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3D Monte Carlo surface-atmosphere radiative transfer modelling with DART

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19	Research highlights:
20	New 3D Monte Carlo surface-atmosphere RT modelling in DART model.
21	A virtual Earth-Atmosphere laboratory for simulating the adjacency effect.
22	Study of the impact of the surface 3D structure on the adjacency effect.
23	Study of the adjacency effect contribution on radiance and albedo at TOC and TOA.
24	

25 Abstract

26 Significant errors can arise if the adjacency effect (*i.e.*, the contribution of neighbouring pixels 27 to the radiance of a pixel) is neglected in the interpretation of remote sensing images. For 28 example, adjacency radiances can account for more than 30% of the signal at the top of the atmosphere (TOA) of a white sand-lined coastline (Bulgarelli and Zibordi, 2018). This paper 29 30 shows that 3D radiative transfer (RT) modelling can quantify this phenomenon. It presents a 31 new 3D Monte Carlo surface-atmosphere RT modelling in the DART RT model, and a resulting 32 virtual 3D Earth-Atmosphere laboratory for accurate simulation of atmospheric RT, including 33 the adjacency effect. It was first validated with the atmosphere model SMART-G for 2D scenes: 34 relative difference is 0.20% in TOA directional reflectance of infinite black surface for solar 35 zenith equal to 60°, and 0.03% in TOA nadir reflectance of a black disc inside infinite white Lambertian surface, for solar zenith equal to 0° and 30°. Then, the adjacency effect on the TOA 36 37 radiance and TOA albedo of a 3D scene was studied for a circular city (radius 2 km) surrounded 38 by a forest (dimension 10 km), for four Sentinel-2A bands (blue, green, red, near infrared). Its 39 contribution to TOA nadir radiance reaches ~20% in the near infrared band, and increases with viewing zenith angle (VZA): ~60% if VZA = 80° . The 3D scene TOA albedo was calculated 40 41 after adapting the DART Bidirectional Reflectance Factor (BRF) camera to simulate TOA 42 radiance for all upward directions at any angular resolution. For Sentinel-2A's four bands, the 43 adjacency effect influences the TOA albedo of the circular city by up to 10% for the green band 44 and up to 27% for the near infrared band, well above the maximum uncertainty 5% usually 45 required in land surface applications. The adjacency effect of the city neighbourhood 3D 46 structure was studied by replacing it by a Lambertian surface with its albedo. The city nadir 47 TOA radiance changed by up to 1.3% with very small change in TOA albedo (< 0.5%). This new modelling greatly improves DART potential for accurate simulation of atmospheric effects. 48 49 It is in the DART version freely available for research and education (https://dart.omp.eu).

51 Key words

52 DART, Monte Carlo, Atmosphere, Adjacency effect, Radiative transfer

53

54 **1 Introduction**

55 From a remote sensing point of view, the adjacency effect is the part of the measured signal 56 due to land surface elements outside the instantaneous field of view (IFOV). This phenomenon 57 is one of the most challenging sources of inaccuracy in the remote sensing study of land surfaces 58 since the advent of high-resolution Earth observation satellites (Kiselev et al., 2015; Liang et 59 al., 2001; Ouaidrari and Vermote, 1999; Pan et al., 2022; Reinersman and Carder, 1995; Sterckx 60 et al., 2015). It depends on many factors: the spectral domain (Dave, 1980), the atmospheric 61 conditions (Reinersman and Carder, 1995), the heterogeneity and anisotropic scattering of the 62 target and its neighbouring land surfaces (Bulgarelli and Zibordi, 2018), and the light source and sensor configurations (Vermote et al., 1997), etc. In the study of (Bulgarelli and Zibordi, 63 64 2018) the adjacency effect reached 30% of the top of atmosphere (TOA) radiance signal at 443 65 nm at 1 km off the coast of northern Adriatic Sea and 15% at 5 km offshore. Therefore, 66 neglecting it can lead to very inaccurate interpretations of remote sensing images.

67

Several methods to study and quantify the adjacency effect have been proposed since the late 1970's. They broadly belong to three groups: (1) empirical methods, (2) point spread function (PSF) based methods and (3) 3D radiative transfer (RT) modelling. Empirical methods (Minomura et al., 2001; Ouaidrari and Vermote, 1999; Richter, 1990) first derive individually the Lambertian reflectance $\rho^{(j)}$ of any pixel *j* from TOA reflectance assuming an infinite homogeneous plane ground, then approximate the adjacency effect on the TOA reflectance as the product of the averaged background reflectance $\langle \rho \rangle$ and the atmospheric diffuse transmittance. $\langle \rho \rangle$ is the reflectance average over a $N \times N$ pixel window around the pixel of interest using the previously computed reflectance $\rho^{(j)}$. Being very fast, empirical methods are often used in operational atmospheric corrections (*e.g.*, Landsat TM). They use windows whose size *N* needs prior experience, mainly depending on the pixel size, the atmospheric condition, and the surface heterogeneity (Richter, 1990).

80

81 In PSF-based methods, the adjacency effect is defined by the atmospheric PSF $f(P, P_0, \Omega_i, \Omega_n)$ that gives the scattering contribution of a land surface point P illuminated in direction Ω_i to the 82 83 observed point P_0 in direction Ω_{ν} . The PSF can be computed analytically using the single 84 scattering approximation (Kiselev et al., 2015; Santer and Schmechtig, 2000) or the two-stream 85 approximation (Mekler and Kaufman, 1980). It can also be derived using a radiosity code 86 (Borel and Gerstl, 1992) or using a Monte Carlo code (Adler-Golden et al., 2008; Miesch et al., 87 2005; Pearce, 1986; Reinersman and Carder, 1995). However, these methods tend to simplify 88 the 3D RT mechanisms (e.g., multiple scattering, 3D surface architecture, atmospheric RT) that 89 give rise to the magnitude of the adjacency radiance.

90

A quantification of the adjacency radiance in remote sensing images needs a unified 3D RT
modelling in a coupled Earth-Atmosphere system. This is increasingly possible as
improvements in 3D RT modelling and computer technology reduce simulation times (Qi et al.,
2019; Ramon et al., 2019; Wang et al., 2022). 3D RT modelling has recently been used to
quantify the adjacency effect (Bulgarelli and Zibordi, 2018; Pan et al., 2022; Sun et al., 2021).

Most 3D RT models are either for the atmosphere and neglect the influence of the 3D structure
and spatial heterogeneity of land surfaces (*e.g.*, 3DMCPOL, SPARTA) (Barlakas et al., 2016;
Cornet et al., 2010) or for land surfaces and neglect the influence of the atmosphere (*e.g.*, librat,

100 raytran) (Govaerts et al., 1996; Lewis, 1999). Coupling a land surface RT model with an 101 atmospheric RT model is often very approximate for simulating the adjacency effect, since it 102 usually supposes a horizontal homogeneous land surface and atmospheric backscattering. This is why DART-FT (Flux-Tracking), the initial version of DART¹ (Gastellu-Etchegorry et al., 103 104 1996), included a radiative coupling mode, between the stratified atmosphere and the 3D land 105 surface (Gascon et al., 2001; Grau and Gastellu-Etchegorry, 2013) instead of a coupling with 106 an atmosphere model like MODTRAN (Berk and Hawes, 2017). DART-FT uses the discrete 107 ordinates method (DOM) (Yin et al., 2013) to simulate the adjacency effect by convolving a pre-computed four-dimensional transfer function $TF_{TOC \rightarrow Z}(\Delta i, \Delta j, \Omega, \Omega')$ that stores the 108 109 incident power in direction Ω' at three image planes Z (any altitude, TOA, and top of canopy: 110 TOC) with Δi line and Δj column shifts relative to point on the TOC plane that gives rise to a 111 unit power in direction Ω . Pre-computing $TF_{TOC \rightarrow Z}$ avoids repeated computations. However, it 112 is only adapted to horizontally homogeneous atmosphere. Also, its efficiency greatly decreases 113 with the increase in the numbers of atmospheric cells, and discrete directions Ω and Ω' , whereas 114 these numbers must be large to accurately simulate the adjacency effect, especially for high-115 resolution remote sensing images of spatially heterogeneous landscapes.

116

Since 2018, a Monte Carlo mode called DART-Lux has been implemented in DART to improve the accuracy and efficiency of simulations of TOC remote sensing images of large-and complex landscapes (Wang et al., 2022). Its end-to-end bidirectional path tracing algorithm samples a group of stochastic paths connecting the light source and the sensor and unbiasedly estimates radiance measurement using the weighted contribution of these path samples. DART-Lux

¹ DART (<u>https://dart.omp.eu</u>) is an ever-evolving radiative transfer model. It simulates the 3D radiative budget, including sun induced chlorophyll fluorescence, and remote sensing (RS) satellite, airborne and in-situ signals (spectroradiometer image, LiDAR FWF, SPL, point cloud) of natural and urban landscapes, from visible to thermal infrared. It is a reference tool for a wide range of RS studies (sensitivity studies, inversion of RS images, design of new RS sensor, etc.). Licenses are free for research and education.

