The Mathematics of Data Representations

Prof. Philipp Grohs

ETH Zurich

Introduction

One of the most pressing challenges in modern science and technology is to cope with the massive amounts of data that are recorded in the digital world we live in today. Indeed, the 21st century is often referred to as the 'century of data' and terms like 'data deluge' and 'big data' are now popular ways to describe this situation. Data can come in very different guises and it can mean several things. One instance which produces heavy loads of data is the internet (think of the $\sim$ 300 million photos uploaded to facebook each day), other examples are wireless communication, stock prices, or medical imaging applications. Taken together, the amount of data which exists is currently estimated to exceed 3000 billion Gigabytes and it is growing fast. Facing these dazzling figures, major data processing tasks, including efficient storage, analysis and transmission, seem all the more challenging. Fortunately, it turns out that most of the time the information content of data is much smaller than its actual storage complexity and there exists great potential for significant compression. For instance the JPEG2000 image compression standard is capable of storing only a small fraction of the bits which would be needed in a naive representation with no distinguishable loss of information, see Figure 1.

Figure 1: Example for image compression. Left: original image. Right: Compressed image only requiring around 5% of the storage required for original image.

How is this possible? The secret lies in finding a smart representation for generic images and this is where mathematics comes into play. For a mathematician data is simply described by a function f. For a black and white image, this function would simply associate to each pixel its brightness or intensity. One idea to reduce complexity and to compress f is to find a dictionary $\{f_i\}_i$ of template signals and to try to represent f as a linear combination of these templates, e.g.

$$f = \sum_i c_i f_i, \quad c_i \in \mathbb{R}.$$

If most values c_i in this representation are zero (or very close to zero) we speak of a 'sparse representation'. In that case the signal can be compressed by storing only the few nonzero coefficients. An example is shown in Figure 2: here an image is represented in a wavelet-dictionary. As we can see, almost all representation coefficients are of neglibible size and we can discard them. This sparse wavelet representation lies behind the JPEG2000 compression standard.

Different types of data possess different characteristic features and thus require different ways for their efficient representation. The following quote from David Donoho, one of the very most successful and innovative figures in the field of mathematical data processing, at the occation of his plenary address at the international conference of mathematics [12] from 2002 pointedly sums this up as follows:

> *Information has its own architecture. Each data source, whether imagery, sound, text, has an inner architecture which we should attempt to discover and exploit for*

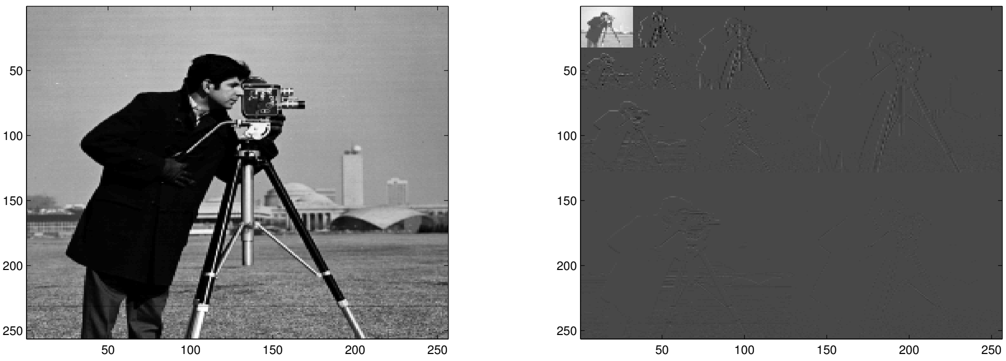

Figure 2: Wavelet representation of image. Left: original image. Right: Representation of the same image in a wavelet representation system. The color coding represents the magnitude of the representation coefficients (c_i) (dark coefficients are close to zero). We see that almost all coefficients are close to zero and can thus be neglected.

