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3DR REVIEW

The High-Numerical Approach for the 3D Sampling Theorem

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Abstract Point-spread-function engineering constitutes an interesting tool for the improvement of the performance of 3D optical imaging devices like high-resolution optical scanning microscopes. Apart from the gains in resolution, which provide an easy method for the estimation of the superresolving abilities of pupil filters, other analytical tools are necessary for the fast computation of the 3D point spread function. Such tools should take into account the non-paraxial nature of microscopy imaging. In this sense, in this paper we report the high numerical-aperture version of the 3D sampling theorem.

Keywords 3D microscopy; sampling expansion; High-NA apodization

1. Introduction

The control of the beam structure in the three-dimensional (3D) region surrounding the focal point of optical systems is an important task in various applications, such as conventional imaging systems[1-2], optical data storage readout heads[3], or in confocal scanning microscopy[4]. Specifically, in confocal microscopes the 3D point spread function (PSF) of the system is a matter of critical interest, so that several efforts to control its shape by the use of radially-symmetric pupil filters have been reported[5-8]. One method for easy calculation of 3D PSF is based in sampling expansions. The use of such method permits the exact calculation of the overall 3D PSF from its value in a series of equidistant values along the optical axis. It is highly relevant, in this sense the paper published by Landgrave and Berriel-Valdos (L&B)[9] which, however, cannot be used in microscopy application since they derive the sampling expansion from paraxial diffraction formulae. In this sense, the aim of this paper is to extend the L&B results to a high-NA context, so that it could be used both, for the easy calculation of the 3D PSF, and also for the design of new superresolving pupil filters. Our study can be the good complement to other recent researches, like the calculation of the PSF of microscopy systems from the measured pupil complex amplitude transmittance[9], or like the evaluation of high-accurate measurements of the 3D intensity PSF[11-12].

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2. Basic theory

As stated by McCutchen[13], the objective, like a cookie cutter, chops a chunk of the spherical wavefront, which can be regarded as a Huygenian source. The amplitude at any point in the vicinity of the focus is calculated by integrating contributions from this source, taking into account their relative phases. To calculate the amplitude distribution in the neighborhood of the focus, we proceed by making use of the first equation of Rayleigh-Sommerfeld[14], which reconstructs the amplitude distribution in the vicinity of the focus as the superposition of the secondary spherical wavelets originated at the spherical wave-front, namely

$$h(P) = -\frac{i}{\lambda} \int_{S_1} U(P_1) \frac{e^{iks}}{s} d^2 S \tag{1}$$

In the geometry under study $\hat{q}$ and $\hat{s}$ are, respectively, the unit vectors from a typical point, P_1, in the emerging wavefront, to the focal point, F, and to the point of observation P. The amplitude of any secondary wavelets is given by

$$U(P_1) = p(P_1) \frac{e^{-ikf}}{f} \tag{2}$$

where p/f is the amplitude of the Hugenian source. The factor $\exp(-ikf)$ is required to move the zero of phase from the Hugenian source, where it would otherwise be, to the geometric focus. In the vicinity of the focus we can approximate

$$\hat{\mathbf{q}}\mathbf{R} \approx s - f \text{ and } d^2 S \approx f\, d^2\Omega \tag{3}$$

where $d^2\Omega$ is the solid angle that $d^2 S$ subtends at F. Then, Eq.(1) can be rewritten as

$$h(\mathbf{R}) = -\frac{i}{\lambda}\int_{\Omega} p(\hat{\mathbf{q}})\, e^{ik\hat{\mathbf{q}}\mathbf{R}}\, d^2\Omega \tag{4}$$

The above equation constitutes the so-called Debye scalar integral representation of strongly focused fields[15], and expresses the field as coherent superposition of monochromatic plane wavefronts. The directions of propagation of the wavefronts fall inside the geometrical cone defined by the focus and the projection of the pupil function onto the spherical principal surface.

Since in most objective lenses the amplitude transmittance of the aperture stop has axial symmetry, it is convenient to express the positions in the reference sphere in terms of a set of spherical coordinates centered at the focus, then

$$\hat{\mathbf{q}} = \left(-\sin\theta\cos\varphi, -\sin\theta\sin\varphi, \cos\theta\right) \tag{5}$$

and

$$d^2\Omega = \sin\theta\, d\theta\, d\varphi \tag{6}$$

Besides, we express the position of point P in terms of a set of cylindrical coordinates centered again at the focus, then

$$\mathbf{R} = \left(r\cos\psi, r\sin\psi, z\right) \tag{7}$$

Therefore, the amplitude distribution in the focal volume can be written as

$$h(r,\psi,z) = -\frac{i}{\lambda}\int_0^{2\pi}\int_0^{\alpha} p(\theta,\varphi)\exp\{-ikr\sin\theta\cos(\varphi-\psi)\}\, e^{ikz\cos\theta}\sin\theta\, d\theta\, d\varphi \tag{8}$$

Assuming axial symmetry for the pupil amplitude transmittance, the focal amplitude has axial symmetry as well,

$$h(r,z) = -i\frac{2\pi}{\lambda}\int_0^{\alpha} p(\theta) J_0(kr\sin\theta)\, e^{ikz\cos\theta}\sin\theta\, d\theta \tag{9}$$

Again in this case is common the use of normalized coordinates, which are defined as

$$\bar{r} = \frac{r\sin\alpha}{\lambda} \text{ and } \bar{z} = \frac{2z\sin^2\alpha/2}{\lambda} \tag{10}$$

