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# 1 3D Monte Carlo differentiable radiative transfer with DART

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12

## 13 **Research highlights:**

14 First derivative (Jacobian) propagation modelling in land surface RT models.

15 Validation of this derivative modelling by the finite difference method.

16 Discussion of the major factors that influence the derivative.

17 Outlook of potential applications of the derivative modelling.

18

19 **Abstract**

20 Understanding the sensitivity of remote sensing (RS) observation to land surface parameters  
21 (e.g., reflectance and temperature) is very important for estimating the accuracy of RS products  
22 and optimizing inversion algorithms. The most precise method for quantifying this sensitivity  
23 is physical modelling of derivative propagation in simulated 3D landscapes. However, to our  
24 knowledge, present land surface radiative transfer models (RTM) do not simulate derivative  
25 propagation. This paper proposes an original “differentiable radiative transfer modelling” that  
26 simulates the derivative propagation in natural and urban landscapes, for reflectance. It is  
27 integrated in the framework of DART RTM. We validated it both analytically and with a finite  
28 difference method applied to a 3D landscape. This new modelling extends the efficiency of 3D  
29 RTMs for sensitivity studies. It is implemented in the DART version freely available for  
30 research and education (<https://dart.omp.eu>).

31  
32 **Key words**

33 DART, Radiative transfer, Derivative, Jacobian, Uncertainty

34

35 **1 Introduction**

36 Only remote sensing (RS) observations enable us to study land surfaces at different spatial and  
37 temporal scales. This is usually done through their inversion with radiative transfer models  
38 (RTM) as surface parameters (*e.g.*, albedo, temperature, leaf area index) or their assimilation  
39 in land surface models (Dickinson, 2008; Liang and Wang, 2019). Quantifying their sensitivity  
40 to surface optical properties is very important to optimize inversion procedures by identifying  
41 influential parameters, optimizing cost functions (Bowyer et al., 2003; Crosetto et al., 2001;  
42 Gupta and Razavi, 2017; Ye and Hill, 2017), and also to estimate the accuracy of RS products  
43 by investigating the error propagation (Gobron et al., 2008; Vermote and Kotchenova, 2008).

44

45 An observation can be viewed as a function  $F=f(\hat{\pi})$  of parameters  $\hat{\pi}=[\pi_1, \pi_2, \dots, \pi_k, \dots, \pi_N]$ .  
 46 Its sensitivity quantification needs to know its derivatives  $\left[\frac{\partial F}{\partial \pi_1}, \frac{\partial F}{\partial \pi_2}, \dots, \frac{\partial F}{\partial \pi_k}, \dots, \frac{\partial F}{\partial \pi_N}\right]$  (Ustinov,  
 47 2015). To compute them with measurements is usually very expensive, if not impossible, due  
 48 to the large amount of data required. RTMs offer an alternative solution because the partial  
 49 derivative of a parameter  $\pi_k$  can be computed as  $\frac{\partial F}{\partial \pi_k} = \frac{f(\pi_1, \pi_2, \dots, \pi_k + \Delta\pi_k, \dots) - f(\pi_1, \pi_2, \dots, \pi_k, \dots)}{\Delta\pi_k}$ , using  
 50 two simulations with a slight shift  $\Delta\pi_k$  of parameter  $\pi_k$ . Zhen et al. (2023) used this finite  
 51 difference method with the 3D RTM DART<sup>1</sup> (Gastellu-Etchegorry et al., 1996; Wang et al.,  
 52 2022) to get the derivatives of Sentinel-2 signal per surface element in each pixel. Similarly,  
 53 Gobron et al. (2008) estimated the uncertainty of MERIS fraction of Absorbed  
 54 Photosynthetically Active Radiation (fAPAR) product by computing the partial derivative of  
 55 fAPAR using a canopy and atmosphere RTM (Vermote et al., 1997). Vermote and Kotchenova  
 56 (2008) estimated the error budget of MODIS surface reflectance product due to uncertainties in  
 57 atmospheric parameters by simulating TOA reflectance with an atmospheric RTM for several  
 58 atmospheric and geometrical scenarios. However, the use of multiple runs of a RTM has two  
 59 drawbacks. (1) It is very expensive if the number of parameters is large, because the number of  
 60 simulations is twice that of parameters. (2) It is noisy with small parameter shift  $\Delta\pi_k$ , and biased  
 61 with large  $\Delta\pi_k$ . A different method is therefore needed to efficiently provide accurate  
 62 derivatives for sensitivity studies.

63

64 In the computer graphics field, Li et al. (2018) proposed the first physically based differentiable  
 65 Monte Carlo ray tracer to compute derivatives over a rendered image with respect to scene

---

<sup>1</sup> DART (<https://dart.omp.eu>) is one of the most accurate and complete 3D radiative transfer models. It simulates the radiative budget and remote sensing signals of natural and urban landscapes, from visible to thermal infrared.

66 parameters such as camera pose, scene geometry, materials, and lighting parameters. Zhang et  
67 al. (2019) designed a comprehensive mathematical framework for physically based  
68 differentiable rendering that computes derivatives for arbitrary differentiable scene changes.  
69 Jakob et al. (2022) and Vicini (2022) improved computation efficiency with respect to scene  
70 parameter optimization. Present research on differentiable renderers is mostly focused on  
71 reconstructing the shape and appearance of real-world objects from very high resolution RGB  
72 images (Ichbiah et al., 2023; Jiang et al., 2020; Luan et al., 2021; Petersen et al., 2022). Salesin  
73 et al. (2024) will adapt these methods for retrieving aerosol size and refractive index in a simple  
74 atmosphere-ocean scene in the future work. However, methods proposed in graphics are usually  
75 not suited to sensitivity studies in the RS domain where the need is derivatives of multi-  
76 spectral/spatial resolution remote sensing signals to surface optical and thermal properties with  
77 consideration of physical mechanisms, such as polarization and solar-induced fluorescence.

78  
79 To our knowledge, land surface RTMs do not simultaneously simulate the RS signal and its  
80 derivatives. This explains at least in part that RTM-based inversion methods (Liang and Wang,  
81 2019) do not use derivatives in optimization methods (Goel and Grier, 1987; Liang and Strahler,  
82 1993), LUT (Look-Up-Table) creation (Darvishzadeh et al., 2008; Weiss et al., 2000) and  
83 machine learning approaches (Abdelmoula et al., 2021; Makhloufi et al., 2021; Miraglio, 2021).

84  
85 This paper presents the first 3D Monte Carlo “land surface differentiable radiative transfer  
86 modelling” that directly computes derivatives for reflectance of each surface element. Section  
87 2 presents the propagation of derivatives and the new formulation of differentiable radiative  
88 transfer. Section 3 describes the implementation of this modelling in the framework of DART  
89 model. Section 4 presents the validation with an analytical method and a finite difference

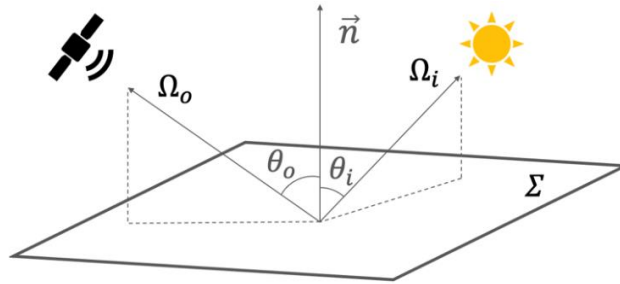
90 method. The major factors that influence the derivative are also discussed. Finally, Section 5  
 91 presents the concluding remarks and the potential applications of this new modelling.