> *applications such as noise removal, signal recovery, data compression, and fast computation.*

So the challenging problem is to find representation systems which are optimally adapted to a given class of signals. It is quite striking that the notion of 'optimality' can be precisely described mathematically and that in many cases one can precisely quantify the interplay between accuracy of a compression and the number ob bits required to represent the compressed data. For this reason mathematics has played and still plays a major role in developing new and efficient algorithms for data processing.

In my research I introduce sophisticated geometric techniques to refine and expand the scope of existing numerical methods for the efficient representation of data. The focus lies both on laying out a rigorous mathematical foundation as well as implementation of the resulting algorithms on a computer. I want to emphasize that the mathematical foundation (e.g. a *proof* that the algorithm works) is at least as important as its efficient implementation – it serves as a safeguard that the algorithm is actually doing what we expect in all cases and that no important information is lost (it is easy to think of examples where such an information loss would have devestating consequences).

I have been able to make progress on problems as diverse as the numerical solution of geometric partial differential equations, geometric multiscale analysis, data compression, the numerical solution of kinetic transport equations, computer aided geometric design and architectural geometry.

In the following sections I describe a few highlights of my past research. The reader will notice that these different projects concern a rather diverse spectrum of problems. What they all have in common is that the key to their solution lies in finding efficient data representations.

Approximation of Manifold-Valued Data

In recent years the numerical approximation and representation of functions which take their values in a curved space (think for instance of data given by directions, assuming its values on the unit sphere) has become increasingly important. For instance in signal processing they appear in medical imaging (Diffusion Tensor MRI [27]), robotics (motion design [25]), chromaticity image denoising [38], and many others, see Figure 3.

All these scenarios have in common that the signal model is given by functions defined on a

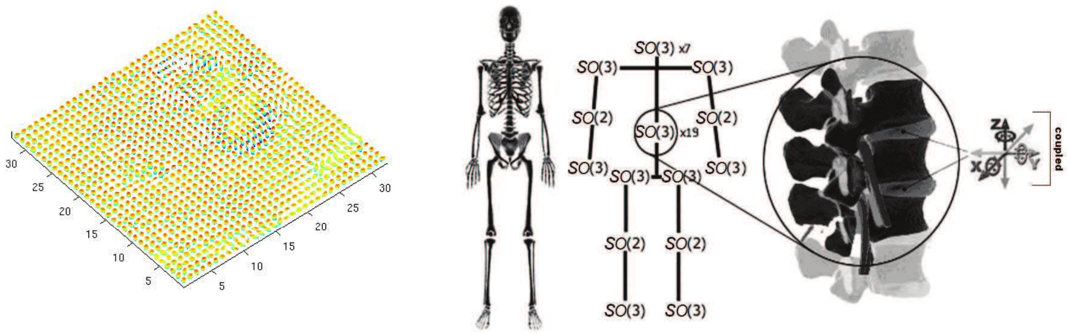

Figure 3: Examples of manifold-valued data. Left: Diffusion Tensor MRI. Here an ellipsoid is attached to each pixel. These ellipsoids describe the directional preferences for the diffusion of water molecules in the brain. This information is used for instance to track brain fibers. Right: Lie Group model of the human spine from [25]. Here the joints of the spine are modeled by rotation matrices.

linear space and assuming its values in a nonlinear manifold (think of an image where not an intensity is attached to each pixel but for instance a direction, a tensor or another geometric object). In order to properly handle such non-linear data, radically new methods that respect the underlying geometric structure, need to be developed. The main difficulty lies in defining geometrically meaningful (in the sense that natural invariances are preserved) algorithms with the desirable properties of linear methods. My research focuses on the problem of developing such algorithms to handle nonstandard data types and on analyzing them theoretically. Due to the additional structure of the data, the necessary mathematical tools to address these problems include classical approximation theory as well as differential geometry. Since this subject lies at the intersection of two different disciplines, many methods in the theoretical analysis have to be developed from scratch. In past research in this field, I have established several final results which now represent the current state-of-the-art in the approximation of manifold-valued data.

