Modeling spatial reflection from an uncoated printing paper using Monte Carlo simulation

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KEYWORDS: Substrate surface, Modelling, Noise, Light scattering, Monte Carlo simulation, Spatial reflection, Printing paper.

SUMMARY: The article deals with Monte Carlo modeling of uncoated printing paper surface based on light reflectance from the surface and on subsurface scattering. The paper surface was simulated using randomly oriented microfacets characterized by a specific parameter, critical azimuthal angle \( \varphi_c \). Determination of the value of \( \varphi_c \) was based on the idea that the standard deviation of the light reflected from a paper surface is not equal to zero, and can be recognized as noise. Noise, i.e. standard deviation of the reflectance measured on actual paper samples, was used for calculating \( \varphi_c \) and, consequently, for obtaining theoretical surface models. The results show a satisfactory agreement with the real paper surfaces and indicate that \( \varphi_c \) can be one of the important parameters in future simulations of this kind.

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Today, despite an increased use of digital media, paper is still one of the favourite media for information distribution. In graphic technology, paper's optical properties are very important, as they differentiate between types of paper according to its purpose. The motivation behind the simulation performed in our study was to describe and anticipate the transport of light through a medium such as paper, and to see the impact light dispersion has on the appearance of paper surface. All real surfaces, those that originate naturally as well as those artificially produced with great care, are rough to some degree. Accordingly, it is of interest and often important to know the extent to which this roughness affects certain physical processes that occur on the surface, particularly the scattering of electromagnetic waves on it or their transmission through it. The scattering of electromagnetic waves from rough surfaces has been actively investigated for over a century, ever since Rayleigh has explored the scattering of monochromatic flat waves that normally fall on the boundary between two different media (Rayleigh 1896). The first theoretical description of scattering of electromagnetic waves from a randomly rough surface was given by Mandel'shtam (1913), in the context of light scattering from the surface of a liquid. Optical and mechanical properties, permeability, etc. directly affect the quality of prints and production experience (Niskanen et al. 1998; Baker 1997).

Paper can be seen as a three-dimensional network consisting primarily of plant fibers, which are held together by hydrogen bonding of the hydroxyl groups of cellulose and hemicelluloses. Other main ingredients include fillers, sizing agents, other functional additives, water and air. Although often regarded as an infinite network in two dimensions, paper is always finite in the z-direction, where there is a clearly defined boundary between the network and the air, while nature and structure of the network at this boundary define the surface of uncoated paper to a great extent. Paper surface is relatively flat, because the fibers are oriented so that they are primarily aligned with the plane of the paper. Various steps must therefore be taken during paper production process to ensure that the surface is really flat and smooth. The surface of paper is extremely important, especially for printing and writing papers. One of its main functions is to accept and transmit printed messages. In mathematical terms, the surface is a plane of zero thickness, and therefore its volume is also equal to zero. But in the technological context, paper surface relates to the specific thickness and volume, which have well-defined and important features.

To improve surface quality, paper or cardboard substrate is after its manufacturing stage often subject to some kind of surface treatment, implementing either surface sizing or pigment coating. Enhanced quality can be focused on optical properties, such as brightness, gloss or opacity; tactile qualities like smoothness, but, most importantly, on the improved print quality. In our study we were modeling three types of uncoated wood-free fine paper designed for multipurpose printing. The tone resolution and reproduction ability of all graphic paper products are significantly conditioned by the way the light scatters in a paper. Light entering the paper between the halftone dots can be scattered in the paper in all directions, but the rays that end up below the dots are absorbed, causing the printed dots to appear larger than intended. This undesirable but unavoidable phenomenon is known in the graphic arts terminology as the dot gain. To manufacture a paper that successfully fulfils the required optical properties, it is necessary to understand the physical principles of the structure and composition of a paper sheet. The theoretical work presented in this article was performed within the frame of the Monte Carlo method (Modrić 2007; 2009), which describes the subsurface transport of light. This is a numerical method for solving mathematical problems based on a random sampling from well-defined probability distributions. Starting from real physical assumptions, the subsurface light scattering in a substrate with a complex structure was modelled (Kubelka, Munk 1931; Emmel 1998; Mourad 2002). For this kind of
problem, where statistics approach offers the best insight and approximation for exact results, the Monte Carlo offers a more flexible approach to the transport of photons in a medium such as paper even though this model has a pure stochastic nature. It turned out to be a feasible quasi experimental approach for the investigation of optical characteristics of paper such as dot gain.