122 results are consistent with those of DART-FT (relative difference < 1%) with simulation times 123 and computer memory reduced by factors over 100 for complex landscapes (without 124 atmosphere). Recently, (Wang and Gastellu-Etchegorry, 2021) designed a hybrid method that 125 couples the Monte Carlo land surface RT and the DOM atmospheric RT to simulate satellite 126 and airborne images. Although fast and accurate for relatively homogeneous land surfaces (e.g., 127 dense forest), this method is inefficient to simulate the adjacency effect, because its DOM 128 atmospheric RT needs small atmospheric voxels. Although usually more efficient than Monte 129 Carlo method for 1D surface-atmosphere coupling (*i.e.*, spatially constant TOC upwelling and 130 downwelling fluxes), the DOM is much less efficient for 3D radiative coupling. Therefore, 131 there was a need to design a Monte Carlo atmospheric RT modelling in DART, in addition to 132 the DOM atmospheric RT.

133

134 This paper presents two improvements of DART-Lux to simulate remote sensing images with 135 accurate account of atmospheric effects (e.g., adjacency effect). 1) A new representation of the 136 Earth-Atmosphere system. 2) A generalization of our initial formulation of RT modelling 137 (Wang et al., 2022) to scenes with surfaces and volumes. In addition, the DART tool (*i.e.*, BRF camera) that simulates the scene TOC radiance at 1° x 1° angular resolution is adapted to any 138 139 altitude level and angular resolution in order to quantify the adjacency effect on the scene 140 radiance and albedo at TOA and TOC. Section 2 summarizes the Monte Carlo modelling of the 141 initial version of DART-Lux for land surfaces. Section 3 presents the new representation of the 142 Earth-Atmosphere system and the new formulation of atmospheric RT modelling. Section 4 143 presents the accuracy assessment of the new modelling and the study of the impact of the 144 adjacency effect on TOA radiance and albedo. Finally, section 5 presents concluding remarks.

146 2 Principles of DART-Lux

147 DART-Lux is an unbiased Monte Carlo method for accurate and efficient simulation of 148 remotely sensed images of large and complex landscapes (Wang et al., 2022). Its features useful 149 for understanding the current work are summarized here. In DART-Lux, the 3D RT problem is 150 described by a multi-dimensional integral and is solved with Monte Carlo integration methods. 151 The radiance $L^{(j)}$ measured at a pixel *j* of the image is an integral over all the possible paths \bar{r} 152 from the light source to pixel *j*:

$$L^{(j)} = \int_{\mathcal{D}} f^{(j)}(\bar{r}) \cdot d\mu(\bar{r}) \tag{1}$$

153 with
$$\mathcal{D} = \bigcup_{n=1}^{\infty} \mathcal{D}_n$$
 the path space, \mathcal{D}_n the set of paths \bar{r}_n of length n , and $\bar{r}_n = r_0 r_1 \dots r_n$ a
154 series of vertices $r_{k=0\dots,n}$ on surfaces $dA(r_k)$ of the scene with r_0 on the sensor and r_n on the
155 light source, $\mu(\mathcal{D}_n) = \int_{\mathcal{D}_n} d\mu(\bar{r}_n) = \int_{\mathcal{D}_n} dA(r_n) \cdot dA(r_{n-1}) \cdots dA(r_0)$ is the area-product of \mathcal{D}_n .
156 The term $f^{(j)}(\bar{r})$ represents the measurement contribution of a path \bar{r} . For a path \bar{r}_n :
 $f^{(j)}(\bar{r}_n) = L_e(r_n \rightarrow r_{n-1}) \cdot G(r_0 \leftrightarrow r_1) \cdot W_e^{(j)}(r_0 \rightarrow r_1) \prod_{k=2}^n f(r_k \rightarrow r_{k-1} \rightarrow r_{k-2}) \cdot G(r_{k-1} \leftrightarrow r_k)$ (2)
157 with $f(r_k \rightarrow r_{k-1} \rightarrow r_{k-2})$ the bidirectional scattering distribution function (BSDF) at vertex r_{k-1} .
158 It is often written as $f(r_k \leftrightarrow r_{k-1} \leftrightarrow r_{k-2})$ if there is Helmholtz reciprocity of scattering. L_e is
159 the radiance emitted by the light source and W_e is the sensor importance function (cf.
160 Appendix A in (Wang et al., 2022)) that transforms incident radiation into radiance.
161 $G(r_{k-1} \leftrightarrow r_k) = V_t(r_{k-1} \leftrightarrow r_k) \cdot \frac{\cos \theta_i^{r_{k-1}} \cos \theta_i^{\sigma_k}}{\|r_{k-1} - r_k\|^2}$ is a geometric term, with $V_t(r_{k-1} \leftrightarrow r_k)$ the
162 visibility function: $V_t(r_{k-1} \leftrightarrow r_k)$ is 1 if r_{k-1} and r_k are mutually visible, and 0 otherwise.
163 $\theta_i^{r_{k-1}}$ is the incident angle at vertex r_{k-1} and $\cos \theta_0^{r_k}$ is the exit angle at vertex r_k .

164

165 The importance sampling method, a major variance reduction technique in Monte Carlo 166 integration (Rubinstein and Kroese, 2016), can unbiasedly estimate $L^{(j)}$ (Eq.) using:

$$F^{(j)} = \frac{f^{(j)}(\bar{r}_n)}{p(\bar{r}_n)}$$
(3)

167 with $F^{(j)}$ an estimate of $L^{(j)}$ and $p(\bar{r}_n)$ the probability of a path sample \bar{r}_n .

168

Eq. (3) indicates that $L^{(j)}$ can be efficiently derived if all paths \bar{r}_n are fast sampled and the 169 estimate $F^{(j)}$ converges with less repetitive scholastic processes. DART-Lux estimates $L^{(j)}$ 170 171 with a robust and rapid bidirectional path tracing method. First, all vertices of two independent paths, one starting from the light source $(\bar{p}_N = p_0, p_1, ..., p_s, ..., p_{N-1})$ and one starting from the 172 sensor $(\bar{q}_N = q_0, q_1, ..., q_t, ..., q_{N-1})$, are connected to get a group of random paths 173 $\bar{r}_{s,t} = p_0, p_1, \dots, p_{s-1}, q_{t-1}, q_{t-2}, \dots, q_0$ (cf. Figure 5 in (Wang et al., 2022)). Then, the multiple 174 importance sampling (MIS) estimator, proposed by (Veach and Guibas, 1997), computes $L^{(j)}$ 175 using a weight $w_{s,t}(\bar{r}_{s,t})$ per path sample $\bar{r}_{s,t}$ (Eq. (4)). In general, a larger weight corresponds 176 177 to a path sample with large probability density function (Wang et al., 2022).

$$F_{\rm MIS}^{(j)} = \sum_{s \ge 0} \sum_{t \ge 0} w_{s,t}(\bar{r}_{s,t}) \cdot \frac{f^{(j)}(\bar{r}_{s,t})}{p(\bar{r}_{s,t})}$$
(4)

178

179 **3** Atmospheric radiative transfer modelling

The initial version of DART-Lux (Wang et al., 2022) simulated RT with a Monte Carlo method for Earth scenes (*i.e.*, landscapes) represented by surfaces (*i.e.*, facets), and with the DOM mode of DART-FT for the atmosphere. As it was not suitable for simulating the adjacency effect, we designed a new representation of the Earth-Atmosphere system and generalized the theorical formulation of DART-Lux to Earth scenes that contain both surfaces and volumes.

185 **3.1** New Earth-Atmosphere system

186 The new Earth-Atmosphere scene (Figure 1) is a square cuboid that contains the atmosphere 187 and a region of interest (ROI) at its bottom centre, surrounded by a horizontal background with

user-defined bi-directional reflectance (e.g., Lambertian, Rahman-Pinty-Verstraete (RPV), 188 189 specular). The ROI is a 3D landscape that includes the observed target. Its topography is 190 smoothly connected to the background by the Bézier triangle (Farin, 2014; Wang et al., 2020). 191 The optical properties of foliar and soil surfaces can be defined using the DART database of 192 optical properties, or computed by the PROSPECT / Fluspect / MARMIT modules (Bablet et 193 al., 2018; Dupiau et al., 2022; Féret et al., 2017; Jacquemoud and Baret, 1990; Vilfan et al., 194 2016). The atmosphere (i.e., gases and, aerosols) is made of horizontally homogeneous and 195 vertically continuous layers with any depths, at any altitudes; default depths are 1 km from 0 to 196 15 km altitude and 5 km from 15 to 50 km altitude. Polynomials from the spline interpolation 197 ensure vertical continuity of optical properties (e.g., extinction coefficient) and temperature 198 within and between layers (Wang and Gastellu-Etchegorry, 2020). Clouds can be imported as 199 3D volumes with defined shape and homogenous properties. The scene default size is 500 km 200 \times 500 km \times 50 km, which is a good approximation of infinite plane-parallel atmosphere with 201 relative difference less than 0.1% (cf. Appendix A). The DART atmosphere database includes 202 six standard gas models (i.e., TROPICAL, MIDLATSUM, MIDLATWIN, SUBARCSUM, 203 SUBARCWIN and USSTD76 (Anderson et al., 1986)) and five standard aerosol models (*i.e.*, 204 Rural, Urban, Maritime, Tropospheric and Fog (Shettle and Fenn, 1979)). These models can be 205 adapted and data (e.g., gas and temperature profiles) can be imported to match actual 206 atmospheric conditions. The methods to compute the atmospheric vertical profiles are detailed 207 in (Wang and Gastellu-Etchegorry, 2020). In this new Earth-Atmosphere scene, the sensor can 208 be anywhere with any orientation and field of view (FOV).



209

Figure 1. The DART-Lux Earth-Atmosphere system: square cuboid filled by the atmosphere and a 3D
landscape (region of interest: ROI) at its bottom centre, surrounded by a horizontal background.
The observed target is in the ROI. Default size: X × Y × Z = 500 km × 500 km × 50 km.