## 92 2 Principles of radiative transfer and its differentiation

### 93 2.1 Radiative transfer and pixel radiance formulation

94 The light transport equation, also called rendering equation (Kajiya, 1986), at a surface  $\Sigma$  with  
 95 bidirectional scattering distribution function (BSDF)  $f_s(r, -\Omega_i \rightarrow \Omega_o)$  at position  $r$ , gives the  
 96 exit radiance  $L(r, \Omega_o)$  [W/m<sup>2</sup>/sr/ $\mu$ m] in direction  $\Omega_o$  as the sum of emitted radiance  $L_e$  and  
 97 radiance due to scattering of incident radiance in direction  $-\Omega_i$  (Figure 1):

$$L(r, \Omega_o) = L_e(r, \Omega_o) + \int_{4\pi} L(r, -\Omega_i) \cdot f_s(r, -\Omega_i \rightarrow \Omega_o) \cdot \cos \theta_i d\Omega_i \quad (1)$$



98  
 99 Figure 1. Light transport at a surface  $\Sigma$  with normal  $\vec{n}$ .  $\theta_i$  is the angle between incident direction  $\Omega_i$   
 100 and  $\vec{n}$ , and  $\theta_o$  is the angle between the exit direction  $\Omega_o$  and  $\vec{n}$ .

101 In absence of volume media, the incident radiation is the exit radiation from the previous  
 102 interaction that is also described by the same light transport equation. Thus, Eq. (1) can be  
 103 recursively expanded to a sum of multiple dimensional integral (Wang et al., 2022). Then, after  
 104 mathematical manipulations with consideration of the optical system (sensor characteristics,  
 105 pixel size, focal distance, observation geometry, *etc.*), for a given pixel,  $j$ , its radiance  $L^{(j)}$  can  
 106 be represented as an integral function of paths  $\vec{r}$  connecting the light source and the sensor:

$$L^{(j)} = \int_{\mathcal{D}} f^{(j)}(\vec{r}) d\mu(\vec{r}) \quad (2)$$

107 with  $f^{(j)}(\bar{r})$  the contribution function,  $\mathcal{D} = \bigcup_{n=1}^{\infty} \mathcal{D}_n$  the path space,  $\mathcal{D}_n$  the set of paths  $\bar{r}_n$  of  
 108 length  $n$ , and  $\bar{r}_n = r_0 r_1 \dots r_n$  a series of vertices  $r_{k=0, \dots, n}$  on surfaces  $dA(r_k)$  of the scene with  
 109  $r_0$  on the sensor and  $r_n$  on the light source (*cf.* Figure 2 in (Wang et al., 2022)).  
 110  $\mu(\mathcal{D}_n) = \int_{\mathcal{D}_n} d\mu(\bar{r}_n) = \int_{\mathcal{D}_n} dA(r_n) \cdot dA(r_{n-1}) \cdots dA(r_0)$  is the area-product of  $\mathcal{D}_n$ .

## 111 2.2 Differentiable radiative transfer

112 Pixel radiance  $L^{(j)}(\hat{\pi})$  is the result of radiation propagation in scenes with parameters  $\hat{\pi} =$   
 113  $[\pi_1, \pi_2, \dots, \pi_k, \dots]$  that can be reflectance, transmittance, emissivity, temperature, surface  
 114 architecture, illumination and observation geometry, *etc.* The aim of differentiable radiative  
 115 transfer is to estimate the partial derivative of  $L^{(j)}$  (Eq. (2)) with respect to any parameter  $\pi_k$ :

$$\frac{\partial L^{(j)}(\hat{\pi})}{\partial \pi_k} = \frac{\partial}{\partial \pi_k} \left[ \int_{\mathcal{D}} f^{(j)}(\bar{r}, \hat{\pi}) d\mu(\bar{r}) \right] \quad (3)$$

116 If the integral contains parameter-dependent discontinuities or if the integration domain  $\mathcal{D}$  is a  
 117 function of  $\hat{\pi}$  (discontinuities at boundary), the derivative operator cannot be directly moved  
 118 inside the integral. Then, the parameter-dependent discontinuities must be specifically treated.  
 119 The Reynolds transport theorem (Reynolds, 1983; Zhang et al., 2019) indicates that a derivative  
 120 of an integral of a function  $f^{(j)}(\bar{r}, \hat{\pi})$  with containing discontinuities depends on the derivative  
 121 of  $f^{(j)}(\bar{r}, \hat{\pi})$ , the boundary motion and internal discontinuities (discontinuities of  $f^{(j)}(\bar{r}, \hat{\pi})$ ):

$$\frac{\partial}{\partial \pi_k} \left[ \int_{\mathcal{D}(\pi_k)} f^{(j)}(\bar{r}, \hat{\pi}) d\mu(\bar{r}) \right] = \int_{\mathcal{D}(\pi_k)} \frac{\partial f^{(j)}(\bar{r}, \hat{\pi})}{\partial \pi_k} d\mu(\bar{r}) + \oint_{\Gamma(\pi_k)} \Delta f^{(j)}(\bar{r}, \hat{\pi}) \cdot \left\langle \frac{\partial \bar{r}}{\partial \pi_k}, \vec{n} \right\rangle d\mu(\bar{r}) \quad (4)$$

122 with  $\Gamma(\pi_k) \in \mathcal{D}(\pi_k)$  the union of the boundary  $\partial \mathcal{D}(\pi_k)$  and the set of parameter-dependent  
 123 interior discontinuities  $\Delta \mathcal{D}(\pi_k)$ , and  $\left\langle \frac{\partial \bar{r}}{\partial \pi_k}, \vec{n} \right\rangle$  the dot product of boundary motion and the  
 124 normal direction at  $\bar{r}$ .  $\Delta f^{(j)}(\bar{r}, \hat{\pi})$  is defined as:

$$125 \quad \Delta f^{(j)}(\bar{r}, \hat{\pi}) = \begin{cases} f^{(j)}(\bar{r}, \hat{\pi}), & \bar{r} \in \partial \mathcal{D}(\pi_k) \\ \lim_{\varepsilon \rightarrow 0} [f^{(j)}(\bar{r} + \varepsilon \cdot \vec{n}, \hat{\pi}) - f^{(j)}(\bar{r} - \varepsilon \cdot \vec{n}, \hat{\pi})], & \bar{r} \in \Delta \mathcal{D}(\pi_k) \end{cases}$$