Important contributions include

- The development of stable multiscale decompositions for manifold-valued data which satisfy the same desirable properties as wavelets for scalar data in [23, 17]. A decomposition is shown in Figure 4. As our results have shown, for piecewise smooth data, most decomposition coefficients are of negligible size which results in substantial compression rates.
- Further, I have obtained a complete solution of the smoothness equivalence conjecture for nonlinear refinement schemes which operate on data in a Riemannian manifold [23, 15, 16], as posed by David Donoho and collaborators in 2005 [39]. Applications for nonlinear refinement schemes include computer graphics and motion design [40]
- In another contribution [22] we introduced a novel denoising and inpainting of corrupted manifold-valued images, see Figure 5 for a particular example. Due to its fast convergence speed (which can be justified rigorously) our algorithm consistently outperforms current state-of-the-art methods, such as [41].
- A more recent research project concerns the numerical approximation of partial differential equations (PDEs) evolving in manifolds. In these cases, the data is not given explicitly to us but implicitly, as the solution of a typically highly complicated nonlinear equation. Such problems arise for instance in the simulation of orientations of magnetic moments in micromagnetism (where the target manifold is the sphere S^2) or directions in nematic crystal models (where we deal with the so-called projective space P^2) [2, 24]. Other examples include variational methods for the processing of manifold-valued signals or nonlinear Cosserat material models which generalize linear elasticity [30, 31].

The numerical approximation of solutions to such PDEs is difficult, and because the relevant function spaces do not possess a linear structure, standard discretization methods cannot be used. Until recently no general method for the numerical approximation of PDEs as described above with proven convergence rate has been available but in the paper [20] we provide a complete convergence theory for the numerical approximation of geometric PDEs by *geodesic finite elements* which have been introduced in earlier work, independently in [19] and [36]. As an example application we obtain the first ever high order approximation method for the harmonic map equation. What our results essentially say is that we can, for the first time ever, exactly quantify how much work (in terms of storage and arithmetic operations to be carried out by a computer) we need to invest in order to compute the exact unknown solution, up to a desired accuracy. A simulation based on geodesic finite elements are shown in Figure 6.

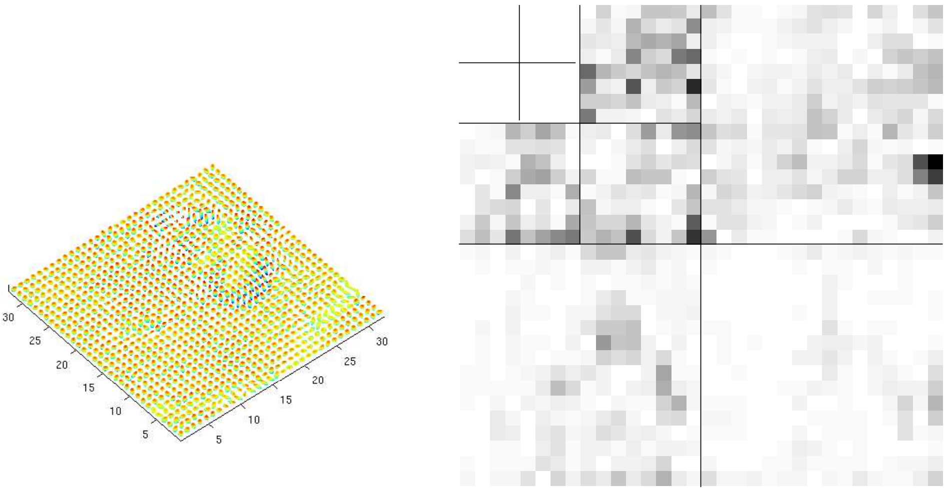

Figure 4: Wavelet decomposition of Diffusion Tensor MRI data $[0,1]^2 \to SPD(3)$, the manifold of symmetric positive definite 3×3 matrices. On the left we see the original image, on the right the magnitude of the transform coefficients which assume their values in the tangent bundle of $SPD(3)$.