The DART BRF camera gives the TOC radiance of the total scene at 1° x 1° angular resolution (Wang et al., 2022). It was adapted in order to give the directional radiance at any altitude from the ground to TOA, for any user-defined angular resolution and scene sub-zones. It provides the directional radiance measured from a user-defined virtual surface Σ . Figure 2 shows its three modes. In mode 1, the BRF camera provides the average directional radiance of Σ measured at Σ . In mode 2, it provides the average directional radiance at a given distance to the centre of Σ . In mode 3, it provides the average directional radiance of Σ measured at a given altitude.



Figure 2. The three modes of the improved BRF camera. They give the radiance from a user-defined surface Σ at altitude H, for any angular resolution and range. Mode 1: average directional radiance measured at Σ . Mode 2: average directional radiance measured at a given distance to the centre of Σ . Mode 3: average directional radiance measured at any user-defined altitude.

227 **3.2** Light transport equation

228 **3.2.1** Radiative transfer equation and its formal solution

Eq. (1) is not adapted to simulate the propagation of radiation in fluids (*e.g.*, atmosphere) and vegetation volumes treated as turbid media. Then, an integro-differential equation gives the change of radiance per unit distance $\frac{dL}{ds}$ in the considered ;medium at location *r* in direction Ω . For fluids, this equation is:

$$\frac{dL(r,\Omega)}{ds} = -\alpha_t(r) \cdot L(r,\Omega) + \frac{\alpha_s(r)}{4\pi} \cdot \int_{4\pi} L(r,\Omega') \cdot P(r,\Omega' \to \Omega) d\Omega' + \frac{dL_e(r,\Omega)}{ds}$$
(5)

with α_t the extinction coefficient and α_s the scattering extinction coefficient. α_t is assumed invariant to rotation: $\alpha_t(r, \Omega) = \alpha_t(r)$, as in a medium filled with microscopically isotropic and mirror-symmetric particles (Mishchenko et al., 2006). The unit normalized scattering phase function $P(r, \Omega' \rightarrow \Omega)$ $(\frac{1}{4\pi} \int_{4\pi} P(r, \Omega' \rightarrow \Omega) d\Omega = 1)$ gives the angular distribution of the scattered power to direction Ω due to the incident power from direction Ω' . The term $\frac{dL_e}{ds}$ is the variation of thermal radiance, *i.e.*, the Planck function, per unit distance. The notation of 239 incident direction Ω' differs for volume and surface scattering: it usually points towards the 240 interaction location in volume scattering and usually points away from the interaction 241 location in surface scattering.

242

Because it is an integro-differential equation, Eq. (5) is transformed to an integral form (Eq. (6)) that a Monte Carlo algorithm can solve. Eq. (6) shows that radiance $L(r, \Omega)$ at a point r in a medium is the sum of (1) radiance $L(r_0, \Omega)$ at r_0 transmitted to r, and (2) cumulated scattering and thermal emission from r_0 to r (Figure 3).

$$L(r,\Omega) = L(r_0,\Omega) \cdot \mathcal{T}(r \leftrightarrow r_0) + \int_0^s \left[\frac{\alpha_s(r')}{4\pi} \int_{4\pi} L(r',\Omega') \cdot P(r',\Omega' \to \Omega) \cdot d\Omega' + \frac{\partial L_e(r',\Omega)}{\partial s'}\right] \cdot \mathcal{T}(r \leftrightarrow r') \cdot ds'$$
(6)

with $s = ||r - r_0||$ the distance between r and r_0 , $r' = r - s'\Omega$ the location at the distance s' from r in direction Ω , and $\mathcal{T}(r \leftrightarrow r_0) = \exp(-\int_0^s \alpha_t(r') ds')$ the transmittance from r_0 to r. The left-right arrow emphasizes the Helmholtz reciprocity principle (i.e., $\mathcal{T}(r_0 \rightarrow r) = \mathcal{T}(r \rightarrow r_0)$).



250

Figure 3. Radiance $L(r, \Omega)$ at *r*. It is the sum of radiance $L(r_0, \Omega)$ at r_0 of a surface Σ that is transmitted to *r*, and radiance due to scattering and thermal emission along the path $\overrightarrow{r_or}$.

253 **3.2.2** Unified light transport equation for the surface and the volume

254 In an infinite medium, Eq. (6) becomes $L(r, \Omega) = \int_0^\infty \frac{\partial L(r', \Omega)}{\partial s'} \cdot \mathcal{T}(r \leftrightarrow r') \cdot ds'$ with:

$$\frac{\partial L(r',\Omega)}{\partial s'} = \int_{4\pi} L\left(r',\Omega\right) \cdot \frac{\alpha_s(r') \cdot P(r',\Omega' \to \Omega)}{4\pi} \cdot d\Omega + \frac{\partial L_e(r',\Omega)}{\partial s'} \tag{7}$$

Eq. (7) becomes an integral over volume *V* by replacing directions with pairs of vertices (*e.g.*, $\Omega \equiv (r' \rightarrow r)$), and solid angle $d\Omega'$ by $\frac{dA(r'')}{\|r'' - r'\|^2}$, and using the visibility function $V_t(r'' \leftrightarrow r')$:

$$\frac{\partial L(r' \to r)}{\partial s'} = \int_{V} \frac{\partial L(r'' \to r')}{\partial s''} \cdot \frac{\alpha_{s}(r') \cdot P(r'' \to r' \to r)}{4\pi} \cdot \frac{V_{t}(r'' \leftrightarrow r') \cdot \mathcal{T}(r'' \leftrightarrow r')}{\|r'' - r'\|^{2}} \cdot dV(r'') + \frac{\partial L_{e}(r' \to r)}{\partial s'} \tag{8}$$

257 Since the derived volume light transport equation (Eq. (8)) and the surface light transport 258 equation (Wang et al., 2022) have a similar formulation, a unified formulation can be used:

$$\tilde{L}(r' \to r) = \tilde{L}_e(r' \to r) + \int_{\mathcal{M}} \tilde{L}(r'' \to r') \cdot \tilde{f}_s(r'' \to r' \to r) \cdot \tilde{G}(r' \leftrightarrow r'') \cdot d\mathcal{M}(r'')$$
(9)

259 with \mathcal{M} a surface A or volume V depending on the material at the vertex. The radiance terms 260 \tilde{L} and \tilde{L}_e correspond to radiance for a surface, and radiance per unit distance for a volume:

261
$$\tilde{L}(r'' \to r') = \begin{cases} L(r'' \to r') & \forall r' \in A \\ \frac{\partial L(r'' \to r')}{\partial s''} & \forall r' \in V \end{cases}$$

262 The scattering distribution function \tilde{f} is either the BSDF for a surface, or the product of the

scattering extinction coefficient and the scattering phase function for a volume:

264
$$\tilde{f}_{s}(r'' \to r' \to r) = \begin{cases} f_{s}(r'' \to r' \to r) & \forall r' \in A \\ \alpha_{s}(r') \cdot \frac{P(r'' \to r' \to r)}{4\pi} & \forall r' \in V \end{cases}$$

265 The generalized geometric term $\tilde{G}(r'\leftrightarrow r'') = V(r'\leftrightarrow r'') \cdot \mathcal{T}(r''\leftrightarrow r') \cdot \frac{\tilde{\mu}_{0}^{r'} \cdot \tilde{\mu}_{i}^{r''}}{\|r''-r'\|^{2}}$ is defined with:

266
$$\tilde{\mu}_{o}^{r'} = \begin{cases} \cos \theta_{o}^{r'} & \forall r' \in A \\ 1, & \forall r' \in V \end{cases} \text{ and } \tilde{\mu}_{i}^{r''} = \begin{cases} \cos \theta_{i}^{r''} & \forall r'' \in A \\ 1, & \forall r'' \in V \end{cases}$$

267 3.2.3 Path integral formulation

In an interaction, the incident radiance is the path attenuated exit radiance from a previous interaction. Therefore, Eq. (9) is iteratively expanded to an infinite sum of multidimensional integrals where each integral is the contribution of a specific scattering order to $\tilde{L}(r_1 \rightarrow r_0)$:

271
$$\tilde{L}(r_1 \to r_0) = \tilde{L}_e(r_1 \to r_0) + \int_{\mathcal{M}} \tilde{L}_e(r_2 \to r_1) \cdot \tilde{f}_s(r_2 \to r_1 \to r_0) \cdot \tilde{G}(r_1 \leftrightarrow r_2) \cdot d\mathcal{M}(r_2)$$

272
$$+ \int_{\mathcal{M}} \int_{\mathcal{M}} \tilde{L}_{e}(r_{3} \rightarrow r_{2}) \cdot \tilde{f}_{s}(r_{3} \rightarrow r_{2} \rightarrow r_{1}) \cdot \tilde{G}(r_{2} \leftrightarrow r_{3}) \cdot \tilde{f}_{s}(r_{2} \rightarrow r_{1} \rightarrow r_{0}) \cdot \tilde{G}(r_{1} \leftrightarrow r_{2}) \cdot d\mathcal{M}(r_{3}) \cdot d\mathcal{M}(r_{2}) + \dots$$

273 Since $r_1 \rightarrow r_0$ is the direction to the sensor, the radiance measurement $L^{(j)}$ at pixel *j* is computed

by integrating $\tilde{L}(r_1 \rightarrow r_0)$ weighted by the importance function $W_e^{(j)}(r_0 \rightarrow r_1)$ of the sensor:

$$\tilde{L}^{(j)} = \int_{A} \int_{\mathcal{M}} W_{e}^{(j)}(r_{0} \rightarrow r_{1}) \cdot \tilde{L}(r_{1} \rightarrow r_{0}) \cdot \tilde{G}(r_{0} \leftrightarrow r_{1}) \cdot d\mathcal{M}(r_{1}) \cdot dA(r_{0})$$
(10)

275 $L^{(j)}$ is a Lebesgue integral over the space $\tilde{\mu}$ of surfaces and volumes of the set of paths $\tilde{\mathcal{D}}$:

$$\tilde{L}^{(j)} = \int_{\widetilde{D}} \tilde{f}^{(j)}(\bar{r}) \cdot d\tilde{\mu}(\bar{r})$$
(11)

276 $\widetilde{\mathcal{D}}_n$ and $\widetilde{\mu}(\widetilde{\mathcal{D}}_n)$ are generalized paths that intersect surfaces and volumes, with $\widetilde{\mathcal{D}}_n$ the multiple 277 cartesian product of the space {*A*, *V*}, since a vertex is either in a volume *V* or on a surface *A*.