Monte Carlo simulation

Below we present a method that describes photon propagation within a substrate. In order to simulate the light transport in a substrate with the Monte Carlo approach, photon packets are sent on a random walk through a virtual paper sample. The technique developed is based on probability distribution, which describes main parameters of the photon packet walk. These parameters are photon packet shift between two events (scattering and/or absorption) defined as step size $s$ (Eq 1) and scattering angles $\phi, \theta$ generated using random numbers. Photon packet history (its motion) is recorded until the packet either abandons the medium or is absorbed in interaction with it.

It is important to realize that scattering is a local phenomenon and that even when each individual scattering event is perfectly diffuse, the arrangement of the totally scattered light need not be perfectly diffuse. It has to be emphasized that the method is of a statistical nature, i.e. it is based on the calculation of a large number of photons paths, resulting in high computer time consumption.

As already mentioned, paper can be regarded as a stochastic three-dimensional structure which mainly consists of fibers mutually connected by hydrogen bonds and of substances that are used as fillers. The characteristics of fibers depend on the type of plant (e.g. hardwoods, softwoods, annual plants) they originate from, and on the way fibers are additionally treated mechanically and chemically during production. In a sheet of paper, the individual scattering agents – the fibers and the filler particles – are so close to one another that multiple scattering becomes important. In the theory of scattering, one starts with a single scattering typical of ensembles with a sufficiently small number of particles whose mutual distance is big enough that each particle can experience an individual scattering event without the influence of the neighbouring particles. The qualitative criterion for the assumption of single scattering is that each particle of the ensemble is influenced by the same input electric field with a negligible influence of the scattered field from other particles in the ensemble.

Paper is in principle a difficult medium for description, due to the fairly diverse optical characteristics of its components. The widely used theory related to the scattering and absorption of light – photons – of particular particles such as fibers or fillers was developed by Kubelka and Munk (1931).

The approach to photon propagation in the frame of the Monte Carlo method applied to paper is based on the work of Phral et al (1989). The object of our investigation is optical behaviour of the multilayer heterogeneous substrate. We treat the surface sizing layer and the substrate as two separate, well-defined layers, in which we exclude from calculation both the reflection of light and the refraction on the layer boundaries where local absorption and scattering conditions are altered. The polarization and the phase of the packet are also neglected. The technique was developed on the basis of the probability distribution that describes the photons’ paths between two events – scattering and/or absorption – and scattering angles. Photon history, i.e. its motion, is recorded until the photon either leaves the medium or is absorbed in the interaction with the medium. The photon can leave the medium, in our case paper, at the lower boundary (light transmission) or at the upper boundary. Through this, information about the subsurface light transport was obtained.

For implementation of this method, a stochastic model is constructed in which the expected variable value (or a combination of variables) is equivalent to the physical value that needs to be determined. The expected value is defined as the mean value of multiple independent samples that represent this random variable. We use random generated numbers, which follow the prior selected normal distribution, to construct the desired array of independent samples.

