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1	A geostationary lightning pseudo-observation generator utilizing
2	low frequency ground-based lightning observations
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#### ABSTRACT

Coincident Geostationary Lightning Mapper (GLM) and National Lightning Detection 11 Network (NLDN) observations are used to build a generator of realistic lightning optical 12 signal in the perspective to simulate Lightning Imager (LI) signal from European NLDN-like 13 observations. Characteristics of GLM and NLDN flashes are used to train different machine 14 learning (ML) models, that predict simulated pseudo-GLM flash extent, flash duration, 15 and event number per flash (targets) from several NLDN flash characteristics. Comparing 16 statistics of observed GLM targets and simulated pseudo-GLM targets, the most suitable 17 ML-based target generators are identified. The simulated targets are then further processed 18 to obtain pseudo-GLM events and flashes. In the perspective of lightning data assimilation, 19 Flash Extent Density (FED) is derived from both observed and simulated GLM data. The 20 best generators simulate accumulated hourly FED sums with a bias of 2% to the observation, 21 while cumulated absolute differences remain of about 22%. A visual comparison reveals that 22 hourly simulated FED features local maxima at the similar geolocations as the FED derived 23 from GLM observations. However, the simulated FED often exceeds the observed FED in 24 regions of convective cores and high flash rates. The accumulated hourly area with FED>025 flashes per  $5 \,\mathrm{km} \times 5 \,\mathrm{km}$  pixel simulated by some pseudo-GLM generators differs by only 7 % 26 to 8% from the observed values. The recommended generator uses a linear Support Vector 27 Regressor (linSVR) to create pseudo-GLM FED. It provides the best balance between target 28 simulation, hourly FED sum, and hourly electrified area. 29

#### <sup>30</sup> 1. Introduction

Lightning is defined as electrical discharges within the atmosphere, more particularly 31 within and between clouds (intra- and intercloud, IC) or between clouds and the ground 32 (CG). Transient lightning phenomena also occur between the cloud and the upper atmo-33 sphere, e.g., Sprites and Jets. While cloud electrification and lightning initiation are still 34 subject of studies, it is widely accepted that cloud ice and graupel are necessary to sepa-35 rate charges within clouds (e.g., Luque et al. 2020; Emersic and Saunders 2020; Lyu et al. 36 2019; Kolmasova et al. 2019; Takahashi et al. 2017; MacGorman and Rust 1998; Brooks 37 et al. 1997). In particular, convection creates favorable conditions for lightning, and the 38 updraft strength can be well correlated to the total lightning rate (e.g., Deierling and Pe-39 tersen 2008). Ávila et al. (2010) found a high correlation between the occurrence of deep 40 convection and lightning over land at a global scale. Hence, lightning is an effective tracer 41 of deep convection. 42

The new generation of geostationary (GEO) satellites carry optical lightning sensors, 43 among other instruments. The Geostationary Lightning Mapper (GLM) of the Geostation-44 ary Operational Environmental Satellite (GOES) R-series, the Lightning Mapping Imager 45 (LMI) on board the Chinese Fengyun-4 satellites (Yang et al. 2017), and the upcoming 46 Meteosat Third Generation Lightning Imager (MTG-LI, Dobber and Grandell 2014) will 47 provide GEO lightning observations at a global scale. This satellite-based, large-scale, con-48 tinuous observation of lightning offers new information for climate monitoring and studies. 49 In addition, the assimilation of GEO lightning data in Numerical Weather Prediction (NWP) 50 can help to improve the initial state of the model. Most of recent lightning data assimilation 51

studies use gridded Flash Extent Density (FED), for example Allen et al. (2016); Fierro
et al. (2019).

To assimilate new observation types in NWP models it is desired to develop an assimilation 54 scheme prior to the instrument launch and data availability. The simulation of appropriate 55 realistic pseudo-observations precedes the development of any assimilation scheme, espe-56 cially when the sensor is not yet in operation. Such synthetic observations can be derived 57 from existing GEO sensors over other regions, i.e., GLM, and ground-based Lightning Lo-58 cating Systems (LLSs). In addition, Low Earth Orbit (LEO) missions such as the Lightning 59 Imaging Sensor (LIS) on the Tropical Rainfall Measurement Mission (TRMM) satellites 60 (e.g., Christian et al. 1999; Cecil et al. 2005) and on board the International Space Sta-61 tion (ISS) (Blakeslee and Koshak 2016; Blakeslee et al. 2020) provide space-based lightning 62 observations. One can also use ground-based networks, e.g., the National Lightning De-63 tection Network (NLDN) (e.g., Cummins and Murphy 2009), Meteorage (e.g., Schulz et al. 64 2016; Erdmann et al. 2020), and Lightning Mapping Arrays (LMAs) (e.g., Rison et al. 1999; 65 Thomas et al. 2004; Coquillat et al. 2019). While the satellite sensors detect visible light 66 of lightning at 777.4 nm, the ground-based networks are operated at different frequencies 67 that match electromagnetic radiation emitted by different lightning processes. NLDN and 68 Meteorage use low frequency (LF) sensors that are most sensitive to discharge processes 69 such as return strokes for CG flashes. Most LF networks can distinguish CG and IC sig-70 nals. The CG flash detection (with return strokes) is usually reliable, whereas the IC flash 71 detection efficiency (DE) increases within the network and for shorter baselines given one 72 LF sensor type (personal communication, Stéphane Pedeboy, 2020/21). Global LF networks 73 have lower DE and accuracy than national and regional LF networks (e.g., Nag et al. 2015). 74 LMA stations sense very high frequency (VHF) signals of lightning leader propagation and 75

<sup>76</sup> allow for 3-dimensional (3D) channel mapping (e.g., Rison et al. 1999). Their drawback is
<sup>77</sup> the limited range. A LMA network provides coverage within a radius of typically a few
<sup>78</sup> hundred kilometers (e.g., Thomas et al. 2004; Koshak et al. 2004; Chmielewski and Bruning
<sup>79</sup> 2016; Coquillat et al. 2019).

Biron et al. (2008) resampled TRMM-LIS data on a MTG-LI-like grid to assess the po-80 tential performance of the MTG-LI with emphasis on the influence of varying minimal de-81 tectable radiant energy. However, this method relying on LEO lightning data is not suitable 82 for producing continuous pseudo-observations in the same area for operational applications 83 because of the poor revisiting time. Stano (2013) demonstrated a simple method to create 84 pseudo-GLM gridded products using LMA data. The pseudo-GLM data served to train 85 forecasters on the use of GLM data products. GLM's Algorithm Working Group (AWG) 86 investigated a transformation function that transforms LMA sources to optical lightning ob-87 servations. The technique combines TRMM-LIS flash statistics and observed LMA flashes 88 (Bateman 2013). The same method was applied by Schultz et al. (2016) to study automated 89 storm tracking and lightning jump algorithms using GLM pseudo-observations. Höller and 90 Betz (2010) present a simple statistical model for transforming stroke-type data of the LF 91 network LINET (Betz et al. 2009) to pseudo-MTG-LI optical events. The statistical rela-92 tions were studied comparing LINET strokes to concurrent TRMM-LIS groups. Then, they 93 created a pixel matrix of the future MTG-LI and used TRMM-LIS statistics of radiance and 94 event number per group to obtain pseudo-MTG-LI events. Their work aimed to propose a 95 statistics-based method to create optical pseudo-observations of lightning from a given set of 96 LF strokes. The available satellite lightning data solely emanated from the LEO TRMM-LIS 97 mission, and in addition the number of cases was fairly limited (705 coincident flashes). 98

Recent studies assessing the GLM performance have shown that the DE varies within the 99 field of view. GLM detects almost 90% of the flashes in the south-eastern USA (e.g., Marc-100 hand et al. 2019; Murphy and Said 2020). The flash DE is statistically lower in other regions 101 like Colorado. Rutledge et al. (2020) showed that the GLM performance depends on the 102 charge structure and the hydrometeor distribution. In particular, electrically "anomalous" 103 storms led to degrading GLM flash DE. The GLM flash DE also depends on the size and 104 duration of flashes. Zhang and Cummins (2020) found that small, short duration flashes are 105 more likely not observed by GLM than larger flashes. 106

This paper introduces in-depth techniques and results of creating GEO lightning pseudo-107 observations. The GEO lightning pseudo-observation generator is developed using NLDN 108 records in the US and can be applied to all NLDN-like ground-based LLSs, e.g., Meteorage 109 in France. One key part of the generator uses machine learning (ML) to relate NLDN-110 like observations to the extent and duration of the generated optical flashes. The generator 111 simulates the GEO lightning pseudo-observations on the flash level including events and thus 112 flash extent. FED grids can be derived from the generated pseudo-observations to serve as 113 assimilation input data. This work prepares in particular the assimilation of pseudo-MTG-114 LI data in the Meteo-France operational mesoscale numerical weather prediction system 115 AROME (Applications de la Recherche à l'Opérationnel à Méso-Echelle) in France. As 116 MTG-LI will produce GLM-like data, and the French Meteorage network observes lightning 117 similarly as NLDN in the US (Erdmann 2020, Chapter II.2.4), the developed GEO lightning 118 pseudo-observation generator can be used to simulate realistic pseudo-MTG-LI data. 119

The main objective of this study is the generation of a realistic GEO lightning FED field. It does not aim at reproducing correctly individual flashes, but the FED product. Therefore, the most important characteristics are the overall flash number and the flash extent. There <sup>123</sup> is no direct dependency of FED on the flash duration and event number per flash, neither
<sup>124</sup> on flash energetics. The developed generator should provide synthetic MTG-LI FED over
<sup>125</sup> France for data assimilation studies (not in the scope of the present paper). The application
<sup>126</sup> in our study is not intended for an operational use even though the developed algorithm
<sup>127</sup> could be used for operational application or for training forecasters and users.

Section 2 introduces both NLDN and GLM instruments. It also describes the dataset with 128 coincident GLM and NLDN flashes. Section 3 explains in-depth the strategy to mimic GLM 129 data from NLDN observations. This includes a 2-part GEO lightning pseudo-observation 130 generator and different ML models to relate GLM and NLDN flash characteristics. Sec-131 tion 4 presents pseudo-GLM observations, their comparison to real GLM observations, and 132 the evaluation of the 2-part generator. FED from real and pseudo-GLM observations is com-133 pared for the different ML-based generators. Finally, recommendations for suitable GEO 134 lightning pseudo-observation generators are given. 135

#### <sup>136</sup> 2. Instruments and Data

GLM and NLDN make use of different lightning detection and locating techniques. This section introduces important specifications of both instruments and the studied dataset. It briefly describes the developed methods to match and compare GLM and NLDN observations, and to infer flash characteristics needed for training ML models.

#### <sup>141</sup> a. Geostationary Lightning Mapper (GLM)

The GLM is an optical sensor on board the GOES R-Series (currently GOES-16 at 75°W and GOES-17 at 137°W). This study uses the GOES-16 GLM data only. The GLM detects total lightning including IC and CG during day and night. Although it cannot directly

distinguish IC from CG signals, Koshak and Solakiewicz (2015) show that some ICs and 145 CGs can be statistically differentiated. Especially due to the difficulty of the detection of 146 daytime lightning against bright, sunlit clouds, thresholds and filters are applied to separate 147 the lightning optical signal from background and other light sources. Lightning is detected 148 in a narrow (1 nm) band centered at the 777.4 nm oxygen line in the near infrared. The 149 wide field-of-view (FOV) image is focused on a high speed Charge Coupled Device (CCD) 150 focal plane with a nearly hemispheric FOV coverage  $(1372 \times 1300 \text{ pixels})$ . The variable pitch 151 pixel CCD allows for resulting pixels of about 8 km at nadir and only 14 km at the edge of 152 the FOV (Goodman et al. 2013). Images are produced continuously and in time frames of 153  $2\,\mathrm{ms}.$ 154

NASA's GLM lightning data algorithm produces Level 2 data with lightning information 155 as events, groups and flashes. The x,y-coordinates of the focal plane are transformed to 156 latitude and longitude coordinates of an estimated cloud top ellipsoid (with a height of 157  $14 \,\mathrm{km}$  at the equator and  $6 \,\mathrm{km}$  at the poles). Bruning et al. (2019) describes the effects of 158 using this ellipsoid on GLM parallax with respect to any known ground-relative reference. 159 GLM events are single illuminated pixels that pass the optical filters and are thus identified 160 as lightning signals. Their location is defined as the center of the illuminated pixel. Adjacent 161 events observed in the same 2 ms time frame are merged to form a group. Next, groups are 162 combined into flashes. NASA's clustering algorithm uses a Weighted Euclidean Distance 163 (WED) with limits of 16.5 km in latitude and longitude direction and 330 ms in time. Two 164 groups with a WED of less than one are assigned to the same flash. The WED criterion is 165 tested for pairs of events with one event in each group (Mach 2020). 166

The reader is referred to Goodman et al. (2013), the GLM Product Performance Guide for Data Users (Koshak et al. 2010), and Goodman et al. (2012) for further information on GLM details. Mach (2020) analyzed the GLM algorithms recently.