278
$$\widetilde{\mathcal{D}}_n = \bigcup_{c \in \{0,1\}^n} (A \times \mathcal{M}_1 \times \dots \times \mathcal{M}_n) \text{, with } \mathcal{M}_k = \begin{cases} A, c_k = 0\\ V, c_k = 1 \end{cases}$$

279
$$\tilde{\mu}(\tilde{\mathcal{D}}_n) = \int_{\mathcal{D}_n} d\mu(\bar{r}_n) = \sum_{c \in \{0,1\}^n} \int_{(A \times \mathcal{M}_1 \times \dots \times \mathcal{M}_n)} dA(r_0) \cdot \prod_{k=1}^n \begin{cases} dA(r_k), \ c_k = 0 \\ dV(r_k), \ c_k = 1 \end{cases}$$

280 with Cartesian product such that $\{0, 1\}^n = \{(c_1, c_2, \dots, c_k, \dots, c_n) | c_k \in \{0, 1\} \forall k \in \{1, 2, \dots, n\} \}.$

281

For example, $\tilde{\mathcal{D}}_1 = (A \times A) + (A \times V)$ describes a surface emission and a volume emission event. $\tilde{\mathcal{D}}_2 = (A \times A \times A) + (A \times A \times V) + (A \times V \times A) + (A \times V \times V)$ describes a surface emission followed by a surface scatter event, a surface emission followed by a volume scatter event, a volume emission followed by a surface scatter event and a volume emission followed by a volume scatter event, and so on. Therefore, integration over $\tilde{\mathcal{D}}_n$ is the sum of 2^n (*n*+1)dimensional integrals.

288

289 The unified contribution function $f^{(j)}(\bar{r}_n)$ uses the unified quantities for both surfaces and 290 volumes in the formulation in Eq. (2):

$$\tilde{f}^{(j)}(\bar{r}_n) = \tilde{L}_e(r_n \to r_{n-1}) \cdot \tilde{G}(r_0 \leftrightarrow r_1) \cdot W_e^{(j)}(r_1 \to r_0) \cdot \prod_{k=2}^n \tilde{f}_s(r_k \to r_{k-1} \to r_{k-2}) \cdot \tilde{G}(r_{k-1} \leftrightarrow r_k) \quad (12)$$

Thus, a unified algorithm handles surface and volume interactions. Differences are only in assessing the effective source emission, scattering distribution function, and geometric term at each vertex r_k according to the material. (Regaieg, 2023) describes its adaptation to vegetation treated as turbid medium.

295

296 3.3 Radiative transfer modelling

297 As the Earth-Atmosphere system (Figure 1) has a huge size (*i.e.*, $X \times Y \times Z = 500 \text{ km} \times 500 \text{ km}$ 298 \times 50 km) compared to ROI, the forward random walk from the light source is inefficient. For 299 example, a ray from a source located 200 km away from the ROI has a very small probability 300 to be scattered into the sensor FOV. In addition, its intersection with a scene element (e.g., a 301 leaf) can be very inaccurate due to computer decimal imprecision. Therefore, because it is time 302 consuming and inaccurate, the forward random walk is deactivated for simulating Monte Carlo 303 surface-atmosphere RT. In short, a random virtual ray is emitted from the sensor, and is 304 connected to the light source after each interaction with a volume or a surface, using a user 305 defined maximal scattering order M to limit the path length. Then, the estimator in Eq. (4) is:

$$F_{\rm IS}^{(j)} = \sum_{n=1}^{\infty} \frac{\tilde{f}^{(j)}(\bar{r}_n)}{p(\bar{r}_n)}$$
(13)

306 3.3.1 Light scattering

307 The sampling of a stochastic path \bar{r}_n and the evaluation of the path contribution $\frac{\tilde{f}^{(j)}(\bar{r}_n)}{p(\bar{r}_n)}$ are 308 detailed here. The scattering direction is sampled with the angular distribution of the exit power 309 due to unit incident power. For surfaces, the probability density function (PDF) for incident 310 direction $-\Omega_i$ (minus sign as Ω_i is defined from the scattering point) and exit direction Ω_o is:

$$p(\Omega_{o}|-\Omega_{i}) = \begin{cases} P^{*} \cdot \frac{\tilde{f}(r, -\Omega_{i} \to \Omega_{o}) \cdot \cos \theta_{o}}{\int_{2\pi} \tilde{f}\left(r, -\Omega_{i} \to \Omega_{o}\right) \cdot \cos \theta_{o} d\Omega_{o}}, & \text{if } (\vec{n} \cdot \Omega_{o}) \cdot (\vec{n} \cdot \Omega_{i}) \ge 0\\ (1 - P^{*}) \cdot \frac{\tilde{f}(r, -\Omega_{i} \to \Omega_{o}) \cdot \cos \theta_{o}}{\int_{2\pi} \tilde{f}\left(r, -\Omega_{i} \to \Omega_{o}\right) \cdot \cos \theta_{o} d\Omega_{o}}, & \text{otherwise} \end{cases}$$
(14)

311 with P^{*} the reflection probability and \vec{n} the surface normal. $p(\Omega_i | -\Omega_o)$ is similarly defined.

312 The conditional PDF of volume scattering (isotropic mirror-symmetric microscopic particles) is:

$$p(\Omega_o|\Omega_i) = \frac{\tilde{f}(r,\Omega_i \to \Omega_o)}{\int_{4\pi} \tilde{f}\left(r,\Omega_i \to \Omega_o\right) d\Omega_o} = \frac{P(r,\Omega_i \to \Omega_o)}{4\pi}$$
(15)

313 with $p(\Omega_i | \Omega_o)$ being similarly defined.

314 Two types of atmospheric scattering implemented in DART are presented here:

315 - *Rayleigh scattering* (particles with diameter d such that $0.002 < \frac{\pi d}{\lambda} < 0.2$) (Petty, 2006) 316 The Rayleigh phase function uses the phase angle γ (cos $\gamma = |\Omega_i \cdot \Omega_o|$) and a depolarization 317 factor δ to consider the influence of molecule anisotropy. δ is a spectral quantity (Bates, 318 1984; Bucholtz, 1995) that decreases from 0.04545 at 0.2 μ m down to 0.02955 at 0.4 μ m, 319 0.02730 at 0.8 μ m, and is nearly constant for longer wavelengths. Its relative influence on 320 Rayleigh scattering phase function of dry air is smaller than 0.1% for wavelengths larger 321 than 0.4 μ m. It is commonly assumed to be equal to 0.0279, as advised by (Young, 1980):

$$P(r, \Omega_i \to \Omega_o) = \frac{3}{2} \cdot \frac{1 - \delta}{2 + \delta} \cdot \left(\frac{1 + \delta}{1 - \delta} + \cos^2 \gamma\right)$$
(16)

322 - *Particle scattering* (particles with diameter d such that $\frac{\pi d}{\lambda} > 0.2$)

323 The double Henyey-Greenstein phase function simulates it, with asymmetry factors $g_1 > 0$

324 (forward scattering) and $g_2 < 0$ (backward scattering) and ratio *a* of forward scattering:

$$P(r, \Omega_i \to \Omega_o) = \frac{a \cdot (1 - g_1^2)}{(1 + g_1^2 - 2g_1 \cdot \cos \gamma)^{3/2}} + \frac{(1 - a) \cdot (1 - g_2^2)}{(1 + g_2^2 - 2g_2 \cdot \cos \gamma)^{3/2}}$$
(17)

325 3.3.2 Light transmission

326 Once an exit direction Ω_o is sampled at r, an intersection test along Ω_o gives the intersected 327 vertex on the nearest surface (Figure 4). If there is no medium in the line of sight, the process 328 continues by sampling the next scattering direction at the intercepted vertex. Otherwise, a free 329 path *S* in the medium is sampled according to the path PDF p(s) and the cumulative 330 distribution function $P_S(s)$ (*i.e.*, $\mathbb{P}(S \le s)$):

$$P_{S}(s) = \mathbb{P}(S \le s) = 1 - \mathcal{T}(s) \text{ and } p(s) = \frac{dP_{S}(s)}{ds} = \alpha_{t}(s) \cdot \mathcal{T}(s)$$
(18)

with $\mathcal{T}(s)$ the transmittance from r to $r + s \cdot \Omega_o$ along Ω_o and $\alpha_t(s)$ the extinction coefficient at $r + s \cdot \Omega_o$. If the signal is modelled for a series of spectral bands, α_t is an average extinction coefficient for all spectral bands.