126 Generally, three types of parameters can change  $\mathcal{D}$  or cause discontinuity in  $f^{(j)}(\bar{r}, \hat{\pi})$ . (1)  
 127 Instrument configuration (*e.g.*, camera position, field of view). (2) Illumination configuration  
 128 (*e.g.*, light position, light size). (3) Land surface architecture (*e.g.*, shape, position). In the  
 129 context of RS applications, our objective is to compute the derivatives of RS image radiance to  
 130 surface optical and thermal properties (*e.g.*, reflectance, transmittance, emissivity, temperature)  
 131 for a given illumination and observation geometry and land surface architecture. Then,  
 132 discontinuity in the integrand and boundary of the integration domain will not be affected by  
 133  $\hat{\pi}$ . Consequently, we can reduce Eq. (4) to Eq. (5).

$$\frac{\partial}{\partial \pi_k} \left[ \int_{\mathcal{D}} f^{(j)}(\bar{r}, \hat{\pi}) d\mu(\bar{r}) \right] = \int_{\mathcal{D}} \frac{\partial f^{(j)}(\bar{r}, \hat{\pi})}{\partial \pi_k} d\mu(\bar{r}) \quad (5)$$

### 134 2.3 Physical interpretation

135 Eq. (5) implies that partial derivatives can propagate in the scene as radiance. This is shown by  
 136 differentiating light transport equation (Eq. (1)), then reformulating it as:

$$\dot{L}(r, \Omega_o) = \dot{L}_e(r, \Omega_o) + \int_{4\pi} \dot{L}(r, -\Omega_i) \cdot f_s(r, -\Omega_i \rightarrow \Omega_o) \cdot \cos \theta_i d\Omega_i \quad (6)$$

137 with  $\dot{L}_e(r, \Omega_o)$  and  $\dot{L}(r, -\Omega_i)$  separately defined as:

$$138 \quad \dot{L}_e(r, \Omega_o) = \frac{\partial L_e(r, \Omega_o)}{\partial \pi_k} + \int_{4\pi} L(r, -\Omega_i) \cdot \frac{\partial f_s(r, -\Omega_i \rightarrow \Omega_o)}{\partial \pi_k} \cdot \cos \theta_i d\Omega_i$$

$$139 \quad \dot{L}(r, -\Omega_i) = \frac{\partial L(r, -\Omega_i)}{\partial \pi_k}$$

140 The transport of derivative (Eq. (6)) has two parts: (1) the emitted differential radiance  $\dot{L}_e(r, \Omega)$   
 141 when emission and BSDF change with parameter  $\pi_k$ ; (2) the scattering of differential radiance  
 142  $\dot{L}(r, \Omega)$  as radiometric quantities. Note that the BSDF must be differentiable. Eq. (6) shows that  
 143 the differentiable light transport equation has the same form as Eq. (1), which implies that the  
 144 transport of radiation and derivative can be evaluated simultaneously.



145 **3 Implementation in DART**

146 The bidirectional path tracing algorithm (Eq. (7)) unbiasedly estimates Eq. (5) for path length  
 147  $n$  from 1 to infinite (*i.e.*, all scattering orders contribute). In short, a light sub-path  $\bar{p}_s =$   
 148  $p_0, \dots, p_s, \dots$  starting from the light source and a sensor sub-path  $\bar{q}_t = q_0, \dots, q_t, \dots$  starting from  
 149 the sensor lens are coupled to generate a group of end-to-end paths, and the derivative estimates  
 150 associated to each path are weighted to evaluate the total derivative measurement.

$$\partial_{\pi_k} F_{MIS}^{(j)} = \sum_{n=1}^{\infty} \sum_{s=0}^{n+1} w_{s,t}(\bar{r}_{s,t}) \cdot \frac{\partial f^{(j)}(\bar{r}_{s,t}) / \partial \pi_k}{p(\bar{r}_{s,t})} \quad (7)$$

151 with

$$w_{s,t}(\bar{r}_{s,t}) = \frac{(p(\bar{r}_{s,t}))^2}{\sum_{s'=0, t'=n-s'+1}^{n+1} (p(\bar{r}_{s',t'}))^2}$$

153 Here, the sum of number of vertices of light and sensor sub-paths always verifies  $s + t = s' +$   
 154  $t' = n + 1$ . This algorithm is detailed in (Wang et al., 2022).

155

156 Automatic differentiation (Kahrmanian, 1953; Wengert, 1964) is commonly used to evaluate  
 157 the partial derivative of a function  $F: \mathbb{R}^n \rightarrow \mathbb{R}^m$ . The key idea is to decompose calculations of  
 158  $F$  into elementary operations (*e.g.*, addition, subtraction, multiplication) to automatically and  
 159 accurately evaluate the partial derivatives of  $m$  outputs with respect to  $n$  inputs (Eq. (8)) through  
 160 the chain rule. Appendix A illustrates an example of automatic differentiation.

$$J_f = \begin{bmatrix} \frac{\partial F_1}{\partial \pi_1} & \dots & \frac{\partial F_1}{\partial \pi_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_m}{\partial \pi_1} & \dots & \frac{\partial F_m}{\partial \pi_n} \end{bmatrix} \quad (8)$$

161

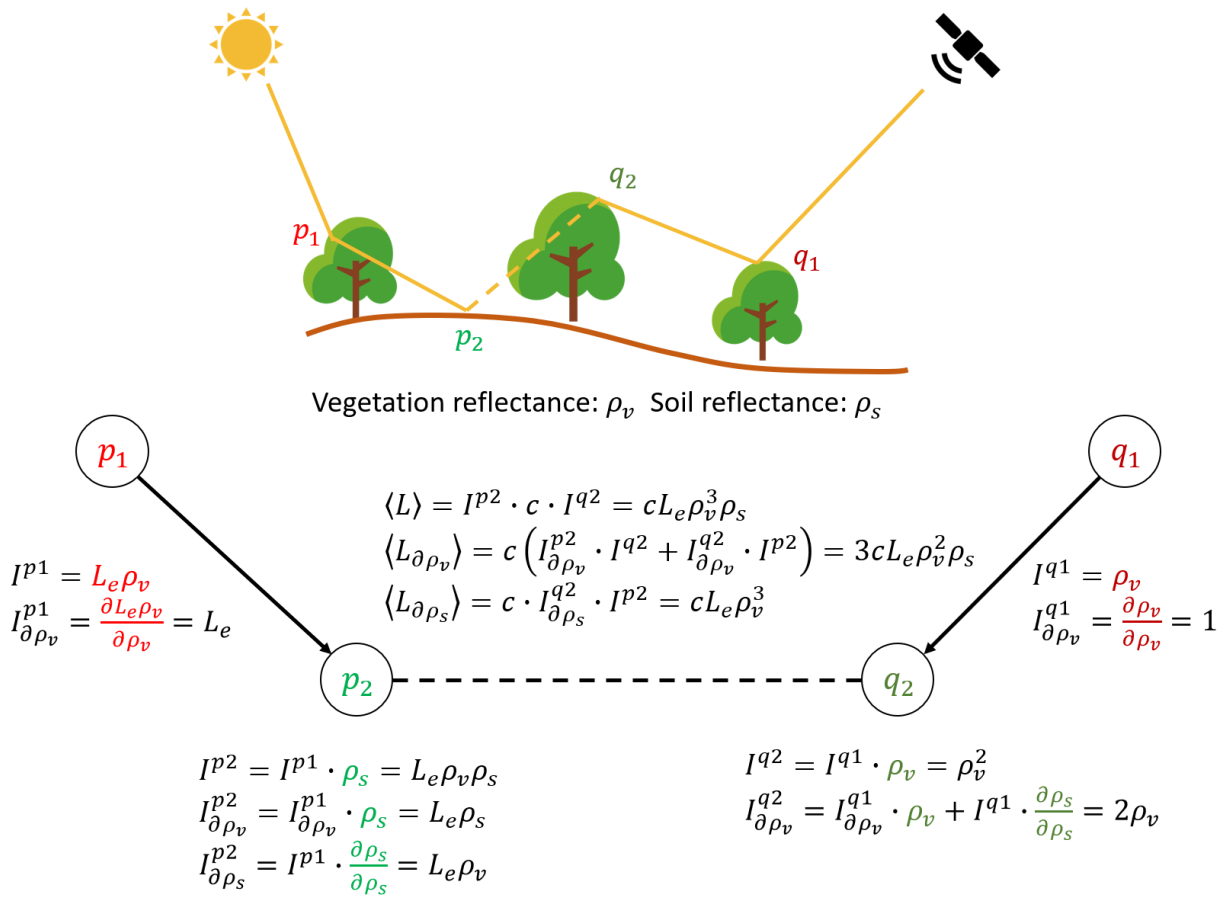
162 Differentiable radiative transfer modelling is a calculation of kind  $F: \mathbb{R}^n \rightarrow \mathbb{R}^1$  for each spectral  
 163 band. Prior knowledge in Monte Carlo radiative transfer modelling enables us to optimize

