Final Activity Report

Summary of the major project achievements over the entire lifetime of the project

The information provided in this section will only be available to ERC staff, to members of the ERC panels, and to the Scientific Council

Explain in a clear manner the work performed during the entire lifetime of the project along the main objectives/activities of the project listed in the Description of Work (DoW). Please indicate the publications linked to these objectives/activities.

Please specify the outcome in terms of:

- research and technological achievements along the main objectives/activities (in line with the DoW)

This presentation refers to the DoW.

A. Catalogue of Prior Information and Test Problems. The priors are so diverse that we could not present them in a unified framework; test problems are described in our publications.

- B. Incorporation of Prior Information.
- Training data for computed tomography (CT) [27,32,33].

Incorporation of training data (images, segmentations, etc.) improves both the reconstruction and the segmentation, and machine learning produces a dictionary that allows a sparse reconstruction. We used non-overlapping patches, a tensor formulation with a very sparse representation, and a novel ap proach to use image texture priors.

• Sparsity priors for electrical impedance tomography (EIT) [5,13,14,15,16,18,22].

We demonstrated that spatial information through sparsity in the spatial domain, together with a spatially varying regularization parameter, can give dramatic improvements in the reconstruction. We used this approach to successfully handle problems with partial boundary information.

• Temporal and spectral priors [1].

New detector technology allows the use of spectral and dynamical information, which calls for new types of priors about material constituents and dynamics. By modeling the measurements and uncer tainties we derived a new algorithm for poor-quality measurements.

• Non-Gaussian noise priors [8,9,25,30,31].

We developed new problem formulations and algorithms based on correct mathematical modeling of the noise in the data. In particular we utilized prior information about non-Gaussian noise and showed how these noise priors improve the computational algorithms and the images.

• Artifact reduction in limited-data problems [29].

Microlocal analysis reveals how measurement conditions associated with incomplete/sparse data in fluence the reconstruction, and we used this insight to reduce artifacts via algorithm modifications, e.g., for region-of-interest problems.

C. Sparsity Priors.

• The role and impact of sparsity for CT [19,20,21].

We used simulation studies to provide a foundation for the use of sparsity in CT where, unlike com pressed sensing, it is not possible give rigorous proofs. We demonstrated that a sparsity constraint – even with highly underdetermined systems – allows full recovery once a sufficient number of data is available.

• Higher-order information as priors, beyond total variation (TV) [7,23].

We developed new methodology that incorporates sparsity on higher-order derivatives with direction

al information. Our anisotropic higher-order techniques are well suited for reconstructing objects with directional features (avoiding the artifacts of classical TV methods) and for segmentation.

- D. Large-Scale Numerical Algorithms. We develop well-defined, robust and efficient algorithms (generic and specific) based on state-of-the-art numerical analysis research.
- Numerical optimization [4,24,34].

Optimization plays a central role for handling complex priors, non-Gaussian noise, and machine learning tasks. We focused on the use of proximal splitting methods and decomposition techniques, and the use of kernel-based regularization.

• Computations with sparse representations [3].

This work focused on the use of accelerated first-order large-scale algorithms for imposing sparsity constraints through the use of a 1-norm constraint.

• Iterative methods [2,6,10,11,12,17,35].

New theory led to improvements in formulations and implementations. We emphasize our semi-convergence analysis of Kaczmarz's method, the examination of the harmful influence of unmatched projector/backprojector pairs, and the use of signal subspace priors.

E. Software Development, Test and Validation [26,28]. These tasks were performed and documented in conjunction with all the tasks in collaboration with specialists in physics, material science, etc. Software is available on our home pages, via publications, and via the packages AIR Tools II (a col lection of algebraic iterative methods) and IR Tools (Krylov subspace methods).

- novel and/or unconventional methodologies

The overall outcome is novel theoretical insight into the role and application of priors, leading to a theoretical and computation framework for including these priors in an optimal way. This was achieved by a number of cases described here.

We expanded the understanding of sparsity priors for CT. Compressed sensing with random sampling has a solid theoretical foundation that does not carry over to CT. We demonstrated via sim ulations that the phase transition property known from compressed sensing also appears in CT. With a sparsity constraint we achieve full recovery once a sufficient number of data are available and we showed how this number depends on the object's complexity. Our results justify why sparsity priors are so successful in CT.