334

Figure 4. Distance sampling schema. *s* is the distance from the start location *r* to the current location $r+s\cdot\Omega_o$ in direction Ω_o . Σ is the nearest surface in the direction of propagation.

337 The probabilistic free path *S* is derived from a random variable $\xi \in [0, 1)$ and an inversion 338 function $S = P_S^{-1}(\xi)$. For a homogeneous medium (*i.e.*, constant α_t in the line of sight):

$$S = P_S^{-1}(\xi) = -\frac{\ln(1-\xi)}{\alpha_t}$$
(19)

Usually, α_t varies in the line of sight, and *S* cannot be derived analytically. Then, the medium is represented by discrete volumes and the free path is sampled with the *Regular Tracking* method (Amanatides and Woo, 1987). For example, for a series of homogeneous segment medium along the line of sight, each one with extinction coefficient α_i and segment length Δs_i :

$$p(s) = \alpha_i \cdot e^{-[\sum_{k=0}^{i-1} \alpha_k \cdot \Delta s_k + \alpha_i \cdot (s \cdot \sum_{k=0}^{i-1} \Delta s_k)]}$$

$$\forall s \in [\sum_{k=0}^{i-1} \Delta s_k, \sum_{k=0}^{i} \Delta s_k]$$

$$P_s(s) = 1 - e^{-[\sum_{k=0}^{i-1} \alpha_k \cdot \Delta s_k + \alpha_i \cdot (s \cdot \sum_{k=0}^{i-1} \Delta s_k)]}$$

$$(20)$$

343 The free path equation $S = P_S^{-1}(\xi)$ is solved recursively until the path optical depth gives the 344 randomly sampled value $-\ln(1 - \xi)$:

$$-\ln(1-\xi) = \sum_{k=0}^{i-1} \alpha_k \cdot \Delta s_k + \alpha_i \cdot \left(S - \sum_{k=0}^{i-1} \Delta s_k\right)$$

Once sampled, if the free path *S* is less than the distance s_{Σ} to the nearest surface (Figure 4), it defines the next scattering event in the medium. If $S \ge s_{\Sigma}$, the sampled vertex is on the nearest surface and the path probability density is multiplied by the probability $\mathbb{P}(S \ge s_{\Sigma}) = \int_{s_{\Sigma}}^{\infty} p(s) ds = \mathcal{T}(s_{\Sigma})$ that the ray will be intercepted by the nearest surface.

350 3.3.3 Measurement evaluation

351 Starting from the sensor, a complete path is created by repeatedly sampling a vertex and free 352 path. In detail, a vertex r_0 on the lens and an emitted virtual ray direction Ω_0 are first sampled 353 using sensor characteristics. Then, a vertex r_k is created by sampling a stochastic exit direction Ω_{k-1} at the vertex r_{k-1} . This sampling depends only on the local incident direction $r_{k-2} \rightarrow r_{k-1}$. 354 355 The free path is always sampled after each bounce. Finally, the last vertex r_n on the light source 356 is generated by uniformly sampling the solid angle subtended by the light source at the previous vertex r_{n-1} . Here the free path is not sampled. Instead, we force the radiation to connect the 357 358 light source to increase the efficiency. The path PDF is evaluated by:

$$p(\bar{r}_n) = p(r_0) \cdot p(r_1|r_0) \cdot \prod_{k=2}^{n-1} p(r_k|r_{k-1}, r_{k-2}) \cdot p(r_n|r_{n-1}) = \prod_{k=0}^n \tilde{p}(r_k)$$
(21)

Eq. (22) shows the expression of PDF p(r_k|r_{k-1}, r_{k-2}, ..., r₀)≡p̃(r_k) for 1<k<n with a reverse
arrow to indicate that it is for backward light transport (*cf.* Appendix C in (Wang et al., 2022)).
PDFs p(r₀)≡p̃(r₀), p(r₁|r₀)≡p̃(r₁) and p(r_n|r_{n-1})≡p̃(r_n) can be derived in a similar way.

$$\tilde{p}(r_k) = \begin{cases}
p(\Omega_{k-1}) \cdot \frac{\mathcal{T}(r_{k-1} \leftrightarrow r_k) \cdot \cos \theta_o^{r_k}}{\|r_{k-1} - r_k\|^2} & \forall r_k \in A \\
p(\Omega_{k-1}) \cdot \frac{\alpha_e(r_k) \cdot \mathcal{T}(r_{k-1} \leftrightarrow r_k)}{\|r_{k-1} - r_k\|^2} & \forall r_k \in V
\end{cases}$$
(22)

362 The contribution function $\tilde{f}^{(j)}(\bar{r}_n)$ is computed as in Eq. (12):

$$F_{\rm IS}^{(j)} = \sum_{n=1}^{\infty} \frac{\tilde{L}_e(r_n \to r_{n-1}) \cdot \tilde{G}(r_0 \leftrightarrow r_1) \cdot W_e^{(j)}(r_0 \to r_1)}{\tilde{p}(r_0) \cdot \tilde{p}(r_1)} \cdot \prod_{k=2}^n \frac{\tilde{f}(r_k \leftrightarrow r_{k-1} \leftrightarrow r_{k-2}) \cdot \tilde{G}(r_{k-1} \leftrightarrow r_k)}{\tilde{p}(r_k)}$$
(23)

Eq. (23) is analysed in Appendix B for a semi-infinite plane parallel atmosphere, illuminated
by parallel sunlight and observed by a TOA orthographic camera. Results are consistent with
the familiar Single Scattering Albedo (SSA) method (Spada et al., 2006).

366

367 4 Model assessment and application

368 DART-Lux already proved to be accurate (Wang et al., 2022) for land surfaces, as compared 369 with Monte Carlo models in the RAMI experiment (Widlowski et al., 2007), and remote sensing 370 and in-situ measurements (Malenovsky et al., 2023, Liu et al., 2023). For example, (Landier et 371 al., 2018) noted a urban TOC albedo (ratio of upward exitance and downward irradiance) 372 relative difference $\approx 2.5\%$ between in-situ measurements and simulations using satellite-derived 373 optical properties of urban elements. This section presents the assessment of DART accuracy 374 for the adjacency effect modelling, including a quantitative study on this effect.

375 4.1 Accuracy assessment

DART accuracy in atmospheric RT modelling, in particular the adjacency effect, was assessed
with the Monte Carlo atmospheric model SMART-G (Ramon et al., 2019), already validated
with the reference MYSTIC model in the International Polarized Radiative Transfer (IPRT)
intercomparison study (https://www.meteo.physik.uni-muenchen.de/~iprt/doku.php). SMARTG is developed by HYGEOS (https://www.hygeos.com) for the French space agency (CNES)

to simulate light propagation in the atmosphere and oceans. Our assessment consists of two phases using atmospheric parameters of case B2 (<u>https://www.meteo.physik.uni-</u> <u>muenchen.de/~iprt/doku.php?id=intercomparisons:b2_absorption</u>) of the IPRT study (Emde et al., 2015). This atmosphere has 30 equal-thickness (1 km) layers, with given absorption and scattering optical thickness per layer. Table 1 shows the DART and SMART-G configurations. 386

- Phase 1 Phase 2 **IPRT** case B2 **IPRT** case B2 **Atmosphere model** Land surface Infinite black surface Black disc (R = 2 km) +Infinite white environment **Solar direction** $SZA = 60^{\circ}$ $SZA = 0^{\circ} and 30^{\circ}$ $SAA = 0^{\circ}$ $SAA = 270^{\circ}$ Sensor altitude 30 km (TOA) 30 km (TOA) Directional reflectance for: Nadir image of the disc: Output VZA $0^{\circ} - 80^{\circ}$ with 5° step Spatial resolution: 10 m VAA $0^{\circ} - 180^{\circ}$ with 5° step Image size: 400×400
- 387 Table 1. Simulation configurations for Phase 1 and Phase 2 comparisons.

2	Q	Q
J	0	0

In phase 1, DART and SMART-G agree (Figure 5): the relative root mean square difference $\epsilon_{\text{DART}}^{\text{SMART-G}} = 0.20\%$ for 629 upward viewing directions (Table 1), by considering $\epsilon_{\text{model}}^{\text{reference}} = \frac{\sqrt{\sum_{i=1}^{N} (\rho_{\text{model}}(i) - \rho_{\text{reference}}(i))^2}}{\sqrt{\sum_{i=1}^{N} \rho_{\text{reference}}(i)^2}}$ (Ende et al., 2015). This small value is mainly due to Monte Carlo noise and rounding errors in calculations. The squared-average TOA reflectance $\sqrt{\frac{\sum_{i=1}^{N} (\rho_{\text{SMART-G}}(i))^2}{N}}$ is 0.04866, with maximum standard deviation $\sigma_{\text{Max}}^{\text{SMART-G}} = 1.1 \times 10^{-5}$ and $\sigma_{\text{Max}}^{\text{DART}} = 3.8 \times 10^{-5}$. It gives composed standard deviation $\sigma_{\text{Max}}^{\text{tot}} = \sqrt{(\sigma_{\text{Max}}^{\text{SMART-G}})^2 + (\sigma_{\text{Max}}^{\text{DART}})^2} = 4.0 \times 10^{-5}$ and maximum tolerated relative difference $\frac{3 \times \sigma_{\text{tot}}}{0.04866} = 0.25\%$, which is a probability of 99.7% the

relative difference $\varepsilon_{DART}^{SMART-G}$ lies in 0.25%. Compared to the proposed reference model MYSTIC 396 in IPRT program, the relative differences are $\epsilon_{DART}^{MYSTIC}=0.21\%$ and $\epsilon_{SMART-G}^{MYSTIC}=0.013\%.$ 397 398