164 conventional automatic differentiation. For example, the final radiance estimate is the sum of a  
165 series of products, *i.e.*, only addition and multiplication operations are concerned. We can  
166 therefore calculate the partial derivatives of each product and add them together (*cf.* Appendix  
167 A). For each product, zero derivatives can be known in advance and only non-zero derivatives  
168 are propagated in the scene (*cf.* Appendix A). In addition, for each product, a change in the  
169 order of computation will not affect the final result. This is a very useful feature, as it allows us  
170 to adapt the automatic differentiation in the framework of bidirectional path tracing.

171

172 Figure 2 illustrates our procedure for computing the derivatives  $\langle \partial L / \partial \rho_v \rangle$  and  $\langle \partial L / \partial \rho_s \rangle$  of a  
173 Monte Carlo radiance estimate  $\langle L(c, \rho_v, \rho_s) \rangle = c L_e \rho_v^3 \rho_s$  for a specific stochastic path in a  
174 schematic landscape with two elements (tree and soil). Estimates will converge to the true  
175 derivatives after sufficient sampling. Here,  $c$  is a geometric connection factor,  $L_e$  is light  
176 emission,  $\rho_v$  is vegetation reflectance and  $\rho_s$  is soil reflectance. A ray starts from the light  
177 source and is scattered at points  $p_1$  and  $p_2$  (light sub-path), a second ray starts from the sensor  
178 and is scattered at points  $q_1$  and  $q_2$  (sensor sub-path). Next, the two sub-paths are connected to  
179 generate a complete path linking the sensor and the source. Note that the connection factor  $c$  is  
180 zero if two vertices are not mutually visible; only complete paths contribute to derivative and  
181 radiance computation. Intermediate radiance and derivative values are computed at each vertex,  
182 with the exact partial derivative being  $3cL_e\rho_v^2\rho_s$  for  $\rho_v$  and  $cL_e\rho_v^3$  for  $\rho_s$  after the connection.  
183 This optimized procedure has been implemented in DART with pixel derivative computed for  
184 each user-defined material (*i.e.*, optical property).

185



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Figure 2. Adapted bidirectional derivatives and radiance computation.  $I$  is an intermediate estimate of the radiance measurement updated after each interaction.  $I_{\partial X}$  is an intermediate estimate of the derivative with respect to variable  $X$ . The product rule ( $\frac{d(uv)}{dx} = u \frac{dv}{dx} + v \frac{du}{dx}$ ) is applied in the connection to get final derivatives.

191

#### 4 Validation and discussion

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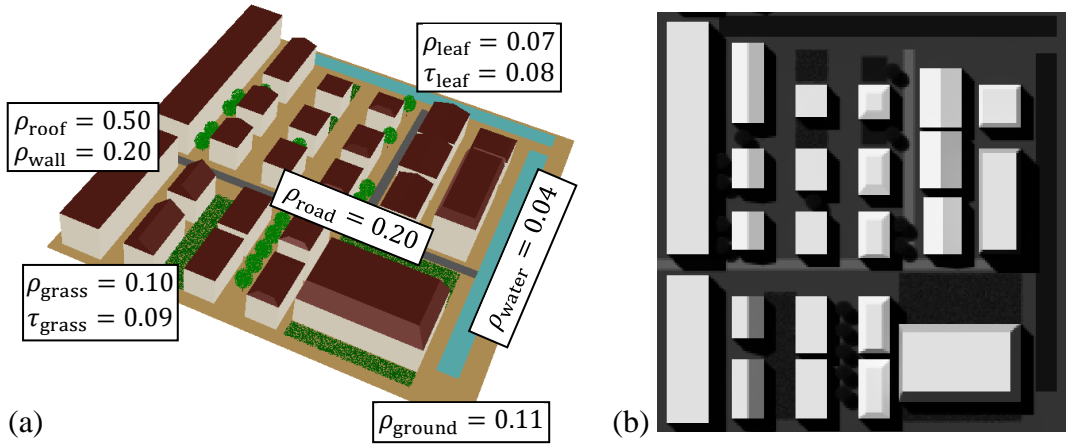
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198

We have validated our modelling using an analytical method and a finite difference method for a 3D urban scene with 7 scene elements (tree, grass, ground, road, wall, roof, water), for solar direction (zenith angle  $\theta_s = 30^\circ$ , azimuth angle  $\varphi_s = 225^\circ$ ), nadir viewing direction, and 1m spatial resolution. Material optical properties are from the DART database (Figure 3). The DART optical property of any scene element can be spatially variable. Here, it is spatially constant (Figure 3) to simplify understanding of our derivative computation. Below, the term "Jacobian" refers to derivative radiance and derivative reflectance products.



200 Figure 3. a) 3D urban model (200 × 200 m) with 7 elements: tree, grass, ground, road, wall, roof, and  
 201 water. Reflectance ( $\rho$ ) and transmittance ( $\tau$ ) are indicated. b) 1m spatial resolution nadir image.