The Monte Carlo simulations of this type are based on the macroscopic optical properties, which are assumed to prevail over small parts of the volume of paper (e.g. cellulose fibers, fillers, adhesives, etc.) (Veatch 1997). A simple variance reduction technique is used to improve the efficiency of the simulations. This technique allows us to simultaneously propagate a number of equivalent photon packets as a package along a path. Each photon packet entering the substrate is associated with a statistical weight $W$ equal to unity. Such description, of course, does not correspond to the actual physical situation, but it gives a reasonable picture of our simulation needs. The packet enters the substrate at the origin of the system and corresponds to collimated narrow beam photon packet (e.g. laser beam). The motion of a single photon packet can be presented with five variables: three spatial coordinates ($x, y, z$) and two angles ($\theta, \phi$), determined relatively with respect to the previous trajectory orientation, which describes the direction of the propagation. We used cylindrical coordinates to determine the position of a photon packet, and two angular variables defined by a line connecting the starting point of a photon and photon itself, to determine the direction of the propagation. The technique developed is based on the probability distribution that describes the distance a photon crosses between the two events (scattering and/or absorption) and scattering angles. Photon packet history (its motion) was recorded until the photon either left the medium or was absorbed in the interaction with the medium. A photon can leave the medium – in our case, paper – at the lower substrate boundary (light transmission) or at the upper one, which we are interested in because it provides information about the subsurface light transport. Individual absorption is determined by comparing a randomly generated number to the albedo. For example, if a random number is larger than the albedo, the packet energy is absorbed and the package vanishes, so the contribution of attenuation in the medium can be registered. After the interaction is
Fig 1. Flowchart illustrating the Monte Carlo simulation algorithm with variable step size for subsurface light scattering in paper. The Monte Carlo simulation program created with MathCad 11 was used to calculate the presented results.
completed, a new set of numbers that determine the path and direction of a new package is generated. The process is repeated until a packet leaves the area. The step size of a photon packet $s$ is the path that the packet passes between two interactions (events) with the substrate, and it can be assumed variable. According to the procedure defined by the model, each step size between photon-substrate interaction position equals:

$$s = \frac{\ln R}{(\mu_a + \mu_s)}$$  \hspace{1cm} (1)$$

where $\xi$ is a random number, and $\mu_a$ and $\mu_s$ are the absorption and scattering coefficients respectively. Each photon has a statistical weight associated to it that decreases from an initial value of 1 as it moves through the substrate, and equals $a$ after $n$ steps, where $a$ is the albedo:

$$a = \frac{\mu_s}{(\mu_a + \mu_s)}$$  \hspace{1cm} (2)$$

Once the photon packet has been moved, it is ready to be scattered. There will be a deflection angle $\theta \in [0,\pi]$ and an azimuthal angle, $\psi \in [0,2\pi]$ to be sampled statistically. The probability distribution for the cosine of the deflection angle, $\cos \theta$, is described by the scattering function that Henyey and Greenstein (1941) originally proposed for galactic scattering:

$$p(\cos \theta) = \frac{1 - g^2}{2(1 + g^2 - 2g\cos \theta)^2}$$  \hspace{1cm} (3)$$

where the anisotropy (asymmetry factor), $g$, equals the averaged $<\cos \theta>$ and has a value between -1 and 1. The parameter $g$ can be adjusted to control the relative amounts of forward and backward scattering in $g(\cos \theta)$; $g = 0$ corresponds to isotropic scattering, and $g \rightarrow \pm 1$ to a highly peaked forward (+) (backward(-)) scattering.

When a photon strikes the surface, a fraction of the photon weight escapes as reflectance and the remaining weight is internally refracted and continues to propagate suffering numerous scattering and absorption events. Eventually, the photon weight drops below a predetermined threshold level of 1% and the simulation for that photon is terminated. In this example, termination occurred when the last significant fraction of the remaining photon weight escaped at the surface at some position which differs from the incoming point. To satisfy the energy conservation law, we used instead single photon packets consisting of a hundred photons.

Parameters of the paper model

The light is scattered at the point of contact between the fibers due to the fact that the transparent wall of an ordinary cellulose fiber exhibits negligible light scattering. Therefore, the coefficient of light scattering can be considered as a measure of connection between the fibers. Mechanical pulp fibers dissipate less than chemical ones due to their lower specific surface.

