Diffraction Shader

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1 Introduction

1.1 Motivation

In Nature, coloring mostly comes from the inherent colors of materials but sometimes colorization has a pure physical origin such as the effect diffraction or interference of light. Both phenomenon are causing the so called structural coloration, which is the production of color through the interaction of visible light with micrioscopically structured surfaces. Color production is die to wave interference with quasiperiodic structures whose periodicity leads to interaction with visible light. Therefore we perceive color when the different wavelengths composing white light are selectively interfered with by matter (absorbed, reflected, refracted, scattered, or diffracted) on their way to our eyes, or when a non-white distribution of light has been emitted. In animals, such as feathers of birds and the scales of butterflies, interference is created by a range of photonic mechanisms, including diffraction grating, selective mirrors, photonic crystals. The connection between microscopic structures and coloration has been observed by Robert Hooke in the early seventeenth centrury. The discovery of the wave nature of light led to the conclusion that the cause for the coloration lies in wave interference.

In the field of computer graphics, many researchers have been attempted rendering of structural colors by formulating a the bidirectional reflectance distribution function (BRDF) for this purpose. But most of the techniques so far, however, are either too slow for interactive rendering or rely on simplifying assumption, like modeling light as rays, to achieve real-time performance, which are not able capturing the essence of diffraction at all.

1.2 Goals

The purpose of this thesis is to simulate realistically by rendering structural colors caused by the effect of diffraction on different biological structures in realtime. We focus on structural colors generated by diffraction gratings, in particular our approach applies to surfaces with quasiperiodic structures at the nanometer scale that can be represented as heighfields. such structures are found on the sehds of snkaes, wings of butterflies or the bodies of various insects. we restrict ourself and focus on different snake skins sheds which are acquired nanoscaled heightfields using atomic force microscopy.

In oder to achieve our rendering purpose we will rely J. Stam's formula-

tion of a BRDF which basically describes the effect of diffraction on a given surface assuming one knows the hightfield of this surface and will further extend this. Appart from Stam's approach, which models the heightfield as a probabilistic superposition of bumps and proceeds to derive an analytical expression for the BRDF, our BRDF representation takes the heightfield from explicit measurement. I.E. in our case, those heightfields are small patches of the microstructured surfaces (in nano-scale) taken by AFM of snake skin patches provided by our collaborators in Geneva.. So this approach is closer to real truth, since we use measured surfaces instead of statistical surface profile.

Therefore, this work can be considered as an extension of J. Stam's derivations for the case one is provided by a explicit height field on a quasiperiodic structure.

Real time performance is achieved with a representation of the formula as a power series over a variable related to the viewing and lighting directions. Values closely related to the coefficients in that power series are precomputed.

The contribution is that this approach is more broadly applicable than the previous work. Although the previously published formula theoretically has this much flexibility already, there is a novel contribution in demonstrating how such generality can be leveraged in practical implementation

1.3 Previous work

stam, hooke, see our paper, see stams paper, see own research.

Robert Hooke = observed connection between microscopic structures and colorisation wave nature of light led to conclusion that the cause for the coloration lies in wave interference.

previous

In computer graphics literature, Stam was the first to develop reflection models based on wave optics called diffraction shaders, that can produce colorful diffraction effects. His approach is based on a far field approximation of the Kirchhof integral. He shows that for surfaces representeted as nanoscale heightfieds it is possible to derive their BRDF as the Fourier transformation of a function of the heightfield. Nevertheless, this formulation is not immediately useful for efficent rendering of measured complex nanostructures since this would require the on-the-fly evaluation of and and integration over Fourier transforms of the heightfield that depend on the light and viewing geometry. In his derivations, Stam models heightfields as probabilistic superpositions

of bumps forming periodic like structures. This provides him an analytical identity for this class of heightfields. However, boplogocal nanostructures are way more complex and do not lend themself to this simplified statistical model.

follow ups

1.4 Overview

The reminder of this thesis is organized as the follows: due to the fact that this thesis has a rather advanced mathematical complexity the first part of chapter 2 introduces some important definitions which are required in order to be able to follow the derivation in the last third of chapter 2. Before starting the derivations a brief summary of J. Stam's Paper about diffraction shaders is provided since this whole thesis is based on his BRDF representation. Our derivations itself are listed step-wiese, whereas there is a final representation provided by the end of chapter 2. Chapter 3 addresses the practical part of this thesis, the implementation of our diffraction model, explaining all precomputation steps and how rendering is preformed in our developed framework for this thesis. Chapter 4 evaluates the validity of our brdf model by rendering the effect of diffraction of a blaze grating for a fixed reflection direction for every indicent directin. Chapter presents the rendering results of our shader for real world paramters, applying our shader on AFM taken snake patches. The thesis is rounded off by providing a conclusion.

2 Theoretical Background

2.1 Definitions

2.1.1 Diffraction

Diffraction is a purely wave-like phenomenon which cannot be modeled using the standard ray theory of light. Interesting diffraction phenomena, however, occur mostly when the surface detail is highly anisotropic, viz. non-isotropic Interference produces colorful effects due to the phase differences caused by a wave traversing thin media of different indices of refraction Diffraction occurs when the surface detail is comparable to the wave- length of light

Light rays passing through a small aperture will begin to diverge and interfere with one another. This becomes more significant as the size of the aperture decreases relative to the wavelength of light passing through, but occurs to some extent for any aperture or concentrated light source.



Since the divergent rays now travel different distances, some move out of phase and begin to interfere with each other — adding in some places and partially or completely canceling out in others. This interference produces a diffraction pattern with peak intensities where the amplitude of the light waves add, and less light where they subtract. If one were to measure the intensity of light reaching each position on a line, the measurements would appear as bands similar to those shown below.



Diffraction refers to various phenomena which occur when a wave encounters an obstacle. In classical physics, the diffraction phenomenon is described as the apparent bending of waves around small obstacles and the spreading out of waves past small openings.

While diffraction occurs whenever propagating waves encounter such changes, its effects are generally most pronounced for waves whose wavelength is roughly similar to the dimensions of the diffracting objects. If the obstructing object provides multiple, closely spaced openings, a complex pattern of varying intensity can result. This is due to the superposition, or interference, of different parts of a wave that travels to the observer by different paths (see diffraction grating).

The effects of diffraction are often seen in everyday life. The most striking examples of diffraction are those that involve light; for example, the closely spaced tracks on a CD or DVD act as a diffraction grating to form the familiar rainbow pattern seen when looking at a disk

In optics, a diffraction grating is an optical component with a periodic structure, which splits and diffracts light into several beams travelling in different directions. The directions of these beams depend on the spacing of the grating and the wavelength of the light so that the grating acts as the dispersive element.

The relationship between the grating spacing and the angles of the incident and diffracted beams of light is known as the grating equation.

Fresnel and Frauenhofer diffraction frauenhofer diffraction = infinite observation distance. In multiple slit patterns each slit produces a diffraction pattern. Hence, multiple slit interference pattern is superimposed over single slit diffraction pattern.

2.1.2 Radiometry

Light is fundamentally a propagation form of enegry, so it is useful to define the SI unit of energy which is joule (J). To aid our intuituin let us describe radiometry in terms of collections of large numbers of photons. A photon can be considered as a quantum of light that has a position, direction of propagation and a wavelength λ measured in nanometers. A photon has a speed c that depends only on the refractive index n of the medium through which it propagates, which allows us do define the frequency $f = \frac{c}{\lambda}$. The amount of energy q carried by a photon is given by the following relationship: $q = hf = \frac{hc}{\lambda}$ where h is the Plank's constant.

Spectral Energy If there is a large collection of photons given, their total energy $Q = \sum_i q_i$ is the sum of each photon q_i . But how is the energy distributed across wavelenghts? One way in order to determine this distribution is

to order all photons by their associated wavelength and then histogramming them, i.e. discretizing the spectrum and combine all photons which will fall into the same interval, i.e. compute the sum for each interval from the energy of all their photons. By dividing such an interval by its length, denoted as Q_{λ} , we get a relatively scaled interval energy energy, which is called sprectral energy and it is an intensive quantity. Intensive quantities can be though of as density functions that tell the density of an extensive quantity at an infinitesimal point.

