

**THE VECTOR SLEPIAN THEORY OF
HIGH NUMERICAL APERTURE
FOCUSING**

PhD thesis booklet

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Background

Focusing coherent light to the smallest possible spot is essential to numerous areas of present-day applied optics, for instance, to laser scanning microscopy, optical lithography, or optical data storage. In these applications, high numerical aperture (NA) focusing systems are usually used, since the diffraction-limited spot size is known to decrease with increasing NA (which itself is proportional to the sine of the angular semi-aperture of the system). There is an increasing demand for controlling finer details of the focal spot as well, e.g. its intensity profile and polarization pattern. This kind of “focal-field engineering” has paved the way to new nanophotonic techniques such as three-dimensional stimulated emission depletion (STED) microscopy [Klar, 2000] and lithography [Klar, 2014] or the determination of the spatial orientation of individual molecules [Novotny, 2001]. Therefore, the role of accurate theoretical models in the design of strongly focused fields cannot be overstated.

Traditional scalar diffraction theory is not suited to describe the focal field of high-NA focusing systems, because vectorial (polarization) effects become significant with increasing NA. In the far-field focusing case (discussed in the thesis), the most widely used vectorial description is the so-called Debye—Wolf integral that represents the focal field as a superposition of homogeneous (vector) plane waves associated to geometrical rays reaching the focal region [Wolf, 1959]. The most important techniques for evaluating the integral itself either rely on fast Fourier transform (FFT) [Leutenegger, 2006] or on various kinds of series expansions [Foreman, 2011]. While FFT-based methods are the winners in terms of computational speed, rapidly converging series expansions may be superior in certain cases, for instance, when one wishes to reduce the number of parameters in an optimization problem.

The so-called multipole theory of focusing [Sheppard, 1997] is one particular theory that relies on a series expansion. It represents the

focal field as a superposition of source-free vector multipole fields that are rigorous solutions to Maxwell’s equations. On the one hand, they have a relatively simple closed form, just as their plane-wave amplitudes described by tangential vector spherical harmonics, which makes them computationally appealing, too. On the other hand, their plane-wave representation consists of homogeneous plane-waves propagating in *all* possible directions, forming pairs of counter-propagating plane waves. Consequently, vector multipole fields are essentially spherical standing waves. As such, they do not resemble usual propagating focused fields, for which the propagation direction of plane-wave components is restricted – to a good approximation – to a spherical cap determined by the angular aperture of the lens (in accordance with the Debye—Wolf theory). We may call this property “directionality” of the focal field [Moore, 2009].

We may assume that focal fields can be approximated using fewer expansion terms in comparison with the multipole approximation, if we choose the basis functions in such a way that they themselves exhibit the directionality dictated by the focusing system [Moore, 2009]. In addition, such basis functions also enable us to invert the Debye—Wolf integral in a straightforward way, because the restrict-edness of plane-wave amplitudes to the above spherical cap is guaranteed.

Goals

The first goal of my PhD work was the creation of vectorial basis functions – starting from a vector spherical harmonics representation – that are well-localized to a spherical cap and can thus serve as a natural basis to approximate plane-wave amplitudes of the Debye—Wolf theory. Moreover, due to the general nature of the problem, the resulting basis functions may be useful to other areas of physics, too.

The second goal was the construction of the focal field basis functions that correspond to the novel plane-wave amplitude basis functions of the previous paragraph and can be used to approximate the focal field.

The third goal was to numerically demonstrate the applicability of the above novel basis functions for forward as well as inverse focusing problems. The former means the calculation of the focal field when the incident field at the entrance pupil is given, while the latter refers to the retrieval of the entrance pupil field that can produce a prescribed focal field. Regarding inverse problems, I placed emphasis on cases where only a prescription on the squared magnitude of the electric field is given in the focal region, because such prescriptions fit real world problems better.