Figure 5: Inpainting and Denoising of $SPD(3)$-valued image with algorithm from [22]. Left: original image. Middle: noisy and lossy image. Right: restored image.

Geometric Multiscale Analysis

For many classes of signals, the topography of information is governed by their singularity structure. To give an example, think of an image. Intuitively it is clear (and this fact has been exploited for several decades) that the major information in most images is contained in its edges. In the introduction we have mentioned the JPEG2000 standard which is based on wavelet

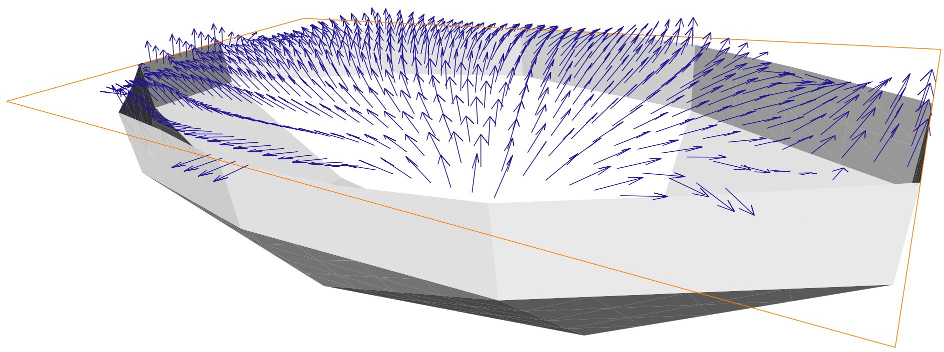

Figure 6: Liquid crystal simulation (Source: O. Sander).

dictionaries. It turns out that these dictionaries are actually suboptimal for the representation of edge singularities, see Figure 7.

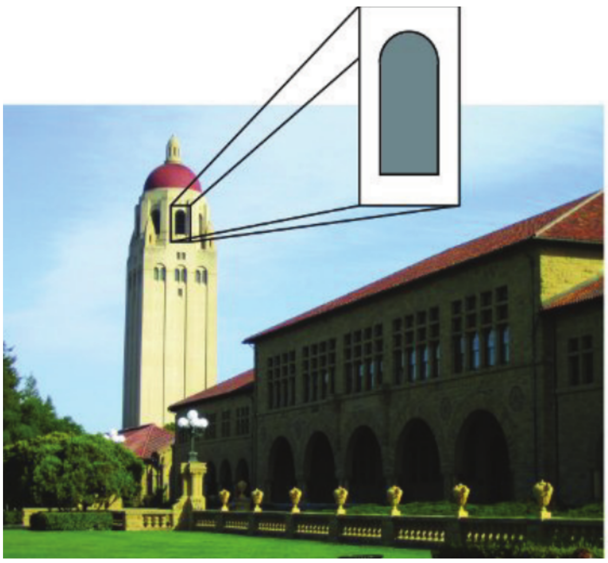

Figure 7: Most information in typical images is contained in its edges.

This and many further examples have lead to the emergence of the research area of geometric multiscale analysis which, roughly speaking, aims at designing optimal representation systems for multidimensional data with curved, anisotropic singularities of intermediate dimension.

A milestone in this area has been the construction of curvelet [9] and shearlet [26] representation systems which are indeed capable of optimally resolving curved singularities in multidimensional data.

Below are some contribution to the research field of geometric multiscale analysis.

- After the breakthrough result [9] new constructions of anisotropic representation systems have been introduced which achieve the same optimal compression rates for images with edge singularities. The recent work [18] introduced the framework of *parabolic molecules* which subsumes all the earlier constructions mentioned above and which established a transference principle of approximation results between any two systems of parabolic molecules. This meta result provides a deeper understanding of the properties a system has to satisfy in order to sparsely approximate anisotropic functions and for effortless proofs of many results which otherwise would require dozens of pages. What these result also show is that the great compression properties of curvelets hold for a much wider class of representation systems.

