); Z.-K. Wang, researcher, (2001 – 2004).

Projects:

1) EPSRC GR/M60804 (1999) – Computational Aeroacoustics;
2) LMS Workshop Grant EGR:hmc:00-0115010L0103 (2000) – Domain Decomposition Methods for Fluid Mechanics;
3) British Council Alliance Franco-British Partnership Programme PN04.043 (2002) – Computational Acoustics;
4) LMS Scheme 8 Grant 81106 (2012) – Workshop on Applied and Numerical Methods: Multiscale Problems.

Temporal motivated decomposition (2001-2012)

Decomposition of the temporal axis initially aimed to achieve parallelisation in the time domain. Members of NAMU began to consider this problem in 2001 with work submitted to RAE2008. Extension of the work based on various transformation methods led to decoupled parametric equations that may be solved concurrently with low complexity coupling at the post-computation

level. Parallelisation in time is achieved by concurrent computation of the parametric equations. Two MSc dissertations and two book chapters [3.4], demonstrate the method. Peers rated the work as of internationally leading quality. This led to a collaborative project in computational finance through FR7 STRIKE [3b] where Greenwich is responsible for the development of distributive multi-scale solution techniques for nonlinear financial problems in commodity markets.

Key UoG personnel involved: N. Kokulan, researcher, joined in 2010; C.-H. Lai, Senior Lecturer and later Professor of Numerical Mathematics; A.K. Parrott, Professor of Computational Science; S. Rout, researcher, (2001 - 2005).

3. References to the research (REF1 submitted staff in **bold**, **REF2 Output)

3.1 Siahaan, A., **Lai, C.-H., & Pericleous, K. (2011). Local convergence of an adaptive scalar method and its application in a nonoverlapping domain decomposition scheme. *Journal of Computational and Applied Mathematics*, *235*(17), 5203–5212. http://dx.doi.org/10.1016/j.cam.2011.05.010 (Impact factor: 0.989)

3.2 Wang, Z. K., Djambazov, G. S., **Lai, C. H., & Pericleous, K. A. (2008). Numerical investigation of a source extraction technique based on an acoustic correction method. *Computers & Mathematics with Applications*, *55*(3), 441–458. http://dx.doi.org/10.1016/j.camwa.2004.08.017 (Impact factor: 2.069)

3.3 X. Jiang, & **Lai, C.-H**. (2009). *Numerical Techniques for Direct and Large-Eddy Simulation*. Boca Raton: CRC Press/Taylor & Francis Group. ISBN 978-1-4200-7578-6 (print), 978-1-4200-7579-3 (ebook). http://dx.doi.org/10.1201/9781420075793 (17 Citations: Google Scholar.)

3.4 **Lai, C.-H**. (2008) Numerical solutions of certain nonlinear models in European options on a distributed computing environment. In M. Ehrhardt (Ed.). *Nonlinear Models in Mathematical Finance: New Research Trends in Option Pricing* (pp. 305-320). New York: Nova Science Publishers, Inc. ISBN: 978-1-60456-931-5, (9 citations: Google Scholar)

Research Grants

3a C.-H. Lai. *OPTWELD – Real-time virtual prototyping tools for OPTimising WELDed products* (TSB/CRD/096 Q20688) http://www.optweld.org.uk/ . TSB, Technology Programme. 01/09/2008 – 31/08/2011; Value funded to Greenwich: £67,000.

R1. 3b C.-H. Lai. *Novel Methods in Computational Finance* (Ref 304617). FP7-People-2012-ITN. Jan-2013 – Dec-2016. €3,582,470 (UoG contribution £329,000). The ITN network STRIKE is led by University of Wuppertal, Germany.

4. Details of the impact

Welding industry benefits from new design process software

The work described above has been successfully applied in the welding industry through the OPTWELD project which ran through 2010. This project resulted in substantial collaboration work with local industry (the TWI Group and the ESI Group) on the implementation of distributed algorithms in the commercial software application 'Sysweld'. An MSc research dissertation, 'Distributed algorithms for heat transfer related problems' by S. Guo, documented the issues surrounding the work and has been widely disseminated in industry. The embedding of the scientific computing techniques, resulting from the research, in welding industry software has led to an easy approach to coupling of subdomains which has significantly enhanced the accuracy and applicability of the software. Research results were also applied to: inverse problems, image processing, pharmacokinetics, and stochastic optimisation and this clearly demonstrated the impact of the numerical frameworks developed in industrial mathematics.