Power Power is the estimated rate of energy production for light sources and is measured in the unit watts, denoted by Q, which is another name for joules per second. Since power is a density over time, it is well defined even when energy production is varying over time. As with enery, we are really intereded in spectral power, measured in W/nm, denoted as Φ_{λ}

Irradiance The term irradiance comes into place when we are interested in how much light hits a given point. In order to answer this question, we must make use of a density function. Let δA a fintie area sensor that is smaller than the light field being measured. The spectral irradiance H is just the power per unit area $\delta \frac{\Phi}{\delta A}$ which is $H = \frac{\delta q}{\delta A \delta t \delta \lambda}$ thus the units of irradiance are $Jm^{-2}s^{-1}(nm)^{-1}$

Radiance Although irradiance tells us how much lighjt is arriving at a point, it tells us little about the direction that light comes from. To measure something something similar to what we see with our eyes we need to be able to associate the quantity how much light with a specific direction.

WIKI: http://en.wikipedia.org/wiki/Radiance Radiance and spectral radiance are measures of the quantity of radiation that passes through or is emitted from a surface and falls within a given solid angle in a specified direction. They are used in radiometry to characterize diffuse emission and reflection of electromagnetic radiation. In astrophysics, radiance is also used to quantify emission of neutrinos and other particles. The SI unit of radiance is watts per steradian per square metre $(W \cdot sr-1 \cdot m-2)$, while that of spectral radiance is $W \cdot sr-1 \cdot m-2 \cdot Hz-1$ or $W \cdot sr-1 \cdot m-3$ depending on whether the spectrum is a function of frequency or of wavelength.

Radiance characterizes total emission or reflection. Radiance is useful because it indicates how much of the power emitted by an emitting or reflecting

surface will be received by an optical system looking at the surface from some angle of view. In this case, the solid angle of interest is the solid angle subtended by the optical system's entrance pupil. Since the eye is an optical system, radiance and its cousin luminance are good indicators of how bright an object will appear. For this reason, radiance and luminance are both sometimes called "brightness". This usage is now discouraged – see Brightness for a discussion. The nonstandard usage of "brightness" for "radiance" persists in some fields, notably laser physics

Def
$$L = \frac{d^2\Phi}{dAd\Omega cos(\theta)} \approx \frac{\Phi}{\Omega Acos(\theta)}$$

2.1.3 BRDF

The bidirectional reflectance distribution function, in short BRDF, denoted as $f_r(w_i, w_r)$ is a four dimensional function that defines how light is reflected at an opaque surface. The function takes a negative incoming light direction, ω_i , and outgoing direction, ω_r , both defined with respect to the surface normal \mathbf{n} and returns the ratio of reflected radiance exiting along ω_r to the irradiance incident on the surface from direction ω_i

$$f_r(w_i, w_r) = \frac{dL_r(w_r)}{dE_i(w_i)} \tag{1}$$

$$= \frac{dL_r(w_r)}{L_i(w_i)cos(\theta_i)dw_i}$$
 (2)

where L is radiance, or power per unit solid-angle-in-the-direction-of-a-ray per unit projected-area-perpendicular-to-the-ray, E is irradiance, or power per unit surface area, and θ_i is the angle between ω_i and the surface normal, **n**. The index i indicates incident light, whereas the index r indicates reflected light.

The reason the function is defined as a quotient of two differentials and not directly as a quotient between the undifferentiated quantities, is because other irradiating light than $d E_i(\omega_i)$, which are of no interest for $f_r(\omega_i, \omega_r)$, might illuminate the surface which would unintentionally affect $L_r(\omega_r)$, whereas $d L_r(\omega_r)$ is only affected by $d E_i(\omega_i)$.

2.1.4 Spectral Rendering

In Computer Graphics, spectral rendering is where a scene's light transport is modeled considering the whole span of wavelengths instead of R,G,B values (still relating on geometric optic, which ignore wave phase). The motivation is that real colors of the physical world are spectrum; trichromatic colors are only inherent to Human Visual System.

CIE color spaces CIE 1931 RGB and CIE 1931 XYZ color spaces are the first mathematically defined color spaces. They were created by the International Commission on Illumination (CIE) in 1931.

The CIE's color matching functions $\bar{x}(\lambda)$, $\bar{y}(\lambda)$ and $\bar{z}(\lambda)$ are the numerical description of the chromatic response of the observer (described above). They can be thought of as the spectral sensitivity curves of three linear light detectors yielding the CIE tristimulus values X, Y and Z. Collectively, these three functions are known as the CIE standard observer.[9]

The tristimulus values for a color with a spectral power distribution $I(\lambda)$, are given in terms of the standard observer by:

are given in terms of the standard observer by: $X = \int_{380}^{780} I(\lambda) \, \overline{x}(\lambda) \, d\lambda \, Y = \int_{380}^{780} I(\lambda) \, \overline{y}(\lambda) \, d\lambda \, Z = \int_{380}^{780} I(\lambda) \, \overline{z}(\lambda) \, d\lambda$ where λ , is the wavelength of the equivalent monochromatic light (measured in nanometers).

2.1.5 Signal

A signal is a function that conveys information about the behavior or attributes of some phenomenon. In the physical world, any quantity exhibiting variation in time or variation in space (such as an image) is potentially a signal that might provide information on the status of a physical system, or convey a message between observers

2.1.6 Fourier Transformation

The Fourier-Transform is a mathematical tool which allows to transform a given function or rather a given signal from defined over a time- (or spatial-) domain into its corresponding frequency-domain.

Let f an measurable function over \mathbb{R}^n . Then, the coninious Fourier Transformation, denoted as FT, $\mathcal{F}\{t\}$ of f is defined as, ignoring all constant factors in the formula:

$$\mathcal{F}\{w\}_{FT} = \int_{\mathcal{R}^n} f(x)e^{-iwt}dt \tag{3}$$

whereas its inverse transform is defined like the following which allows us to obtain back the original signal:

$$\mathcal{F}\{w\}_{FT}^{-1} = \int_{\mathbb{R}} \mathcal{F}\{w\} e^{iwt} dt \tag{4}$$

By using fourier analysis, which is the approach to approximate any function by sums of simpler trigonometric functions, we gain the so called discrete time fourier transform (in short DTFT). The DTFT operates on a discrete function. Usually, such an input function is often created by diitally sampling a continius function. The DTFT itself is operation on a discretized signal on a continious, periodic frequency domain and looks like the following:

$$\mathcal{F}\{w\}_{DFT} = \sum_{-\infty}^{\infty} f(x)e^{(-iwk)}$$
 (5)

we can further discretize the frequency domain and will get then the discrete fourier transformation (in short DFT) of the input signal:

$$\mathcal{F}\{w\}_{DFT} = \sum_{n=0}^{N-1} f(x)e^{(-iw_n k)}$$
 (6)

Where the angular frequency w_n is defined like the following $w_n = \frac{2\pi n}{N}$ and N is the number of samples within an equidistant periode sampling.

2.1.7 Convolution

$$(f * g)(t) = \int_{\mathcal{R}^n} f(t)g(t - x)dx \tag{7}$$

Note that the Fourier transform of the convolution of two functions is the product of their Fourier transforms. This is equivalent to the fact that Convolution in spatial domain is equivalent to multiplication in frequency domain. Therefore, the inverse Fourier transform of the product of two Fourier transforms is the convolution of the two inverse Fourier transforms

2.1.8 Taylor Series

Taylor series is a representation of a function as an infinite sum of terms that are calculated from the values of the function's derivatives at a single point.

The Taylor series of a real or complex-valued function f(x) that is infinitely differentiable at a real or complex number a is the power series:

$$\mathcal{T}(f;a)(x) = \sum_{n=0}^{\infty} \frac{f^n(a)}{n!} (x-a)^n$$
 (8)

2.2 Thesis Basis: J.Stam's Paper about Diffraction Shader

GOAL main task in the theory of diffraction is to solve this wave equation for different geometries. we are interested in computing the reflected waves from various types of surfaces

abstract: before: most reflection models empirically or based on ray-theory of light. now: new reflection model based on wave theory modeling the effect of diffraction

In his Paper Diffraction Shader, Jos Stam derives a BRDF which modeling the effect of diffraction for various analytical anistropic reflaction models using the scalar Kirchof theory and the theory of random processes. By employing the so called scalar wave theory of diffraction [source 5 in stams paper] in which a wave is assumed to be a complex valued scalar. It's noteworthy, that stam's BRDF formulation does not take into account the polarization of the light. Fortunately, light sources like sunlight and light bulbs are unpilarizaed. In our simulations we will always assume we have given i directional light source, i.e. sunlight. Hence, we can use stam's model for our derivations

A further assumption in Stam's Paper is, the emanated waves from the source are stationary, which implies the wave is a superposition of independent monochromatic waves. This implies that each wave is associated to a definite wavelangth lambda. However, sunlight once again fulfills this fact.