#### <sup>170</sup> b. The National Lightning Detection Network (NLDN)

The NLDN (Cummins and Murphy 2009) consists of more than 100 Vaisala LS7002 ground 171 sensors in the contiguous US (CONUS). It detects LF electromagnetic signals generated by 172 fast lightning discharges such as return strokes or by intracloud components. Due to a 173 combination of magnetic direction finding and time-of-arrival techniques, only two sensors 174 are needed to construct the horizontal location (latitude and longitude, no altitude) and 175 time of a signal. NLDN locates total lightning, including CG and IC discharges. According 176 to Vaisala (2013), up to 95% and better than 50% of all CG and IC lightning, respectively, 177 is detected. Zhu et al. (2016) found that one third of 153 IC pulses were detected by NLDN, 178 and 86 % were classified correctly. NLDN detected 92 % of 367 return strokes, and also 92 %179 were correctly classified as CG. The median location accuracy approaches 250 m for CG 180 strokes in the interior of the network. Lightning can be located at long range  $(1500 \,\mathrm{km})$ , 181 but the location accuracy in the interior of the network is significantly higher than outside. 182 NLDN measures also the peak amplitude of the LF source. NLDN data used in this study 183 include time (resolved at 1 ms), the location as latitude and longitude, the peak amplitude 184 [kA], the polarity, the type (CG or IC) of the LF source, and quality parameters, e.g., the 185 location error ellipse axes. Although Vaisala merges strokes to flashes (within 10 km and 186 1s), this study retrieves NLDN flash level data using the algorithm developed by Erdmann 187 et al. (2020) for Meteorage records in France. Hence, pulses/strokes are merged into a flash 188

if they occur within both 20 km and 0.4 s. The dataset is not further separated in this work,
and the term *pulse/stroke* is used to represent all NLDN detections on the stroke-pulse level.

#### <sup>191</sup> c. Database for the current study

The general dataset consists of six months of GLM and NLDN records, from March 15, 2018 to September 15, 2018. NLDN data were provided in a region between 30°N and 35°N and 95°W and 82°W. GLM data before 26 September 2018 need a time-of-flight (TOF) correction that takes into account the time lightning photons need to travel from the cloud tops (approximated at 10 km of altitude) to the GLM orbit. Our study applies a dynamical TOF correction with values ranging from 122.8 ms to 124.9 ms in the region of interest.

In order to handle the large amount of GLM data and hence to limit the data processing 198 time, a reduction of the 6-month dataset was necessary. The complete lightning dataset is 199 studied to identify lightning-active days (start and end at 00 UTC), defined by the number 200 of GLM flashes and the number of GLM events. Ten days with significant lightning activity 201 and different storm types during both day and night are selected. Table 1 summarizes the 202 number of GLM events and flashes as well as NLDN pulses and strokes and flashes recorded 203 in the region during each of the ten selected days. Table 1 also states the dominant weather 204 situation during each of the ten days. At least one day per month is selected to represent 205 possible climatological differences of the lightning within the region. All further analyses 206 use these ten days in order to reduce the immense amount of GLM event scale data. The 207 resulting dataset comprises 1,133,671 GLM flashes and 1,115,675 NLDN flashes. Missing 208 data is identified through an analysis of instrument activity during 20s time windows equal 209 to those of the GLM L2 data files. The amount of flashes is reduced to 1,132,051 GLM flashes 210

and 1,115,585 NLDN flashes due to possible<sup>1</sup> short periods of instrument inactivity. Hence, 211 the difference in the number of observed flashes is less than 2% of the flash counts, and both 212 instruments operated continuously during the selected days. As the effect of downtimes of 213 an instrument can be disregarded, the following analysis uses all available data. Three 214 among the ten days are chosen to test the generators with uncorrelated data and to assess 215 the variability in the results (test days). The test days (07 April 2018, 26 May 2018, and 216 31 July 2018) feature both thermally driven convection and dynamic forcing at air mass 217 boundaries. In the following, the different weather regimes with different lightning activity 218 are briefly described for the test days as the final FED product is in fact only analyzed for 219 these three days. 220

For instance on 07 April 2018, the weather was dominated by a major cold front that traversed the region from northwest to southeast. Temperatures dropped by about 10 K behind the front. The strong dynamic forcing caused a mesoscale convective system (MCS) with linear structure. This system produced the vast majority of flashes observed during the test period of 07 April 2018 until it left the studied region at about 12 UTC.

226 May 2018 was characterized by relatively warm surface temperatures with slightly
227 decreasing temperatures from west to east within the region. Moisture was induced into
228 the region by a weak tropical depression over Cuba and later southern Florida. Convection
229 occurred mainly in the local afternoon as a result of surface heating. Well defined cells
230 formed and propagated slowly southward in the cyclonic flow.

 $<sup>^{1}</sup>$ We do not know instrument downtimes from the data. Data may come with flags, but they do not give reliable information about the instrument status. We used a two-step approach to identify downtimes; (i) the flash DE is less than 50 % and (ii) the number of flashes observed is less than 10 % of the reference LLS.

Daytime temperatures widely exceeded 30 °C and remained at about 25 °C at night within the region on 31 July 2018. Moisture was advected into the region from the Gulf of Mexico while a dry line approached from the northwest. A multicell storm cluster formed in the convergence zone at local nighttime and propagated eastward driven by a short baroclinic wave aloft. The second peak of lightning activity results from thermal convection in the eastern portion of the region before the dry air moved in and inhibited further convection.

#### <sup>237</sup> d. Data processing algorithms – Flash scale data and identification of matches

NLDN and GLM observe lightning independently of each other. The comparison of the two LLSs needs, however, coincident observations. This work uses the matching algorithm introduced by Erdmann et al. (2020). Coincident observations are defined at the flash scale for flashes within 20 km and 1.0 s. The criteria are tested for any pair of events and pulses/strokes. Two parent flashes are matched if one event (pulse/stroke) meets both the spatial and the temporal criteria to any pulse/stroke (event) of the given flash. The algorithm does not analyze the flash mean position but the event and pulse/stroke locations.

GLM flash level data are included in the GLM L2 science data and emanate from NASA's 245 GLM L2 clustering algorithm. Mach (2020) found recently that NASA's GLM clustering 246 algorithm was quite stable for different spatial and temporal merging criteria (mainly for 247 storms with flash rates below about 40 flashes per minute). In the present study, the perfor-248 mance of NASA's GLM L2 clustering algorithm for one hour on May 26 was investigated. 249 NASA's L2 GLM clustering algorithm succeeded to merge many events and to detect large 250 flashes. The GLM operational algorithm still limits the maximum size of flashes due to 251 computational restrictions. However, such cases are rare and hardly influence the data 252 generators as statistical approaches are used for both training and testing here. 253

The matching of GLM and NLDN flashes (for the 10-day dataset) leads to 948,872 GLM 254 and 971,102 NLDN flashes with match. Some flashes from one system are matched to more 255 than one flash in the other system, and it happens more often that one GLM flash matches 256 multiple NLDN flashes than vice versa. Considering the total number of GLM (NLDN) 257 flashes, the relative flash DE is defined as ratio of flashes observed by both given and 258 reference LLSs to the total number of flashes observed by the reference LLS. It yields 87.0%259 (of 1,115,585 NLDN flashes) and 83.8% (of 1,132,051 GLM flashes) for GLM and NLDN, 260 respectively. Figure 1 illustrates the flash DE of both GLM and NLDN within the studied 261 region, along with 2D density of observed flash centroids (gray iso-contour). The flash DE 262 remains consistent within the entire domain. The local minimum in the northeast is caused 263 by a low number of observed flashes for the two  $1^{\circ} \times 1^{\circ}$  pixels in Figure 1. The high flash DE 264 of GLM agrees with the results of Marchand et al. (2019), who found the GLM DE relative 265 to ground-based Earth Networks Total Lightning Network (ENTLN) flashes exceeding 80% 266 for most of the southeastern CONUS. They used 35 km and 330 ms as spatial and temporal 267 matching criteria, respectively. Murphy and Said (2020) compared among others GLM and 268 NLDN relative DE, matching flashes within 20 km between GLM flash centroids and the 269 first NLDN pulse/stroke per flash and 200 ms between the flash time windows between the 270 start and end times, and report similar flash DE values on the large scale in the southeastern 271 CONUS. A new approach to the GLM flash DE and false alarm ratio (FAR) is introduced by 272 Bateman and Mach (2020); Bateman et al. (2021): combining several ground-based networks 273 to provide reference data, and using coarse matching criteria of 50 km and 10 min, they found 274 flash DE of over 90% and FAR just above 5% for the GLM on GOES-16. 275

#### 276 3. Methods

This section defines the concepts and the strategy to generate GEO pseudo lightning 277 observations. The methods are designed to use NLDN data and evaluated using real GLM 278 observations. MTG-LI will provide total lightning observations with similar data structure 279 as GLM observations. It will also consist of events, groups, and flashes. Although MTG-280 LI's spatial resolution  $(4.5 \,\mathrm{km} \text{ at nadir versus } 8.0 \,\mathrm{km} \text{ at nadir})$  and the temporal resolution 281 (1 ms versus 2 ms) will be higher than those of GLM, the methods presented here can still 282 be applied to simulate MTG-LI observations. A comparison of ISS-LIS records over the 283 domain of this study (USA) and the target region (France) revealed statistically similar 284 flash characteristics (Erdmann 2020, thesis, Chapter II.1-2). In addition, for both regions 285 of interest, statistics on NLDN and Meteorage LF lightning observations relative to ISS-LIS 286 records were consistent. The FED as explained in the following section is simulated on a 287  $5 \,\mathrm{km} \times 5 \,\mathrm{km}$  resolution grid approximating the MTG-LI grid. 288

#### <sup>289</sup> a. Definition of the Flash Extent Density (FED)

Flash extent density is a gridded product, summing over a given time integration period, 290 the projections of the location of flash components, e.g., events and pulses/strokes on a 291 given regular grid mesh. FED pixels with any lightning observation are identified, while 292 pixels with multiple observations (e.g., multiple NLDN pulses/strokes) are counted once per 293 flash. This gives a grid of pixels with either lightning (value 1) or no lightning (value 0) for 294 each flash. The FED product considers all flashes within a given time integration period 295 and sums up the occurrence of flash components per pixel. Hence, the FED product can 296 have values greater than or equal to one flash per pixel. It shows the spatial distribution of 297

lightning activity within the given time period. For example, the propagation of convective
cores can be tracked over several successive time integration periods.

The FED in this study is calculated on a regular latitude longitude grid with an average 300 pixel size of  $5 \,\mathrm{km} \times 5 \,\mathrm{km}$ . To obtain the regular latitude longitude grid, the distance of 301 5 km is transformed to latitudinal and longitudinal distance as of the pixel at the center 302 of the study region. Appendix A describes the details to transform GEO pixel grid to the 303 regular FED grid. In the present study, FEDs are analyzed per 60 min time integration 304 periods. The 1-hour period maintains information to locate tracks of convective cores and 305 most electrified regions while it is also long enough to capture several storms distributed 306 within the full domain. There might be, however, multiple storms at one location during 307 60 min. The FED integration period can be changed as needed since our GEO lightning 308 pseudo-observation generator simulates data at the flash level. The sum of multiple short 309 FED periods is equal to the FED of a corresponding long period, but the computation of one 310 long period is more efficient. Hence, this work simulates FED per hour for computational 311 reasons. It should be mentioned, however, that other FED time integration periods are 312 currently under investigation, and the assimilation of MTG-LI will use a shorter FED time 313 integration period. 314

#### <sup>315</sup> b. Work flow – The simulation of GEO pseudo-observations of FED

The simulation of pseudo-GLM flashes from NLDN observations is performed in 2 parts. First, our GEO lightning pseudo-observation generator uses the flash database with the coincident GLM and NLDN flashes and their characteristics. This part called target generator employs ML techniques. It is based on statistical relationships between the NLDN characteristics (features) and the characteristics of the concurrently observed GLM flashes (targets). The target generator is detailed in the following section. This part is conducted using different approaches, which will be explained thereafter. They include simple linear regressions as well as more sophisticated ML models. The second part of the GEO lightning pseudo-observation generator, described in the last section here, simulates pseudo-GLM events using the simulated GLM flash characteristics.