- Data with anisotropic singularities not only appears in images but also typical solutions of a particular class of partial differential equations, so-called transport PDEs exhibit these features. Equations of this type appear for instance in the numerical discretization of kinetic transport equations (modeling e.g. gas dynamics or radiative transport, see below) and in phase contrast imaging. In [21] we used a different kind of representation system, so called ridgelets, for the representation of solutions of transport equations. This construction lets us, for the first time, solve such equations in optimal complexity. Given a prescribed error tolerance we can exactly quantify the amount of work (arithmetic operations) to be carried out to represent the sought solution up to this tolerance. Again, the relation between accuracy and computational effort turns out to be optimal and in particular vastly superior to previous methods.

Kinetic Transport Equations

This project is concerned with the Boltzmann equation, derived by Ludwig Boltzmann in 1872 to describe the statistical behavior of the dynamics of a dilute gas. Even though the Boltzmann equation has its origins in the area of statistical physics, it has by now transcended this purpose and is nowadays widely used whenever a fully microscopic deterministic description of a multi-particle system is too costly or not informative and a macroscopic (fluid-dynamic) description is too inaccurate to reliably model the actual behavior. Applications of interest include the description of the collective behavior of species in socio-economic models, various probabilistic models in population biology and molecular biology, high energy physics, hydrodynamics or plasma modeling. Related equations are the so-called 'master equation' in chemistry or the radiative transport equation. Often, particular interest lies in the extraction of macroscopic quantities which are usually given as velocity moments of the probability density u which solves the Boltzmann equation.

The mathematical and computational challenges posed by the Boltzmann equation (and its many variants) are formidable. n recent years a number of attempts have been made towards design and development of efficient solvers but no satisfactory methods with provably optimal convergence rates have been found as of today.

Again, the key to an efficient solution of the Boltzmann equation is to find a suitable representation system which is well adapted to the equations and which captures accurately the main features of typical solutions. In [14] we have constructed such a representation system and designed and implemented an efficient algorithm for the numerical solution of the Boltzmann equation. This algorithm is the first of its kind in the sense that it captures the main physical properties of the exact equation, while possessing very good approximation properties. A simulation is shown in Figure 8.

Discrete Differential Geometry

The goal to design arbitrary freeform surfaces comes with a number of challenges (good structural properties, low cost, ...). To overcome some of them it has proven beneficial to utilize concepts of classical differential geometry. In fact the connection between freeform architecture and geometry has been so fruitful in the past few years that it has ignited the flourishing research area of architectural geometry [32].

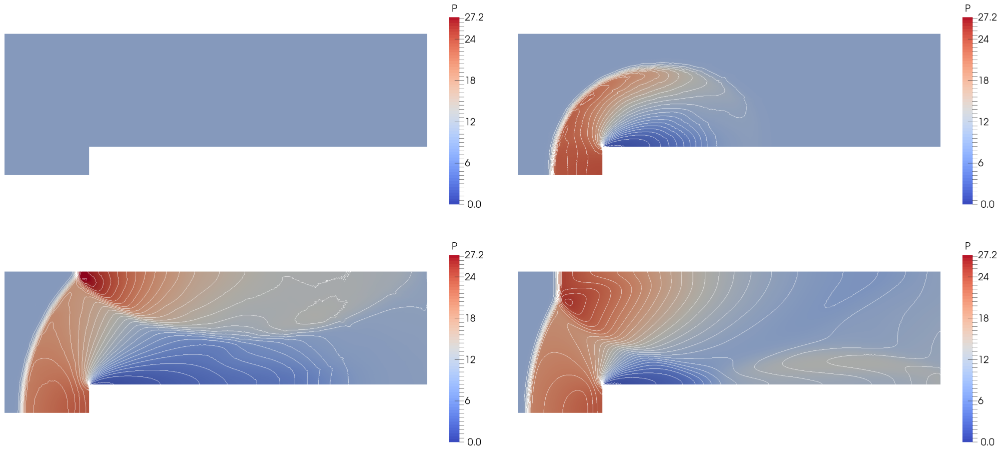

Figure 8: Simulation of the evolution of the air pressure in the Mach 3 wind tunnel experiment. The simulation is based on a polar spectral discretization of the Boltzmann equation. Joint work with S. Pintarelli and R. Hiptmair (ETHZ).