Mention Helmolth equation, which has the solution $k = \frac{2\pi}{\lambda}$ which is the wavenumber

Based on his these previous assumptions and applying Stam starts his derviations by applying the so called Kirchhoff integral, which is relating the reflected field to the incoming field. This equation is a formalization of Huygen's well-known principle that states that if one knows the wavefront at a given moment, the wave at a later time can be deduced by considering

each point on the first wave as the source of a new disturbance, i.e. once the field $\psi_1 = e^{ik\mathbf{x}\cdot\mathbf{s}\mathbf{s}}$ on the surface is known, the field everywhere ψ_2 else away from the surface can be computed. More precisely, we want to compute the wave ψ_2 equal to the reflection of an incoming planar monochromatic wave $\psi_1 = e^{ikk_1*x}$ traveling in the direction k_1 from a surface S. Mathematically this can be formulized the following:

$$\psi_2 = \frac{ike^{iKR}}{4\pi R} (F\mathbf{v} - \mathbf{p}) \cdot \int_S \mathbf{\hat{n}} e^{ik\mathbf{v} \cdot \mathbf{s}d\mathbf{s}}$$
(9)

In applied optics, when dealing with scattered waves, one does use differential scattering cross-section rather than defining a BRDF which has the following identity:

$$\sigma^{0} = 4\pi \lim_{R \to 0} R^{2} \frac{\langle |\psi_{2}|^{2} \rangle}{\langle |\psi_{1}|^{2} \rangle}$$
 (10)

Relationship between the BRDF and the scattering cross section is the follwing:

The relationship between the BRDF and the scattering cross section can be shown to be equal to $BRDF = \frac{1}{4\pi} \frac{1}{A} \frac{\sigma^0}{cos(\theta_1)cos(\theta_2)}$ Wheras $\theta_1 a$ and θ_2 are the angles that the vectors $\hat{k_1}$ and $\hat{k_2}$ make with the vertical direction.

ADD FIGURE for k1, k2

where R is the disance from the center of the patch to the receiving point x_p , $\hat{\mathbf{n}}$ is the normal of the surface at s and the vectors:

$$\mathbf{v} = \hat{\mathbf{k}_1} - \hat{\mathbf{k}_1} = (u, v, w)$$

$$p=\hat{k_1}+\hat{k_1}$$

During his derivations, Stam provides a analytical representation for the Kirchhoff integral by using his assumptions. He restricts himself to the reflaction of waves from height fields h(x,y) with the assumption that the surface is defined as an elevation over the (x,y) plane using the surface plane approximation.

Which will lead him to the following identity for the Kirchhoff integral

$$\mathbf{I}(ku,kv) = \int \int \frac{1}{ikw} (-p_x, -p_y, ikwp)$$
 (11)

wheras stam formulates for a hightfield auxiliary function $p(x,y) = e^{iwkh(x,y)}$ where $w = -(cos(\theta_i) + cos(\theta_r))$ and θ_i and θ_r are the angles of incident and reflected directions with the surface normal (ADD picture) and the wavenumber $k = \frac{2\pi}{\lambda}$

$$p(x,y) = e^{ikwh(x,y)} \tag{12}$$

We the observation that the integral is a Fourier transform by -iku and -ikv which will lead us to his final derivation, using the identity of BRDF, and computing the limes:

$$BRDF_{\lambda}(w_i, w_r) = \frac{k^2 F^2 G}{4\pi^2 A w^2} \langle |P(ku, kv)|^2 \rangle$$
 (13)

 $BRDF_{\lambda}(w_i,w_r)$ is BRDF where wavelength λ w_i and w_r are incident and reflected normalized directions vectors, pointing away from the given surface. Which can be written, using the fourier transform (FT) P(u,v) = F(p)(u,v), as: $BRDF_{\lambda}(w_i,w_r) = \frac{F^2G}{\lambda^2Aw^2}abs(P(\frac{u}{\lambda},\frac{v}{\lambda}))^2$ where F represents the Fresnel term, uv,v,w are derived from the incident and reflected directions as $(u,v,w) = -\omega_i - \omega_r$, abs(P) represents the expected valuess of a random variable X and A is an area of integration on the surface that is considered to contribute to diffraction, G is the geometry term which is $G = \frac{(1-\hat{\mathbf{k_1}}\cdot\hat{\mathbf{k_2}})^2}{cos(\theta_1)cos(\theta_2)}$

and P(x,y) is the Fourier transform (FT) of the function p(x,y) from above. This identity for the BRDF is the starting point for our derivations.

2.3 Derivations

2.3.1 BRDF formulation

EXPLAIN: Why do we want a formulation for $L_{\lambda}(w_r)$ in some words. what does it represent?

Definition of
$$BRDF(w_i, w_r) := f_r(w_i, w_r) = \frac{dL_r(w_r)}{dE_i(w_i)} = \frac{dL_r(w_r)}{L_i(w_i)\cos(\theta_i)dw_i}$$

Hence, we can dervie the following expression:

$$f_r(w_i, w_r) = \frac{dL_r(w_r)}{L_i(w_i)cos(\theta_i)dw_i}$$

$$=> f_r(w_i, w_r)L_i(w_i)cos(\theta_i)dw_i = dL_r(w_r)$$

$$=> \int_{\Omega} f_r(w_i, w_r)L_i(w_i)cos(\theta_i)dw_i = \int_{\Omega} dL_r(w_r)$$

$$=> L_r(w_r) = \int_{\Omega} f_r(w_i, w_r)L_i(w_i)cos(\theta_i)dw_i$$

We assume, that our incident light is a directional light source like sunlight and therefore its radiance is given as $L_{\lambda}(w) = I(\lambda)\delta(w - w_i)$ where $I(\lambda)$ is the intensity of the relative spectral power for the wavelength λ . Thus we get for our the brdf formulation:

$$L_{\lambda}(w_r) = \int_{\Omega} BRDF_{\lambda}(w_i, w_r) L_{\lambda}(w_i) cos(\theta_i) dw_i$$

$$= BRDF_{\lambda}(w_i, w_r) I(\lambda) cos(\theta_i)$$
(15)

where w_i is the solid angle for the incoming light, θ_i is the angle of incidence, w_r is the solid angle for the reflected light, λ wavelength, Ω is the hemisphre we of integration for the incomming light. Radiance reflected by given surface in given direction: $L_{\lambda}(w_i)$ is the incomming radiance, $L_{\lambda}(w_r)$ is the reflected radiance

For the $BRDF(w_i, w_r)$ we are going to use the formulation dervied by Stam described above which looks like this using the fact that wavenumber $k = \frac{2\pi}{\lambda}$:

$$BRDF(w_{i}, w_{r}) = \frac{k^{2}F^{2}G}{4\pi^{2}Aw^{2}} \langle |P(ku, kv)|^{2} \rangle$$

$$= \frac{k^{2}F^{2}(1 - \hat{\mathbf{k_{1}}} \cdot \hat{\mathbf{k_{2}}})}{cos(\theta_{1})cos(\theta_{2})4\pi^{2}Aw^{2}} \langle |P(ku, kv)|^{2} \rangle$$

$$= \frac{4\pi^{2}F^{2}(1 - \hat{\mathbf{k_{1}}} \cdot \hat{\mathbf{k_{2}}})}{cos(\theta_{1})cos(\theta_{2})4\pi^{2}A\lambda^{2}w^{2}} \langle |P(ku, kv)|^{2} \rangle$$

$$= \frac{F(w_{i}, w_{r})^{2}(1 - \hat{\mathbf{k_{1}}} \cdot \hat{\mathbf{k_{2}}})}{cos(\theta_{1})cos(\theta_{2})A\lambda^{2}w^{2}} \langle |P(ku, kv)|^{2} \rangle$$

where $\hat{\mathbf{k_t}}$ represents a unit vector whose spherical coordinates are given by the solid angle t. Since we are going to integrate over a sphere Ω we can write the component $w = (\cos(\theta_i) + \cos(\theta_r))$ SHOW WHY WE ARE ALLOWED TO WRITE IT LIKE THIS => SPHERICAL COORDINATES DIFFERENCE $(k_1 - k_2) = (u, v, w)$ and so on. this our identity for $L_r(w_r)$ will lead us to the following identity using our identity:

$$\begin{split} L_{\lambda}(w_{r}) &= \frac{F(w_{i}, w_{r})^{2}(1 - \hat{\mathbf{k_{1}}} \cdot \hat{\mathbf{k_{2}}})^{2}}{A\lambda^{2}cos(\theta_{i})cos(\theta_{r})(cos(\theta_{i}) + cos(\theta_{r}))^{2}} \langle \left| P_{cont}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^{2} \rangle cos(\theta_{i})I(\lambda) \\ &= I(\lambda) \frac{F(w_{i}, w_{r})^{2}(1 - \hat{\mathbf{k_{1}}} \cdot \hat{\mathbf{k_{2}}})^{2}}{\lambda^{2}A(cos(\theta_{i}) + cos(\theta_{r}))^{2}cos(\theta_{r})} \langle \left| P_{cont}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^{2} \rangle \\ &= I(\lambda) \frac{F(w_{i}, w_{r})^{2}(1 - \hat{\mathbf{k_{1}}} \cdot \hat{\mathbf{k_{2}}})^{2}}{\lambda^{2}A(cos(\theta_{i}) + cos(\theta_{r}))^{2}cos(\theta_{r})} \langle \left| T_{0}^{2}P_{dtft}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^{2} \rangle \end{split}$$