#### 202 4.1 Comparison with the analytical method

203 The comparison is done for single scattering, because the analytical computation of RS radiance  
 204 derivatives with respect to optical properties is only possible for single scattering. For a flat  
 205 Lambertian surface (reflectance  $\rho$ , normal  $\bar{\Omega}_n$ ) and direct sunlight (horizontal irradiance  $E_s$ ,

206 direction  $\bar{\Omega}_s(\theta_s, \varphi_s)$ ), the single scattered radiance in viewing direction  $\Omega_v$  is

$$207 L(\Omega_v) = \frac{\rho \cdot E_s |\bar{\Omega}_s \cdot \bar{\Omega}_n|}{\pi \cos \theta_s}, \text{ and } \frac{\partial L(\Omega_v)}{\partial \rho} = \frac{E_s |\bar{\Omega}_s \cdot \bar{\Omega}_n|}{\pi \cos \theta_s}, \text{ which is } \frac{\text{Observed radiance}}{\text{Parameter of interest}}.$$

208 the reflectance for an opaque material. For translucent materials (*e.g.*, foliar element), it is the  
 209 sum of reflectance and transmittance (*i.e.*, single scattering albedo). The analytical Jacobian

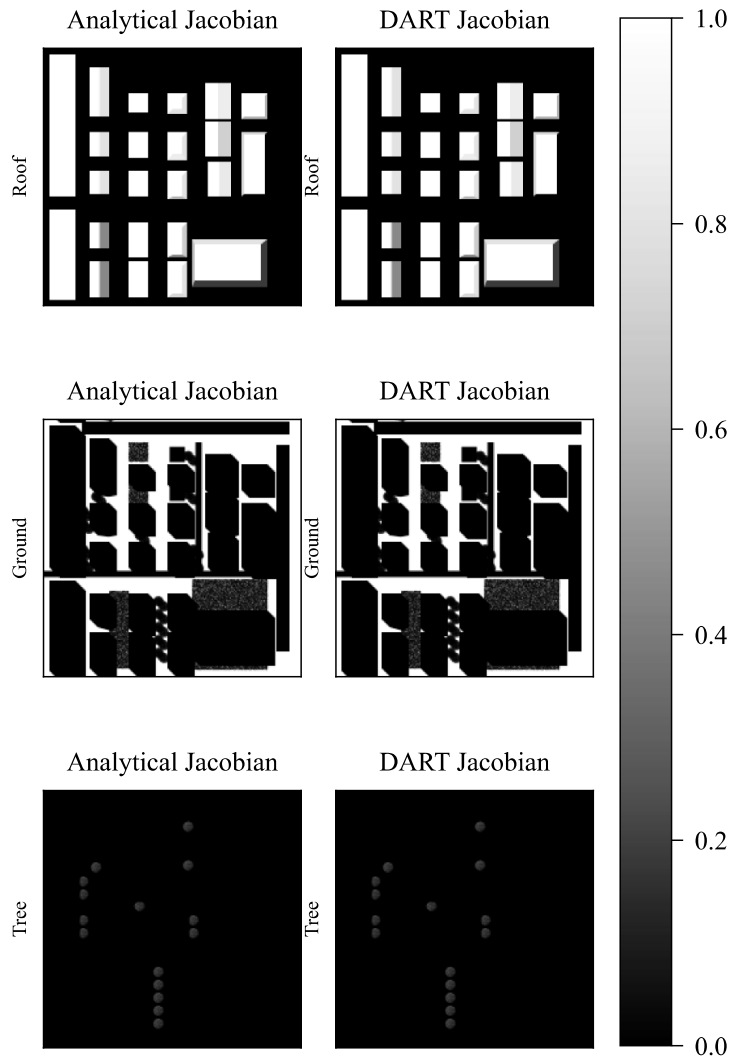
210 reflectance image is  $\frac{\text{DART single scattering Bidirectional Reflectance Factor (BRF) image}}{\text{Parameter of interest}} = \frac{|\bar{\Omega}_s \cdot \bar{\Omega}_n|}{\cos \theta_s}$ . We

211 verified the equality of the analytical and DART Jacobian reflectance images. Figure 4 shows

212 the analytical and DART Jacobian reflectance images for the roof, tree, and ground scene

213 elements, and Figure 5 shows their pixelwise comparison: coefficients of determination = 1 and

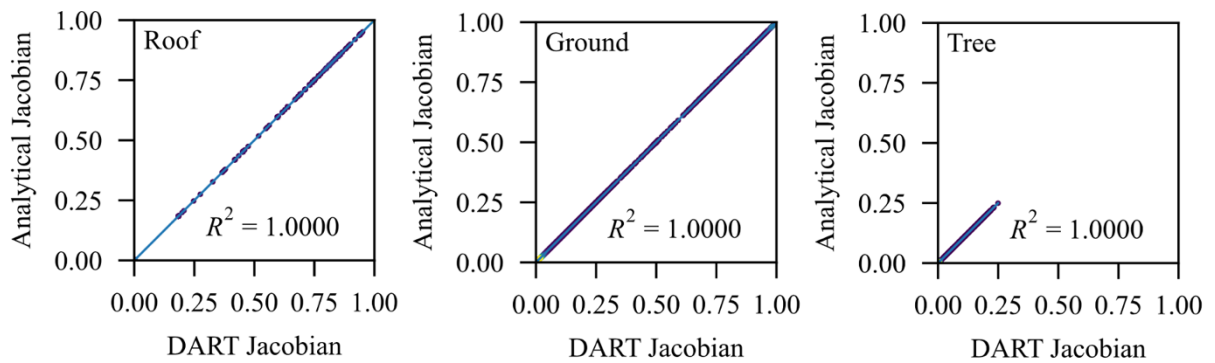
214 RMSE = 0 for all scene elements.



215

216 Figure 4. Single scattering analytical (left) and DART (right) Jacobian roof, ground and tree  
 217 reflectance images. Roof Jacobians depend on the configuration {roof slope, sun direction}.

218



219

220 Figure 5. Pixelwise comparison between single scattering DART and analytical Jacobian reflectance  
 221 images for roof, ground and tree. Coefficients of determination are indicated.

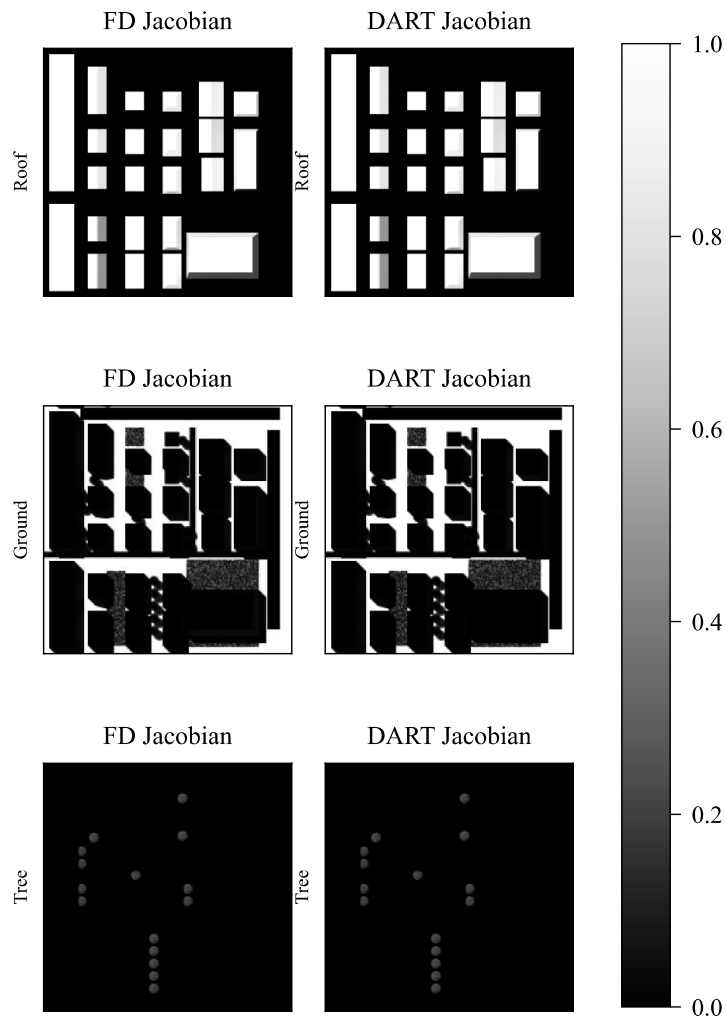
222 **4.2 Comparison with the finite difference method**