#### <sup>326</sup> 1) SIMULATE PSEUDO-GLM FLASH CHARACTERISTICS

Coincident NLDN and GLM flashes are analyzed regarding their characteristics including 327 the flash extent and flash duration (both GLM and NLDN) as well as the event number per 328 flash (GLM) or pulse/stroke number (NLDN) per flash. The flash extent is a characteristic 329 distance for the illuminated area for GLM or simply the distance between point sources for 330 NLDN. It sums up the distance between the lowest and highest latitude (the North-South 331 [NS] extent) and the distance between lowest and highest longitude (the West-East [WE] 332 extent) of events or pulses/strokes of the flash. GLM flash extent relies on the pixel center 333 position but does not include the pixel extensions. Single pixel GLM flashes and single 334 pulse/stroke NLDN flashes have an extent of 0.0 km. Flash duration is defined as the time 335 between the frames; therefore, a single frame features a flash duration of 0.0 s, i.e., GLM 336 flashes with all events at the same time and NLDN flashes with all pulses/strokes at the 337 same time. The maximum and mean signal strengths, defined from the LF peak currents 338 and radiant energies as measured by NLDN and GLM, respectively, are evaluated per flash 339 to represent flash energetics. In addition, a CG stroke ratio is calculated for NLDN flashes 340 dividing the number of CG strokes of the flash by the total pulse/stroke number. Previous 341 studies (e.g., Thomas et al. 2000; Marchand et al. 2019; Erdmann et al. 2020; Murphy and 342 Said 2020; Rutledge et al. 2020) found that characteristics of flashes observed by optical 343

<sup>344</sup> satellite LLSs depend among others on the flash altitude. Flash components identified as
<sup>345</sup> CG strokes propagate on average at lower altitudes than the IC components. In total,
<sup>346</sup> there are 5 GLM flash characteristics (flash duration, event number per flash, flash extent,
<sup>347</sup> mean and maximum event radiant energy per flash) and 6 NLDN flash characteristics (flash
<sup>348</sup> duration, pulse/stroke number per flash, flash extent, mean and maximum LF amplitude per
<sup>349</sup> flash, CG stroke ratio). Details on the distributions of the flash characteristics are provided
<sup>350</sup> by Erdmann (2020, Chapter II.3.4).

Linear regressions between any two GLM and NLDN flash characteristics showed that 351 GLM flash duration has Pearson correlation coefficients R above 0.64 to NLDN flash duration 352 and the number of pulses/strokes per flash. GLM event number per flash and GLM flash 353 extent feature R of 0.08 to 0.43 to the complete set of features. Mean and maximum event 354 radiant energies per GLM flash are not correlated to any NLDN flash characteristic on the 355 flash scale and then not relevant for synthetic FED generation. Hence, they are excluded 356 from the ML targets. The remaining targets are GLM flash duration, event number per 357 flash, and flash extent. 358

Building the GEO lightning pseudo-observation generator requires independent generator 359 building (GB) and generator testing (GT) data for the generator design and for the veri-360 fication of the generated product, i.e., the FED, respectively. The split of our dataset is 361 illustrated in Figure 2. The GB data consist of seven days and the GT data of the remaining 362 3 days (test days) of the full dataset (see Section 2.c and Table 1). The GB includes an 363 ML part. Here, only matched flashes are considered in order to compare feature and target 364 values (see Figure 2). Features (input data) of the ML are the six NLDN characteristics, 365 and targets (output data) are GLM flash duration, event number per flash, and flash extent. 366 Feature and target sample sizes are given as the number of matched flashes detected by 367

GLM and NLDN, respectively, and are not equal in general (Section 2.d). Since training 368 the ML models requires the same sample size for the features and targets, two (or more) 369 flashes matched to the same flash of the other LLS are merged, and characteristics of the 370 merged flashes are combined. The resulting ML data (dark orange in Figure 2) consist of 371 672,794 flashes, each sample with six NLDN features and three GLM targets. The ML part 372 further splits this set of ML data randomly into independent ML training and ML validation 373 data at a ratio of 90% to 10%. The ML models are thus trained with 605,515 flashes. The 374 ML validation data serves to calculate goodness-of-fit scores for each applied ML technique. 375 Then, the different ML models are compared and the model parameters (e.g., the number 376 of trees or the number of neural network layers, see Appendix B.a) are tuned based on the 377 scores. The 3-day GT dataset is used to evaluate each generator as a whole including the ML 378 and event generation parts. The test exercise exploits both observed GLM and generated, 379 NLDN-based pseudo-GLM datasets as two independent populations. 380

The generator simulates one pseudo-GLM flash for each observed NLDN flash. Thereby, 381 it is assumed that flashes detected by GLM only and detected by NLDN only compensate 382 each other. The assumption was justified as (i) GLM and NLDN feature flash DEs on the 383 same order, (ii) both GLM-only and NLDN-only flashes were smaller in extent and shorter 384 in duration than the flashes with coincident observations (see also e.g., Zhang and Cummins 385 2020; Erdmann et al. 2020), and (iii) most GLM-only and NLDN-only flashes were found in 386 the same regions in proximity to convective cores where high flash rates were observed (as 387 in Zhang and Cummins 2020). The overall GLM and NLDN flash numbers (see Table 1) 388 vary by only a few percent. However, it can be seen that there are days and cases where 389 NLDN detects more flashes than GLM, i.e., 07 Apr. and 14 Apr. and other days where 390 GLM detected more flashes than NLDN, i.e., 26 May, 03 Jun., and 07 Aug. 391

Here, only GLM flashes will be simulated and only if there are NLDN records. The al-392 gorithms do not distinguish potential NLDN flashes that would not be detected by GLM. 393 In addition, there is no algorithm developed to create flashes only detected by GLM. For 394 those two configurations, developing dedicated algorithms would require taking into account 395 the microphysical properties of the cloud profiles, but also a model that would generate the 396 lightning activity as realistically as possible to mimic GLM-only and NLDN-only flashes. 397 The goal of the lightning generator is to provide synthetic LI records with a better represen-398 tativeness than what has been used so far, knowing that there are some limitations in our 399 models, to develop a new proof of concept to assimilate space-based lightning observations. 400 Another aspect concerns the detection of optical flashes at day and night. One can consider 401 to develop a GEO pseudo-observation generator for both day and nighttime with potentially 402 different relations between LF flash characteristics and GEO flash characteristics. However, 403 as this paper includes a variety of methods and the first approach to use ML techniques to 404 simulate GEO flashes, day and nighttime flashes are not separated. This also is the case for 405 flashes over land and sea. 406

The aforementioned assumption means that flashes detected by NLDN only are treated similarly to those coincidently detected by both NLDN and GLM. As the number of NLDNonly flashes is significantly lower than the number of NLDN flashes with GLM match (given a GLM flash DE relative to NLDN of 87% for the full 10-day dataset), the assumption only affects about 13% of the simulated flashes. Statistics of GLM targets and FED fields inferred from the generated pseudo-GLM flashes are compared to those from all observed GLM flashes during the 3 days.

The comparisons of statistics of the observed and simulated targets include the distribution mean, median, minimum, and maximum. The root mean squared error (RMSE) between

characteristics of individual (simulated and real) GLM flashes is also computed, but only for 416 the 295,313 NLDN flashes with GLM match (representing a GLM flash DE of 86.7% for the 417 test days). The evaluation makes an addition use of two statistical scores that are defined for 418 the cumulative (in fact empirical) distribution functions (CDFs): the Kolmogorov-Smirnov 419 statistic (KS, Massey 1951) and the Cramér-von Mises criterion (CvM, Anderson 1962) 420 measure the distance between the observed and simulated CDFs of the targets. Both the 421 KS and the CvM tests can verify the null-hypothesis that two samples belong to the same 422 population. 423

### 424 2) ML-based target generators relating NLDN flash characteristics to 425 GLM flash characteristics

The previous sections explained that our GEO lightning pseudo-observation generator consists of 2 parts, the ML-based target generator and the simulation of GEO pseudoevents. Appendix B.a briefly describes the different ML models used in the ML-based part of this generator. The ML-based algorithms relate NLDN flash characteristics to GLM flash characteristics in this work. Hence, all ML models are supervised models with the same training data. The models emanate from Python's scikit-learn library (sklearn, Pedregosa et al. 2011).

This study uses seven different ML model types (details in Appendix B.a): Multivariate linear regressions (LinReg), third-degree polynomial regressions (Poly), Extra Trees Regressors (ETR) as a form of Random Forests, Bagging with k-nearest neighbor regressors (BAGR KNN), Multilayer Perceptron neural networks (MLP), linear Support Vector Regressors (linSVR), and Histogram Gradient Boosting Regressors (HGBR).

#### 438 3) Multi-Step Approach

Targets of a multi-target ML training can be correlated, e.g., GLM event number per flash 439 is strongly correlated to GLM flash extent with R of 0.74. To the best knowledge of the 440 authors, models of Python's sklearn library do not take advantage of correlations between 441 targets. Indeed, the so-called single target (ST) approaches do not consider correlations 442 between targets, however, such correlations can help to improve the skill of ML models and 443 thus the prediction of the generators. Borchani et al. (2015) summarize methods to deal with 444 multi-target regressions and take advantage of correlations between targets. Their paper 445 compares the ST approach to multiple multi-target approaches, e.g., multi-target regressor 446 stacking (MTRS), regression chains (RC), multi-output support vector regression, multi-447 target regression trees, and rule methods. Spyromitros-Xioufis et al. (2016) introduced the 448 stacked ST (SST) and ensemble RC (ERC). These methods can be computationally complex 449 with high memory costs (Mastelini et al. 2019). As Aguiar et al. (2019) state, choosing the 450 most suitable approach needs previous testing and depends on the task. The methods cited 451 here are computationally expensive. 452

The flow chart in Figure 3 shows a computationally efficient multi-target approach that simplifies the SST. As a starting point, there are NLDN features and GLM targets as input for the ML training. The approach combines ST models (Figure 3a) of three classes (colored) for the training. The application case only uses the NLDN features as first input. Therefore, a multi-step approach is required. An application example is shown in Figure 3b. More details about our approach can be found in Appendix C.

<sup>459</sup> In summary, the multi-step approach modifies the ML input feature set selection and thus <sup>460</sup> the configuration of the corresponding generator. It is a form of multi-target regression that <sup>461</sup> can take advantage of correlations between the ML targets. Appendix B.b summarizes the
<sup>462</sup> available feature set selections for the ML as different configurations of generators. Figure 3b
<sup>463</sup> shows just one example of the application that is also detailed in Appendix C. Section 4 will
<sup>464</sup> demonstrate whether the additional GLM pseudo-features can help to tune the pseudo-GLM
<sup>465</sup> simulation towards observed GLM data.

#### 466 4) Applied Scaling Methods

467 This study normalizes features to the [0,1] range with a Min-Max-scaler:

$$X_N = \frac{X - \min X}{\max X - \min X} \tag{1}$$

where X is a data vector,  $\min X$  and  $\max X$  define the minimum and maximum of X, respectively, and the resulting normalization  $X_N$  ranges from 0 to 1.

The targets are scaled with a common standard-scaler (also called z-value scaling) defined as

$$Z = \frac{X - \operatorname{mean} X}{\operatorname{std} X} \tag{2}$$

where X is a data vector, mean X and std X are the mean and the standard deviation of  $X_{73}$  X, respectively. The resulting standardization Z is centered around 0.

The Min-Max-Scaler is an alternative standardization method that is more robust to small standard deviations and for different feature ranges than the common standard-scaler (sklearn documentation).