 P_{cont} is the continious inverse Fourier transform for the taylor seies of our hight-field representing the nano structure, i.e. $P(k,l) = \mathcal{F}^{-1}\{p\}(k,l)$ and P_{dtft} is the dicrete-time inverse Fourier Transform for the same problem domain and T_0 the sampling distance for the discretization pf p(x,y) assuming equal and uniform sampling in both dimensions x,y.

2.3.2 Relative BRDF

reason why relative brdf: In order to scale the reflactiance such that we are able to texture. convex combination reflectance with texture. Scale illumination.

Let us examine what $L_{\lambda}(w_r)$ will be for $w_r = w_0 := (0,0,*)$ i.e. specular reflection case, denoted as $L_{\lambda}^{spec}(w_0)$. When we know the expression for $L_{\lambda}^{spec}(w_0)$ we would be able to compute the relative reflected radiance for our problem by simply dividing $L_{\lambda}(w_r)$ by $L_{\lambda}^{spec}(w_0)$, denoted as

$$\rho_{\lambda}(w_i, w_r) = \frac{L_{\lambda}(w_r)}{L_{\lambda}^{spec}(w_0)} \tag{16}$$

But first, let us derive the following expression:

$$\begin{split} F(w_0, w_0)^2 &(1 - \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix})^2 \\ L_{\lambda}^{spec}(w_0) &= I(\lambda) \frac{\lambda^2 A(\cos(0) + \cos(0))^2 \cos(0)}{\lambda^2 A(\cos(0) + \cos(0))^2 \cos(0)} \langle \left| T_0^2 P_{dtft}(0, 0) \right|^2 \rangle \\ &= I(\lambda) \frac{F(w_0, w_0)^2 (1 + 1)^2}{\lambda^2 A (1 + 1)^2 1} \left| T_0^2 N_{sample} \right|^2 \\ &= I(\lambda) \frac{F(w_0, w_0)^2}{\lambda^2 A} \left| T_0^2 N_{sample} \right|^2 \end{split}$$

Where $N_{samples}$ is the number of samples of the dtft.

Thus, we can plug our last derived expression into the definition for the relative reflectance radiance in the direction w_r and will get:

$$\begin{split} \rho_{\lambda}(w_{i},w_{r}) &= \frac{L_{\lambda}(w_{r})}{L_{\lambda}^{spec}(w_{0})} \\ &= \frac{I(\lambda) \frac{F(w_{i},w_{r})^{2}(1-\hat{\mathbf{k_{1}}}\cdot\hat{\mathbf{k_{2}}})^{2}}{\lambda^{2}A(\cos(\theta_{i})+\cos(\theta_{r}))^{2}\cos(\theta_{r})} \langle \left| T_{0}^{2}P_{dtft}(\frac{2\pi u}{\lambda},\frac{2\pi v}{\lambda}) \right|^{2} \rangle}{I(\lambda) \frac{F(w_{0},w_{0})^{2}}{\lambda^{2}A} \left| T_{0}^{2}N_{sample} \right|^{2}} \\ &= \frac{F^{2}(w_{i},w_{r})(1-\hat{\mathbf{k_{1}}}\cdot\hat{\mathbf{k_{2}}})^{2}}{F^{2}(w_{0},w_{0})(\cos(\theta_{i})+\cos(\theta_{r}))^{2}\cos(\theta_{r})} \langle \left| \frac{P_{dtft}(\frac{2\pi u}{\lambda},\frac{2\pi v}{\lambda})}{N_{samples}} \right|^{2} \rangle \end{split}$$

for simplification and a better overview, let us introduce the following expression, the so called gain factor

$$C(w_i, w_r) = \frac{F^2(w_i, w_r)(1 - \hat{\mathbf{k_1}} \cdot \hat{\mathbf{k_2}})^2}{F^2(w_0, w_0)(\cos(\theta_i) + \cos(\theta_r))^2 \cos(\theta_r) N_{samples}^2}$$
(17)

Using this substitute, we will end up with the following expression for the relative reflectance radiance

$$\rho_{\lambda}(w_i, w_r) = C(w_i, w_r) \langle \left| P_{dtft}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^2 \rangle$$
 (18)

using the previous definition for the relative reflectance radiance $\rho_{\lambda}(w_i, w_r) = \frac{L_{\lambda}(w_r)}{L_{\lambda}^{spec}(w_0)}$ which we can rearrange to the expression

$$L_{\lambda}(w_r) = \rho_{\lambda}(w_i, w_r) L_{\lambda}^{spec}(w_0)$$
(19)

Let us choose $L_{\lambda}^{spec}(w_0) = S(\lambda)$ such that is has the same pforifle as the relative spectral power distribution of CIE Standard Illuminant D65. Further, when integration over λ for a specular surface we should get CIE_XYZ values corresponding to the white point for D65

the corresponding tristimulus values using CIE color matching functions for the CIE_XYZ values look like:

SEE HOW THIS DEFINITION DIFFERS FROM THE WIKIDEF AND HOW WE COULD END UP WITH A SIMILAR DEFINITION.

$$X = \int_{\lambda} L_{\lambda}(w_r) \overline{x}(\lambda) d\lambda \tag{20}$$

$$Y = \int_{\lambda} L_{\lambda}(w_r)\overline{y}(\lambda)d\lambda \tag{21}$$

$$Z = \int_{\lambda} L_{\lambda}(w_r)\overline{z}(\lambda)d\lambda \tag{22}$$

where \overline{x} , \overline{y} , \overline{z} are the color matching functions

Using our last finding for $L_{\lambda}(w_r)$ and the definition for the tristimulus values we can actually derive an expression for computing the colors for our brdf model. Since X, Y, Z are defined similarly, it satisfies to derive an explicit expression for just one tristimulus term, for example X. The other two will look the same, except the we have to replace all X with Y or Z respectively. Therefore, we get:

$$X = \int_{\lambda} L_{\lambda}(w_{r})\overline{x}(\lambda)d\lambda$$

$$= \int_{\lambda} \rho_{\lambda}(w_{i}, w_{r}) L_{\lambda}^{spec}(w_{0})\overline{x}(\lambda)d\lambda$$

$$= \int_{\lambda} \rho_{\lambda}(w_{i}, w_{r})S(\lambda)\overline{x}(\lambda)d\lambda$$

$$= \int_{\lambda} C(w_{i}, w_{r}) \left\langle \left| P_{dtft}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^{2} \right\rangle S(\lambda)\overline{x}(\lambda)d\lambda$$

$$= C(w_{i}, w_{r}) \int_{\lambda} \left\langle \left| P_{dtft}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^{2} \right\rangle S(\lambda)\overline{x}(\lambda)d\lambda$$

$$= C(w_{i}, w_{r}) \int_{\lambda} \left\langle \left| P_{dtft}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^{2} \right\rangle S_{x}(\lambda)d\lambda$$

Where we used the definition $S_x(\lambda)\overline{x}(\lambda)$ in the last step.

