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A numerical approximation of the Huygens-Fresnel integral – Simulations of a rough wetting problem ☆

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ABSTRACT

Computing numerical approximations of the Huygens-Fresnel principle in three dimensions is demanding in terms of time and hardware, but thanks to massive parallelization in GPGPU-enabled graphics cards these computations can be sped up considerably. Our newly developed software framework is capable of simulating many wave propagation-related problems. Although it was initially intended to generate laser speckle images for various real physical setups used to measure the surface roughness of sheet metal and/or the oil film thickness upon it, it turned out to also be suitable for larger setups and apertures. This paper gives a short overview of the underlying physical and mathematical concepts and elaborates on the strengths and weaknesses of the numerics. We describe the theoretical background of rough wetting and the core parts of the software. Further, we present several test cases using apertures and their known Fraunhofer diffraction patterns and objective speckle patterns generated for rough surfaces.

1. Introduction and motivation

Corrosion of iron and its alloys, commonly termed “rust”, can be a serious problem in automotive sheet metal production. In finished products, the metal is usually coated by varnish or some other protective coating. Prior to this, the metal is often protected by a thin film of oil, whose thickness is of concern to sheet steel manufacturers: a minimum thickness is required for protective purposes, but excessive thickness affects subsequent processes and incurs unnecessary costs.

Numerous methods for determining the layer thickness of fluids on smooth surfaces exist, for example, techniques based on changes in capacitance [1], Raman backscattering [2], the temperature gradient [3], or ultrasound [4]. However, if the surface is rough and the film thickness is in the range of its roughness, the film fills in the pits and grooves of the surface such that adhesive forces between the materials and cohesive forces within the film reach an equilibrium. Since film thickness varies greatly over small distances, integral effects such as changes in capacitance, or principles based on long wavelength radiation, yield unreliable results due to their relatively low spatial resolutions.

The theory of *rough wetting* appears to offer a solution, as Andelman et al. [5,6] established a connection between the profile of the surface/fluid interface of an oil-covered rough plane and the profile of the fluid/air interface atop. It was found that the liquid acts as a low-pass filter to the underlying surface roughness: the wet surface appears to become smoother as the film thickness increases, and roughness measurements can provide information about film thickness.

Evaluations by Lettner and Zagar [7] focused on laser speckle techniques [8,9] to measure surface roughness and thus oil film thickness locally. Various measurement setups were devised and thoroughly tested, but their

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adjustment and evaluation proved to be tedious. The wish to simulate experimental outcomes soon arose and led to the development of the custom software toolbox presented in this paper.

Numerical laser speckle simulations, such as those given by Goodman [10] and Equis and Jacquot [11], often use relations in the Fourier domain which make inherent use of the Huygens-Fresnel principle under a paraxial approximation. Since diffuse reflections of laser light on a rough surface do not satisfy this assumption, a numerical approximation of the Huygens-Fresnel principle in the spatial domain forms the core part of our approach. It involves a summation over all elements of an electromagnetic field within an aperture plane to compute the field in a single arbitrary location in another plane of interest. Only mild approximations are used which affect the computed result: a discretization of both electromagnetic fields and the use of finite precision arithmetics [12].

Laser-speckle-related simulations require high spatial resolutions in the order of the wavelength used (e.g., 550 nm for green light), which results in relatively large matrix sizes when using realistic dimensions for the setup. Sequential computations on a CPU proved unfeasible due to the long time needed to solve even simple problems; for instance, we estimated that solving the wave propagation from a 2000×2000 points source aperture to a 512×512 points destination field would take a week. However, the free software toolbox “GPUmat[1]” for Matlab[2] provides a convenient way to access the general-purpose computational capabilities of the graphics processing units of Nvidia CUDA™ enabled graphics cards. Depending on the size of the problem, it speeds up calculation by at least a factor of 20–50. The GPU-accelerated[3] solver finished above example problem in approximately 6 h 36 times faster than the same algorithm running on its Intel® Core™2 Q9550 @ 2.83 GHz host CPU.

This paper extends an IMEKO TC2 conference article [13], and presents the physical models and principles which were used to simulate the wave propagation of monochromatic light, the validation of the simulation results, and a short conclusion.

2. Rough surfaces

In this section, a short introduction to the theory of rough wetting is followed by an algorithm for defining an artificial surface.