Some generators perform well with unscaled data (i.e., direct input of data with physical units) used as a reference input method during the ML part. All results presented in this paper are re-scaled to physical units.

#### 480 5) GENERATE PSEUDO-GLM EVENTS

The studied domain is separated into regular adjustable size latitude-longitude pixels that 481 represent the pseudo-GLM pixel matrix. Any given latitude-longitude position is projected 482 on that pixel matrix to determine the corresponding pixel and thus the shape of one pseudo-483 GLM event. Using a regular grid simplifies and speeds up the simulation of pseudo-GLM 484 events significantly. Each regularly shaped pseudo-GLM event covers an area equal to the 485 average size of the observed, irregularly shaped GLM events in the region of interest. Ana-486 lyzing simulations built on this regular pseudo-GLM grid should lead to statistically similar 487 results as for the irregular grid of the GLM observations. 488

The target generator of the GEO lightning pseudo-observation generator simulates the 489 targets based on the given NLDN flash characteristics. These pseudo-GLM targets provide 490 the information to derive individual pseudo-GLM events. As the target generator may 491 produce targets with values smaller than the observed (and physical) limits, the targets are 492 adjusted to account for the known thresholds. For instance, negative flash extent and flash 493 duration are set to zero, and there are at least 2 pseudo-GLM events per flash in accordance 494 with NASA GLM data processing (Mach 2020). Pseudo-GLM flash NS and WE extents are 495 calculated based on the simulated pseudo-GLM flash extent applying the same ratio as the 496 NS and WE extents of the corresponding NLDN flash. If the NLDN flash contains a single 497 pulse or stroke, the NS to WE ratio is set to one. 498

First, the locations of pseudo-GLM events are generated. Using the simulated pseudo-GLM flash extent and its NS and WE components, a rectangular sub-domain on the pseudo-GLM pixel matrix is defined. The center of this sub-domain houses the NLDN flash position centroid and the corresponding pixel constitutes the first event of the pseudo-GLM flash.

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Any pixel within the sub-domain may also become a pseudo-GLM event of this pseudo-503 GLM flash. Three constraints have been designed to generate subsequent pseudo-GLM 504 events: (i) each event of the flash has at least one adjacent or diagonal neighbor within 505 one flash, thus, avoiding spatial gaps; (ii) pixels are primarily selected starting at the first 506 event and propagating (meaning increasing distance to the first event) towards the sub-507 domain border to approximate the simulated flash extent; and (iii) additional pixels can be 508 selected randomly within the rectangular area until the simulated event number is reached. 509 In consequence one single pixel of the sub-domain can contain more than one pseudo-GLM 510 event. Since pixels of the sub-domain are not guaranteed to contain a pseudo-GLM event, 511 this random selection also affects the final FED product. 512

Then, the pseudo-GLM events get time stamped. In the present study, the matching of 513 GLM and NLDN flashes revealed that the median time offset between the mean time of a 514 given NLDN flash and the mean time of the matched GLM flash was about 8 ms. The NLDN 515 and GLM average flash duration were 0.24 s and 0.39 s, respectively. Hence, the mean time 516 of matched NLDN and GLM flashes are relatively close while GLM flashes last on average 517 longer than NLDN flashes. As a consequence, the mean time of the NLDN flash defines the 518 mean time of the pseudo-GLM flash that is also the time stamp of the first pseudo-GLM 519 event. Our generator is built to generate realistic FED fields. Only the spatial distribution 520 of the events is needed to infer FED. Hence, the temporal occurrences of pseudo-events are 521 uniformly and arbitrary distributed during the duration of one flash. Pseudo-event times 522 are then rounded to the time frames of the mimicked GEO LLS, i.e., to 2-ms-frames for 523 pseudo-GLM data. The only constraint is that any adjacent pixel occurs within 330 ms (i.e., 524 the time criterion to separated flashes in NASA's GLM L2 algorithm). One 2-ms-frame 525 contains often several pseudo-GLM events. 526

#### 527 4. Results

Figure 4 shows the example of one simulated pseudo-GLM flash created with the final 528 GEO lightning pseudo-observation generator based on a linSVR model, the corresponding 529 GLM and NLDN observations, and the observed and simulated GLM flash characteristics. 530 One can see the difference between the real GLM grid and the regular pseudo-GLM grid of 531 the simulation (Figure 4(c)). The difference between observed and simulated flash extent 532 is within the size of one GLM pixel for this example. The simulated flash duration exceeds 533 the observed flash duration significantly. There is also an overestimation of the number of 534 GLM events by the generator. 535

Results are obtained from the 3-day test dataset. It contains 340,712 NLDN flashes that 536 are used to simulate the same number of pseudo-GLM flashes. Statistics of the pseudo-GLM 537 flashes are compared to the statistics of all 338,579 observed GLM flashes. First, the distri-538 butions of the simulated and observed GLM flash extent, flash duration, and event number 539 per flash are compared. The best target generators are used to simulate pseudo-GLM events 540 and eventually compute the pseudo-FED product. The FED is analyzed statistically for both 541 observed and simulated GLM data of the three test days. The minimum discrepancy between 542 observation and simulation will indicate the most suitable target generator configuration for 543 the final GEO lightning pseudo-observation generator. 544

# a. Evaluating the target generators – Distributions of GLM flash extent, flash duration and event number per flash

In a general sense, a wide range of values is observed for all target distributions. The GLM flash duration ranged from 0.0 s to 16.4 s. Observed GLM flashes comprised between <sup>549</sup> 2 and 1395 events. The test data features GLM flash extent between 0 km and 277 km. The <sup>550</sup> target generators should handle these ranges of values and predict target statistics similar <sup>551</sup> to the statistics of observed GLM flashes.

Table 2 summarizes the findings, with statistics, the KS, and the CvM of the distributions of observed and simulated GLM flash duration, event number per flash, and flash extent for the full 3-day test data. The table contains distribution statistics for the respective target generator with smallest difference between observed and simulated characteristics over the test period. Results for the *linSVR num* ext(a) plus generator are shown as reference. Statistics of the simulated pseudo-GLM and the observed distributions are referred to as simulated statistics and observed statistics, respectively.

This analysis was also conducted for each test day. The results are presented in Appendix D.a.

The majority of the target generators features mean values similar to the observed means 561 for all three target characteristics. The simulated medians, however, exceed the observed 562 medians in most cases, especially for the number of events per flash, suggesting a tendency 563 to overestimate the target values. The previously described behavior is true for all but the 564 linSVR-based generators. linSVR filters the dataset in advance to build the prediction on the 565 support vectors (Appendix B.a. (vi)). That results (in this study) in lower differences between 566 the simulated and observed median values as compared to using the other ML model types. 567 The mean values of *linSVR*-based predictions, are, however, often smaller than the observed 568 mean, especially for the event number per flash. Table 2 demonstrates this behavior of 569 linSVR-based generators. To detail one example, the recommended linSVR-based generator 570 (see Section 4.b, bold in Table 2) underestimates median and mean flash extent by about 571 4.5% and 11.7%, respectively. The mean event number per flash is also underestimated 572

<sup>573</sup> by about 29.6%, however, the median event number per flash is overestimated by 20%. <sup>574</sup> The linSVR-based generator creates, compared to the observations, not enough flashes with <sup>575</sup> an event number in the tails of the distribution, i.e., close to the observed minimum and <sup>576</sup> maximum event numbers. Hence, it cannot mimic the full range of the observed event <sup>577</sup> numbers per flash. This linSVR-based generator still outperforms all other generators with <sup>578</sup> respect to the median considering the full 3-day test data.

Some general conclusions can be drawn regarding the generator performances for the ob-579 served range and variability of the target values. The target generator minimum often 580 approximates or slightly exceeds the observed minimum, whereas the maximum is under-581 estimated in most cases. This particular behavior can even be seen for the best target 582 generators (Table 2) because the number of small flashes with characteristics close to the 583 minimum observed target values is relatively high. The rare, highest observed values are 584 often underrepresented in the statistical approach. It is further found that observed GLM 585 flash statistics can vary for a given set of the six observed NLDN features. This is the case 586 as our six NLDN features cannot completely explain the range of target values even if the 587 statistics derived here are significant in terms of the large sample size. The large values of 588 the RMSE per flash in Table 2 and also Appendix D.a result from the deterministic nature of 589 the ML models in combination with this lack of information in the features, e.g., cloud prop-590 erties. The RMSE values of the GLM flash extent are similar to the mean values, whereas 591 they reach twice the mean for both GLM flash duration and event number per flash. Here, 592 the optimization of our GEO lightning pseudo-observation generator for FED that depends 593 mostly on the flash extent is evident. A relatively wide range of target values is in particular 594 found for small NLDN flashes with NLDN pulse/stroke number, extent, and duration near 595 the lower end of the distributions (not shown). Large (meaning long extent, long duration, 596

and many pulses/strokes or events) NLDN flashes usually coincide with large GLM flashes. 597 As the NLDN features are somewhat correlated to the GLM targets, the high RMSE due to 598 a small NLDN flash as input also leads to a high RMSE when predicting small GLM flashes. 599 KS and CvM assign a quantitative value to measure the distance between two samples. 600 While KS is normalized (values of 0 to 1), the CvM value depends in general on the distance 601 between simulated and observed CDFs and the sample size. As the sample size is kept con-602 stant for all generators, CvM in fact provides a common measure of the agreement between 603 observed and simulated targets. Both KS and CvM feature lower values for the GLM flash 604 duration than for both the GLM flash extent and the GLM event number per flash consid-605 ering the full test dataset (Table 2). This result is in accordance with the strong correlation 606 coefficients between observed GLM flash duration and NLDN features (see also Section 1). 607 KS and CvM for the flash duration rely mainly on the underestimation of long duration 608 flashes. As an exception, the recommended linSVR num ext(a) plus generator not only 609 underestimates the maximum flash duration but also cannot produce single-frame flashes. 610 Therefore, KS and CvM are higher for the flash duration than for the flash extent here<sup>2</sup>. KS 611 and CvM reach their highest values, i.e., when comparing the 3 target distributions, for the 612 GLM event number per flash, for which the weakest correlations to features were observed. 613 The presented selection of generator performance for the 3-day test data and each test day 614 (Appendix D.a) indicate that the choice of a suitable target generator can be situational. The 615 objective now is to find a configuration that best approximates the observed GLM flashes 616 and target distributions. Therefore, the differences between the simulated and observed 617

<sup>&</sup>lt;sup>2</sup>It can be noticed from Table 2 that this linSVR-based generator also overestimates the minima of event number per flash and flash extent. For those two targets, the simulated maxima are closer to the observed maxima than for the best performing generator in Table 2 causing overall similar and even lower KS and CvM for the linSVR num ext(a) plus.

statistics (i.e., mean, median, minimum, maximum, RMSE, KS, CvM) are calculated and 618 normalized for each statistic. The normalization divides each absolute difference by the 619 maximum absolute difference of all target generators for a given statistic. A value of 1 620 represents the worst target generator for the given statistic, while a value of 0 indicates 621 no difference to the observation. In addition, and to summarize all the information, the 622 so-called Normalized Difference Average (NDA) is introduced to average the normalized 623 absolute differences and scores for a given generator. The perfect generator would yield an 624 NDA of zero. NDAs of the target generators can be directly compared in order to identify 625 the highest performer. NDA is calculated per target and for all three targets overall. 626

Overall NDAs for all three targets range from 0.35 for the *linSVR num ext raw* generator to 627 0.87 for the MLP num ext(a) raw generator. The best (i.e., lowest NDA) 24 target generators 628 all use a linSVR, and the performance of the best target generators varies only within the 629 range of uncertainty given in Section 1. For example, the difference between the 1st and 10th 630 ranked target generator is only 0.04 NDA. The NDA ranking of target generators reveals 631 a clustering explained by the ML model type, with *linSVR*-based generators performing 632 the best, followed by BAGR KNN dist-based, ETR-based, and polynomial regression-based 633 generators. MLP- and HGBR-based generators exhibit the highest NDAs. 634

The generators yielding the lowest NDA values are mostly those using the multi-step approach. In addition, the use of all six (*plus*, Appendix B.b) instead of only four (*default*) NLDN features improved the performance of the majority of tested generators. The feature and target scaling had little effect on the generator performance, although scaling is usually recommended for ML applications. The ML model type has in fact the highest impact on the simulation of pseudo-GLM flashes and thus on the target generator performance.