Recent research in architectural geometry has identified class of discrete surfaces, so-called Edge Offset meshes (quadrilateral meshes with planar faces, possessing a combinatorially equivalent offset mesh with planar faces and parallel edges with a fixed edge distance), as particularly desirable for applications [35], see Figure 9.

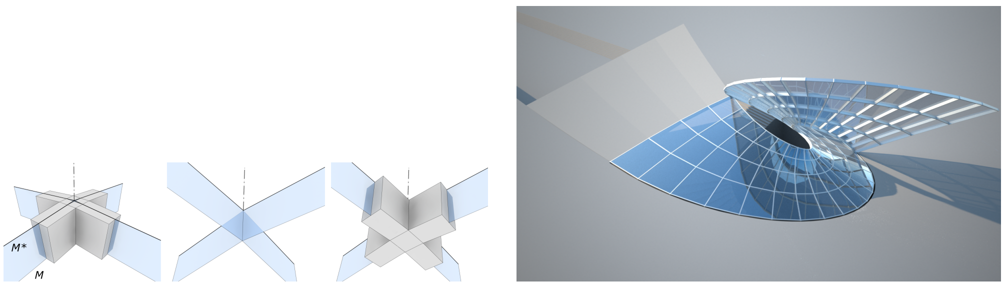

Figure 9: Left: Edge offset meshes are attractive candidates for architectural design since they give rise to the cleanest possible nodes in a supporting structure with beams of constant height Right: Architectural design based on discrete Enneper-type Laguerre minimal surface from [33].

This class of discrete surfaces a natural entity of a specific kind of geometry, so called Laguerre geometry. In view of form finding e.g. for architecture it is often useful to look for surfaces which are extremals of certain geometric energies. My research in this direction has focused on so-called Laguerre minimal (L-minimal) surfaces which arise as local extrema of a natural Laguerre geometric energy. We have studied these surfaces mathematically in [34] and [37] and constructed an algorithm for the efficient discrete representations of those as edge offset meshes which can then be used for architectural design in [33].

Acknowledgement

I would like to thank the department of mathematics for nominating me for the Latsis prize. This in itself is a huge honor for me. I am very grateful to the Latsis foundation for their effort in promoting science at a national and international level. Last but not least I am immensely indebted to all my collaborators, my former mentors and my students for providing me with so much inspiration and making my life as a researcher exciting. Thank you!

References

[1] P. Absil, R. Mahony, and R. Sepulchre. *Optimization algorithms on matrix manifolds.* Princeton University Press, 2009.

[2] F. Alouges. A new algorithm for computing liquid crystal stable configurations: the harmonic mapping case. *SIAM Journal on Numerical Analysis*, 34(5):1708–1726, 1997.

[3] D. Amsallem, J. Cortial, K. Carlberg, and C. Farhat. A method for interpolating on manifolds structural dynamics reduced-order models. *International Journal for Numerical Methods in Engineering*, 80(9):12411258, 2009.

[4] D. Amsallem, J. Cortial, and C. Farhat. Towards real-time computational-fluid-dynamics-based aeroelastic computations using a database of reduced-order information. *American Institute of Aeronautics and Astronautics Journal*, 48(9):2029–2037, 2010.

[5] D. Amsallem and C. Farhat. Interpolation method for adapting reduced-order models and application to aeroelasticity. *American Institute of Aeronautics and Astronautics Journal*, 46(7):1803–1813, 2008.