In our approach, we used the fact that the standard deviation of reflectance – noise – is not equal to zero even for an unprinted paper, so we measured the reflectance of three types of office paper commonly used in digital printing: NAVIGATOR 80g, ARCPRIINT 120g and SPLENDORGEL 115g, and compared it with the modelled one.

The following results were calculated based on some typical values of paper properties, which have been retrieved from the literature (Alava, Niskanen 2006; Mark 1984; van der Reyden et al 1993; Dyer 2004; Ek et al. 2009). We chose a trade-off paper composition that corresponds to the available data, while still being simple enough not to consume excessive computer time.

In our calculations we used the "paper" consisting of chemical pulp, fillers, surface sizing and air (although the number of components was not limited by the software) in the amounts represented as weight ratios shown in Table 1. Of course, the composition of the actual papers whose reflectance was measured is a commercial secret, but the composition used in our modelled paper gave fairly good results, as demonstrated by the modelled reflectance profiles of paper prints (Atkinson 1997). The refractive index ($n$) of the surface sizing layer was chosen to be that of starch, i.e. 1.47.

Fig. 2. Example of calculated photon trajectory (virtual walk) for a) transmission and b) reflection. Photon packet penetrated at the $(0,0,0)$ coordinate into the substrate of arbitrarily chosen thickness of 1 see Fig 2a). Circles represent positions of scattering and/or absorption events. Dimensions in figures are shown in arbitrary units (note different scales of the Z axis in the figures).
Table 1. Numerical data for one of our "papers" consisting of four components: filler, chemical pulp, sizing agent (starch) and air.

<table>
<thead>
<tr>
<th>Component</th>
<th>Weight ratio, %</th>
<th>Asimmetry factor ((q_i)), (\cdot)</th>
<th>Scattering coefficient ((\mu_s)), m(^2)/kg</th>
<th>Absorption coefficient ((\mu_a)), m(^2)/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Wavelength ((\lambda)), nm</td>
<td>Wavelength ((\lambda)), nm</td>
<td></td>
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<tr>
<td>Filler</td>
<td>10</td>
<td>0.7</td>
<td>25</td>
<td>25</td>
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<td></td>
<td></td>
<td>25</td>
<td>25</td>
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<td></td>
<td>0.5</td>
<td>0.5</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>0.5</td>
<td>0.5</td>
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<tr>
<td>Chemical pulp</td>
<td>69</td>
<td>0.75</td>
<td>25</td>
<td>108</td>
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<td></td>
<td></td>
<td></td>
<td>115</td>
<td>110</td>
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<td></td>
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<td></td>
<td>29</td>
<td>6</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>Surface sizing agent</td>
<td>9</td>
<td>0.02</td>
<td>30</td>
<td>30</td>
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<td></td>
<td></td>
<td></td>
<td>30</td>
<td>30</td>
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<td></td>
<td></td>
<td></td>
<td>0.02</td>
<td>0.02</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>0.02</td>
<td>0.02</td>
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<tr>
<td>Air</td>
<td>12</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<td></td>
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<td>0</td>
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</table>

Determining the parameter values in the substrate surface model

Several excellent review articles were written on the subject of numerical algorithms for the modelling of scattering from rough surfaces (Adams, Brown 1999; Atkinson 1997; Sallard, Sentenac 2001), while an overview of surface modelling using the concept of microfacet is given in Maretić et al. (2010) and Žitinski et al. (2008). In this model, a crucial parameter is the critical azimuthal angle \(\theta_c\), the angle that defines paper roughness. The model is based on the fact that the surface of a printing paper is "bombarded" with photon packets, where each packet falls on a microfacet, which has a random orientation in the plane of the paper and position on its surface (Fig 3). The main challenge with the model was to determine the optimum value of the \(\theta_c\); the model is defined by the size of a microfacet so we had to find a compromise between the number of microfacets and the number of photon packets which had to be sufficiently large for a correct simulation due to our stochastic approach.