223 Derivatives of full radiative transfer modelling with single and multiple scatterings cannot be  
 224 computed analytically due to the complex formulation of light transport equation in 3D scenes.

225 As already stated, the finite difference (FD) method can provide approximate partial derivatives:

$$\frac{\partial f(\pi_1, \pi_2, \pi_3, \dots)}{\partial \pi_1} = \frac{f(\pi_1 + h\pi_1, \pi_2, \pi_3, \dots) - f(\pi_1 - h\pi_1, \pi_2, \pi_3, \dots)}{2h\pi_1} \quad (9)$$

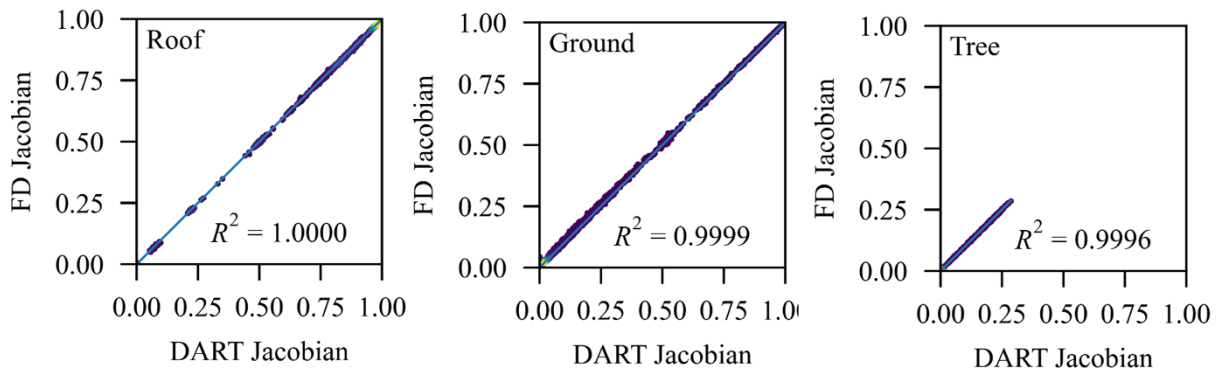
226 Here,  $h = 10\%$ . It is a compromise, because a large  $h$  value tends to induce a biased derivative  
 227 while a small  $h$  value tends to induce a noisy derivative with Monte Carlo noise close to the  
 228 term  $f(\pi_1 + h\pi_1, \pi_2, \pi_3, \dots) - f(\pi_1 - h\pi_1, \pi_2, \pi_3, \dots)$ . Fourteen simulations were run to compute  
 229 the FD Jacobians of the seven scene elements using Eq. (9). The resulting FD and DART  
 230 reflectance Jacobian images appeared to be very close (*cf.* Figure 6 for roof, ground and tree).



231  
 232 Figure 6. Roof, ground and tree FD (left) and DART (right) reflectance Jacobian images.

233

234 The pixelwise comparison of the FD and DART Jacobian reflectance images (Figure 7 and  
 235 Table 1) stresses a very good agreement: coefficients of determination above 0.9995, and  
 236 relative RMSE of derivatives for all scene elements visible to sensor below 0.02%, except for  
 237 walls (relative RMSE = 0.4%), which is explained by the fact that they are not directly visible  
 238 in nadir images. The small differences are mostly due to (1) the Monte Carlo noise in DART  
 239 Jacobian images and (2) the approximation of the FD method.



240

241 Figure 7. Pixelwise comparison of roof, ground and tree DART and FD Jacobian images. Coefficients  
 242 of determination are indicated.

243

Table 1. RMSE and relative RMSE of DART and FD Jacobian images.

Element	Roof	Ground	Tree	Grass	Road	Wall	Water
RMSE	0.0012	0.0048	0.0005	0.0014	0.0006	0.0101	0.0018
rRMSE	0.001%	0.005%	0.010%	0.013%	0.002%	0.400%	0.003%