[6] D. Amsallem and C. Farhat. An online method for interpolating linear parametric reduced-order models. *SIAM Journal on Scientific Computing*, 33(5):2169–2198, 2011.

[7] B. G. Bodmann, G. Kutyniok, and X. Zhuang. Gabor shearlets. *arXiv preprint arXiv:1303.6556*, 2013.

[8] L. Borup and M. Nielsen. Frame decomposition of decomposition spaces. *Journal of Fourier Analysis and Applications*, 1:39 – 70, 2007.

[9] E. J. Candès and D. L. Donoho. New tight frames of curvelets and optimal representations of objects with C^2 singularities. *Communications in Pure and Applied Mathematics*, 56:219–266, 2004.

[10] S. Dahlke, G. Steidl, and G. Teschke. Shearlet coorbit spaces: compactly supported analyzing shearlets, traces and embeddings. *Journal of Fourier Analysis and Applications*, 17(6):1232–1255, 2011.

[11] M. Do and M. Vetterli. The contourlet transform: an efficient directional multiresolution image representation. *IEEE Transactions on Image Processing*, 14:2091–2106, 2005.

[12] D. L. Donoho. Emerging applications of geometric multiscale analysis. *Proceedings of the ICM 2002*, 1:209–233, 2002.

[13] A. Edelman, T. Arias, and S. Smith. The geometry of algorithms with orthogonality constraints. *SIAM Journal on Matrix Analysis and Applications*, 20(2):303–353, 1998.

[14] E. Fonn, P. Grohs, and R. Hiptmair. Hyperbolic cross approximation for the spatially homogenous Boltzmann equation. *IMA Journal of Numerical Analysis*, 2014. Accepted subject to Major Revision. Preprint available from `http://www.sam.math.ethz.ch/~pgrohs/files/doc.pdf`.

[15] P. Grohs. Smoothness equivalence properties of univariate subdivision schemes and their projection analogues. *Numerische Mathematik*, 113(2):163–180, 2009. DOI: `http://dx.doi.org/10.1007/s00211-009-0231-9`.

[16] P. Grohs. A general proximity analysis of nonlinear subdivision schemes. *SIAM Journal on Mathematical Analysis*, 42:729–750, 2010. DOI: `http://dx.doi.org/10.1137/09075963X`.

[17] P. Grohs. Stability of manifold-valued subdivision schemes and multiscale transformations. *Constructive Approximation*, 32:569–596, 2010. DOI: http://dx.doi.org/10.1007/s00365-010-9085-8.

[18] P. Grohs. Tree approximation with anisotropic decompositions. *Applied and Computational Harmonic Analysis*, 33:44–57, 2012. DOI: http://dx.doi.org/10.1016/j.acha.2011.09.004.

[19] P. Grohs. Quasiinterpolation for Riemannian data. *IMA Journal of Numerical Analysis*, 33:849–874, 2013. DOI: http://dx.doi.org/10.1093/imanum/drs026.

[20] P. Grohs, H. Hardering, and O. Sander. Optimal a priori discretization error bounds for geodesic finite elements. *Foundations of Computational Mathematics*, 2015. In press. Available as SAM Report 2013-16, ETH Zürich, http://www.sam.math.ethz.ch/sam_reports/reports_final/reports2013/2013-16.pdf.

[21] P. Grohs and A. Obermeier. Optimal adaptive ridgelet schemes for linear transport equations. 2014. Submitted. Available as SAM Report 2014-21, ETH Zürich, http://www.sam.math.ethz.ch/sam_reports/reports_final/reports2014/2014-21.pdf.

[22] P. Grohs and M. Sprecher. Total variation regularization by iteratively reweighted least squares on hadamard spaces and riemannian manifolds. 2014. Submitted. Preprint available from http://www.sam.math.ethz.ch/~pgrohs/files/irls.pdf.