2.1. Rough wetting

Complete wetting with zero contact angle describes a thin layer of liquid completely covering a solid surface [14,15], as shown in Fig. 1. The solid surface $\zeta_S(\boldsymbol{\rho})$ is specified for each vector $\boldsymbol{\rho} = \{\xi, \eta\}$ in a two-dimensional reference plane [5]. Andelman et al. determined the liquid/vapor interface $\zeta_L(\boldsymbol{\rho})$ above the solid surface by minimizing

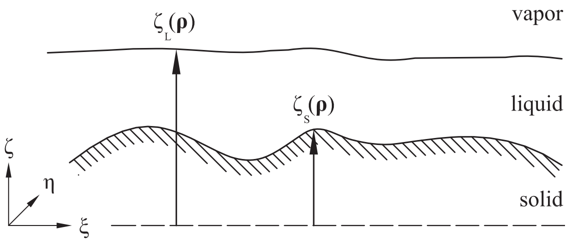

Fig. 1. A liquid film between vapor and a rough solid surface. The solid/liquid and liquid/vapor interfaces are at heights $\zeta_S(\boldsymbol{\rho})$ and $\zeta_L(\boldsymbol{\rho})$ above the $\{\xi, \eta, 0\}$ reference plane [5], respectively.

the free energy **F**, which consists of solid/vapor, solid/liquid, and liquid/vapor surface tensions, molecular interactions between the solid and the liquid surfaces, and the chemical potential of the film. Linearization of the resulting integro-differential equation yields

$$\tilde{\zeta}_L(\mathbf{q}) = \tilde{\zeta}_S(\mathbf{q})\tilde{K}(\mathbf{q})/(1 + \mathbf{q}^2\chi^2), \tag{1}$$

where $\mathbf{q}$ is a frequency in periods/meter, $\tilde{\zeta}_L(\mathbf{q})$, $\tilde{\zeta}_S(\mathbf{q})$, and $\tilde{K}(\mathbf{q})$ are the Fourier transforms of the liquid/vapor interface, the solid/liquid interface, and a convolution kernel $K(\boldsymbol{\rho})$, containing energy-related terms, and χ is the surface tension-dependent *healing length*. Eq. (1) acts as a low-pass filter on $\tilde{\zeta}_S(\mathbf{q})$, which means that great differences in the undulation of the metal surface are damped and the liquid surface becomes smoother with increasing film thickness.

2.2. An artificial surface

Next, a surface $\zeta_{S,\mathrm{art}}(\boldsymbol{\rho})$ must be generated for the proposed simulation model. It is defined in a two step process where first an artificial Fourier transform $\tilde{\zeta}_{S0}(\mathbf{q})$ of the surface determines most of its spectral properties, and subsequent scaling in the spatial domain guarantees a specified surface roughness. The spectrum for all frequencies $\mathbf{q}$ is given by

$$|\tilde{\zeta}_{S0}(\mathbf{q})| = a(\mathbf{q}), \tag{2}$$

$$\angle(\tilde{\zeta}_{S0}(\mathbf{q})) \sim \mathcal{U}(-\pi, \pi), \tag{3}$$

$$\tilde{\zeta}_{S0}(\mathbf{q}) = \tilde{\zeta}^*_{S0}(-\mathbf{q}), \tag{4}$$

where $a(\mathbf{q}) : \mathbb{R}^2 \to \mathbb{R}$ in Eq. (2) may be an arbitrary functional which acts only on the magnitude of $\tilde{\zeta}_{S,\mathrm{art}}(\mathbf{q})$ (e.g., the kernel of a low-pass filter) to approximate the frequency content of a real surface. The complex phase of each component of the spectrum is distributed randomly on the unit circle via relation (3). The uniform distribution $\mathcal{U}(-\pi, \pi)$ on the interval $[-\pi, \pi)$ ensures that a random surface is generated. Finally, the symmetry condition in Eq. (4) guarantees $\zeta_{S0}(\boldsymbol{\rho}) \in \mathbb{R}$.

In the simplest case, the functional $a(\mathbf{q})$ is the kernel of a rotationally symmetric Gaussian low-pass filter [16]

$$a(\mathbf{q}) = \exp(-|\mathbf{q}|/(2\sigma^2)),$$

where σ is the standard deviation of the Gaussian curve. In a more sophisticated approach, the functional depends on the direction of the vector $\mathbf{q} = \{q_1, q_2\}$ in order to simulate

[1] http://sourceforge.net/projects/gpumat/.

[2] http://www.mathworks.com/.

[3] A Zotac NVIDIA GeForce 580 AMP! graphics card was used.