399 In phase 2, we determined the horizontal profiles of average TOA reflectance of the black disc² from its centre to its edge, with a step of 0.1 km, for two solar directions³ (SZA = 0° and SZA 400 401 $= 30^{\circ}$) (Figure 6). The adjacency effect clearly increases from the centre to the edge of the disc. 402 The relative root mean square difference is 0.033% for SZA = 0° and 0.032% for SZA = 30° . 403 These small differences are due to Monte Carlo noise and rounding error in calculations. Indeed, the average TOA nadir reflectance of the disc is 0.137 for SZA = 0° and 0.114 for SZA = 30° , 404 while DART and SMART-G maximum standard deviations are $\sigma_{MAX}^{SMART-G} = 6 \times 10^{-6}$ and 405 $\sigma_{\text{MAX}}^{\text{DART}} = 1.8 \times 10^{-5}$. Then, composed standard deviation $\sigma_{\text{MAX}}^{\text{tot}} = \sqrt{\left(\sigma_{\text{MAX}}^{\text{SMART-G}}\right)^2 + \left(\sigma_{\text{MAX}}^{\text{DART}}\right)^2} = 1.9 \times 10^{-5}$. 406 10^{-5} and maximum tolerated relative difference $\frac{3 \times \sigma_{\text{tot}}}{0.114} = 0.05\%$. 407







Figure 5. DART and SMART-G TOA directional reflectance and difference in phase 1, from left to 410 right. Simulation parameters are indicated in Table 1.

² In phase 2, DART simulates a nadir 400 x 400 image with spatial resolution of 10 m while SMART-G simulates $1.6 \ge 10^5$ sensors that are positioned at each pixel center of the image.

³ The solar direction in DART is defined as a vector in local coordinates pointing towards the sun. Azimuth is measured from the north-south axis in an anticlockwise manner.



412 Figure 6. DART and SMART-G TOA reflectance value and difference from centre to edge of black
413 disc for sun zenith angle (SZA) = 0° and 30°. Simulation parameters are in Table 1.

415 **4.2 3D** modelling of the adjacency effect

416 **4.2.1 The experiment**

417 The influence of the adjacency effect on target radiance and albedo is shown for four Sentinel-2A bands: blue (B: $\lambda = 0.4924 \,\mu\text{m}$, $\Delta \lambda = 0.066 \,\mu\text{m}$), green (G: $\lambda = 0.5598 \,\mu\text{m}$, $\Delta \lambda = 0.036 \,\mu\text{m}$, 418 419 red (R: $\lambda = 0.6646 \,\mu\text{m}, \Delta \lambda = 0.031 \,\mu\text{m}$) and near infrared (NIR: $\lambda = 0.8328 \,\mu\text{m}, \Delta \lambda = 0.106 \,\mu\text{m}$). 420 The atmosphere is defined by the USSTD76 gas model, and the Rural aerosol model. Table 2 421 gives its vertical scattering and absorption optical depth per band. Solar zenith and azimuth 422 angles are $\theta_s = 30^\circ$ and $\varphi_s = 270^\circ$, respectively. The target is a circular city with a 2 km radius 423 in a 3D neighbourhood of 10 km sides inside a 500 km square Lambertian plane background 424 (Figure 7). The city has 55828 houses in regular rows (tiled roofs, concrete wall) and streets 425 (asphalt roads), with optical properties of urban materials (e.g., asphalt, concrete, tile) from the

- 426 SLUM (http://www.met.reading.ac.uk/micromet/LUMA/SLUM.html) and ECOSTRESS
- 427 (https://speclib.jpl.nasa.gov) libraries. Two cases are considered (Figure 8):
- 428 3D case (Figure 8): the neighbourhood is a $10 \text{ km} \times 10 \text{ km}$ 3D forest with 1553504 nearly-
- 429 randomly located Tilia cordata trees at five growing stages, with homogeneous understory.
- 430 The tree models and optical properties, including those of the understory, are from the
- 431 RAMI experiment (https://rami-benchmark.jrc.ec.europa.eu/_www/index.php).
- 432 1D case: the neighbourhood is a 10 km x 10 km Lambertian plane with the TOC albedo of
- 433 the forest. DART computes the TOC albedo of the forest and city for subzones $(1 \text{ km} \times 1 \text{ mm})$
- 434 km at city centre and $2 \text{ km} \times 2 \text{ km}$ in top-left forest, in Figure 7).

Table 2. Atmosphere vertical scattering and absorption optical depth (OD), and city and forest TOCalbedos, for four Sentinel-2A bands.

Band	Wavelength	Scattering OD	Absorption OD	City TOC albedo	Forest TOC albedo
В	0.4924 μm	0.501	0.030	0.06	0.03
G	0.5598 μm	0.392	0.058	0.07	0.07
R	0.6646 µm	0.286	0.036	0.010	0.03
NIR	0.8328 μm	0.189	0.045	0.100	0.42



Figure 7. 3D case. a) Target: circular city of 2 km radius with 55828 houses spaced 15 m apart in a 10 \times 10 km forest with 1553504 quasi-randomly distributed Tilia cordata trees at five growing stages, spaced \approx 5 m apart). b) DART created house. b) Example of Tilia cordata: TICO 5.



Figure 8. Two cases: city (*i.e.*, target) in a neighbourhood that is a forest (a: 3D case) or a Lambertian
plane with the forest TOC albedo (b: 1D case). The two cases have the same background.

444 4.2.2 Adjacency effect on TOA nadir radiance

The adjacency effect is evaluated as the difference of two simulations, one with the 1D/3D neighbourhood and the background and the other one with the neighbourhood and background as flat black surfaces. Figure 9 shows the TOA nadir adjacency NIR radiance $L_{adj}(x, y)$ and $L_{adj}(r)$ of the city with 1D (a) and 3D (b) neighbourhood, with *r* the distance from the city

449 centre to the edge (r = 2 km). L_{adj} increases from the city centre. It is larger for the 3D 450 neighbourhood than for the 1D neighbourhoods, although both have the same TOC albedo. This 451 is mostly due to the forest anisotropic reflectance.





Figure 9. Adjacency radiance L_{adj} in the nadir TOA images for the 1D (a) and 3D (b) neighbourhoods at NIR band. $L_{adj}(r)$ greatly increases with distance r from the city centre to the edge. $L_{adj}(r)$ is the average for all pixels $L_{adj}(x, y)$ in the ring $[r, r+\Delta r]$ with $\Delta r=0.1$ km (Table 3).

Table 3 shows nadir L_{adj} at city centre and edge, and its relative contribution $\zeta_{L_{adj}} = L_{adj}/L_{TOA}$ 456 to TOA radiance for four Sentinel-2A bands. L_{adj} is $\approx 2-3$ times larger at the edge of the city 457 than at its centre, for all bands. It reaches ~20% in the NIR band. L_{adj} and $\zeta_{L_{adj}}$ increase with 458 the neighbour TOC albedo and the importance of atmospheric scattering. For example, $\zeta_{L_{adj}}$ is 459 460 more than 5 times larger in NIR band than in the red band because the forest TOC albedo is 461 more than 12 times larger in the NIR band than in the red band. Also, $\zeta_{L_{adi}}$ is more than 1.5 462 times larger in the blue band than in the red band, although the TOC albedo of the forest is 463 similar, because the atmosphere scatters more in the blue band than in the red band (cf. 464 atmospheric scattering optical depth in Table 2). The study of adjacency effect under different 465 aerosol loadings in the Appendix C confirms this point. We also note that the impact of 3D

466 structure on the adjacency radiance is maximal in the NIR band, the $\zeta_{L_{adj}}$ values of the 1D and 467 3D cases differ by 0.3% at the city centre and by 1.3% at the city edge.

468 Table 3. Adjacency radiance L_{adj} (W/m²/sr/ μ m) and its relative contribution $\zeta_{L_{adj}} = L_{adj}/L_{TOA}$ (%) to

469

total TOA nadir radiance at the city centre and edge, for the four Sentinel-2A bands.

		1D neig	ghbour		3D neighbour			
	Centre		Edge		Centre		Edge	
	$L_{\rm adj}$	$\zeta_{L_{ m adj}}$	$L_{\rm adj}$	$\zeta_{L_{ m adj}}$	$L_{\rm adj}$	$\zeta_{L_{ m adj}}$	$L_{\rm adj}$	$\zeta_{L_{ m adj}}$
В	1.4	2.2%	2.5	4.2%	1.4	2.3%	2.8	4.7%
G	1.8	3.6%	3.9	8.0%	1.9	3.9%	4.4	9.0%
R	0.4	0.9%	1.1	2.5%	0.4	1.0%	1.2	2.8%
NIR	1.7	5.5%	6.1	17.5%	1.8	5.8%	6.6	18.8%

470

471 **4.2.3** Adjacency effect on directional radiance and albedo

472 The TOA albedo of the city centre and the edge are simulated using the BRF camera (Figure 2) 473 in mode 3, for a user-defined plane ($\Delta x = \Delta y = 100$ m) with altitude H=15 m, mode 3 to obtain 474 the TOA signal and mode 1 to obtain the TOC signal. Figure 10 shows the directional 475 distributions of TOA radiance L_{TOA} , adjacency radiance L_{adj} and its relative contribution $\zeta_{L_{adj}}$. 476 at the city centre and edge, for the NIR band. L_{TOA} tends to be larger in the backward directions 477 due to the hot-spot effect of the 3D land surface and is smaller in the forward directions due to 478 the observation of the shadows of the city buildings. L_{adi} increases with the obliquity of the 479 observation directions. For example, $\zeta_{L_{adj}}$ can be as high as 60% for directions with VZA = 80°, 480 because increasing the "sensor-city" path (*i.e.*, larger atmospheric optical depth for observation) 481 decreases the city signal and increases the city neighbourhood signal by atmospheric scattering.