2.3.3 Taylour approximation for BRDF

Based on J. Stam's Paper about Diffraction shaders we will show that there is an approximation of his equation (5), $\mathbf{p}(\mathbf{x},\mathbf{y})$, for a explicitly given heightfield $\mathbf{h}(\mathbf{x},\mathbf{y})$. This approximation is achieved by using Taylor-Series and using this identity we will further be able to approximate the Fourier-Transformation of $\mathbf{p}(\mathbf{x},\mathbf{y})$, denoted as $\mathbf{P}(\mathbf{u},\mathbf{v})$. Finally we will give an error bound for this approximation. Finally, we will put our new found identity into our so far found relative BRDF representation.

Taylor Series of p Given $p(x,y)=e^{ikwh(x,y)}$ form Stam's Paper where h(x,y) is here a given heightfield. Also given the definition $e^y=1+y+\frac{y^2}{2!}+\frac{y^3}{3!}+...=\sum_{n=0}^{\infty}\frac{y^n}{n!}$ where y can be real or even complex valued - note this identity can either be derived by power series or by Taylor-Series (using the derivatives of the exp-function and developing the Taylor-Series around the point a=0). Let us now set y=ikwh(x,y) where i is the imaginary number. For simplification, let us denote h(x,y) as h. It follows by our previous stated identities: $e^y=1+(ikwh)+\frac{1}{2!}(ikwh)^2+\frac{1}{3!}(ikwh)^3+...=\sum_{n=0}^{\infty}\frac{(ikwh)^n}{n!}$. Hence it holds $p(x,y)=\sum_{n=0}^{\infty}\frac{(ikwh(x,y))^n}{n!}$.

Fourier Transformation of function p Let us now compute the Fourier Transformation of p(x,y) form above: $\mathcal{F} \{p\} (u,v) = \mathcal{F} \left\{ \sum_{n=0}^{\infty} \frac{(ikwh(x,y))^n}{n!} . \right\} = \mathcal{F}^{lin\,Operator}$ $\sum_{n=0}^{\infty} \mathcal{F} \left\{ \frac{(ikwh(x,y))^n}{n!} \right\} = \sum_{n=0}^{\infty} \frac{(ikwh)^n}{n!} \mathcal{F} \{h(x,y)^n\}. \text{ Hence it follows: } P(\alpha,\beta) = \sum_{n=0}^{\infty} \frac{(ikwh)^n}{n!} \mathcal{F} \{h^n\} (\alpha,\beta).$

NB: $\mathcal{F}\{h^n\}$ (u,v) denotes the two dimensional Fourier Transformation of p(x,y) and can be numerically computed by the two dimensional **DFT** or rather by the two dimensional **FFT** over h(x,y).

Approximation of function P Next we are going to look for an $N \in \mathbb{N}$ s.t. $\sum_{n=0}^{N} \frac{(ikwh)^n}{n!} \mathcal{F}\{h^n\}(\alpha,\beta) \approx P(\alpha,\beta)$. is a good approximation. We have to prove two things:

- 1. Show that there exist such an $N \in \mathbb{N}$ s.t the approximation holds true.
- 2. Find a value for B s.t. this approximation is below a certain error bound, for example machine precision ϵ .

Proof Sketch of 1. By the **ratio test** (see [1]) we can show that the series $\sum_{n=0}^{N} \frac{(ikwh)^n}{n!} \mathcal{F}\{h^n\}(\alpha,\beta)$ converges absolutely:

Proof: Consider $\sum_{k=0}^{\infty} \frac{y^n}{n!}$ where $a_k = \frac{y^k}{k!}$. By the definition of the ratio test for series it follows: $\forall y : limsup_{k\to\infty} |\frac{a_{k+1}}{a_k}| = limsup_{k\to\infty} \frac{y}{k+1} = 0$

Thus this series converges absolutely, no matter what value we will pick for y.

Part 2: Find such an N Let $f(x) = e^x$. We can formulate its Taylor-Series, stated above. Let $P_n(x)$ denote the n-th Taylor-Polinomial, $P_n(x) = \sum_{k=0}^n \frac{f^{(k)}(a)}{k!} (x-a)^k$, where a is our developing point (here, in this case a=0). We can define the error of the n-th Taylor-Polinomial to be $E_n(x) = f(x) - P_n(x)$. That error is the actual value minus the Taylor polinomial. It holds true: $|E_n(x)| = |f(x) - P_n(x)|$. By using the Lagrangien Error Bound (see source [2]) it follows: $|E_n(x)| \leq \frac{M}{(n+1)!} |x-a|^{n+1}$ with a=0, where M is some value satisfying $|f^{(n+1)}(x)| \leq M$ on the interval I = [a,x]. Since we are interested in an upper bound of the error and since a is known, we can reformulate the interval as $I = [0, x_{max}]$, where $x_{max} = |i| * k_{max} * w_{max} * h_{max}$, since we are interested in computing an error bound for $e^{ikwh(x,y)}$.

From Stam's Paper about diffraction shader we know some paramters for the length, width and height for a given sample patch, i.e. heightfield h(x,y) and when using those parameters are able to find a explicit number for x_{max} .

Facts we are using from Stam's Paper:

- Height of bump: 0.15micro meters
- Width of a bump: 0.5micro meters
- Length of a bump: 1micro meters
- $k = \frac{2\pi}{\lambda}$ is the wavenumber and $\lambda \in [\lambda_{min}, \lambda_{max}]$ its wavelength hence $k_{max} = \frac{2\pi}{\lambda_{min}}$
- w is a component of the vector $\vec{v} = \vec{k_1} \vec{k_2} = (u, v, w)$, where $\vec{k_1}$ and $\vec{k_2}$ are **normalized** direction vectors and this each component can have a value in range [-2, 2].
- for simplification, assume $[\lambda_{min}, \lambda_{max}] = [400nm, 700nm]$.

Hence $x_{max} = |i| * k_{max} * w_{max} * h_{max} = k_{max} * w_{max} * h_{max} = 2 * (\frac{2\pi}{4*10^{-7}m}) * 1.5 * 10^{-7} = 1.5\pi$ and it follows for our intervall $I = [0, 1.5\pi]$. Next we are going to find the value for M. Since the exponential function is monoton growing (on the interval I) and and the derivative of the \exp function is the exp function itself, we can find such an M: $M = e^{x_{max}} = exp(1.5\pi)$ and $|f^{(n+1)}(x)| \leq M$ holds. With $|E_n(x_{max})| \leq \frac{M}{(n+1)!} |x_{max} - a|^{n+1} = \frac{exp(1.5\pi)*(1.5\pi)^{n+1}}{(n+1)!}$ we now can find a value of n for a given bound, i.e. we can find an value of $N \in \mathbb{N}$ s.t. $\frac{exp(1.5\pi)*(1.5\pi)^{N+1}}{(N+1)!} \leq \epsilon$. With Octave/Matlab we can see:

- if N=20 then $\epsilon \approx 2.9950 * 10^{-4}$
- if N=25 then $\epsilon \approx 8.8150 * 10^{-8}$
- if N=30 then $\epsilon \approx 1.0050 * 10^{-11}$

Conclusion With this approach we have that $\sum_{n=0}^{25} \frac{(ikwh)^n}{n!} \mathcal{F}\{h^n\}$ (α,β) is an approximation of P(u,v) with error $\epsilon \approx 8.8150 * 10^{-8}$. This means we can precompute 25 Fourier Transformations (for example via FFT2) and then sum them up in order to approximate P(u,v) and $\epsilon \approx 8.8150 * 10^{-8}$. This approach will allow us to speed up our shader. Furthermore we see that when we just take 5 more iterations, we will reduce the error bound to the dimension of 10^{-11} .

Using $P_{dtft} = \mathcal{F}^{-1}\{p\}(u,v)$ definied in the section of the taylor approximationwe get for the tristumulus value X, we will get:

$$X = C(w_i, w_r) \int_{\lambda} \left\langle \left| P_{dtft}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^2 \right\rangle S_x(\lambda) d\lambda$$

= $C(w_i, w_r) \int_{\lambda} \left| \sum_{n=0}^{N} \frac{(wk)^n}{n!} \mathcal{F}^{-1} \{i^n h^n\} (\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda}) \right|^2 S_x(\lambda) d\lambda$

2.3.4 Sampling: Gaussian Window

why this identity works: The DFT of a discrete heightfield patch is equivalent to the DTFT of an infinitely periodic function consisting of replicas of the same discrete patch. By windowing with a window function that is zero outside the central replica, the convolution of either the DFT or the DTFT of heightfield with the fourier transfrom of the window becomes equivalent.