Dissemination of findings in aero-acoustics and inverse problems

Work in the area of domain decomposition methods started with applications in aero-acoustics and inverse problems in 1996 with Djambazov, and later with Palansuriya, Wang, L. Lai, Siahaan, Tian, Kokulan. The most important recent publication disseminating important results in the concept of acoustic correction methods for the extraction of disparate scales can be found in [3.2]. In relation to this work, C. Lai and other former students explored the concept of a wider class of methods known as the defect correction method for multi-scale problems. C. Lai solicited a special issue, published in June 2008, entitled 'Mathematical and Computational Aspects of Multi-Scale Problems'

with the *Journal of Algorithms and Technology*, ISSN 1748-3018, while attending the World Congress on Computational Mechanics, Los Angeles, 2006. During an academic visit to China in July 2008, Lai gave an invited seminar entitled 'Some new results of the acoustic correction method for the extraction of sound signals' at Dalian University of Technology. C. Lai visited Prof. P. Lin and Dr D. Trucu, Dundee University, in order to exchange experiences in multi-scale methods and gave a talk entitled 'On the acoustic correction method for extracting sound signals' during March 2009. In May 2009 C. Lai was in discussion with Dr A. Rona, Leicester University, on a joint Marie Currie Network proposal to FR7 fund, and gave a talk there entitled 'On the acoustic correction method for extracting sound signals'. This was recently funded under FP7-People-2012-ITN AeroTraNet (Ref 317142) in which Greenwich has secured a share of £257,000 funding. Lai was also invited to give an invited talk at the 2nd Belgian Mathematical Society and London Mathematical Society Conference, Catholic University of Leuven, the Netherlands on the topic 'On high order schemes and defect correction methods'. The work was summarised and presented at 16th International Conference on Sound and Vibration, Krackow, July 2009, and at World Congress on Computational Mechanics 2010, July 2010, Sydney. Lai gave a talk to University of Essex in May 2011 entitled 'On high order schemes and defect correction methods in CFD software'. A joint Essex, Greenwich, and Hertfordshire Workshop on Applied and Numerical Methods: Multiscale Problems, June 2012, was funded through LMS Scheme 8 Grant 811062. The work in the acoustic correction method and high order schemes mentioned above led to significant contribution to the book listed in [3.3]. It is extremely exciting to see that this book is being used as one of the texts and references for numerical techniques for LES at Lancaster and Greenwich. The PhD student, L. Lai, recently completed his thesis in this area with a generalised framework using defect correction.

Coupling of black box engineering software

Building on the early research experience in domain decomposition methods before 2008, NAMU has been engaged in the TSB project described in [3a] on a domain decomposition method for the coupling of black box engineering software using the concept of the defect equation. Here the main contribution is to allow work at different locations and sites using different software being coupled to form a final piece of work. At the same time Siahaan has been working on the theory of the convergence of a quasi-Newton method showing that the coupling using the defect equation converges to the solution, though very slowly. This is an extremely encouraging theoretical result and Siahaan has also improved the method so that convergence is speeded up as demonstrated in his PhD thesis in June 2011. The theoretical work is summarised in [3.1].

Temporal and scale parallel algorithms

NAMU has a long history of developing **temporal and scale parallel algorithms**. In particular Lai and Parrott have been involved in such work before joining the university in 1989 and 1993 respectively. Previous work with an application in computational finance submitted in the last RAE was demonstrated by Lai and Parrott in the paper entitled 'A distributed algorithm for European options with nonlinear volatility', *Computers and Mathematics with Applications*, **49**, 885-894, 2005. This work helped to attract the funding described in R6 for ITN-STRIKE. Recent activities and work concentrated on induced parallel and distributive properties into mathematical models/formulations so that a nonlinear financial option problem which is intrinsically sequential may process parallel properties. Typical techniques used here are transformation methods summarised in two recent MSc dissertations at Greenwich:

1) N. Natkunam, Numerical analysis of the diffusion equation using Laplace transform, 2009.
2) M.T. Tarawneh, Theoretical performance analysis of parallel algorithms and applications to differential equations, 2009.