TOA exitance M_{TOA} is the hemispherical integral of the directional average upward TOA 483 radiance of a surface at TOC level. TOA albedo \mathcal{A}_{TOA} is the ratio of TOA exitance M_{TOA} to 484 TOA irradiance E_{TOA} . Table 4 shows the contribution \mathcal{A}_{adj}^{Z} (altitude level Z can be TOC or 485 TOA) due to the adjacency effect and its relative importance $\zeta_{\mathcal{A}_{adj}^Z} = \mathcal{A}_{adj}^Z / \mathcal{A}_Z$ at the city centre 486 and edge, for the four Sentinel-2A bands. $\zeta_{\mathcal{A}_{adj}^{TOA}}$ is usually larger than 5%, the maximum TOC 487 488 advised by the Global Climate Observing System (GCOS: albedo uncertainty 489 https://gcos.wmo.int/en/essential-climate-variables/albedo/). Therefore, the adjacency effect 490 can be a significant source of uncertainty for the interpretation of TOC albedo from RS images 491 if they are not corrected by the atmospheric correction algorithm. Here, the large TOC albedo of the neighbour forest in the NIR can increase \mathcal{A}_{adj}^{TOA} up to 0.035 (*i.e.*, 28.1% of the total TOA 492 493 albedo). Although it impacts the directional radiance, the 3D structure of the neighbourhood only slightly influences \mathcal{A}_{adj}^{TOA} : the difference of \mathcal{A}_{adj}^{TOA} between 1D and 3D neighbour case is 494 495 less than 0.8% for all four bands.





City centre City edge	
Chy churc Chy cuge	



Figure 10. Angular plots of TOA total radiance L_{TOA} , radiance L_{adj} due to the adjacency effect, and relative contribution $\zeta_{L_{adj}}$ at the city centre and edge. NIR band. a) 1D neighbour. b) 3D neighbour.

500 Table 4. Adjacency TOA albedo \mathcal{A}_{adj}^{TOA} and its percentage contribution $\zeta_{\mathcal{A}_{adj}^{TOA}} = \mathcal{A}_{adj}^{TOA} / \mathcal{A}_{TOA}$ (%) to 501 total TOA albedo at the city centre and edge, for four Sentinel-2A bands.

		1D nei	ghbour			3D nei	ghbour	
	Centre		Edge		Cer	Centre		lge
	$\mathcal{A}_{\mathrm{adj}}^{\mathrm{TOA}}$	$\zeta_{\mathcal{A}_{\mathrm{adj}}^{\mathrm{TOA}}}$	$\mathcal{A}_{\mathrm{adj}}^{\mathrm{TOA}}$	$\zeta_{\mathcal{A}_{\mathrm{adj}}^{\mathrm{TOA}}}$	$\mathcal{A}_{\mathrm{adj}}^{\mathrm{TOA}}$	$\zeta_{\mathcal{A}_{\mathrm{adj}}^{\mathrm{TOA}}}$	$\mathcal{A}_{\mathrm{adj}}^{\mathrm{TOA}}$	$\zeta_{\mathcal{A}_{\mathrm{adj}}^{\mathrm{TOA}}}$
В	0.004	3.8%	0.006	4.9%	0.005	3.9%	0.007	5.2%
G	0.008	7.4%	0.010	10.1%	0.008	7.6%	0.011	10.6%
R	0.003	2.6%	0.004	3.9%	0.003	2.6%	0.004	4.1%
NIR	0.021	18.6%	0.033	27.3%	0.022	19.0%	0.035	28.1%

502

The influence of the adjacency effect is smaller on the TOC irradiance and TOC exitance than 503 504 on the TOA exitance. Its relative contribution to local TOC albedo A_{TOC} is even smaller 505 because it contributes in a similar way to TOC exitance M_{TOC} and irradiance E_{TOC}: it is only 506 about 0.13% at NIR band, 0.01% at the red band, 0.03% at the green band and 0.03% at the 507 blue band. Table 5 shows M_{TOC} , E_{TOC} and A_{TOC} at NIR band as well as their respective increases Δ_{adj}^{TOC} due to the adjacency effect, at the city centre and edge, for 1D and 3D neighbour 508 cases. The ratio of the components Δ_{adj}^{TOC} to M_{TOC} and E_{TOC} is close to \mathcal{A}_{TOC} (*i.e.*, $\Delta_{adj}^{M_{TOC}}$ / 509 $\Delta_{\rm adi}^{\rm E_{\rm TOC}} \approx \mathcal{A}_{\rm TOC}).$ 510

511 Table 5. TOC exitance M_{TOC} (W/m²/ μ m), irradiance E_{TOC} (W/m²/ μ m) and albedo \mathcal{A}_{TOC} at NIR band 512 as well as their component Δ_{adj}^{TOC} due to the adjacency effect. E_{TOC} is the integral of directional 513 radiance captured by a fisheye camera looking upward and placed at the city centre and edge.

		1D neig	ghbour		3D neighbour			
-	Cei	ntre	Ed	ge	Cer	ntre	Ed	lge
	Total	Δ_{adj}^{TOC}	Total	$\Delta_{ m adj}^{ m TOC}$	Total	Δ_{adj}^{TOC}	Total	Δ_{adj}^{TOC}
M _{TOC}	87.67	0.92	87.87	1.06	87.67	0.91	87.88	1.07
E _{TOC}	857.99	8.90	858.24	9.26	858.03	8.94	858.33	9.35
$\mathcal{A}_{ ext{TOC}}$	0.1022	0.0000	0.1024	0.0001	0.1022	0.0000	0.1024	0.0001

515 **5 Concluding remarks**

516 This paper presents the new 3D Monte Carlo modelling of surface-atmosphere RT in DART as 517 an extension and adaptation of the initial light transport theory to scenes that comprise surfaces 518 and volumes. It also presents a new Earth-Atmosphere system. It is designed to simulate 519 accurate remote sensing observations and their atmospheric contributions, including those due 520 to the adjacency effect. The default setting of this Earth-Atmosphere system (*i.e.*, $X \times Y \times Z =$ 521 $500 \text{ km} \times 500 \text{ km} \times 50 \text{ km}$) is consistent (relative error < 0.1%) with a quasi-infinite parallel 522 atmosphere. Its dimensions can be easily adapted to any experimental context. Its atmospheric 523 RT modelling has been successfully evaluated with SMART-G with an atmosphere defined in 524 the IPRT program. The relative root mean square difference of TOA reflectance is 0.20% for 629 upward viewing directions from VZA = 0° to 80° for infinite black surface, and 0.03% for 525 the points on the radius of a black disc inside infinite white environment. These differences are 526 527 mainly due to Monte Carlo noise and the roundoff error of computing.

This new DART modelling is very well adapted to study the influence of the adjacency effect 529 530 on remotely sensed radiance of land surfaces at any altitude. We studied this influence for a 531 scene made up of a target city (radius 2 km) surrounded by a forest (dimension 10 km), for four 532 Sentinel-2A bands (blue, green, red, NIR). Results allow one to quantify the increase of the 533 adjacency effect with larger TOC albedo of the neighbouring forest and atmospheric scattering. 534 In our experiment, the adjacency effect contributes up to $\sim 5.5\%$ at the city centre and up to 535 ~20% at the city edge to the TOA nadir NIR radiance, which is more than 5 times larger than 536 that at red band (\sim 1% at the city centre and \sim 3% at the city edge). It is explained by the fact 537 that the forest TOC albedo at NIR band is more than 12 times larger than in the red band. The 538 adjacency effect in the blue band is 1.5 times larger than that of the red band at the city centre 539 and edge although forest TOC albedo is similar in the blue and red bands, because the 540 atmosphere scatters more in the blue band than in the red band. The 3D structure of the 541 neighbouring forest also plays a role because it drives the angular distribution of the radiation 542 scattered by the neighbourhood of the city. Compared to the 1D Lambertian neighbour case, it 543 can induce a difference of adjacency contribution up to 1.3% for the edge of the city for the 544 NIR band.

545

546 The BRF camera of DART has been adapted to the new Earth-Atmosphere system in order to 547 simulate the hemispherical distribution of the upward radiance, then to compute the 548 corresponding albedo at a given altitude, a key parameter reflecting the radiative balance. 549 Results show that the adjacency contribution increases if the observing direction is more 550 inclined. In our virtual experiment, at observing zenith equal to 80°, the adjacency contribution 551 in the NIR band can represent up to 60% of the TOA radiance. The increased TOA albedo due 552 to adjacency effect for the four Sentinel-2A bands considered is generally larger than the 553 required maximum TOC albedo uncertainty 5% in applications as reported in GCOS. For example, the proportion of adjacency albedo in total TOA albedo can reach 10% in the green
band and 27% in the NIR band. The anisotropic reflectance of the forest that surrounds the city
influences the TOA radiance of the city, but only slightly influences the TOA albedo of the city.
The adjacency effect changes TOC irradiance but hardly changes the TOC albedo since the
adjacency effect increases both the TOC irradiance and exitance.