[23] P. Grohs and J. Wallner. Interpolatory wavelets for manifold-valued data. *Applied and Computational Harmonic Analysis*, 27(3):325–333, 2009. DOI: http://dx.doi.org/10.1016/j.acha.2009.05.005.

[24] R. Hardt, D. Kinderlehrer, and F. Lin. Existence and partial regularity of static liquid crystal configurations. *Communications in mathematical physics*, 105(4):547–570, 1986.

[25] V. Ivancevic. Symplectic rotational geometry in human biomechanics. *SIAM review*, 46(3):455–474, 2004.

[26] G. Kutyniok and D. Labate. *Shearlets: Multiscale Analysis for Multivariate Data*, chapter Introduction to Shearlets, pages 1–38. Birkhäuser, 2012.

[27] D. Le Bihan, J.-F. Mangin, C. Poupon, C. A. Clark, S. Pappata, N. Molko, and H. Chabriat. Diffusion tensor imaging: concepts and applications. *Journal of magnetic resonance imaging*, 13(4):534–546, 2001.

[28] A. Marthinsen. Interpolation in Lie Groups. *SIAM Journal on Numerical Analysis*, 37(1):269–285, 1999.

[29] A. Myers. Good vibrations: Stanford engineers put a damper on 'aeroelastic flutter', 2011. news.stanford.edu/news/2011/march/airplane-aeroelastic-flutter-032411.html.

[30] P. Neff. A geometrically exact Cosserat shell-model including size effects, avoiding degeneracy in the thin shell limit. Existence of minimizers for zero Cosserat couple modulus. *Mathematical Models and Methods in Applied Sciences*, 17(3):363–392, 2007.

[31] P. Neff. A geometrically exact planar Cosserat shell-model with microstructure: Existence of minimizers for zero Cosserat couple modulus. *Mathematical Models and Methods in Applied Sciences*, 17: 363–392, 2007.

[32] H. Pottmann, A. Asperl, M. Hofer, and A. Kilian. *Architectural Geometry*. Bentley Institute Press, 2007.

[33] H. Pottmann, P. Grohs, and B. Blaschitz. Edge offset meshes in Laguerre geometry. *Advances in Computational Mathematics*, 33:45–73, 2010. DOI: `http://dx.doi.org/10.1007/s10444-009-9119-6`.

[34] H. Pottmann, P. Grohs, and N. Mitra. Laguerre minimal surfaces, isotropic geometry and linear elasticity. *Advances in Computational Mathematics*, 31:391–419, 2009. DOI: `http://dx.doi.org/10.1007/s10444-008-9076-5`.

[35] H. Pottmann, Y. Liu, J. Wallner, A. I. Bobenko, and W. Wang. Geometry of multi-layer freeform structures for architecture. *ACM Transactions on Graphics*, 25(3):1–11, 2007.

[36] O. Sander. Geodesic finite elements for Cosserat rods. *International Journal for Numerical Methods in Engineering*, 82(13):1645–1670, 2010.

[37] M. Skopenkov, H. Pottmann, and P. Grohs. Ruled Laguerre minimal surfaces. *Mathematische Zeitschrift*, 272(1):646–674, 2012. DOI: `http://dx.doi.org/10.1007/s00209-011-0953-0`.

[38] B. Tang, G. Sapiro, and V. Caselles. Color image enhancement via chromaticity diffusion. *IEEE Transactions on Image Processing*, 10(5):701–707, 2001.

[39] I. Ur Rahman, I. Drori, V. C. Stodden, D. Donoho, and P. Schröder. Multiscale representations for manifold-valued data. *Multiscale Modeling and Simulation*, 4(4):1201–1232, 2005.

[40] J. Wallner and H. Pottmann. Intrinsic subdivision with smooth limits for graphics and animation. *ACM Transactions on Graphics (TOG)*, 25(2):356–374, 2006.

[41] A. Weinmann, L. Demaret, and M. Storath. Total variation regularization for manifold-valued data. *arXiv preprint arXiv:1312.7710*, 2013.