We developed a novel algorithm for EIT with a spatially varying regularization parameter, where the solution's sparsity is guided by spatial priors. This improves the reconstruction, especially for prob lems with partial boundary information. We proved that details are guaranteed to be detected from noisy data based. In a study of depth resolution, we also proved how the reconstruction's resolution depends on the distance to the measured part of the boundary; these are the first rigorous results sup porting the intuition that reconstructions are better close to the measurements.

Training data take the form of images and segmentation classes. Machine learning produces a dic tionary from the training data, and by expressing the reconstruction as a sparse combination of the dictionary elements we can handle very underdetermined problems. We developed a novel algorithm that uses non-overlapping image patches and a tensor-basis formulation that allows a very sparse rep resentation – this work is mentioned on the front page of SIAM News. We also developed a novel ap proach for handling joint reconstruction/segmentations using training textures.

Priors can also be expressed as signal subspaces that represent wanted features. We demonstrated the power of this approach and developed two novel algorithms LBAS and R3GMRES, based on Krylov subspace methods, which include such priors.

We provided a novel framework that takes into account the problem's specific non-Gaussian noise statistics (e.g., impulse, multiplicative or Cauchy). In our new models and algorithms we extract more relevant information related to the noise, and the numerical computations become more robust.

We emphasize our novel use of anisotropic higher-order regularization, such as directional total gen eralized variation.

Our collaboration with experts of microlocal analysis for CT led to insight how incomplete or limited data deteriorate the reconstruction. We used this insight to reduce artifacts via algorithm modifica tions. This is used in the study of flow in porous media and in a new sparse-view region-of-interest method for underwater pipeline inspection.

Research teams outside the mathematical communities occasionally lack a solid background in nu merical analysis, so they often rely on heuristics and traditions. Our research provides well-defined, robust and efficient computational algorithms based on state-of-the-art numerical analysis research. We made rigorous statements about the methods, their convergence, and the properties of the recon structions.

We gave semi-convergence analysis of the regularizing properties of algebraic iterative methods; our paper on Kaczmarz's method is in the "highlight collection" of Inverse Problems. We also gave a new theoretical and experimental examination of the harmful influence of unmatched projector/backprojector pairs.

Our novel contribution in numerical optimization is the use of kernel-based regularization and empir ical Bayes to infer model parameters from data, thus carrying techniques from system identification over to inverse problems. We also established a link between the optimization framework and iterat ive reconstruction methods allowing us to generalize them, e.g., to handle Poisson noise.

- inter and cross disciplinary developments

X-ray tomography has many applications in science, engineering, and medicine. To ensure a focused effort, our research in the present project was almost entirely devoted to problems in materials science – a research area that receives much attention due to new and forthcoming European measure ment facilities, such as MAX IV and ESS in Lund and European XFEL in Hamburg. For image processing and segmentation we relied upon expertise in the department's image analysis section, resulting in the novel methods for joint reconstruction and segmentation – and providing the foundation for current and future collaboration in this area. In addition we formed a novel collaboration with researchers in image processing from Copenhagen University's department of computer science.

Within the Technical University we established joint projects on phase contrast X-ray imaging with the Department of Physics and the Department of Energy Conversion and Storage. These collaborations led to new algorithms such as a combined phase-retrieval/reconstruction method utilizing total variation, and iterative algorithms for phase-wrapping and geometric alignment. We also collaborate with DTU Physics on velocity-space tomography in fusion plasma physics and mapping of grain ori entations in materials science.

Access to real data sets is crucial for test and validation of our algorithms, and we acknowledge the fruitful collaborations with the experts at DTU's Imaging Industry Portal (www.imaging.dtu.dk) who provided ordinary as well as spectral and dynamical CT data, our partners in the Danish "Alliance for Imaging and Modelling of Energy Applications" (www.cinema-dsf.dk), and the computational imaging experts at Manchester University's School of Mathematics and X-Ray Imaging Facility (www.mxif.manchester.ac.uk) and at CWI in Amsterdam (www.cwi.nl). In return we provided these collaborators with mathematical and numerical insight into their computational reconstruction al gorithms.