Let $window_g$ denote the gaussian window with $4\sigma_s$ μm where $\sigma_f = \frac{1}{2\pi\sigma_s}$ let us further substitute $\mathbf{t}(\mathbf{x},\mathbf{y}) = i^n h(x,y)^n$

$$\mathcal{F}_{dtft}^{-1}\{\mathbf{t}\}(u,v) = \mathcal{F}_{fft}^{-1}\{\mathbf{t}\}(u,v)window_g(\sigma_f)$$
 (23)

Therefore we can deduce the following expression from this:

$$\mathcal{F}_{dtft}^{-1}\{\mathbf{t}\}(u,v) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_{fft}^{-1}\{\mathbf{t}\}(w_{u},w_{v})\phi(u-w_{u},v-w_{v})dw_{u}dw_{v}
= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{i} \sum_{j} F_{fft}^{-1}\{\mathbf{t}\}(w_{u},w_{v})\delta(w_{u}-w_{i},w_{v}-w_{j})\phi(u-w_{u},v-w_{v})dw_{u}dw_{v}
= \sum_{i} \sum_{j} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_{fft}^{-1}\{\mathbf{t}\}(w_{u},w_{v})\delta(w_{u}-w_{i},w_{v}-w_{j})\phi(u-w_{u},v-w_{v})dw_{u}dw_{v}
= \sum_{i} \sum_{j} F_{fft}^{-1}\{\mathbf{t}\}(w_{u},w_{v})\phi(u-w_{u},v-w_{v})$$

where
$$\phi(x,y) = \pi e^{-\frac{x^2+y^2}{2\sigma_f^2}}$$

2.3.5 Aplitude smooting

Let us consider the so called 1-dimensional Box-function with length T which is defined as the following: ADD AN IMAGE OF BOXFUNCTION

$$Box(x) = \begin{cases} 1 & \text{if } x \le T \\ 0 & \text{if } else \end{cases}$$

We assume, that our given heighfield can be represented as a 2-dimensional box-function. Note that we can use any explicit given constrainted 2-dimensional function and will get some identities like we get from the box-function.

Further we are assuming that we can model the overall surface be assuming this heighfield being distributed in a periodic manor. Therfore, the whole surface can be represented like this $f(x) = \sum_{n=0}^{N} Box(x+nT_1,y+mT_2)$ assuming the given heighfield has the dimensions T_1 by T_2 . But let us first consider the 1-dimensional Box-function case before deriving an identity for the Fourier transform of our 2-dimensional Box-function, i.e. the fourier transform of our heighfield.

Note: A function f periodic with periode T means: $\forall x \in \mathcal{R} : Box(x) = Box(x+T)$

A so called bump can be represented by our 1-dimensional Box-function. We assume periodicity which is equaivalent to: $f(x) = \sum_{n=0}^{N} Box(x + nT)$

We are insterested in the 1-dimensional inverse Fourier transform of the 1-dimensional Box-function:

$$\mathcal{F}^{-1}{f}(w) = \int f(x)e^{iwx}dx$$

$$= \int_{-\infty}^{\infty} \sum_{n=0}^{N} Box(x+nT)e^{iwx}dx$$

$$= \sum_{n=0}^{N} \int_{-\infty}^{\infty} Box(x+nT)e^{iwx}dx$$

Next, apply the following substituation x + nT = y which will lead us to:

$$x = y - nT$$
$$dx = dy$$

Plugging this substituation back to the equation from above we will get

$$\mathcal{F}^{-1}\{f\}(w) = \int f(x)e^{iwx}dx$$

$$= \sum_{n=0}^{N} \int_{-\infty}^{\infty} Box(y)e^{iw(y-nT)}dy$$

$$= \sum_{n=0}^{N} e^{-iwnT} \int_{-\infty}^{\infty} Box(y)e^{iwy}dy$$

$$= \sum_{n=0}^{N} e^{-iwnT} \mathcal{F}\{f\}(w)$$

$$= \mathcal{F}^{-1}\{f\}(w) \sum_{n=0}^{N} e^{-iwnT}$$

We used the fact that the term e^{-iwnT} is a constant when integrating along dy and the identity for the inverse Fourier transform of the Box function. Next, let us consider $\sum_{n=0}^{N} e^{-uwnT}$ further:

$$\sum_{n=0}^{N} e^{-uwnT} = \sum_{n=0}^{N} (e^{-uwT})^{n}$$
$$= \frac{1 - e^{iwT(N+1)}}{1 - e^{-iwT}}$$

We recognize the geometric series identity for the left-handside of this equation. Since our series is bounded we can derive our right-handside.

Since e^{-ix} is a complex number and every complex number can be written in its polar form, i.e. $e^{-ix} = cos(x) + isin(x)$ we can go even further, using the trigonometric idententities that cos(-x) = cos(x) and sin(-x) = -sin(x):

$$\frac{1 - e^{iwT(N+1)}}{1 - e^{-iwT}} = \frac{1 - \cos(wT(N+1)) + i\sin(wT(N+1))}{1 - \cos(wT) + i\sin(wT)}$$

Which is still a complex number (p+iq). Every complex number can be written as a fraction of two complex numbers. This means that the complex number (p+iq) can be written as $(p+iq) = \frac{(a+ib)}{(c+id)}$ for any (a+ib), (c+iq) $id) \neq 0$. For our case, let us use the following substituations:

$$a := 1 - cos(wT(N+1)) \qquad b = sin(wT(N+1)) \qquad (24)$$

$$c = 1 - cos(wT) \qquad d = sin(wT) \qquad (25)$$

$$c = 1 - \cos(wT) \qquad \qquad d = \sin(wT) \tag{25}$$

hence it follows $\frac{1-e^{iwT(N+1)}}{1-e^{-iwT}} = \frac{(a+ib)}{(c+id)}$. By rearanging the terms it follows (a+ib) = (c+id)(p+iq) and multiplying the right handside out we get the following system of equations:

$$(cp - dq) = a \tag{26}$$

$$(dp + cq) = b (27)$$

Which gives lead us we some further math (trick: mult first eq. by c and 2nd by d, then adding them together using distributivity and we have the identity for p for example, similar for q) to

$$p = \frac{(ac + bd)}{c^2 + d^2} \tag{28}$$

$$q = \frac{(bc + ad)}{c^2 + d^2} \tag{29}$$

Putting our substituation for a, b, c, d back into the current representation for p and q and using some trigonometric identities, this we then get:

$$p = \frac{1}{2} + \frac{1}{2} \left(\frac{\cos(wTN) - \cos(wT(N+1))}{1 - \cos(wT)} \right)$$
 (30)

$$q = \frac{\sin(wT(N+1)) - \sin(wTN) - \sin(wT)}{2(1 - \cos(wT))}$$
(31)

Since we have seen, that $\sum_{n=0}^{N} e^{-uwnT}$ is a complex number and can be written as (p+iq) and we know now the explicit identity for those p and q we get for the 1-dimensional Fourier transform of the 1-dimensional Boxfunction the following final identity:

$$\mathcal{F}^{-1}{f}(w) = \mathcal{F}^{-1}{f}(w) \sum_{n=0}^{N} e^{-iwnT}$$
$$= (p+iq)\mathcal{F}^{-1}{Box}(w)$$

In oder to derive next a identity for the Fourier transform for our 2-dim heighfield, we can proceed similarly, the only fact which changes is, that we are now in a 2-dimensional domain, i.e. we are about to compute a two-dimensional Fourier transform: Let us again us again a Box-function, this time a 2-dimensional Box-function Box(x,y) just for the sake of convenience.