Methods

My method of choice for constructing vectorial basis functions localized to a spherical cap was the solution of Slepian's concentration problem for bandlimited tangential vector fields.

Slepian and his colleagues pioneered in the 1960s in the investigation of the concentration problem of square-integrable bandlimited functions defined on the real line, i.e. the search for a bandlimited function (in the Fourier sense) whose „energy” (the integral of its squared magnitude) is maximally contained within a finite subinterval of its domain. Solving this variational problem actually yielded a whole set of orthonormal functions, a subset of which exhibited excellent concentration property with respect to the above interval [Slepian, 1961].

Later, Slepian's concentration problem was adapted to scalar fields defined over the sphere [Grünbaum, 1982; Simons, 2006]. Studying this problem provided valuable ideas for the solution of the

concentration problem of bandlimited *vector* fields tangential to the sphere.

Focal fields calculated using the new focal field basis functions introduced in the thesis (the so-called „vector Slepian multipole fields”) were validated with help of the Debye—Wolf integral mentioned above.

New scientific results

1. I have solved the Slepian concentration problem of bandlimited tangential vector fields within a spherical cap by reducing it to eigenvalue problems of fixed-order concentration matrices in the vector spherical harmonics basis $\{\mathbf{Y}_{lm}(\theta, \phi), \mathbf{Z}_{lm}(\theta, \phi)\}$. The eigenvectors contain the expansion coefficients of the solutions of the concentration problem (the so-called vector Slepian harmonics). I have shown that (1) the eigenvalue spectrum exhibits the step-like shape that is characteristic to Slepian concentration problems in general, and that (2) the vector Slepian harmonics obtained are doubly orthogonal.

Related publication: [1]

2. I have constructed alternative solutions to the Slepian concentration problem of bandlimited tangential vector fields within a spherical cap by solving the eigenvalue problems of fixed-order concentration matrices in the mixed vector spherical harmonic basis $\{\mathbf{Q}_{lm}^+(\theta, \phi), \mathbf{Q}_{lm}^-(\theta, \phi)\}$. I have shown that in this latter formalism, (1) the vector concentration problem reduces to a scalar problem, the so-called vector-related scalar concentration problem; (2) vector Slepian harmonics can be written in a product form that involves the Sheppard—Török functions $F_{lm}(\cos \theta)$. I have proposed an efficient computational method for the numerical evaluation of vector Slepian harmonics, which is based on special relations of the Sheppard—Török functions I have discovered (an explicit formula for the lowest degree functions and a three-term recurrence relation).

Related publications: [2, 5]

3. I have shown that in the Sheppard—Török basis, the matrix J_m of the differential operator \mathcal{J}_m is tridiagonal (sparse) and commutes under matrix multiplication with the dense fixed-order concentration matrix K_m of the vector-related scalar concentration problem. By solving the eigenvalue problem of sparse matrices J_m , the expansion coefficients of vector Slepian harmonics can be computed with a lower computational cost than using the corresponding dense fixed-order concentration matrices K_m . Unlike matrices K_m , matrices J_m have a simple eigenvalue spectrum, hence their eigenvalue problem can be solved using double precision arithmetic and does not exhibit the numerical instability associated with the eigenvalue problem of concentration matrices.

Related publication: [5]

4. Using vector Slepian harmonics as plane-wave amplitudes, I have defined novel vector Slepian multipole fields, which represent the associated focal fields and are rigorous solutions to the source-free vector Helmholtz equation. I have used vector Slepian multipole fields and vector Slepian harmonics as basis functions to approximate strongly focused fields and their plane-wave amplitudes, respectively. I have shown that with help of the above vector Slepian functions, one can achieve \mathcal{L}^2 -approximation errors of the same order of magnitude – compared to a vector spherical harmonic and vector multipole field approximation, respectively, having the same bandlimit – using a significantly smaller number of expansion terms. The number of terms is approximately given by the sum of partial Shannon numbers associated with the orders involved in the above approximations.