Figure 5 visualizes the statistics of all tested target generators for the flash extent as the 641 most impactful characteristic on FED. It groups the results for each statistic by ML model 642 type. Seven ML model types were used to build the generators (Section 2 and Table B1 643 except RF). Each distribution contains the results of 28 generators using this ML model 644 type including 7 feature set selections and 2 optional attributes (Appendix B.b., Table B2). 645 Figure 5 shows these results as normalized differences and scores for the 3 test days combined. 646 It reveals that the boxplot minima for the linSVR type generators are the closest to zero 647 for most statistics. BAGR KNN dist-based generators feature the second lowest values of 648 KS and CvM. The finding is supported by results for each test day (Appendix D.a) showing 649 best performances for the targets by BAGRN KNN dist-based generators on 07 April 2018 650 and by *linSVR*-based generators on 26 May and 31 July 2018. Some boxplots exhibit a 651 wide range of outcomes. The range shows that all ML model types are sensitive to the 652 configuration. The NDA of the best generator, i.e., linSVR num ext(a2), equals 0.28. The 653 associated outcomes for flash duration and event number per flash statistics (AppendixD.b) 654 confirm linSVR-based generators as most suitable to simulate GLM targets for the entire 655 test period. Hence, results for the individul targets agree with the overall NDA analysis. 656

#### 657 1) CONFIDENCE IN THE RESULTS

The confidence in the outcomes is evaluated for the two parts of the GEO lightning pseudo-observation generator. The uncertainty of the outcomes is expressed as the range of outcomes given the same configuration. First, (only) three selected generators with constant configuration are trained 10 times using the same full training dataset (for computational efficiency). Herewith, the training variability of the ML model is assessed. The selected generators are *BAGR KNN dist num plus*, *MLP alpha8 num raw*, and *linSVR num ext(a)* 

plus. They are labeled by their ML model type as BAGR KNN dist. MLP, and linSVR. 664 respectively. Figure 6 shows the distributions (boxplots) of targets for the full test data 665 for the 3 generators (x-axis) each trained 10 times for pseudo-GLM flash duration (a), 666 pseudo-GLM number of event per flash (b), and pseudo-GLM flash extent (c), respectively. 667 The predicted target range of the 10 trained generators is smaller than the variability due 668 to different ML model types and due to different configurations of one ML type. The 10 669 BAGR KNN dist based simulations feature a very narrow range of outcomes for all statistics. 670 The 10 trainings of both this linSVR and this MLP yield a range of values of 0.2 to 0.4 671 normalized absolute difference for most statistics. The range of the minimum event number 672 per flash (Figure 6b) and the minimum flash extent (Figure 6c) reaches about 0.5 and up 673 to 0.7 for the linSVR and MLP-based generators, respectively. This range is in the order 674 of magnitude as the variability enforced by using different ML model types. The range of 675 normalized absolute difference for the maximum event number predicted based on 10 equally 676 configured *linSVR* models is also about 0.6. In addition, the range of normalized absolute 677 differences is always wider for the mean than for the median. Despite a relatively high 678 uncertainty in some statistics, the overall trends as described in the previous section remain 679 valid. Statistics sensitive to distribution outliers, i.e., the mean and minimum, exhibit higher 680 uncertainties due to the GB than more robust statistics, i.e., the median, KS, and CvM. 681 Some target generators, i.e., the BAGR KNN dist-based one, appear to provide very robust 682 predictions. The uncertainty range is usually smaller than the overall range of values for 683 each statistic. 684

The test of the variability in the results enforced by the second part of the GEO lightning pseudo-observation generator, i.e., generating pseudo-GLM events (not shown) is much

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<sup>667</sup> smaller than for the ML part. Hence, the overall range of targets for a given generator <sup>668</sup> configuration is similar to those shown in Figure 6.

#### b. Evaluating observed and simulated Flash extent density (FED)

<sup>600</sup> Hourly FED maps are calculated for both GLM observed and simulated flashes. They will <sup>601</sup> be referred to as observed and simulated FED, respectively, in the following. The evaluation <sup>602</sup> includes the hourly FED summed-up over the domain (termed FED sum), the electrified <sup>603</sup> areas defined as pixels with positive FED (i.e., greater than 0 flashes per  $5 \text{ km} \times 5 \text{ km}$  pixel <sup>604</sup> per hour), and a visual inspection of convective cores. As the choice of the ML model type <sup>605</sup> has the highest impact on the overall performance of the GEO lightning pseudo-observation <sup>606</sup> generator, the results are mainly discussed with respect to the ML model types.

Figure 7 presents the observed FED (a) to the simulated FED of 3 selected generator 697 configurations (b-d) for the example of 26 May 2018, 20:00 to 21:00 UTC. The 3 generator 698 configurations represent a selection of the variety of tested generators with different ML 699 model types, feature set selections, and scaling, as detailed below (see also Appendix B). 700 Simulated FED fields capture the coarse geographical distribution of the observed FED. 701 One can identify the most active regions (highest FED values), that are situated at similar 702 locations for the observed and simulated FEDs. The numbers in the top corners of the 703 panels (a)-(d) indicate the number of lightning pixels with FED>0 flashes per  $5 \text{ km} \times 5 \text{ km}$ 704 pixel per hour on the left and the FED sum on the right. The product of the number of 705 lightning pixels and the area per pixel yields the electrified area. The linSVR (num ext(a)) 706 plus, Table B2) in Figure 7b uses GLM duration as additional feature when simulating GLM 707 number, and then GLM duration and GLM event number to simulate GLM extent. This 708 *linSVR*-based generator performs among the best for the simulation of GLM targets overall, 709

and it appears to be among the best also for the FED sum. It underestimated the electrified 710 area in most cases (as in the example in Figure 7a,b). The *MLP*-based simulation (num 711 raw, Table B2) of the FED of Figure 7c uses unscaled features and targets. GLM flash 712 extent and flash duration relate only to 4 NLDN features (without mean amplitude and CG 713 stroke ratio). The attribute *num* means that pseudo-GLM flash duration and flash extent 714 are obtained directly from ST approaches. Those simulated targets serve as pseudo-features 715 to derive the pseudo-GLM event number. This *MLP*-based generator performs among the 716 best for the electrified area, but overestimates GLM flash extent, GLM event number per 717 flash, and eventually the FED sum. Figure 7d maps the FED as simulated by the BAGR718 KNN dist based generator (num plus, Table B2) that uses all six NLDN features and the 719 num method (see above). It is the best performing generator using the BAGR KNN dist 720 ML model type. Although this generator overestimates the target medians and the FED 721 sum, it belongs to the best 25% of generators for both FED sum and and electrified area. It 722 performed best for 07 April 2018 test case with the dominant squall line that produced most 723 of the large-extent lightning flashes. In general, all 3 generators overestimate the 1-hour 724 FED sum in Figure 7. The *linSVR*-based generator simulates an FED sum significantly 725 closer to the observed FED sum than using both the MLP and the BAGR KNN dist. The 726 linSVR, however, underestimates the number of lightning pixels, that is best simulated by 727 the *MLP*-based generator here. 728

The results are further investigated for the 3-day test period by comparing pixel-to-pixel simulated and observed hourly FED. Figure 8 shows the 2D-histograms, computed for the entire 3-day test dataset, for the same linSVR (a), MLP (b), and BAGR KNN dist (c) based generators as used in Figure 7. In general, the Pearson correlation coefficients R of 0.91 to 0.92 indicate well correlated distributions of observed and simulated FED. Figure 8 also <sup>734</sup> shows the range of simulated FED is wider than the range of observed FED (grey box). The <sup>735</sup> corresponding trend to overestimate the FED in the simulation is proofed by the regression <sup>736</sup> lines (light green) that feature steeper slopes than the equal-value line (black). In particular, <sup>737</sup> the *MLP*-based (Figure 8b) and the *BAGR KNN dist* based generator (Figure 8c) overes-<sup>738</sup> timate the FED usually more than the *linSVR*-based generator (Figure 8a). Y-intercepts <sup>739</sup> near 0 indicate good agreement for regions without lightning activity. These findings agree <sup>740</sup> with the example in Figure 7.

To summarize and quantify the evaluation of both FED sum and electrified area, the metrics normalized difference  $D_{real}$  and absolute normalized difference  $D_{abs}$  are defined:

(a) 
$$D_{real} = \frac{\sum_{n=1}^{H} S_n - O_n}{\sum_{n=1}^{H} O_n}$$
 and (b)  $D_{abs} = \frac{\sum_{n=1}^{H} |S_n - O_n|}{\sum_{n=1}^{H} O_n}$  (3)

where  $S_n$  is the simulated hourly FED sum or electrified area,  $O_n$  is the observed hourly FED sum or electrified area, and H is the total number of time steps (here 72 hours).  $D_{real}$ and  $D_{abs}$  can be used to compare the different GEO lightning pseudo-observation generators and identify the generator with the lowest difference to the observation.

All 196 generators are evaluated for  $D_{real}$  and  $D_{abs}$  of both FED sum and electrified area. As the ML part of the generator enforces significantly higher differences than the derivation of pseudo-GLM events (the second part), again results are mainly discussed regarding the different ML configurations.

 $D_{real}$  and  $D_{abs}$  are calculated for the 3-day test period. For the FED sum, the 28 linSVRbased generators tested are ranked as best 28 configurations in the comparison, i.e., lowest  $D_{abs}$ . Table 3 presents the results for the best 20 and worst 5 generators as ranked by  $D_{abs}$  of FED sum. The best GEO lightning pseudo-observation generators exhibit an  $D_{abs}$  of 22% to 25%, while  $D_{real}$  is close to zero, i.e., balance between situations with over- and underestimated FED sum. The worst generators (some of MLP and ETR based configurations) lead to almost twice as high FED sum as the observed values. Similar, positive values of both  $D_{real}$  and  $D_{abs}$  for the FED sum mean that most generators overestimate the FED sum. This agrees well with Figure 8. The exception is found for the linSVR type generators that often underestimate the FED sum with  $D_{real}$  ranging from -22% to +39%. Figure 8a shows one example of a linSVR with positive  $D_{real}$ .

As mentioned, the best 28 generators for the FED sum are all of type linSVR. The best 10 generators use the multi-step approach (*num* and *num ext*, Table 3). The use of mean LF amplitude and CG fraction (*plus*) as additional NLDN features has a minor effect on the simulation of FED sum.

Results for the electrified area are in general closer to the observation than the FED sum. 766 They are shown in Table 4 for the best 20 and worst 5 generators as ranked by  $D_{abs}$  of the 767 electrified area. The generators with the lowest  $D_{abs}$ , HGBR type, differ absolutely by about 768 7.5% from the observed electrified area. The vast majority of all tested target generators 769 underestimate the electrified area (negative  $D_{real}$ ). Multiple generators of various types 770 feature  $D_{abs}$  of less than 10%, e.g., using HGBR, Poly, BAGR KNN dist, ETR, or MLP 771 models. The *linSVR*-based generators, that performed best for the FED sum, exhibit the 772 highest differences to the observation here with  $D_{abs}$  from 15% to 35% (all with negative 773  $D_{real}$ ). For example, the best performer for the FED sum is ranked as third worst for the 774 electrified area with a high underestimation of the area. 775

The best 20 generators for the electrified area take advantage of the multi-step approach in 15 cases. Also 15 of those 20 ML-based generators use all NLDN features (Table 4). Comparing only the *linSVR*-based generators, all 10 leading generators use 6 rather than
only 4 NLDN features. This result strengthens the meaning of including all NLDN features
and of the multi-step approach.