This work expands the potential of DART to study and correct atmospheric effects in remote sensing images through the consideration of realistic landscapes with their spatial heterogeneity, 3D architecture, topography, *etc.* It also helps quantifying the error in the fast methods that estimate approximately the adjacency effect.

564

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569 Appendix A. The default atmosphere dimension

570 The default parameters (e.g., 50 km altitude, $500 \text{ km} \times 500 \text{ km}$ atmosphere horizontal dimension) 571 of the new Earth - Atmosphere system (cf. section 3.1) were derived from sensitivity studies in 572 order to be optimal in usual configurations. For example, larger dimensions improve accuracy but increase simulation time. The optimal altitude was determined using MODTRAN as a 573 574 reference. Considered an atmosphere characterized by the USSTD76 gas model and the Rural 575 aerosol model, TOC albedo equal to 0.5, 2721 bands from 0.32 to $2.5 \,\mu$ m, nadir solar and viewing directions, and sensors at 40 km, 45 km, 50 km, 55 km, 60 km and 70 km altitudes. 576 577 The relative differences ε between sensor and MODTRAN spectra are very small and decrease 578 with altitude (Figure A.1, Table A.1). For the selected 50 km altitude $\varepsilon = 0.07\%$.



579

Figure A.1. MODTRAN TOA radiance spectra at seven sensor altitudes (40 km, 45 km, 50 km, 55 km, 60 km, 70 km, 100 km). TOC albedo is 0.5. USSTD76 atmosphere model with rural aerosols.

583Table A.1. Mean relative error ε of radiance spectra at six sensor altitudes (Figure A.1) compared to584the reference radiance spectrum of a sensor at 100 km altitude.

Sensor altitude	40 km	45 km	50 km	55 km	60 km	70 km
8	0.17%	0.07%	0.07%	0.06%	0.03%	0.01%

The optimal horizontal dimension D_{XY} of the atmosphere volume was studied using a DART simulation with $D_{XY} = 10000$ km as a reference, for a TOC albedo equal to 0.5, an atmosphere characterized by the USSTD76 gas model and rural aerosol model, and nadir solar and viewing directions. D_{XY} was set to 20 km, 50 km, 100 km, 200 km, 500 km, and 10000 km. Figure A.2 shows that a small D_{XY} value (*e.g.*, 20 km) leads to a large underestimate of TOA reflectance in the visible domain. Table A.2 shows the average relative error ε for each D_{XY} value. $D_{XY} =$ 500 km is a good approximation for an infinite parallel atmosphere because ε =0.08%.



593

Figure A.2. DART TOA nadir reflectance for five atmosphere horizontal dimensions D_{XY} (20 km, 50 km, 100 km, 200 km, 500 km). TOC albedo is 0.5. USSTD76 atmosphere model with rural aerosols. The reference is for D_{XY} =10000 km.

597

598 Table A.2. The mean relative error ε of all DART TOA nadir reflectance spectra (Figure A.2) 599 compared to the reference spectrum simulated with $D_{XY} = 10000$ km.

	D_{XY}	 D _{XY}	20 km	50 km	100 km	200 km	500 km
ε 7.74% 3.59% 0.55% 0.45% 0.0	Е	ε	7.74%	3.59%	0.55%	0.45%	0.08%

601 Appendix B. Radiance estimate for a semi-infinite atmosphere

602 For the semi-infinite plane-parallel atmosphere, illuminated by parallel sunlight and observed

603 by an orthographic camera, the radiance estimate $F_{\text{IS}}^{(j)} = \sum_{n=1}^{\infty} \left[\frac{\tilde{L}_e(r_n \to r_{n-1}) \cdot \tilde{G}(r_0 \leftrightarrow r_1) \cdot W_e^{(j)}(r_0 \to r_1)}{\tilde{p}(r_0) \cdot \tilde{p}(r_1)} \cdot \right]$

604
$$\prod_{k=2}^{n} \frac{\tilde{f}_{s}(r_{k} \to r_{k-1} \to r_{k-2}) \cdot \tilde{G}(r_{k-1} \leftrightarrow r_{k})}{\tilde{p}(r_{k})}$$
 (Eq. (23)) can be simplified since all vertices, except those at

the light source and sensor, are in the medium, we have:

$$606 \qquad \qquad \frac{\tilde{G}(r_0 \leftrightarrow r_1) \cdot W_e^{(j)}(r_0 \to r_1)}{\tilde{p}(r_0) \cdot \tilde{p}(r_1)} = \frac{\mathcal{T}(r_0 \leftrightarrow r_1) \cdot \frac{\cos \theta_i^{r_0}}{\|r_0 - r_1\|^2} \cdot \frac{\delta(\Omega_0 - \Omega_d)}{A_{\text{img}}}}{\frac{1}{A_{\text{img}}} \cdot \frac{\delta(\Omega_0 - \Omega_d)}{\|r_0 - r_1\|^2} \cdot \alpha_e(r_0 \to r_1) \cdot \mathcal{T}(r_0 \leftrightarrow r_1)} = \frac{1}{\alpha_e(r_0 \to r_1)}$$

$$607 \qquad \qquad \frac{\tilde{f}_{s}(r_{k} \to r_{k-1} \to r_{k-2}) \cdot \tilde{G}(r_{k-1} \leftrightarrow r_{k})}{\tilde{p}(r_{k})} = \frac{\alpha_{s}(r_{k} \to r_{k-1}) \cdot \frac{P(r_{k} \to r_{k-1} \to r_{k-2})}{4\pi} \cdot \frac{P(r_{k} \to r_{k-1} \to r_{k-2})}{\|r_{k-1} - r_{k}\|^{2}}}{\frac{P(r_{k} \to r_{k-1} \to r_{k-2})}{4\pi} \cdot \frac{\alpha_{e}(r_{k-1} \to r_{k-1})}{\|r_{k-1} - r_{k}\|^{2}}} = \frac{\alpha_{s}(r_{k} \to r_{k-1})}{\alpha_{e}(r_{k-1} \to r_{k})}$$

608 Besides, the direct connection of the light source indicates:

$$609 \qquad \frac{\tilde{L}_e(r_n \to r_{n-1}) \cdot \tilde{f}_s(r_n \to r_{n-1} \to r_{n-2}) \cdot \tilde{G}(r_{n-1} \leftrightarrow r_n)}{\tilde{p}(r_n)}$$

610
$$= \frac{E_s \cdot \delta(\Omega_{n-1} - \Omega_s) \cdot \alpha_s(r_n \to r_{n-1}) \cdot \frac{P(r_n \to r_{n-1} \to r_{n-2})}{4\pi} \cdot \frac{\mathcal{T}(r_{n-1} \leftrightarrow r_n)}{\|r_{n-1} - r_n\|^2}}{\delta(\Omega_{n-1} - \Omega_s) \cdot \frac{\cos \theta_o^{r_n}}{\|r_{n-1} - r_n\|^2}}$$

611
$$= E_s \cdot \alpha_s(r_n \to r_{n-1}) \cdot \mathcal{T}(r_{n-1} \leftrightarrow r_n) \cdot \frac{P(r_n \to r_{n-1} \to r_{n-2})}{4\pi}$$

612 with E_s the solar constant at TOA, and Ω_s the solar direction.

613

Assuming that atmospheric constituents are isotropic, extinction coefficients depend only on
location. After a few mathematical manipulations, we obtain a form consistent with the SSA
method in (Spada et al., 2006):

617
$$F_{\mathrm{IS}}^{(j)} = \sum_{n=1}^{\infty} \left[E_s \cdot \mathcal{T}(r_n \leftrightarrow r_{n-1}) \cdot \frac{P(r_n \to r_{n-1} \to r_{n-2})}{4\pi} \cdot \prod_{k=1}^{n-1} \frac{\alpha_s(r_k)}{\alpha_e(r_k)} \right]$$

619 Appendix C. Adjacency effect under different aerosol loadings

620 The adjacency effect is mostly due to scene elements at short distance if the aerosol optical 621 depth (AOD) is high, and at greater distances if the AOD is small (Houborg and McCabe, 2016). 622 Here, we consider TOA reflectance for different AODs. The scene is a black disc with radius equal to 2 km surrounded by an infinite white environment. The atmosphere is characterized 623 624 by a USSTD76 gas model and a Rural aerosol model. $SZA = 30^{\circ}$ and $SAA = 270^{\circ}$. Figure C.1 625 shows the TOA adjacency reflectance of the disc as a function of distance from the disc centre 626 to edge for four different AODs. The AOD in DART was scaled by a so-called multiplicative factor applied to the aerosol vertical profile. For example, a factor equal to 0.5 means the 627 628 resulted AOD is the AOD of Rural aerosol model multiplied by 0.5. Four factors were 629 considered: 0, 0.5, 1 and 5. Figure C.1 shows that the adjacency effect decreases at the disc 630 centre if AOD increases. The trend is more complex on the disc border: an AOD increase leads 631 to an increase of the adjacency effect if AOD is low (i.e., factor less or equal to 1), and to a 632 decrease of the adjacency effect if the AOD is very high (i.e., factor 5).

633



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Figure C.1. TOA adjacency reflectance from the centre to border of the black disc, for fourdifferent aerosol loadings.

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