$$\mathcal{F}^{-1}\{f\}(w_{1},w_{2}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{n_{2}=0}^{N_{1}} \sum_{n_{2}=0}^{N_{2}} Box(x_{1} + n_{1}T_{1}, x_{2} + n_{2}T_{2})e^{iw(x_{1}+x_{2})}dx_{1}dx_{2}$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{n_{2}=0}^{N_{1}} \sum_{n_{2}=0}^{N_{2}} Box(y_{1},y_{2})e^{iw((y_{1}-n_{1}T_{1})+(y_{2}+n_{2}T_{2}))}dx_{1}dx_{2}$$

$$= \sum_{n_{2}=0}^{N_{1}} \sum_{n_{2}=0}^{N_{2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} Box(y_{1},y_{2})e^{iw(y_{1}+y_{2})}e^{-iw(n_{1}T_{1}+n_{2}T_{2})}dy_{1}dy_{2}$$

$$= \sum_{n_{2}=0}^{N_{1}} \sum_{n_{2}=0}^{N_{2}} e^{-iw(n_{1}T_{1}+n_{2}T_{2})} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} Box(y_{1},y_{2})e^{iw(y_{1}+y_{2})}dy_{1}dy_{2}$$

$$= \left(\sum_{n_{2}=0}^{N_{1}} \sum_{n_{2}=0}^{N_{2}} e^{-iw(n_{1}T_{1}+n_{2}T_{2})}\right) \mathcal{F}^{-1}\{Box\}(w_{1},w_{2})$$

$$= \left(\sum_{n_{2}=0}^{N_{1}} e^{-iwn_{1}T_{1}}\right) \left(\sum_{n_{2}=0}^{N_{2}} e^{-iwn_{2}T_{2}}\right) \mathcal{F}^{-1}\{Box\}(w_{1},w_{2})$$

$$= (p_{1}+iq_{1})(p_{2}+iq_{2})\mathcal{F}^{-1}\{Box\}(w_{1},w_{2})$$

$$= (p_{1}p_{2}-q_{1}q_{2})+i(p_{1}p_{2}+q_{1}q_{2}))\mathcal{F}^{-1}\{Box\}(w_{1},w_{2})$$

$$= (p+iq)\mathcal{F}^{-1}\{Box\}(w_{1},w_{2})$$

Where we define $p := (p_1p_2 - q_1q_2)$ and $q := (p_1p_2 + q_1q_2)$. For this identity we used green's integration rule which allowed us to split the double integral to the product of two single integrations. Also, we used the definition of the 2-dimensional inverse Fourer transform of the Box-function. We applied the same substituation like we did in for the 1 dimensional case, but this time twice, once for each variable seperately. The last step, substituting with p and q will be useful later in the implementation. The insight should be, that the product of two complex numbers is again a complex number. We will have to compute the absolute value of $\mathcal{F}^{-1}\{f\}(w_1, w_2)$ which will then be equal $(p^2 + q^2)^{\frac{1}{2}} |\mathcal{F}^{-1}\{Box\}(w_1, w_2)|$

2.3.6 Final Expression

As the last step of our series of derivations, we plug all our findings together to one big equation in order to compute the colors in the CIE_XYZ colorspace:

For a given heigh-field h(x,y), representing a small patch of the nanostructure of our surface, the resulting CIE_XYZ caused by the effect of diffraction can be computed like the following: Let $P(u, v, \lambda) = F_{fft}^{-1} \{i^n h^n\} (\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda})$

Let
$$P(u, v, \lambda) = F_{fft}^{-1}\{i^n h^n\}(\frac{2\pi u}{\lambda}, \frac{2\pi v}{\lambda})$$

$$\begin{pmatrix}
X \\
X \\
Z
\end{pmatrix} = C(w_i, w_r) \int_{\lambda} \sum_{n=0}^{N} \frac{(wk)^n}{n!} \sum_{r} \sum_{s} |P(u - w_r, v - w_s, \lambda)|^2$$

$$\phi(u - w_r, v - w_s) \begin{pmatrix} S_x(\lambda) \\ S_y(\lambda) \\ S_z(\lambda) \end{pmatrix} d\lambda$$
(32)

where $\phi(x,y)=\pi e^{-rac{x^2+y^2}{2\sigma_f^2}}$ is the gaussian window, where w_s and w_r are ... explain them

3 Implementation

how to discretize from final derivation to computation? what do we have to precompute, what during runtime? how does the final algorithm look like explain shaders: vertex(geometriy, precomp) - and fragment-shader(in local space-tspace) how from cie_xyz to cie_rgb how gamma correction how texturing can we do better? our approaches

TODO: explain that there is the jrtr and the scene code - what are their responsibilities.

shader

show schema: scene data => GPU=[Vertex processing, modeling and viewing transformation => Projection => Rasterization, fragment processing, visibility] => image

In computergraphics, we are interested in synthesizing 2d images from a given scene containing our 3d geometries by using so called shader programs. This process is dentonoted as rendering. The purpose of shader programs, which are executed directly on the GPU hardware device, is to compute the colorization and illumination of the objects living in our scene. All these computations happen in several stages and depend on the provided scene-input parameters like the camera, light sources, objects material constants and the desired rendering effect one is interested in to model. The shader stages are implemented sequencially as small little programs, the so called vertex-, geometry- and fragment-shaders. Those stages are applied within the rendering pipeline sequencially.

Our shaders which we use are written in a highlevel language called GLSL, the OpengGL Shading Language. The decission for using OpenGL has been made since my underlying framework, which is responsible for the precomputation of all scene date, is based on another framework, written in Java using JOGL in oder to communicate with the GPU and is also responsible to precompute all the relevant scene data. This framework, the so called jrtr framework, has been developed as an exercise during the class computer graphics held by M. Zwicker which I attended in autumn 2012. The framework itself has been used and further extended during this thesis quite a lot. All necessary input data required for our java framework in order to perfrom the shading is precomputed by using Matlab. This is basically addressing all the required precomputations for the provided heigh-fields, refering to computation of the inverse two dimensional Fourier transformations which are further explained within this chapter. The matlab scripts themself rely on

the provided snake nano-scaled sheds images, taken by AFM.

SHOW ARCHITECTURE GRAPHIC from CG

It's noteworthy that all the vertices are processed within the vertex-shader, whereas the fragement shader's responsibility is to perfrom pixelwise rendering, using the input from the vertex shader. Just remember, fragements are determined by a triple of vertices, hence each pixel has assigned a trilinear interpolated value of all input parameters of its spanning vertices. Usually, all necessary transformations are applied vertex-wise, considering the vertex-shader as the precomputation stage for the later rendering within the rendering pipeline, in the fragment-shader. In the geometry shader, new vertices around a considered vertex can be created, this is useful for debugging - displaying normals graphically for example.

In this part of thesis we are going to explain how we render our BRDF formulation derived in the last section in practice. all the necessary computations in order to simulate the effect of diffraction are performed within a fragment shader. This implies that we are modeling the effect of diffraction pixelwise and hence the overall modeling quality and computional pace depends on rendering window's resolution.

By the end of this chapter we will have seen how our how our render works, what we have to precompute and how our shaders work.

3.1 Precomputations in Matlab

Our first task is to precompute the inverse two dimensional discrete fourier transformations of a given snake shed patch of interest taken by AFM. For that purpose we have written a small matlab script which offers a huge collection of mathematically, nummerically fast and stable alforithmes. Our matlab script reads a given image, which is representing a nano-sclaed heightfield, and computes its inverse two dimensional DFT by using matlab's internel inverse fast fourier transformation function, denoted by ifft2. Note that we only require once color channel of the input image since the input image is representing an heightfield, encoded by just one color. Basically, we are interested in computing the ifft2 for different powers of the input image since our taylor series approximation for the overall computation relies on this. Keep in mind that taking the fourier transformation of an arbitrary function will result in a complex valued output which imples that we will get a complex value for each pixel of our input image. Therefore, for each input image we get as many output images, representing the two dimensional in-

verse fourier transformation, as the minimal amount of taylor terms required for a well-enough approximation. In order to store our output images, we have to use 2 color channels instead just one like it was for the given input image. As an optimization step, we do not directly store images, rather we output binary files which contain all RGB values for each pixel in a row first, coloumn last format. This allows us to have much higher precission for the output values and also it does not waste any color channels. Note that we have scaled each pixel value in a range between 0 and 1. Therefore, we have to remember store four scaling factors for each output image as well, which are the real and imaginary minimum and maximum values. Later, using linear interpolation within the shaderm we will get back the image's original values.

Say something about shifting - the centering why required? list code

3.2 Our Java Renderer

based on cg class...

3.2.1 Scene

what is its purpose

explain geometry computation explain light(source) setup explain factories explain camera setup explain how materials are stored explain how assigned to jrtr

3.2.2 jrtr Framework

rendering synthesis of 2d images from 3d scene description. rendering algorithms interpret data structures that represent scenes using geometric primitives, matrial properties and lights. Input: Data structures that represent scene (geometry, material properties, lights, virtual camera) Output: 2d images (array of pixels - RGB for each pixel)

focus of computer graphics: interactive rendering in order to produce images within a short periode of time which should be as photorealistic as possible - depending on applied shading apporach.

in class(framework) - build own 3d rendering engine

rendering 3d models: camera simulation, interactive viewing, lighting, shading, modeling: triangle meshes, smotth surfaces java base code, openGL

3.0,

explain how this will work explain how passed to glsl shader - see computer graphics slides maybe show schematically the architecture

3.3 GLSL Diffraction Shader

explain vertex shader and fragment shader and how they are related. show rendering pipeline image

review fragment- and vertex-shader

start using the final findings from chapter 2 and substitute explain how all the components are computed and why they are computed like this.