Noise as a measure for determining the parameters of the surface model

Image noise is a random variation of brightness or colour information in images produced by the imaging system which may add noise to the signal and may not be able to resolve all of the features of the original signal. There can be many causes of noise and these can be thought of as a noise variable. Often it is a random variable. Even a beam of photons from the light source contains noise (quantum noise). Noise reduction to zero can be compared to the cooling to the temperature of absolute zero. Natural laws do not allow us to do this, so the best we can do is to measure and understand the causes of noise in an imaging system, so that it can be reduced as much as possible. There are three sources of noise in the generation of prints (pictures). The first one is the paper itself, and it reflects the fact that an unprinted paper has a non-zero standard deviation of reflection. This parameter is called granularity \(\sigma_p\) (p for paper) and has the largest contribution to granularity of an image at the maximum reflection \(R_{max}\). The second contribution comes from the ink covered surface; this granularity – \(\sigma_i\) (i for ink) – is caused primarily by the variability in the ink material. This contribution is absent in our case, because there is no ink on paper, so we will consider \(\sigma_i = 0\). Thirdly, in addition to paper reflectance variability, the sensor (IAS) also has its noise. This noise from the IAS is represented as a standard deviation referred to as \(\sigma_{IAS}\).

Both experience and theory indicate that system variability is generally amplified by the slope, \(\gamma\), of the system TTF (tone transfer function). Adding this system variability to the total noise gives us the equation for the total system variance:

\[
\sigma_{tot} = \sqrt{\sigma_p^2 + \gamma \cdot \sigma_{IAS}^2}
\]
The granularity computation averages together all the reflectance data within 42µm x 42µm square tiles. The graininess value is the standard deviation of these tiles. However, graininess excludes reflectance variation on a size scale larger than 250µm. The math describing this process is given in the ISO standard 13660 (Briggs et al. 1999; 2005). By adjusting the value of $\sigma_{IAS}$, we should be able to fit our experimental data.

Measured reflectance values (Fig 5) were compared with those obtained for the three versions of the paper modelled with different critical azimuthal angles $\alpha_c$ (Fig 6, Fig 7). Papers are marked as Paper I, with $\alpha_c = 0^\circ$, Paper II with $\alpha_c = 30^\circ$ and Paper III with $\alpha_c = 50^\circ$. Calculations suggest that the critical azimuthal angle $\alpha_c = 50^\circ$ gives better results compared to those using the two lower angles, i.e. the biggest similarity to the actual paper Navigator.

In the measured signal (reflectance) of white paper, it is obvious that noise is present, and consists of the above mentioned components. Considering that the measured noise is by an order of magnitude smaller than the calculated one, which does not include the component that comes from the sensors, we can conclude that the impact of sensors is small and that the measured noise can be compared with the modelled one. From the table in Fig 7 it is evident that the model gives a satisfactory mean reflectance and noise. Fig 6 shows a comparison

<table>
<thead>
<tr>
<th>Paper</th>
<th>Mean reflectance</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Navigator 80 g/m²</td>
<td>0.748</td>
<td>0.029</td>
</tr>
<tr>
<td>Splendorgel 115 g/m²</td>
<td>0.747</td>
<td>0.030</td>
</tr>
<tr>
<td>Arcoprint 120 g/m²</td>
<td>0.763</td>
<td>0.025</td>
</tr>
</tbody>
</table>

Fig 5. Measured reflectance profiles (above) and the corresponding data (below) for the three investigated papers.