The computational cost of our multi-step approach is still higher than the ST approach, 781 however, only needed for the training of the generator. The application of trained multi-782 step generators is relatively fast, i.e., similar duration as applying ST generators. The 783 best generator without multi-step approach (linSVR(a) raw) exhibits  $D_{abs}$  more than 14% 784 higher than the best generator for the FED sum (Table 3). In addition,  $D_{real}$  exceeds 23 % 785 indicating that the FED sum is mostly overestimated. FED sum simulation is most sensitive 786 to the choice of the generator and, hence, particularly important to obtain realistic synthetic 787 FED. The multi-step approach helps in particular to obtain more realistic FED sum than 788 ST-based generators. For the electrified area, however, generators not using the multi-step 789 approach can perform as well as the best generators (Table 4). If only electrified area is 790 of interest, common ST models can be used. The multi-step generator linSVR num ext(a)791 plus is successfully applied to simulate GLM FED (Section 4) and also MTG-LI FED over 792 France (not in the present paper). 793

The recommended GEO lightning pseudo-observation generator balances the simulation 794 of all pseudo-GLM target distributions, FED sum, and electrified area. It is named *linSVR* 795 num ext(a) plus generator. This configuration features an overall NDA of 0.39, and an  $D_{abs}$ 796 to observed FED sum and electrified area of 24.9% and 21.3%, respectively. This generator 797 used all available features and utilizes the multi-step approach. First, GLM flash duration is 798 predicted from all six NLDN features, and then used as additional pseudo-feature to predict 799 the event number per flash. Finally, the pseudo-GLM flash extent is simulated from NLDN 800 features and the pseudo-features GLM flash duration and event number. Both features and 801 targets are scaled (Section 4). The linSVR ML technique is more time-efficient than the 802

MLP and bagging-based, e.g., *BAGR KNN dist* and *ETR*, techniques for the training and also needs less disk space to be stored. These are two other advantages of the *linSVR num* ext(a) plus generator.

Figure 9 presents hourly FED sum (a) and electrified area (b) with the overall value (1) and 806 the difference to the observation (2) for 31 July 2018 test case. The observed FED and results 807 for the 10 generators with lowest  $D_{abs}$  are plotted. Figure 9(a) includes in addition results of 808 the best generator for electrified area (lime), and Figure 9(b) the results of the best generator 809 for FED sum (orange). The figure also shows the number of hourly simulated pseudo-GLM 810 flashes (histogram). Similar figures for the other two test days are also evaluated but not 811 shown here because identical conclusions are drawn. The absolute values (Figure 9 panels 812 1) show that the FED sum (a) reacts directly to the number of (simulated) flashes. The 813 electrified area curves (b) appear to have a time offset relative to changes in the flash number, 814 suggesting that within 1 h a lower number of relatively large flashes can electrify a similar 815 area as a higher number of smaller flashes. An increasing (decreasing) flash rate during the 816 development (decay) of convective storms does not automatically mean a larger (smaller) 817 electrified area, since even less flashes can still illuminate a large portion of the cloud via 818 scattering. The simulated FED adapts this behavior very well. In particular, the simulated 819 FED features similar hours with highest FED and electrified area as the observed FED. 820

It is observed that the simulated FED sum usually exceeds the corresponding observation during the phases of highest flash amounts within the region (Figure 9a). This could mean that NLDN detects significantly more flashes than GLM during these times, and thus the number of simulated flashes is significantly higher than the number of observed GLM flashes. These findings agree with Zhang and Cummins (2020), who found that the GLM <sup>826</sup> DE decreases for high flash rates and with shorter extent and duration flashes, which are <sup>827</sup> observed during the mature phase of a thunderstorm.

It should be noted that the absolute values (Figure 9a1 and b1) and difference to the 828 observation (Figure 9a2 and b2) for the FED sum (Figure 9a) have the same order of 829 magnitude. In contrast, the difference (9b2) is one order of magnitude smaller than the 830 absolute values (Figure 9b1) for the electrified area. Hence, the difference to observed FED 831 and also the spread between generators with different configurations are much greater for 832 the FED sum than for the electrified area. Therefore, it is decided to put more weights 833 on the ranking of the FED sum than on the ranking of generators by electrified area when 834 choosing the recommended generator. Eventually, the linSVR-based generator returns as 835 the recommendation in an overall evaluation context. If, however, for a certain objective 836 the electrified area is most important, several HGBR, MLP or even ETR based generators 837 perform better than the recommended *linSVR*-based generator. 838

In a Monte Carlo approach, FEDs for 10 of in total 100 realizations of the recommended 839 linSVR generator are calculated for the three test days. Figure 10 illustrate the median 840 (line) and range (shaded) of FED sum and electrified area on 31 July 2021. The variability of 841 both the FED sum and the electrified area has the same order of magnitude as the difference 842 between the leading generators (Figure 9). Figure 10 also confirms that the linSVR-based 843 generator tends to underestimate the electrified area. The vast majority of the time, all 10 844 realizations simulate lower electrified area than the GLM observations indicate. However, 845 all 10 realizations remain relatively close to the observed FED sum at most times (except 846 for the cases with intense convection, as discussed earlier). It should be noted that this 847 linSVR-based generator does not appear among the best 10 generators for the electrified 848 area (Figure 9b). 849

#### **5.** Summary

This study analyzed in detail the simulation of GEO lightning pseudo-observations in two parts: First pseudo-GLM flash characteristics are simulated and then pseudo-GLM events are derived. The data generator uses only LF ground-based data. There is no additional cloud information used in the generator. The entire process is non-trivial because relations (correlations) between characteristics of coincident LF ground-based and optical satellite lightning observations are often weak at the flash scale.

A multivariate analysis using several features and targets is conducted to achieve more robust flash characteristics. Simulated GEO flash characteristics (targets) are obtained via machine learning (ML) models. Targets include GLM flash extent, GLM flash duration, GLM event number per flash. An independent test data set is then introduced to compare the statistics of simulated pseudo-GEO flashes to the observed GEO, i.e., GLM, flash characteristics. In a second part, the simulated targets are used to mimic individual GEO events on a regular latitude longitude grid.

After testing different ML models used in the first part of our generator, a linear SVR (linSVR) based GEO lightning pseudo-observation generator is recommended. The results of multiple linSVR configurations turned out to be similar. In more detail, our recommendation is to use a linSVR with feature and target scaling, that uses all NLDN and pseudo-GLM features in a multi-step approach.

The type of the ML model chosen in the first part of our GEO lightning pseudo-observation generated has a major impact on the simulated flashes. In fact, the performance ranking of tested target generators reveals clusters per ML model type. Whereas the vast majority of generators produces pseudo-GLM flashes with flash characteristic means close to the

observed ones, they simultaneously overestimate the medians of flash characteristics. There-873 fore, they produce insufficient small flashes as compared to the GLM observations. Only 874 linSVR-based generators were able to simulate pseudo-GLM flash characteristics with dis-875 tribution medians close to the observation for the 3-day test dataset. This gain is achieved 876 at the expense of slightly underestimating the target means. It is then found that FED 877 sums from linSVR-based generators are closer to the observed FED sum than for all other 878 generators, however, the electrified area is at least 10 % smaller than the observed electrified 879 area. 880

Besides the type of the ML model, the set of features and the feature scaling impact the results. In particular, including (pseudo) GLM flash characteristics in the set of features improved the predictions of most ML models as target generators and thus the overall performance of the GEO lightning pseudo-observation generator.

In general, generators that perform well for the FED sum exhibit high  $D_{abs}$  for the electrified area and vice versa. For example, the best generator for the electrified area with  $D_{abs}$  $(D_{real})$  of 7% (-2%) highly overestimates the FED in most cases with  $D_{abs}$  and  $D_{real}$  of 75% and 72%, respectively. On the other hand, the best generator for the FED sum with  $D_{abs}$  ( $D_{real}$ ) of 22% (2%) always underestimates the electrified area with  $D_{abs}$  ( $D_{real}$ ) of 27% (-27%). Figure 9 illustrates this finding on the example of test day 31 July 2020.

The developed GEO lightning pseudo-observation generator provides exactly one pseudo-GEO flash for each LF flash. It does not distinguish whether an LF flash, i.e., an NLDN flash, is detected by the GEO LLS, i.e., GLM. During the application of the generator, there is no information whether a given NLDN flash could be detected by the GEO LLS. Additional assumptions, e.g., using flash characteristics, would then be needed to distinguish the LF flashes with and without GEO match. In addition, our GEO lightning data generator

does not include a specific part to simulate GEO flashes that are not directly coincident to 897 any LF flash. Here, the pragmatic approach of using all LF flashes as input is justified 898 with similar flash DE of the LF (i.e., NLDN) and the GEO (i.e., GLM) LLS thus giving 899 overall similar amounts of GLM and NLDN flashes. Then, NLDN and GLM flashes without 900 any coincident observation are analyzed. They are referred to as NLDN-only and GLM-901 only flashes, respectively. It was observed that both the NLDN-only and GLM-only flashes 902 occurred mostly in proximity to the convective cores and regions of overall high flash rates. 903 The number of observed GLM-only and NLDN-only flashes was in general of the same order 904 of magnitude. It is assumed that pseudo-GLM flashes simulated from the NLDN-only flashes 905 substitute the observed GLM-only flashes. It should be mentioned that some simulated 906 pseudo-GLM flashes might overlap as the pseudo-GLM flash extent is usually greater than 907 the NLDN flash extent. Overlapping pseudo-GLM should actually be merged, however, this 908 is not further studied here. As one possible consequence, the simulated pseudo-GLM FED 909 can be somewhat higher than the observed GLM FED (as seen for most configurations of 910 generators). In particular, the simulated hourly FED values are often higher than observed 911 in situations when many NLDN flashes were observed. On the other hand, lower simulated 912 than observed FED at the rim of cells indicate that NLDN flashes cannot represent the 913 scattering of light as seen by GLM. Peterson et al. (2020) showed that optically detected 914 flashes can appear large near storm edges due to light reflected off nearby clouds. Simulated 915 FED (based on NLDN observations) could then be closer to the actual flash channel extent 916 as derived from LMA-type observations than the observed FED, especially at the rim of 917 cells. Nevertheless, the simulation might differ from what the satellite sensor sees. 918

<sup>919</sup> Our methodology is configured and refined for NLDN Vaisala sensors. NLDN flash statis-<sup>920</sup> tics were compared to coincident GLM flashes and their extent, duration, and event number. For an application in other regions than the US and/or with different LF networks, NLDN operational specification and observations might be compared with the ones of the other LF network in order to identify the necessity for adapting the input data. This comparison can be of direct (e.g., NLDN and GLD360) or indirect (e.g., NLDN and Meteorage compared to ISS-LIS as common reference) nature.

The studied dataset is limited to a region in the SE USA and for the months of March 926 to September. GLM features high flash DE (e.g., Marchand et al. 2019; Murphy and Said 927 2020) in this region satisfying our objective to build a high-fidelity generator to simulate GEO 928 lightning data. However, the limited dataset lacks winter storms that may have different 929 characteristics. For the application of our generator in Europe, this should be a minor 930 limitation as winter storms rarely occur here. Taszarek et al. (2020) found that 3.6%931 of flashes over Europe occurred during the European winter. Wintertime flashes might 932 be important over SE Europe and the Mediterranean Sea. The performance of the data 933 generator will depend on the LF network performance, e.g., flash DE. Realistic data can 934 only be expected in regions where the LF network provides good coverage. The simulated 935 data are, thus, restricted by the quality and range of the LF data input. The SE US region 936 features mostly normal polarity storms while storms with different charge structure occur 937 more often in other parts of the US. For example, Rutledge et al. (2020) show that flash 938 characteristics and GLM flash DE are altered for storms with anomalous charge structure. 939 In addition, the data used to train our GEO lightning data generator were recorded in 940 this region well covered and far from the edges of the GLM's (on GOES-16) field of view. 941 Simulating data of a GEO LLS near the edges of the field of view needs caution regarding 942 parallax effects and an increase in the area one event covers. 943

The GLM data includes a parallax correction. Our GEO lightning pseudo-observation generator assumes that GLM observations are correctly located. The simulated flashes are placed according to the LF lightning data. If the GEO LLS that should be mimicked uses a different parallax correction than GLM, an adaption may become necessary to obtain realistic data of this LLS.

A comparison of GLM and NLDN during day and night, and for intra-cloud (IC) and cloud-to-ground (CG) flashes revealed similar relationships between NLDN and GLM flash characteristics. The dataset for the ML includes all observed flashes, without a separation of these flash types. In addition, all applied ML models aim to optimize average characteristics. This study uses deterministic approaches without a definition of a confidence interval of the outcomes. As one result, the tails of the characteristics' distributions, e.g., exceptionally small flashes, are underrepresented in the simulation compared to the observation.