3.3.1 Vertex Shader

The first computional stage within our rendering pipeline is computing all necessary per vertex data. Those computations are preformed in the vertex shader. In our case, we compute for any vertex of our current geometry the direction vectors k1 and k2 described like previousely in the tangent space. Initially all input data lives in its own space. Hence, we first have to transfrom all input data into the same space in order to use it for later computations within the fragment shader. We are going to transform k1 and k2 into the so called tangent space which. Furthermore, we have also to realign our local coordinate system. This is why there is an rodrigues rotation also involved. In order to avoid scaling issues and since we are only interested in the direction of the vectors k1 and k2, we have to normalize them, too. Last, we also output the position of the current vertex transfomed into the projective camera space.

explain cop_w modelM other shader assigned inputs

3.3.2 Fragment Shader

The purpose of a fragment shader is to render per fragment. A fragment is spaned by three vertices of a given mesh. For each pixel within all the output from the vertex shaders of its corresponding vertices is then trilinearly interpolated, depending on the pixel's position within the fragment, and passed into its fragment shader program. Furthermore, there can be additional input be assigned which is not directly interpolated from the output of vertex shader programs. Our fragment shader just relies on k1 and k2 from its vertex

Algorithm 1 Vertex diffraction shader

```
foreach Vertex \ v \in Shape \ do
vec3N = normalize(modelM * vec4(normal, 0.0)).xyz
vec3T = normalize(modelM * vec4(tangent, 0.0)).xyz
T = rotateRodrigues(T, N, phi)
vec3B = normalize(cross(N, T))
vec3Pos = ((cop_w - position)).xyz
vec4lightDir = (directionArray[0])
lightDir = normalize(lightDir)
l = projectVectorOnTo(lightDir, TangentSpace)
p = projectVectorOnTo(Pos, TangentSpace)
normalize(l); normalize(p)
gl_Position = projection * modelview * position
end for
```

shaders for the computation of the effect of diffraction. There are some values preliminarily assigned to our fragment shader during the opgengl setup within our java program, like all references to the image buffers, containing the fourier transformations, the number of taylor step approximations, the minimal and maximal wavelength, other lookup values like the scaling factors, a reference to a lookup table containing the cie xyz color weights for our wavelength domain and other scaling constants.

tell how we are going to sample - uniformly along lambda - explain draw-back of this approach - explain possible solutions for this issue. maybe refer to reference shader or leave this for the disscusion part.

one which basically samples the whole lambda space using a gaussian window. This shader will be modeling the effect of diffraction completely but will also be rather slow. The other shader will use a gaussian window too but will just use a few wavenumber for the sampling process. Furthermore, this shader will thread specularity seperatly as a special case which will be more like an approximation.

Algorithm 2 Fragment diffraction shader

```
foreach Pixel p \in Fragment do
   INIT BRDF_{XYZ}, BRDF_{RGB} TO vec4(0.0)
   (u, v, w) = \hat{\mathbf{k_1}} - \hat{\mathbf{k_2}}
   for (\lambda = \lambda_{min}; \lambda \leq \lambda_{max}; \lambda = \lambda + \lambda_{step}) do
       xyzWeights = getClrMatchingFnWeights(\lambda)
       lookupCoord = getLookupCoord(u, v, \lambda)
       INIT P TO vec2(0.0)
       k = \frac{2\pi}{\lambda}
       for (n = 0 \text{ TO } MAXTAYLORTERMS) do
           taylorScaleF = \frac{(kw)^n}{n!}
           INIT F_{fft} TO vec2(0.0)
           anchor X = int(floor(center.x + lookupCoord.x * fftImWidth)
           anchorY = int(floor(center.y + lookupCoord.y * fftImHeight)
           for (i = (anchorX - winW) \text{ TO } (anchorX + winW + 1)) \text{ do}
               for (j = (anchorY - winW) TO (anchorY + winW + 1)) do
                   dist = getDistVecFromOriginFor(i, j)
                   position = getLocalLookUp(i, j, n)
                   fftVal = getRescaledFourierTextureValueAt(position)
                   fftVal *= getGaussWeightAtDistance(dist)
                   F_{fft} += fftVal
               end for
           end for
           P += taylorScaleF * F_{fft}
       xyzPixelColor += dot(vec3(|P|^2), xyzWeights)
   end for
   BRDF_{XYZ} = xyzPixelColor * C(\hat{\mathbf{k_1}}, \hat{\mathbf{k_2}}) * shadowF
   BRDF_{RGB}.xyz = D_{65} * M_{XYZ-RGB} * BRDF_{XYZ}.xyz
   BRDF_{RGB} = gammaCorrect(BRDF_{RGB})
end for
```

4 Data Acquisition and Evaluation

what is this chapter about how is evaluation perfromed our shader

4.1 Diffraction Grating

Gratings may be of the reflective or transmissive type, analogous to a mirror or lens respectively. A grating has a zero-order mode (where m=0), in which there is no diffraction and a ray of light behaves according to the laws of reflection and refraction the same as with a mirror or lens respectively.

An idealised grating is considered here which is made up of a set of slits of spacing d, that must be wider than the wavelength of interest to cause diffraction. Assuming a plane wave of wavelength with normal incidence (perpendicular to the grating), each slit in the grating acts as a quasi pointsource from which light propagates in all directions (although this is typically limited to a hemisphere). After light interacts with the grating, the diffracted light is composed of the sum of interfering wave components emanating from each slit in the grating. At any given point in space through which diffracted light may pass, the path length to each slit in the grating will vary. Since the path length varies, generally, so will the phases of the waves at that point from each of the slits, and thus will add or subtract from one another to create peaks and valleys, through the phenomenon of additive and destructive interference. When the path difference between the light from adjacent slits is equal to half the wavelength, /2, the waves will all be out of phase, and thus will cancel each other to create points of minimum intensity. Similarly, when the path difference is , the phases will add together and maxima will occur. The maxima occur at angles m, which satisfy the relationship dsin m/=|m|where m is the angle between the diffracted ray and the grating's normal vector, and d is the distance from the center of one slit to the center of the adjacent slit, and m is an integer representing the propagation-mode of interest.

Thus, when light is normally incident on the grating, the diffracted light will have maxima at angles θ_m given by:

$$dsin(\theta_m) = m\lambda$$

It is straightforward to show that if a plane wave is incident at any arbitrary angle i, the grating equation becomes:

$$d(sin(\theta_i) + sin(\theta_m)) = m\lambda$$

When solved for the diffracted angle maxima, the equation is:

$$sin(\theta_m) = \left(\frac{m\lambda}{d} - sin(\theta_i)\right)$$

The light that corresponds to direct transmission (or specular reflection in the case of a reflection grating) is called the zero order, and is denoted m = 0. The other maxima occur at angles which are represented by non-zero integers m. Note that m can be positive or negative, resulting in diffracted orders on both sides of the zero order beam.

This derivation of the grating equation is based on an idealised grating. However, the relationship between the angles of the diffracted beams, the grating spacing and the wavelength of the light apply to any regular structure of the same spacing, because the phase relationship between light scattered from adjacent elements of the grating remains the same. The detailed distribution of the diffracted light depends on the detailed structure of the grating elements as well as on the number of elements in the grating, but it will always give maxima in the directions given by the grating equation.

$$\forall \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3 : \exists r \in [0, \infty) \exists \phi \in [0, 2\pi] \exists \theta \in [0, \pi] \text{ s.t.}$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} rsin(\theta)cos(\phi) \\ rsin(\theta)sin(\phi) \\ rcos(\theta) \end{pmatrix}$$

4.2 Snake Skin Parameters

5 Results

differece of this shader compared to evaluation shader

6 Conclusion

explain why we did our derivations explain why our approach is a good idea explain how the straight foreward approach would behave compared to our approach, computing the fourier transformations straight away. explain what we achieved, summary say something about draw-backs and about limitations of current apporach say something about the ongoing paper

6.1 Further Work

6.1.1 Sources

- [1] http://en.wikipedia.org/wiki/Ratio_test
- [2] http://math.jasonbhill.com/courses/fall-2010-math-2300-005/lectures/taylor-polynomial-error-bounds