So that we can write the amplitude distribution in the focal volume as

$$h(\bar{r},\bar{z}) = -i\frac{2\pi}{\lambda}\exp\left\{i\pi\frac{\bar{z}}{\sin^2\alpha/2}\right\} \int_0^{\alpha} p(\theta) J_0\left(2\pi\bar{r}\frac{\sin\theta}{\sin\alpha}\right)\exp\left\{-i2\pi\bar{z}\frac{\sin^2\theta/2}{\sin^2\alpha/2}\right\}\sin\theta\, d\theta \tag{11}$$

We must recall at this point that on the projection of the incident plane wavefront onto the emanated spherical wavefront, see Figure 1, energy consideration should be taken into account. Most microscope objectives are designed to fulfill the aplanatic condition, also known as sine condition, in order to produce images with transverse invariance[16-17]. In this case an anodizing factor $g(\theta) = \sqrt{\cos\theta}$ should be included in the integrand of Eq.11. This equation is exact for scalar wave and is a good approximation for light if the NA is small enough so that different parts of the arriving wavefront do not have their polarizations significantly twisted relative to one another on the way to focus.

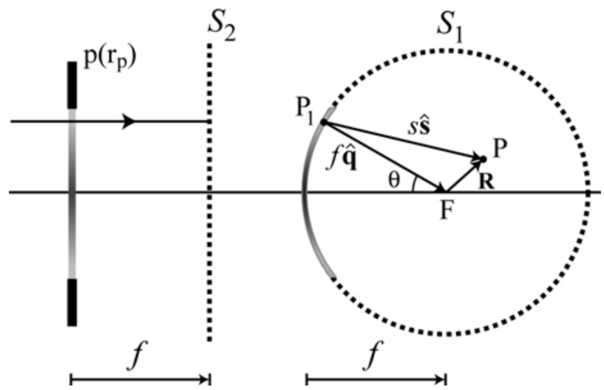

Fig. 1 When a high-NA objective is illuminated by a plane wave, the amplitude transmittance of the aperture stop is projected onto the spherical principal surface.

3. Sampling expansion

PSF engineering constitutes an interesting tool for the improvement of the performance of optical microscopes. Apart from the gains in resolution, which provide an easy method for the estimation of the superresolving abilities of pupil filters, other analytical tools are necessary for the fast computation of the 3D PSF. Sampling expansions of the PSF have been used in the past for the computation of 2D or even 3D diffraction patterns[18-19], but always within the frame of the paraxial approximation. In order to be able to use such tool for calculation of 3D PSF of optical microscopes, it is necessary to extend the L&B[9,] approach to a non-paraxial context. To this end, we start be rewriting Eq. (11) as

$$h(\bar{r},\bar{z}) = -i\frac{2\pi}{\lambda}\int_{\cos\alpha}^{1} p(\cos\theta) J_0\left(2\pi\bar{r}\frac{\sin\theta}{\sin\alpha}\right)\exp\left\{i2\pi\bar{z}\frac{\cos\theta}{2\sin^2\alpha/2}\right\} d(\cos\theta) \tag{12}$$

Let us suppose, next that the kernel of the above transformation

$$K(\theta;\bar{r},\bar{z}) = J_0\left(2\pi\bar{r}\frac{\sin\theta}{\sin\alpha}\right)\exp\left\{i2\pi\bar{z}\frac{\cos\theta}{2\sin^2\alpha/2}\right\} \tag{13}$$

can be expanded in Fourier series as

$$K(\theta;\bar{r},\bar{z}) = \sum_{m=-\infty}^{\infty} f_m(\bar{r},\bar{z})\, K(\theta;0,m) \tag{14}$$

In such case,

$$h(\bar{r},\bar{z}) = -i\frac{2\pi}{\lambda}\sum_{m=-\infty}^{\infty} f_m(\bar{r},\bar{z})\, h(0,m) \tag{15}$$

Following the L&B approach, now the problem consists in finding the coefficients of the kernel expansion. To solve this problem we notice the following orthogonal property,

$$\int_{\cos\alpha}^{1} K(\theta;0,m)K^{*}(\theta;0,m')d(\cos\theta)=(1-\cos\alpha)\delta_{m,m'} \tag{16}$$

which permits us to find that

$$f_{\mathrm{m}}(\bar{r},\bar{z})=\frac{\int_{\cos\alpha}^{1} K(\theta;\bar{r},\bar{z})K^{*}(\theta;0,m)d(\cos\theta)}{1-\cos\alpha}=\frac{h_{\mathrm{C}}(\bar{r},\bar{z}-m)}{1-\cos\alpha} \tag{17}$$

where $h_{\mathrm{C}}(\bar{r},\bar{z})$ is the 3D PSF corresponding to the circular aperture. Finally we obtain

$$h(\bar{r},\bar{z})=-i\frac{2\pi}{\lambda(1-\cos\theta)}\sum_{m=-\infty}^{\infty} h_{\mathrm{C}}(\bar{r},\bar{z}-m)h(0,m) \tag{18}$$

This important formula, which represents the non-paraxial form of the axial sampling theorem, indicates that the 3D amplitude PSF of an optical microscope, in which a pupil filter has been inserted in the objective aperture, results from the coherent superposition of an infinite number of axially-shifted PSFs that correspond to the circular aperture. The shifts are equal to integer numbers. The weighting-factor set of this superposition is obtained by sampling the axial PSF of the pupil filter in the axial nulls of a circular-aperture PSF.

4. Conclusion

In this paper it is derived, for the first time we believe, the non-paraxial form of the 3D sampling theorem. On the basis of the Debye diffraction theory we have obtained a very simple expansion for the calculation of focal amplitude distribution of tightly focused beams. This is very useful since such amplitude distribution constitute the point spread function of modern optical microscopes. This formula can be useful, as well, for the calculation of the binary version of purely-absorbing amplitude modulation elements as done, in a paraxial context in Ref [22].

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