<sup>956</sup> Supplementary data might improve the present GEO lightning data generator. Cloud <sup>957</sup> information and brightness temperature data could provide additional features for the ML, <sup>958</sup> e.g., cloud top height, and also information about more likely scattering directions, e.g, in <sup>959</sup> anvils of convective clouds or in stratiform cloud lightning. (Doppler-)Radar data would <sup>960</sup> provide even more versatile possibilities to include cloud structures, dynamics and micro-<sup>961</sup> physics.

Data availability statement. NLDN data are available from Vaisala, and data as presented
 in this paper were provided by Ronald L. Holle.

GLM data are in general available from NOAA: GOES-R Algorithm Working Group and GOES-R Series Program, (2018): NOAA GOES-R Series Geostationary Lightning Mapper (GLM) Level 2 Lightning Detection: Events, Groups, and Flashes. Flash and Event subsets <sup>967</sup> used. NOAA National Centers for Environmental Information. doi:10.7289/V5KH0KK6.
<sup>968</sup> Access date: 01 November 2018. The GLM data as presented in this paper were downloaded
<sup>969</sup> from the French AERIS/ICARE Data and Services Center of the Université de Lille where
<sup>970</sup> the files were stored 19 April 2018.

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<sup>983</sup> The authors declare that there is no conflict of interests.

### APPENDIX A

### 985

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# GEO pixel slicing for FED

Deriving FED requires knowledge about flash locations or, in case of satellite observations, the positions of lightning data pixels. GLM products do not come with this necessary information. Therefore, the real GLM grid is reconstructed locating the centers of all events

of the full half-year dataset. This large dataset was used to ensure that the reconstruction 989 of the GLM grid would be complete, i.e., there was at least one event at each GLM pixel. A 990 time invariant real GLM grid is assumed. As individual pixels appear to wobble locally with 991 time and do not appear on a regular grid; due to micro-vibrations of the satellite platform, 992 spacecraft jitter, and variable pitch CCD; a k-means-clustering analysis is performed to 993 identify the statistical mean location of each pixel center. Corner points of pixels are then 994 defined as the mean locations between the centers of the 4 pixels adjacent to each point. It 995 is assumed that corner points can be connected by straight lines in order to represent the 996 pixel shapes. This assumption is not entirely true, as the regular CCD grid is projected on 997 the Earth (more precisely, on the cloud top ellipsoid, Section 2.a), however, the FED should 998 be less impacted by this assumption than by assuming a regular GLM grid. Shapes of GLM 999 events do usually not match the FED grid pixel shapes. One GLM event with average side 1000 length of 8.7 km can overlap multiple FED pixels with side length of 5 km to some part. 1001 The fractions of the GLM event within each pixel of the FED grid are summed up while 1002 integrating over the time period. This slicing of GLM events reduces the effect of producing 1003 gaps or double counts of GLM pixel when transformed to the regular FED grid, as recently 1004 described by Bruning et al. (2019). 1005

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#### APPENDIX B

1007

### Definitions of the machine learning (ML) algorithms

1008 a. ML model types

This section defines the seven ML model types that are trained in the study. The basic idea of each ML model type is introduced, and specifications and important parameters for their tuning are briefly described. As mentioned in Section 2, Python's sklearn-package is used. Model names are given as they appear in the sklearn library and documentation (https://scikit-learn.org/stable/) that provides further details.

(i) Multivariate Linear Regression. The first approach is the most commonly used linear regression sklearn.linear\_model.LinearRegression. It is applied simultaneously to all features and targets and is, thus, a multivariate linear regression (LinReg). The algorithm seeks for the minimum sum of squared errors between the features and the targets by using linear functions. It is an ordinary least square fit in a space with dimensions equal to the number of features times the number of targets.

(*ii*) Multivariate Polynomial Regression. The Polynomial Regression (Poly) is an adjustment to the multivariate linear regression. It fits a polynomial of degree 3 (rather than a linear function) to minimize the sum of squares between predicted targets and the corresponding observations in the validation dataset. The cubic polynomial model is chosen based on the initial correlation analysis with relations between any one feature and one target. The low polynomial degree allows fast computation.

(iii) Random Forest Regressor. A Random Forest (RF) is a ML algorithm using boot-1026 strapping and applying single decision trees to each bootstrap sample. The overall result 1027 is the average of the outcomes of all the decision trees. The minimum leaf size defines the 1028 minimum size at the end of the decision tree. A specific form of the RF is called Extra Trees 1029 sklearn.ensemble.ExtraTreesRegressor (ETR, Geurts et al. 2006). ETR enforces randomness 1030 by not only selected random features in each subset but also splits depending on the best 1031 randomly produced thresholds instead of looking for the most distinctive threshold (as in 1032 RF). ETR usually reduces the variance and increases the bias of the model compared to 1033

*RF.* In general, a higher number of trees improves the performance but also the computation 1034 time. Our RF implementation uses a ETR model with 50 decision trees. The number of 1035 decision trees results from a sensitivity test (ETRs with 5, 10, 20, 50, 100, and 500 trees were 1036 tested) between performance as  $R^2$ -score (see skilearn documentation) and computational 1037 effort. Here, the GB dataset with independent ML training and validation (i.e., calculating 1038 the  $R^2$ -scores) data (see Section 1) is used. The minimum leaf size is set to two, i.e., a 1039 remaining sample of two data points defines the end of the branch. Single point leaf size 1040 would increase the variability of the trees and would lead to a higher likelihood of overfitting. 1041

(iv) Bagging Regressor with k-Nearest Neighbor Regressor. Bootstrap Aggregation, short 1042 Bagging (Breiman 1996), uses subsamples drawn by bootstrapping from the entire dataset. 1043 This step is similar to the RF regressor. The algorithm used to treat the subsamples can, 1044 however, be chosen (not always a decision tree). This paper applies the bagging regressor 1045 sklearn.ensemble.BaggingRegressor combined with a K-Nearest Neighbor (KNN) regressor 1046 (e.g., Altman 1992) sklearn.neighbors.KNeighborsRegressor on each of 50 subsamples. The 1047 number of neighbors to use by default is set to the 5 closest points and distance weighting is 1048 applied for Euclidean distances. The KNN finds closest neighbors with a K-dimensional tree 1049 (KD tree) method (Bentley 1975). It reduces the number of distance calculations compared 1050 to a brute-force approach calculating distances between all data points. The KNN regressor 1051 in combination with distance weighting should represent the actual range of the subsample 1052 training data better than a decision tree (as used in RF and ETR). The expense might be 1053 an increase in overfitting of the data. 1054

(v) Multilayer Perceptron Neural Network. MultiLayer Perceptrons (MLPs) are a form of Neural Networks in supervised ML (Glorot and Bengio 2010). They consist of differ-

ent layers of neurons, where the input layer neurons represent the features and the output 1057 layer neurons represent the simulated targets. An adjustable number of hidden layers can 1058 connect the input and output layers. Each neuron initially transforms the values from the 1059 previous layer in a weighted linear summation. Then, a (non-)linear activation function 1060 is used. Parameters of our *MLP* model sklearn.neural\_network.MLPRegressor were deter-1061 mined after testing different configurations to balance computation time and accuracy. It 1062 uses one hidden layer with 50 neurons. The activation function is the rectified linear unit 1063 function. Additionally, an early stopping criterion is applied if there is no improvement 1064 over 20 consecutive iterations. The early stopping requires splitting the training dataset 1065 randomly, whereby 10% are used to verify the improvement of the model and 90% remain 1066 as actual training dataset. The tolerance for the stopping criteria is reduced from default 1067  $10^{-4}$  to  $10^{-8}$  to allow a higher number of iterations. The alpha parameter for the L2 penalty 1068 was also reduced from default  $10^{-4}$  to  $10^{-8}$  after testing different values. The lower alpha 1069 led to faster training while maintaining the model skill. This change is indicated by naming 1070 alpha8 of the MLP-based generators. Furthermore, the default Adam solver (Kingma and 1071 Ba 2014) and a constant learning rate are used, along with adjusted parameters beta (0.7), 1072 beta2 (0.9), and epsilon  $(10^{-10})$  for the decay rates and the numerical stability in the Adam 1073 solver. 1074

(vi) Support Vector Regressor. The Support Vector Regressor (SVR) is based on Support Vector Machine (SVM) algorithms. A set of hyper-planes is constructed. Therefore, a defined kernel function is applied to achieve a separation of data clusters (by the hyper-planes) for the regression. The kernel function can be a linear or non-linear function (i.e., polynomial or Radial Basis Function). Linear SVR (linSVR) is faster and uses less memory than

SVR with non-linear kernel-functions. Non-linear SVR provides usually better separation 1080 of different clusters in the data and thus a higher score than linear SVR. The distances of 1081 the nearest data points to the hyper-planes (so-called functional margins) are maximized. 1082 Points with a larger functional margin lead to less uncertainty for the prediction than data 1083 close to the hyper-planes. SVM in general analyzes all data while the cost function (L1) 1084 loss) depends on a subset of the training data, referred to as support vectors. Support 1085 vectors are a set of data points with some distance from the target values that still allow 1086 the correct prediction. The systematic reduction of the training data makes this model type 1087 fundamentally different from the remaining model types of this study. Further information 1088 is also provided by Smola and Schölkopf (2004). 1089

<sup>1090</sup> Due to our large sample size (672,794 flashes), only the linSVR sklearn.svm.LinearSVR is <sup>1091</sup> used in this study in its default configuration. As for the *MLP*, an early stopping criterion <sup>1092</sup> is used for a lack of improvement between consecutive iterations.

(vii) Histogram-based Gradient Boosting Regression Tree. Boosting is, besides bagging, 1093 another approach to reduce overfitting of ML models. It combines an ensemble of 1094 The Histogram Gradient Boosting Regression weak learners to one strong learner. 1095 sklearn.ensemble.HistGradientBoostingRegressor (HGBR) is much faster than regular Gra-1096 dient Boosting Regressors. Data is first binned into 256 integer-valued bins. The algorithm 1097 can then leverage histograms instead of relying on sorted continuous values when building 1098 the decision trees. The number of splitting points is reduced and the algorithm becomes 1099 time efficient, inspired by LightGBM (Ke et al. 2017). The first step of the HGBR averages 1100 the target values and calculates residuals (average difference of observation to prediction) 1101 with a least-squares loss function. Based on these residuals, a small decision tree is built, 1102

along with a learning rate. The learning rate limits the influence of a single small decision tree in the final ensemble to avoid overfitting. Then, new predictions are computed using the averages and the decision tree for residuals. Based on new predictions, new residuals are calculated and a new decision tree is created. The final model combines several of these decision trees to pull the target averages towards the observations. The used maximum number of iteration is 500 and the early stopping criteria kicks in after 50 iterations without significant improvement of the loss value.

## <sup>1110</sup> b. Naming convention for the GEO lightning pseudo-observation generator configurations

This section defines the meaning of names given to different configurations of a target 1111 generator. The names and abbreviations of the ML model types can be found in Table B1. 1112 The given ML model types are used in the first part of the GEO lightning pseudo-observation 1113 generator referred to as target generator<sup>3</sup>. Table B2 summarizes the feature usage that is 1114 available for each ML model type available for the target generator. The feature set selections 1115 indicate whether a single-target or multi-step approach is used. The feature set selection 1116 called *NLDN* is the default configuration as described. Generators with extension of only 1117 *default, plus, raw,* or *raw plus* are single-step approaches, i.e., using 3 times the model of class 1118 (1) in Figure 3. Multi-step simulations always simulate the GLM flash duration in the first 1119 step here. The order of the targets number of events per flash and the GLM flash extent is 1120 not fixed. The extension *num* indicates one additional step only for the pseudo-GLM event 1121 number per flash using the pseudo-GLM flash duration as pseudo-feature. GEO lightning 1122 pseudo-observation generator configurations with extension num ext and num ext(a) have 1123 two additional steps using different pseudo-features as shown in Table B2. The num ext(a2)1124

<sup>&</sup>lt;sup>3</sup>RF is included in the table for completeness. Only ETR as a special RF model is used in the study.

generators use only the GLM flash duration as pseudo-feature, thus two models of class (2) as of Figure 3.