Lai visited the School of Mathematical Sciences, University of Liverpool, in May 2010 while on an external examination role, and presented the above work. He also took the opportunity of World Congress on Computational Mechanics 2010 to visit the Mathematics Department, University of Canberra, Australia, where he disseminated the above work in July 2010. Further research work generated two book chapters in books, one with applications to computational finance, as described in [3.4], and the other a general concept on induced parallel properties, as below:

C.-H. Lai. On transformation methods and the induced parallel properties for the temporal domain, in **Substructuring Techniques and Domain Decomposition Methods**, ed F. Magoules, ISBN: 1759-3158 (doi: 10.4203/csets.24.3), Saxe-Coburg Publications, Stirlingshire, UK, 45-70, 2010.

Lai was invited to be the external examiner for a PhD thesis on temporal parallelisation at the

University of Claude Bernard Lyon I in July 2011. Knowing such impact in academia through the above work, financial and market analysts are interested to know more about how temporal parallel algorithms would affect the computational efficiency in derivative analysis and prediction of prices. Discussion of collaboration with Wuppertal University, Deutsche Postbank, and other financial organisations resulted to the FR7 project linking these partners as described in [3b].

5. Sources to corroborate the impact

S.1 Collaboration work with local industry, TWI Group and ESI Group, on the implementation of distributed algorithms for the commercial software Sysweld. http://www.optweld.org.uk/home/optweld_overview.pdf). Techniques based in defect correction and coupling of subdomains have been embedded into the parallel software design.

S.2 Lai was invited to be the external examiner for a PhD thesis on temporal parallelisation at the University of Claude Bernard Lyon I in July 2011. Discussion of collaboration with Wuppertal University and several financial organisations, including Deutsche Postbank, resulted to an industrial and academia collaborative project in FR7 as described in [R6].

S.3 A special issue highlighting industrial collaborative work with hospitals in pharmacokinetics and other applications in medical sciences: Computer methods in pharmacy related research, *Journal of Algorithms and Computational Technology*, **2** (1), 2011.

In relation to temporal scale decomposition, Lai applied inverse problem techniques for some pharmacokinetic models and developed an intrinsic parallel method:
L. Liu, C.-H. Lai, S.-D. Zhou, F. Xie, H.-W. Lu. PKAIN: An artificial immune network for parameter optimisation in pharmacokinetics. *Modelling in Medicine and Biology VIII*, 277 – 286, WIT Press, ISSN 1747-4885, 2009.

L. Liu, C.-H. Lai, S.-D. Zhou, F. Xie, R. Lu. Two level time-domain decomposition based distributed method for numerical solutions of pharmacokinetic models. *Computers in Biology and Medicine, 41,* 221 – 227, 2011. (doi:10.1016/j.compbiomed.2011.02.003)

S.4 DCABES (Distributed Computing and Algorithms for Business, Engineering, and Sciences) is a research and industrial network exploring modern mathematical tools related to distributed and parallel algorithms and their roles in industry. The network was initiated by the University of Greenwich and Wuhan University of Science and Technology, Wuhan, China, and started long before NAMU was established and has been running since 2001 when the first international conference was held in Wuhan, China: http://www.dcabes.org. Lai is now one of the two co-chairs of the steering committee of DCABES which looks after the annual conference – International Conference on Distributed Computing and Applications to Business, Engineering, and Sciences. Proceedings of the annual conference are now being published by IEEE.

S.5 Lai is also a visiting professor at Buckingham University: http://www.buckingham.ac.uk/directory/professor-choi-hong-lai/; Jiangnan University, China; and Fuzhou University: http://cmcs.fzu.edu.cn/glwz/, China. He is also an honorary professor at Wuhan University of Science and Techology, Wuhan, China. The main role of such visiting professorships is to promote joint research collaborations in various areas of numerical analysis and scientific computing for industrial related applications.

S.6 NAMU has close ties with Fuzhou University in the area of applied computing and applications. Lai is one of two co-directors of Fuzhou-Greenwich Applied Computing R & D Centre (http://cmcs.fzu.edu.cn/glwz/). One of the roles that NAMU undertakes is to consolidate collaborations with Chinese industry in image processing amongst other areas.

S.7 Recently NAMU has hosted the visit of Prof. Shidah Mohd-Ali, Malaysian Science University to work in the area of domain decomposition methods. Lai is nominated by Malaysian Science University as a member of their external supervision team for one PhD student who works in domain decomposition method.

S.8 Lai has taken up external supervision of a PhD student at University of Hertfordshire in the area of computational finance.

S.9 The concept of defect correction method and multi-scale problems is included in the final year course: Methods of Nonlinear Mathematics (Course code MATH1133) which will be used in the training programme provided through the FR7 project described in [R6].