We also acknowledge collaboration with leading experts in microlocal analysis for CT, Prof. Jürgen Frikel (OTH Regensburg) and Prof. Todd Quinto (Tufts University), both of whom spent extended visits in our research group and contributed to our teaching and research – especially in the area of ar tifact reduction. In return they benefited from access to our computational expertise and various CT data in materials science. In this connection we emphasize our ongoing collaboration with FORCE Technology (forcetechnology.com) on region-of-interest CT for underwater pipeline inspection.

- knowledge and technology transfer

In addition to the items listed below, transfer takes place through the collaborations mentioned in the previous section and through research visits abroad and visitors coming to DTU – see the next section.

Courses, workshops, and conference attendance:

- Sixth International Conference on Scale Space and Variational Methods in Computer Vision, 2017
- Workshop: Sparse Tomo Days, 2014
- Workshop: HD-Tomo Days, 2016
- Workshop: Computational Inverse Problems Insight and Algorithms, 2017
- Two seminars by Prof. Todd Quinto: What you can see in limited data tomography, Inverse Scale Space Decomposition; 2016.
- Four seminars by Prof. Jürgen Frikel: Mathematics of computerized tomography, Basic concepts of microlocal analysis, Microlocal analysis of limited angle reconstruction in tomography, and On the use of highly directional representations in incomplete data tomography; 2015–2016
- Five seminars by Prof. Bill Lionheart: Sufficient data for stable reconstruction, Ray transforms, EIT for beginners, Rich tomography, and Inverse problems in security screening; 2013–2014
- Online short-course Algebraic Iterative Reconstruction Methods
- COST training school Algebraic Reconstruction Methods in Tomography, 2016
- COST training school Scientific Computing for Computed Tomography, 2017
- Master course Computational Science in Imaging, once every year
- PhD course Inverse Problems with Applications in Tomography and Imaging (with Copenhagen University), 2014
- PhD course Introduction to Inverse Problems, once every year
- PhD course PDE-Constrained Optimization, once every second year
- PhD course (Joint with COST) Scientific Computing for Computed Tomography, 2017
- PhD course Convex Optimization, 2017
- PhD course Computational Uncertainty Quantification for Inverse Problems, 2017

The members of our research group are highly visible through publications and participation in many international conferences and workshops. The PI was invited speaker at:

- Manchester Image Reconstruction and Analysis, 2012
- UCL Centre for Inverse Problems: Opening Meeting, London, 2013
- Lorentz Center: Advanced X-Ray Tomography, Leiden, 2014.
- Distinguished Lecture, Scientific Computing and Imaging Institute, University of Utah, 2014
- Householder Symposium on Numerical Linear Algebra, Belgium, 2014.
- Oberwolfach Workshop on Mathematics and Algorithms in Tomography, 2014
- Celebration in Honor of D. P. O'Leary, SIAM Conf. on Appl. Lin. Alg., Atlanta, 2015
- Mathematical Imaging and Emerging Modalities, Osnabrück, 2016
- Numerical Linear Algebra and Applications, Luminy, 2016
- International Conf. on Scale Space and Variational Methods in Computer Vision, Kolding, 2017

Martin S. Andersen was invited speaker at:

- 20th Conf. International Linear Algebra Society (ILAS), 2016
- Workshop on Convex and Real Time Optimization, Denmark, 2016

Public-domain software and data:

• Multiple-kernel regularization; ring reduction – Martin S. Andersen (www2.compute.dtu.dk/~mskan/software.html)

- Handling non-Gaussian noise Yiqiu Dong (www2.compute.dtu.dk/~yido/Links.html)
- Iterative regularization methods Per Christian Hansen (2 submitted packages: AIR Tools II and IR Tools)
- DLCT-Toolbox, a Matlab package for the dictionary learning approach to tomograhic image recon struction, written by Sara Soltani (www2.compute.dtu.dk/~pcha/HDtomo/DLCT-ToolBox.zip)
- DTGV-Reg, a Matlab package for Directional Total Variation (DTV) and Directional Total Gener alized Variation (DTGV) regularization, written by Rasmus Dalgas Kongskov: (www2.compute.dtu.dk/~pcha/HDtomo/DTGV-Reg.zip)
- Data from: Jørgensen & Sidky, How little data is enough? Phase-diagram analysis of sparsity-regularized X-ray computed tomography (DOI: 10.5061/dryad.3jg57)
- SparseBeads Dataset for benchmarking of sparsity-regularized reconstruction methods Jakob Sauer Jørgensen et al. (https://zenodo.org/record/290117)