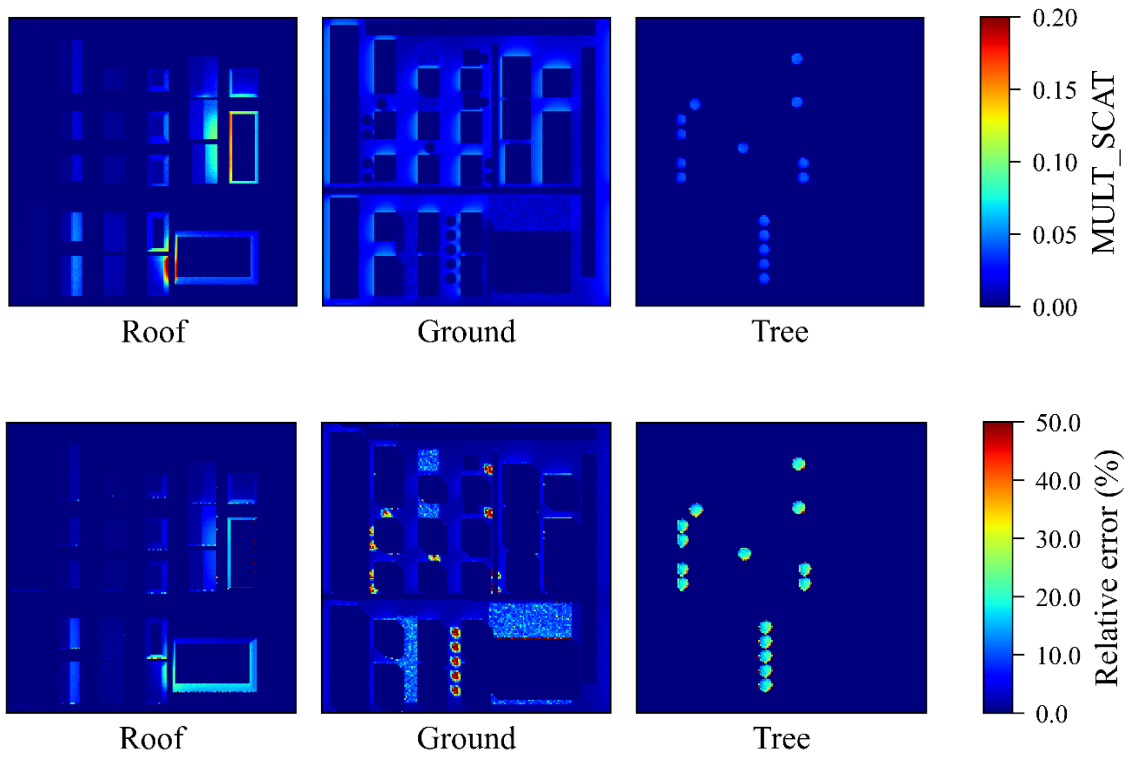
244

### 245 4.3 Discussion

246 **Which factors do impact pixel derivatives?** Figure 6 highlights three major factors: surface  
 247 orientation, masking effect, and multiple scattering. Examples are presented below. 1) Although  
 248 all roofs have the same optical properties, the sunny roofs (*i.e.*, roofs orientated towards the sun)  
 249 have larger derivatives than less sunny roofs. Values in Figure 4 are in agreement with the  
 250 single scattering derivative expression  $\frac{|\bar{\Omega}_s \cdot \bar{\Omega}_n|}{\cos \theta_s}$  of plane Lambertian surfaces with orientation  $\bar{\Omega}_n$ .

251 Indeed, most sunlit roofs have the highest  $|\bar{\Omega}_s \cdot \bar{\Omega}_n|$ . 2) All ground surfaces have the same  
 252 orientation, but those below grass and tree crowns has lower derivatives. 3) Multiple scattering  
 253 explains that ground pixels close to 3D scene elements (*e.g.*, walls or tree crown) tends to have  
 254 larger derivatives. Figure 8 illustrates this. It shows Jacobian images due to multiple scattering  
 255 (*i.e.*, difference of full and 1<sup>st</sup> scattering Jacobian images in Figure 6 and Figure 4, respectively).  
 256 Here, multiple scattering can increase derivatives by as much as 20%, especially for less sunny  
 257 areas. Furthermore, being the original mechanism of the Jacobian image for "walls" and  
 258 majority source of non-linearity of parameter and observation, it implies the large relative error  
 259 between DART and FD Jacobian images for walls (Table 1).

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263 Figure 8. Roof, ground and tree DART Jacobian images due to multiple scattering (MUL\_SCAT) (top)  
 264 and relative error (%) of single scattering DART Jacobian (bottom).

265



266 **Can single scattering Jacobian be useful?** It is very interesting in terms of computation  
267 efficiency, but is exact only for a theoretical flat landscape (Figure 4). The relative difference  
268 of DART full and single scattering Jacobians images (Figure 8) is less than 5% for most roof  
269 and ground pixels, and very large ( $> 50\%$ ) for shaded areas and also ground under vegetation  
270 because vegetation attenuates and scatters the ground signal. The relative error is also around  
271 20% for tree crown derivatives. These errors are even larger if scene elements have larger  
272 optical properties, which is commonly the case in the near infrared domain, especially for  
273 vegetation. Therefore, the single scattering Jacobian is not suitable for most sensitivity studies.

## 274 **5 Conclusions and perspectives**

275 This paper presents the first differentiable land surface 3D RTM. It computes Jacobian radiance  
276 and reflectance images and has been implemented in the framework of DART model. We have  
277 validated it by both an analytical method and a FD method for a schematic urban scene with  
278 trees, buildings, grass, etc. Results show very good agreement (*i.e.*, coefficient of determination  
279  $< 0.9995$ , relative RMSE  $< 0.02\%$ ) for scene elements directly visible in a nadir image. We  
280 showed that surface orientation, shadow and multiple scattering impact derivatives and  
281 estimated the accuracy of single scattering derivatives. By computing Jacobian images during  
282 the run of the RTM, our modelling avoids running multiple times the RTM and reduces Monte  
283 Carlo errors compared to the FD Jacobian modelling, which offers new avenues in sensitivity  
284 and inversion methods. One particular example is the significant acceleration of DART 3D  
285 RTM-based inversion procedure proposed in (Zhen et al., 2023). It also enables us to calculate  
286 the error propagation from surface optical properties to simulated RS signals, and to estimate  
287 the uncertainty of RS products through back propagation of derivatives if the sensor  
288 uncertainties are known. We note that although this paper presents the reflectance case, the  
289 proposed theory and derivative propagation can also be used for computing derivatives of many

290 other parameters than reflectance. For example, we recently extended DART differentiable  
291 modelling to compute Jacobian images for emissivity and temperature.

292

### 293 **Acknowledgement**

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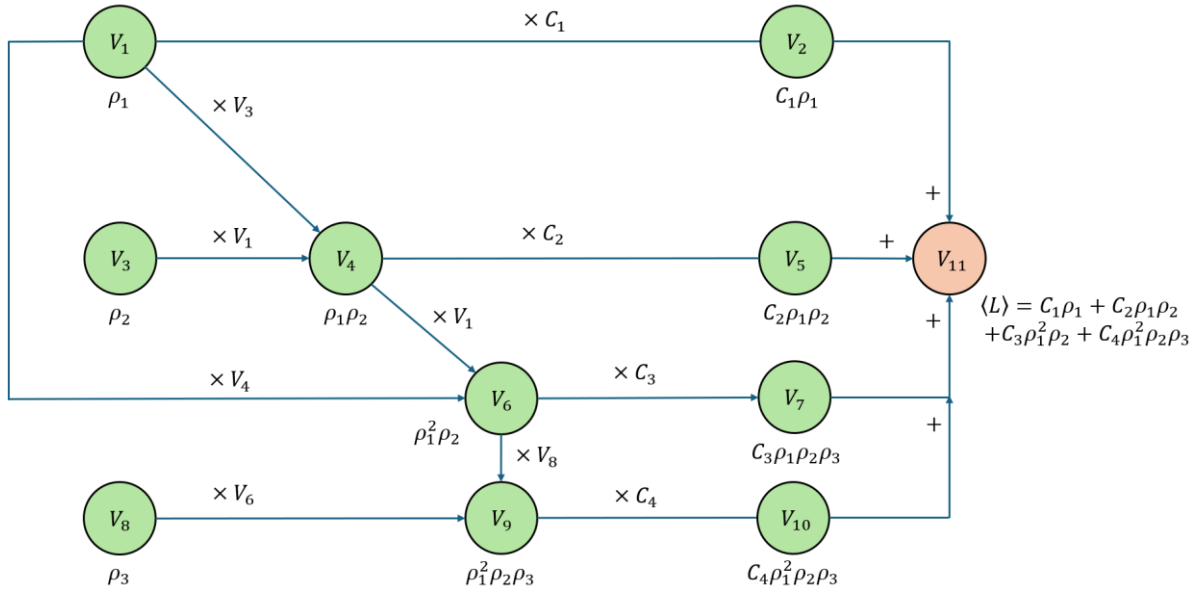
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376 **Appendix A. Automatic differentiation and DART implementation**



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Figure A.1. Wengert list: graphical representation of the elementary operations for a single Monte Carlo radiance estimate, with indication of the vertices  $V_{1-11}$ . Here, a ray starts from the camera, is scattered successively at surfaces with Lambertian reflectance values  $\rho_1, \rho_2, \rho_1, \rho_3$ . A second ray is sent to the light source from each interaction, with connection factors  $C_1, C_2, C_3, C_4$  that represent the radiation of the light source and the illumination geometry.