Fig 6. Pseudo 3D images of the a) measured reflectance from Navigator paper and the modelled surface reflectances - b), c), and d) obtained with critical azimuthal angles $\alpha_c = 0^\circ$, 30$^\circ$, and 50$^\circ$, respectively.
between the measured and the calculated reflectance profiles of a paper presented in pseudo 3D display. Noise reduction in calculated reflectances might be partly achieved by increasing the number of photon packets that model these reflectances. This is clearly seen in Fig 8, which represents calculated surface reflectances using pseudo 3D display of surfaces generated with the same parameter $\varphi_c$, but with a different number of photon packets.

It should be noted that by increasing the number of photon packets that randomly fall on the surface of the paper, the number of surface microfacets is increased, causing too fine segmentation of the surface (see Fig 9). In fact, in the model, there is no size limit for microfacets, and surface area reduction with increased number of photon packets occurs. This area reduction causes the modelled surface to appear smoother regardless of the possibly large critical azimuthal angle $\varphi_c$ used in calculations. This approach requires a compromise between the requirements for such a large number of photon packets in the simulation on the one hand, and a realistic description of the paper surface on the other. The model captures only the point on the paper surface where the microfacet is generated, and calculates only the angle at which the package enters (Fig 3). The distribution of points on the surface where the packets fall was obtained randomly (Fig 4). For each incoming point, the described procedure generates angles, but the surface area of a microfacet is not determined. One can only determine its average size if the total area of the paper is divided by the number of incoming packets. Fig demonstrates a change in the paper surface structure by increasing the number of photon packets that simulate its surface reflectance. It is obvious that an increase in the number of packets results in a smoother surface (bottom figure), which can be easily understood if we compare this result with a sandpaper. Sandpaper with smaller abrasive particles appears smoother, although particles themselves can be extremely sharp.

However, from Fig 6 it is evident that a lower critical azimuthal angle $\varphi_c$ generates much lower noise, which gives us guidelines for modelling the paper surface.

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**Fig 7.** Measured – Navigator 80 g/m$^2$ – and calculated reflectance profiles (left) and the corresponding data (right). Reflectances were calculated at three different values of $\varphi_c$.

**Fig 8.** Calculated pseudo 3D surface reflectance obtained with two different numbers of photon packets: a) $2 \times 10^5$ and b) $2 \times 10^6$.

**Fig 9.** Illustration of the increase in paper surface smoothness through reduction of the areas of individual microfacets at the constant critical azimuthal angle. It should be noted that, in the model, as opposed to the illustration, the size of the microfacets is not constant.
Conclusions

This paper summarizes the possibilities of a realistic modelling of a substrate surface based on experimentally acquired data. To obtain a realistic description, we have used the noise that we recognize as the standard deviation of the substrate reflectance. This noise is inherent to every surface, and provides information about its optical properties, thus enabling one to discriminate among different surfaces. Noise is a characteristic of an image that is otherwise undesirable, and the impact of which image analysis tries to reduce to its minimum. In our model (Modrić 2007; 2009) which is stochastic in nature, its presence is normal. Those noise parameters that appear in our model enable us to realistically describe the media observed. However, the determination of the numerical values of these parameters is a problem, and the method presented is one of the ways for a simpler and physically plausible determination of the appropriate parameter values. The method presented opens up many questions related to the model itself, and provides guidance for future work. In the future, it will be necessary to define a finite size of the microfacet in the model (according to the paper type) to prevent the smoothing of the surface of the substrate with increasing number of photon packets.

This model gives the possibility for “experimenting” with different combinations of paper components without physically producing the real paper, which is often expensive and time consuming. By easily changing the composition and the amount of each paper component, this model can be used to study the optical properties of recycled papers. All paper components, such as mechanical and/or chemical pulp, whiteners, fillers, other additives etc., affect the way the light is scattered in paper and influences its surface properties. As also demonstrated by our findings, the paper appearance is not only the consequence of its surface, but of its subsurface structure, too.

Literature


Dyer T. J. (2004): Elucidating the Formation and Chemistry of Chromophores during Kraft Pulping, PhD thesis, Institute of Paper Science and Technology; Atlanta, Georgia


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