- enhancing the immediate research environment

Perhaps the largest impact of the ERC grant was the establishment and consolidation of the Inverse Problems and Tomography group in department's Section for Scientific Computing – see the next section. Along with this, we could attract additional funding from the Danish Research Council, from DTU and Marie Skłodowska Curie Actions, and from the Otto Mønsted Foundation in Denmark. On a larger scale, the ERC grant allowed the group and the department to play a large role within DTU's strategic research plan towards increased activities in industrial and scientific use of tomography. The second largest impact of the grant was the creation of an inspiring and internationally oriented research environment for this group. Due to the large size of the group, we can work in an interdis ciplinary fashion among its members and benefit from our diversity – ranging from theory to com puter implementations and applications. Weekly research seminars – and occasionally workshops – were given interchangeably by students, group members and research visitors. All this created an in spiring environment for our BSc, MSc and PhD students.

All group members (PhD students, Post Docs and faculty) could easily perform short or long re search visits abroad (this is mandatory for our PhD students), providing inspiration for new research topics and building a very strong international network. Research visits were paid to, among others, Linköping University, Helsinki University, University of Lübeck, CWI in Amsterdam, Universität Mainz, Johannes Kepler University Linz, Universität Wien, Emory University, Stanford University, UCLA, Tufts University, Cambridge University, University College London, Peking University, and Japan's National Institute of Informatics.

Due to our large research group and our many activities, we obtained substantial national and interna tional visibility and recognition. In 2015 Prof. Per Christian Hansen was named a SIAM Fellow for his contributions to algorithms for rank-deficient and discrete ill-posed problems and regularization techniques.

We were able to attract more than 40 visitors, many of them coming several times, specifically doing research with us and/or giving seminars about their work for the benefit of the group and the depart ment. Among the regular visiting professors are Joost Batenburg, CWI; Tommy Elfving, Linköping; Tobias Lasser, TUM; James G. Nagy, Emory; Carola-Bibiane Schönlieb, Cambridge; Mila Nikolova, Paris-Saclay; Gabriele Steidl, Kaiserslautern; Raymond Chan, Hong Kong.

We hosted a number of students from abroad who spent part of their studies MSc or PhD with us:

- Simon Hubmer, Johannes Kepler University, Linz
- Julia Mrongowius, University of Lübeck
- · David Franck, TUM
- Gabriele Stocchino, University of Padua
- Yunyi Hu, Emory University
- Jin-jin Mei, UESTC, China
- Arne Bechensteen, University of Toulouse

The project allowed us to continue and expand our long-term collaboration with DTU's Computing Center (www.hpc.dtu.dk); we benefited from their HPC competences to develop new high-performance CT software that utilizes GPU computing.

- establishment and/or consolidation of the research group and team composition

Assistant Professors, Post Docs, and PhD students were all hired after international postings with equal gender opportunity, in order to create the best team. All members of the team are affiliated with the Department of Applied Mathematics and Computer Science (DTU Compute) at the Technical University of Denmark.

Faculty members related the project team:

- Associate Professor Martin S. Andersen (funded by the project during his Post Doc)
- Associate Professor Yiqiu Dong (fully funded by the project)
- Professor Per Christian Hansen Principal Investigator
- Associate Professor Mirza Karamehmedovic
- Associate Professor Kim Knudsen

Post Docs related to the project (* = funded by the project):

- Martin S. Andersen*, Post Doc project: Practical optimal first-order methods, 2012–2014 (now As sociate Professor at DTU Compute)
- Jürgen Frikel, Post Doc project: Insights and algorithms for incomplete data tomography, 2015–2016 (now Full Professor at OTH Regensburg) funded by the H C Ørsted COFUND program.
- Lauri Harhanen*, Post Doc project: Formulation and application of priors in spectral CT, 2015–2016 (now with KaVo Kerr, Finland)
- Jakob Sauer Jørgensen*, Post Doc project: Computations with sparse representations, 2013–2017 (now with Manchester University)
- Hans Martin Kjer*, Post Doc project: Joint CT reconstruction and segmentation, 2016–2017 (now in a joint position with DTU Compute and Danish Research Centre for Magnetic Resonance) Visiting professors during the project (both funded by grants from the Otto Mønsted Foundation):
- Professor Bill Lionheart, Manchester University, 2013–2014
- Professor Todd Quinto, Tufts University, 2016 –2017

Honorary professors associated with the group:

- Prof. Jan S. Hesthaven, EPFL
- Prof. Samuli Siltanen, Helsinki University

Due to the prestige and success of the ERC grant it was possible to substantially expand and consol idate the department's team working on inverse problems, and thus ensure a strong new generation of researchers in this research field at DTU. The three new faculty members are Associate Professors Martin S. Andersen, Yiqiu Dong and Mirza Karamehmedovic.