Related publication: [1]

5. By representing the focused field as a linear combination of vector Slepian multipole fields, I have proposed a general approach to solving the inverse problem of high numerical aperture focusing in an approximate way, i.e. computing an electric field at the entrance pupil of the focusing system that produces a prescribed focal field. Importantly, I have demonstrated that this method is also well-suited to inverse optimization problems where only the squared magnitude of the electric field is specified inside a given volume in the focal region.

Related publications: [3, 4]

Utilization of the results

As demonstrated in the thesis, vector Slepian harmonics and multipole fields are a useful tool when solving forward and inverse problems of focusing. In addition, since vector Slepian harmonics form a basis of square-integrable bandlimited tangential vector fields over the sphere, their applicability goes beyond the field of optics. They can be used, for instance, in any least-squares fitting problem where vectorial measurement data are noisy and only available inside a spherical cap region [Plattner, 2015].

It is important to note that vector Slepian harmonics have been introduced independently by A. Plattner and F. J. Simons [Plattner, 2012; Plattner, 2014], too. They extended the the concentration problem to regions other than the spherical cap, too, and also solved it for the radial direction. This broader set of vector Slepian functions (that also includes radial functions) can be used efficiently in various potential-field estimation problems in geophysics, which are based on measurement data of the potential gradient [Plattner, 2015].

Simons and Plattner referred to the computational method of Thesis Point No. 3 (that relies on matrices J_m) as an „exciting discovery” in the second edition of the *Handbook of Geomathematics* [Simons, 2015]. They also pointed out that – for a spherical cap region – „calculations are always fast and [numerically] stable” when using matrices J_m .

Publications related to the thesis statements

- [1] [K. Jahn](#) and N. Bokor. “Vector Slepian basis functions with optimal energy concentration in high numerical aperture focusing,” *Opt. Commun.* **285**(8), 2028–2038 (2012).
DOI: 10.1016/j.optcom.2011.11.107
- [2] [K. Jahn](#) and N. Bokor. “The connection between tightly focused beams and the concentration problem on the sphere,” in: *Proceedings of the PhD Conference organised by the Doctoral School of Physics of the Faculty of Natural Sciences, Budapest University of Technology and Economics (June 22, 2012)*. Ed. by G. Mihály (Doctoral School of Physics of the Faculty of Natural Sciences, Budapest, Hungary, 2012). 10–13. ISBN: 978-963-313-065-0
- [3] [K. Jahn](#) and N. Bokor. “Vector Slepian functions and the inverse problem of high numerical aperture focusing,” in: *Optical Systems Design 2012*. Ed. by L. Mazuray *et al.* Vol. 8550. Proc. SPIE (2012). 855038.
DOI: 10.1117/12.979311
- [4] [K. Jahn](#) and N. Bokor. “Solving the inverse problem of high numerical aperture focusing using vector Slepian harmonics and vector Slepian multipole fields,” *Opt. Commun.* **288**, 13–16 (2013).
DOI: 10.1016/j.optcom.2012.09.051
- [5] [K. Jahn](#) and N. Bokor. “Revisiting the Concentration Problem of Vector Fields within a Spherical Cap: A Commuting Differential Operator Solution,” *J. Fourier Anal. Appl.* **20**(2), 421–451 (2014).
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Further publications

- [6] K. Jahn and N. Bokor. “Intensity control of the focal spot by vectorial beam shaping,” *Opt. Commun.* **283**(24), 4859–4865 (2010).
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- [9] H. Kumagai, Y. Iketaki, K. Jahn, and N. Bokor. “Fabrication of two-color annular hybrid wave plate for three-dimensional super-resolution microscopy,” in: *Three-Dimensional and Multidimensional Microscopy: Image Acquisition and Processing XXIII*. Ed. by T. G. Brown, C. J. Cogswell, and T. Wilson. Vol. 9713. Proc. SPIE (2016). 971311.
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