389

$$\dot{V}_i = \partial V_i / \partial \rho = \sum_{p \in \text{sons}(i)} \frac{\partial V_i}{\partial V_p} \cdot \frac{\partial V_p}{\partial \rho}$$

390

391

392

for each vertex. Here,  $p \in \text{sons}(i)$  means all son vertices of  $V_i$ , *i.e.*, all vertices  $V_p$  that are used to compute the value of vertex  $V_i$ . A step-by-step calculation from the first to the last vertex is shown below. This procedure also works reversely. In DART differentiable radiative transfer

393 modelling, only non-zero derivatives are computed and propagated, which avoids many  
 394 redundant computations compared to the classic automatic differentiation. Derivatives  
 395 computed in DART modelling are indicated in blue. In this demonstration case, only 13  
 396 derivatives over 23 are computed.  
 397

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$\frac{\partial V_1}{\partial \rho_1} = 1 \quad \frac{\partial V_2}{\partial \rho_1} = \frac{\partial V_2}{\partial V_1} \frac{\partial V_1}{\partial \rho_1} = C_1 \quad \frac{\partial V_3}{\partial \rho_1} = 0$ $\frac{\partial V_1}{\partial \rho_2} = 0, \quad \frac{\partial V_2}{\partial \rho_2} = \frac{\partial V_2}{\partial V_1} \frac{\partial V_1}{\partial \rho_2} = 0, \quad \frac{\partial V_3}{\partial \rho_2} = 1$ $\frac{\partial V_1}{\partial \rho_3} = 0 \quad \frac{\partial V_2}{\partial \rho_3} = \frac{\partial V_2}{\partial V_1} \frac{\partial V_1}{\partial \rho_3} = 0 \quad \frac{\partial V_3}{\partial \rho_3} = 0$	$\frac{\partial V_4}{\partial \rho_1} = \frac{\partial V_4}{\partial V_1} \frac{\partial V_1}{\partial \rho_1} + \frac{\partial V_4}{\partial V_3} \frac{\partial V_3}{\partial \rho_1} = \rho_2$ $\frac{\partial V_4}{\partial \rho_2} = \frac{\partial V_4}{\partial V_1} \frac{\partial V_1}{\partial \rho_2} + \frac{\partial V_4}{\partial V_3} \frac{\partial V_3}{\partial \rho_2} = \rho_1$ $\frac{\partial V_4}{\partial \rho_3} = \frac{\partial V_4}{\partial V_1} \frac{\partial V_1}{\partial \rho_3} + \frac{\partial V_4}{\partial V_3} \frac{\partial V_3}{\partial \rho_3} = 0$
$\frac{\partial V_5}{\partial \rho_1} = \frac{\partial V_5}{\partial V_4} \frac{\partial V_4}{\partial \rho_1} = C_2 \rho_2$ $\frac{\partial V_5}{\partial \rho_2} = \frac{\partial V_5}{\partial V_4} \frac{\partial V_4}{\partial \rho_2} = C_2 \rho_1$ $\frac{\partial V_5}{\partial \rho_3} = \frac{\partial V_5}{\partial V_4} \frac{\partial V_4}{\partial \rho_3} = 0$	$\frac{\partial V_6}{\partial \rho_1} = \frac{\partial V_6}{\partial V_1} \frac{\partial V_1}{\partial \rho_1} + \frac{\partial V_6}{\partial V_4} \frac{\partial V_4}{\partial \rho_1} = 2\rho_1\rho_2$ $\frac{\partial V_6}{\partial \rho_2} = \frac{\partial V_6}{\partial V_1} \frac{\partial V_1}{\partial \rho_2} + \frac{\partial V_6}{\partial V_4} \frac{\partial V_4}{\partial \rho_2} = \rho_1^2$ $\frac{\partial V_6}{\partial \rho_3} = \frac{\partial V_6}{\partial V_1} \frac{\partial V_1}{\partial \rho_3} + \frac{\partial V_6}{\partial V_4} \frac{\partial V_4}{\partial \rho_3} = 0$
$\frac{\partial V_7}{\partial \rho_1} = \frac{\partial V_7}{\partial V_6} \frac{\partial V_6}{\partial \rho_1} = 2C_3\rho_1\rho_2 \quad \frac{\partial V_8}{\partial \rho_1} = 0$ $\frac{\partial V_7}{\partial \rho_2} = \frac{\partial V_7}{\partial V_6} \frac{\partial V_6}{\partial \rho_2} = C_3\rho_1^2, \quad \frac{\partial V_8}{\partial \rho_2} = 0$ $\frac{\partial V_7}{\partial \rho_3} = \frac{\partial V_7}{\partial V_6} \frac{\partial V_6}{\partial \rho_3} = 0 \quad \frac{\partial V_8}{\partial \rho_3} = 1$	$\frac{\partial V_9}{\partial \rho_1} = \frac{\partial V_9}{\partial V_6} \frac{\partial V_6}{\partial \rho_1} + \frac{\partial V_9}{\partial V_8} \frac{\partial V_8}{\partial \rho_1} = 2\rho_1\rho_2\rho_3$ $\frac{\partial V_9}{\partial \rho_2} = \frac{\partial V_9}{\partial V_6} \frac{\partial V_6}{\partial \rho_2} + \frac{\partial V_9}{\partial V_8} \frac{\partial V_8}{\partial \rho_2} = \rho_1^2\rho_3$ $\frac{\partial V_9}{\partial \rho_3} = \frac{\partial V_9}{\partial V_6} \frac{\partial V_6}{\partial \rho_3} + \frac{\partial V_9}{\partial V_8} \frac{\partial V_8}{\partial \rho_3} = \rho_1^2\rho_2$
$\frac{\partial V_{10}}{\partial \rho_1} = \frac{\partial V_{10}}{\partial V_9} \frac{\partial V_9}{\partial \rho_1} = 2C_4\rho_1\rho_2\rho_3$ $\frac{\partial V_{10}}{\partial \rho_2} = \frac{\partial V_{10}}{\partial V_9} \frac{\partial V_9}{\partial \rho_2} = C_4\rho_1^2\rho_3$ $\frac{\partial V_{10}}{\partial \rho_3} = \frac{\partial V_{10}}{\partial V_9} \frac{\partial V_9}{\partial \rho_3} = C_4\rho_1^2\rho_2$	$\frac{\partial V_{11}}{\partial \rho_1} = C_1 + C_2\rho_2 + 2C_3\rho_1\rho_2 + 2C_4\rho_1\rho_2\rho_3$ $\frac{\partial V_{11}}{\partial \rho_2} = C_2\rho_1 + C_3\rho_1^2 + C_4\rho_1^2\rho_3$ $\frac{\partial V_{11}}{\partial \rho_3} = C_4\rho_1^2\rho_2$

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