- others

The work carried out during the last part of the project is not yet published. Therefore we include here a list of accepted papers and papers in review.

Accepted Papers:

L. Borg, J. S. Jørgensen, J. Frikel, and J. Sporring, Reduction of variable-truncation artifacts from beam occlusion during in situ X-ray tomography, Measurement Science and Technology, to appear. V. A. Dahl, A. B. Dahl, and P. C. Hansen, Computing segmentations directly from X-ray projection data via parametric deformable curves, Measurement Science and Technology, to appear. T. Elfving and P. C. Hansen, Unmatched projector/backprojector pairs: perturbation and convergence

T. Elfving and P. C. Hansen, Unmatched projector/backprojector pairs: perturbation and convergence analysis, SIAM J. Sci. Comp., to appear.

- P. C. Hansen and J. S. Jørgensen, AIR Tools II: Algebraic iterative reconstruction methods, improved implementation, Numerical Algorithms, to appear.
- J. S. Jørgensen, S. B. Coban, W. R. B Lionheart, S. A. McDonald, and P. J. Withers, SparseBeads Data: Benchmarking sparsity-regularized computed tomography, Measurement Science and Technology, to appear.
- T. Ramos, J. S. Jørgensen, and J. W. Andreasen, Automated angular and translational tomographic alignment and application to phase-contrast imaging, Journal of the Optical Society of America A, to appear.

Papers in Review:

- G. Bal, K. Hoffmann, and Kim Knudsen, Propagation of singularities for linearised hybrid data im pedance tomography, submitted to Inverse Problems.
- L. Borg, J. Frikel, J. S. Jørgensen, and E. T. Quinto, Characterizing artifacts in X-ray CT for arbitrary limited data, submitted.
- Y. Dong, P. C. Hansen, and H. M. Kjer, Joint CT reconstruction and segmentation with discriminat ive dictionary learning, submitted to IEEE Trans. Comput. Imaging.
- S. Gazzola, P. C. Hansen, and J. G. Nagy, IR Tools A MATLAB package of iterative regularization methods and large-scale test problems, submitted to Numerical Algorithms.
- Y. Hu, J. G. Nagy, J. Zhang, and M. S. Andersen, Iterative methods for polyenergetic image recon struction, submitted to IEEE Trans. Comput. Imaging.
- R. D. Kongskov, Y. Dong, and K. Knudsen, Directional total generalized variation regularization, submitted to SIAM J. Imaging Sciences.
- N. A. B. Riis, J. Frøsig, Y. Dong, and P. C. Hansen, Limited-data X-ray T for underwater pipeline in spection, submitted to Inverse Problems.
- M. F. Schmidt, M. Benning, and C.-B. Schönlieb, Inverse scale space decomposition, submitted to Inverse Problems.

Technical Reports:

- L. Borg, J. Frikel, J. S. Jørgensen, and E. T. Quinto, Theorems that characterize artifacts for arbitrary limited X-ray CT data, Technical Report arXiv:1707.03055.
- L. Borg, J. S. Jørgensen, and J. Sporring, Towards characterizing and reducing artifacts caused by varying projection truncation, Technical Report 2017/1, Department of Computer Science, University of Copenhagen, 2017.
- M. Burger, Y. Dong, and F. Sciacchitano, Bregman cost for non-Gaussian noise, DTU Compute Technical Report 2016-8.
- Y. Dong and T.-Z. Huang, Image fusion and denoising using fractional-order gradient information, Technical Report 2017-05.
- P. C. Hansen and K. Abe, LBAS: Lanczos Bidiagonalization with Subspace Augmentation for Discrete Inverse Problems; Technical Report 2017-03.
- R. D. Kongskov and Y. Dong, Tomographic reconstruction methods for decomposing directional components, Technical Report 2017-04.
- M. Romanov, A. B. Dahl, Y. Dong, and P. C. Hansen, Relaxed Simultaneous Tomographic Recon struction and Segmentation with Class Priors for Poisson Noise, DTU Compute Technical Report 2015-6.
- M. Romanov, P. C. Hansen, and A. B. Dahl, A Parameter Choice Method for Simultaneous Recon struction and Segmentation, DTU Compute Technical Report 2015-5.
- S. Soltani, Studies of Sensitivity in the Dictionary Learning Approach to Computed Tomography: Simplifying the Reconstruction Problem, Rotation, and Scale, DTU Compute Technical Report 2015-4, July 2, 2015.
- P. Weiss, P. Escande, and Y. Dong, Contrast Invariant SNR, DTU Compute Technical Report

2016-09.

Project No.: 291405 Ref: 291405_HD-Tomo_Final_Activity_Report14_20170929_092836_CET.pdf

Page 10

Publishable brief summary of the achievement of the project

This section, which should not exceed 1 page (approx. 600 words), might be used for dissemination of the project progress/results to the general public/scientific community. For this reason, please do not reproduce here the project abstract, which is already available in CORDIS.

Stand alone description of the project and its outcomes

With computed tomography (CT) we can see inside objects – we send signals through an object and measure the response, from which we compute an image of the object's interior. Medical doctors can look for cancer, physicists can study microscopic details of new materials, engineers can identify in ternal defects in pipes, and security personnel can inspect luggage for suspicious items.

It is of vital importance that the images are as sharp, detailed and reliable as possible, so scientists, engineers, doctors etc. can make the correct decisions. To achieve high-definition tomography – sharper images with more reliable details – we must use prior information consisting of accumulated knowledge about the object.

Overall Outcome: Insight and Framework

Previous efforts were often based on ad-hoc techniques and naive algorithms with limited applica tions and ill-defined results. This project focused on obtaining deeper insight and developing a rigor ous framework. We carefully analyzed the underlying mathematical problems and algorithms, and we developed new theory that provides better understanding of their challenges and possibilities. This insight allowed us to develop a solid framework for precisely formulated CT algorithms that compute much more well-defined results. We laid the groundwork for the next generation of rigor ously defined algorithms that will further optimize the use of prior information.

The road to this insight involved specific case studies related to the formulation and use of prior in formation, involving such applications as X-ray phase-contrast tomography, fusion plasma physics, and underwater pipeline inspection. Below we list the highlights of these cases.

Understanding of Sparsity for Low-Dose CT

We characterize how the prior information that an object is "simple" – in mathematical terms, sparse – allows us to compute reliable images from very limited data, and we show that the sufficient amount of CT data depends in a simple way on the sparsity. This is essential in medical and engineer ing CT where one must minimize the X-ray dose and shorten measurement time.

Superior Localization in Electrical Impedance Tomography

By incorporation the prior information that the details stand out from the background, we can now compute images with superior localization and contrast. Moreover we developed new theory that, for the first time, precisely describes the obtainable resolution and the optimal measurement configura tion. This is essential in industrial process monitoring where measurement constraints often limit the amount of data.

Superior Use of Textural Training Images

For textural images, we developed a new mathematical and computational framework that is superior to other methods for limited-data. It is particularly suited for computing reliable segmentations of these images. To do this we use prior information in the form of training images that the computed image must resemble.

Novel Convergence Analysis of Iterative Methods

We developed novel theoretical insight into the advantages and limitations of the iterative methods that are required for 3D tomography computations. This insight guided the development of new soft ware suited for many-core and GPU computers, as well as public-domain software with model imple mentations of these algorithms.

Correct Handling of Noise

We formulate correct mathematical models for the measurement noise and we develop new computa tional algorithms especially suited for using prior information about non-Gaussian noise. We show that these noise priors improve both the algorithms and the images, compared to the standard algorithms that are based on cruder models.

Novel Use of Prior Information about Structure

Structural prior information states that the image contains visual structures, e.g., texture along certain directions. Incorporation of this kind of information prompted us to develop new anisotropic higher-order techniques that avoid the unwanted artifacts of traditional methods (such as total variation).

Project No.: 291405