The attributes define a modification of the feature set selections with binary character. 1127 The *plus* attribute indicates that NLDN LF amplitude and CG fraction are added to the list 1128 of features. Attribute raw means that no feature and target scaling were used. Combinations 1129 of the given feature set selections and attributes are possible, e.g., an unscaled model with 1130 NLDN mean LF amplitude and CG stroke ratio as additional features that uses the GLM 1131 flash duration as pseudo-feature for the event number per flash gets the extension num(a)1132 raw plus. The total number of generator configurations equals 196: There are 7 ML model 1133 types (Table B1 except RF). For each ML model type there are 7 feature set selections 1134 resulting from the single and multi-step approaches, and for each combination of ML model 1135 and feature set selection again 4 different attribute usages (Table B2), i.e., none, *plus*, *raw*, 1136 or raw plus. The 196 generator configurations (28 for each ML model type) define the base 1137 for the statistical results presented in Section 4. 1138

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APPENDIX C

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#### The multi-target multi-step approach

This section describes a multi-target regression that simplifies the idea of the stacked single target (SST) approach (Spyromitros-Xioufis et al. 2016). In this study, there are six NLDN features (as physical input) and three GLM targets (as physical simulated variables) per sample, i.e., per flash. The three GLM targets are denoted  $T_i$ ,  $T_j$ , and  $T_k$ .  $T_i$  can represent any of the 3 targets. The indexes i, j, k indicate the order of obtaining the final targets. Targets that are used like features are referred to as pseudo-features, i.e.,  $T_j$  and  $T_k$  in Figure 3a. With this dataset, there are in general 4 different ways to simulate the target  $T_i$ .

The 4 ST models are shown as the training part in Figure 3a. There are 3 classes of models: 1148 Yellow is the model class (1) without pseudo-features, gray indicates model class (2) using 1149 1 pseudo-feature, and the red for model class (3) uses 2 pseudo-features. The model  $M_{\rightarrow i}$ 1150 constitutes the common ML model, i.e., class (1), with only the NLDN features as input. 1151 One (i.e.,  $T_j$  or  $T_k$ ) or two (i.e.,  $T_j$  and  $T_k$ ) of the three targets can be added to the input as 1152 pseudo-features in order to simulate the target  $T_i$ . The resulting models  $M_{j\to i}$  (using  $T_j$  as 1153 pseudo-feature),  $M_{k\to i}$  (using  $T_k$  with the features), and  $M_{j,k\to i}$  (using  $T_j$  and  $T_k$  with the 1154 features) may indeed take advantage of correlations between the predicted target and the 1155 targets that are used as pseudo-features. 1156

The application case only uses the NLDN features as first input. Therefore, a multi-step 1157 approach is required. Figure 3b presents the example application for a 3-step approach 1158 that first predicts the pseudo-GLM flash duration, then the pseudo-GLM event number 1159 per flash, and finally the pseudo-GLM flash extent. This configuration is denoted num 1160 ext(a) (see Table B2 for details on the configuration naming). The first step,  $M_{\rightarrow i}$ , uses 1161 the NLDN features and predicts the first pseudo-GLM characteristic  $M_{\rightarrow i}$  (NLDN), i.e., 1162 pseudo-GLM flash duration. The second step,  $M_{i \to j}$ , uses the NLDN features and the result 1163 of the first step,  $M_{\rightarrow i}$  (NLDN), i.e., the pseudo-feature GLM flash duration. This model of 1164 class (2) predicts the second pseudo-GLM characteristic  $M_{i \to j} [NLDN, M_{\to i} (NLDN)]$ , i.e., 1165 the pseudo-GLM event number per flash. Both predicted pseudo-GLM characteristics (i.e., 1166 GLM flash duration and event number per flash) can then be used as pseudo-features to 1167 predict the third target with the class (3) model  $M_{i,j\to k}$ . Hence, the final target prediction 1168  $M_{i,j \to k} \langle NLDN, M_{i \to j} [NLDN, M_{\to i} (NLDN)] \rangle$  depends on the NLDN features and both 1169 previous predictions for this configuration. In general, a model of class (3) can also use two 1170 pseudo-features produced by two models of class (1). Also, 2 models of class (2) could be 1171

<sup>1172</sup> used to simulate the remaining 2 targets after the first step. Utilizing 3 times a model of <sup>1173</sup> class (1) is equal to the common ML ST approach. Hence, several combinations of models <sup>1174</sup> of different classes are possible and have been investigated here.

The ML training for the multi-step approach can be performed in parallel for the models 1175  $M_{\rightarrow i}, M_{i \rightarrow i}$ , and  $M_{i,k \rightarrow i}$ . The approach can use all ML model types as the training creates 1176 independent learners. Our multi-step approach adapts the idea of the SST, but uses GLM 1177 observations instead of simulated pseudo-GLM targets during the ML training. A trained 1178 generator can be applied even if the observations are not available using the corresponding 1179 pseudo-observation in their place. This method assumes similarity between observations and 1180 pseudo-observations, however, the pseudo-observations only approximate the real observa-1181 tions. Our approach does not propagate errors in successive steps. However, the training is 1182 more efficient than for an SST approach as all generator parts can be trained simultaneously 1183 rather than waiting for the pseudo-observations to be created. Computational efficiency was 1184 necessary due to the large number of generators tested in this paper and in the perspective 1185 of an operational-like application. The results (Section 4) showed that our multi-step ap-1186 proach aids in simulating realistic pseudo-GLM observations and the performance is often 1187 better than with using common ST models without pseudo-features. 1188

Although the correlations between the NLDN features and both GLM flash extent and event number per flash are relatively weak, the NLDN features improve the prediction during each step as seen through feature drop tests (not shown). Indeed, all features have a positive effect on the model score. Due to strong correlations between GLM flash duration and NLDN features flash duration and pulse/stroke number, and to reduce the number of ML-based target generators, only the multi-step approaches which predict the GLM flash duration in the first step  $(M_{\rightarrow i})$  are considered. There remains only one model of class (2) in Figure 3a

and three ways to simulate a target  $T_i$ . The GLM flash duration is also weakly correlated 1196 to both GLM flash extent and event number (R of about 0.10 and 0.17), and GLM flash 1197 extent and event number per flash are well correlated (R of about 0.74). Thus, the first 1198 step always provides the pseudo-GLM flash duration from the NLDN flash characteristics 1199 as features. The second step uses the simulated flash duration in addition to the NLDN 1200 features to simulate one or both of pseudo-GLM flash extent and event number per flash. 1201 The pseudo-feature used in model class (2) (Figure 3) is fixed in this paper to be flash 1202 duration leaving only one realization of model class (2) to simulate a second target. To 1203 further reduce the number of multi-step configurations, the approaches that simulate the 1204 flash extent but not the event number per flash through a multi-step process are not further 1205 considered since (i) GLM flash duration shows weaker correlation with GLM flash extent 1206 than with the event number per flash and (ii) the ST approach for event number per flash 1207 from NLDN features exhibits the lowest skill of the three targets. A potential third step may 1208 simulate the last GLM target based on NLDN features and the two remaining simulated 1209 pseudo-GLM characteristics as additional pseudo-features. The paper describes generator 1210 configurations using only the GLM duration (strongest correlations) or using GLM duration 1211 and a second target as additional pseudo-features to simulate the remaining target (GLM 1212 flash extent or event number per flash). 1213

Our multi-step approach aims at producing more realistic pseudo-GLM flash extent and event number per flash than using the NLDN features alone. The NLDN features also remain important as the correlations between some targets are weak.

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#### APPENDIX D

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Supplementary results for each test day and target distribution statistic

This section contains detailed results for each test day that are presented in the main paper for the combined 3-day period. The second part includes the Figures and analysis of the normalized difference between distribution statistics of observed and simulated GLM flash duration and event per flash. The results are presented in a similar way as for the flash extent statistics in the main paper.

#### <sup>1224</sup> a. Target generator results for each test day

Tables D1, D2, and D3 present the results for 07 April 2018, 26 May 2018, and 31 July 1225 2018, respectively. As explained for Table 2 with results for the 3 days combined, the 1226 tables show the observed statistics for each target distribution, the outcomes using the 1227 best performing generator, and statistics of data simulated with the linSVR num ext(a)1228 plus recommended generator. The most common behavior of the target generators exibitis 1229 simulated mean values close to the observation statistics of the three target distribution. 1230 Median values are usually underestimated by the target generators as seen in Tables D2 and 1231 D3. Results for the 07 April 2018 test case differ from the general behavior (Table D1). That 1232 day saw exceptionally large flashes with high event numbers per flash that likely occurred 1233 within the MCS and the squall line. As a consequence, the ML-based target generators 1234 underestimated the means of the observed flash characteristics for that test case, but the 1235 medians of simulated and observed targets are similar. 1236

The results for each test day resample the results for the combined 3-day test data (see Table 2) overall. Minimum values are often only slightly overestimated for the three targets, while the simulated maxima cannot reach the observed maxima for none of the targets and on none of the 3 test days (Tables D1 to D3). *linSVR*-based target generator outperform all other generator types on 26 May an on 31 July 2020. On April 07 with extensively

large flashes, different BAGR KNN dist-based generators are found as best performers for 1242 all three targets (Table D1). The choice of the most suitable generator appears to be 1243 situational, i.e., there is no generator that performs better than all other generators in all 1244 cases. The recommended linSVR num ext(a) plus (bold in Tables D1 to D3) performs on 1245 one level with best generator for the event number per flash and flash extent on 26 May 1246 an on 31 July 2020. The event number per flash is significantly underestimated by this 1247 linSVR-based generator on 07 April 2020 for the mentioned reason. The flash extent, as 1248 most important target for the FED, is also underestimated on that day, however, the CvM 1249 is only about half of the CvM for event number per flash meaning a more realistic simulation 1250 of the flash extent distribution than the event number per flash distribution. 1251

# b. Normalized statistics for difference between observation and simualation for GLM flash duration and event number per flash

Figures D1 and D2 group the results for each statistic by the seven ML model types. As explained in Section 4.a, each distribution contains the results of 28 generators (see also Appendix B.b, Table B2).

Figure D1 shows the normalized differences and scores of different target generators for the GLM flash duration for the 3 test days combined. The GLM flash duration distribution is equally well simulated by a variety of ML-based target generators as the narrow spread of the medians (green line) indicates. In detail, a linSVR-based generator and a MLPbased generator can predict the mean well, a MLP-based generator and an ETR-based generator are best for the maximum, while a linSVR-based generator exhibits the lowest differences for the median as well as both KS and CvM scores. In total, a linSVR-based target generator (linSVR num ext raw) best approximates the observed distribution of the GLM flash duration in this comparison with an NDA value of 0.30.

For the GLM event number per flash in Figure D2, *linSVR* and *BAGR KNN dist* models 1266 make the best target generators. The lowest NDA of 0.45 is obtained for several linSVR1267 and BAGR KNN dist-based generators, e.g., linSVR num ext(a) raw plus and BAGR KNN 1268 dist num ext raw. For test day 07 April 2018 (a dominant mesoscale system with above-1269 average mean and median GLM event numbers per flash), all generators underestimated the 1270 event number per flash. As generators using a linSVR usually predict lower values than the 127 other generators, they underestimate the observed statistics even more on 07 April 2018. 1272 Nevertheless, for the full test data, there are linSVR-based generators that predict the mean 1273 event number equally well as the best target generator, i.e., MLP-based, as demonstrated 1274 by the lower whiskers in Figure D2. LinSVR-based generators are again most suitable to 1275 predict the event number distribution median. 1276

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1558		the best generator for each target on 31 July 2018. The recom-
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TABLE 1. Study dates (year 2018) with the amounts of GLM and NLDN data. The three rightmost columns indicate whether the data are used for ML-based generator building (GB) or the generator test (GT) part, the time of most lightning activity in the region (D: local daytime, N: local nighttime), and the primary forcing (Trigger) for storm development and lightning.

Date	number of GLM events	number of GLM flashes	number of NLDN pulses, strokes	number of NLDN flashes	Usage	Time	Trigger
19 Mar	4,053,599	79,420	315,854	78,351	GB	D+N	cyclone, cold front
29 Mar	2,611,064	35,822	122,772	37,931	GB	D+N	stationary front, MCS
07 Apr	5,854,407	94,447	494,686	113,978	GT	D+N	short wave trough, front
14 Apr	8,610,567	142,587	729,622	169,181	GB	D+N	cold front
26 May	4,364,985	130,632	422,193	120,608	GT	D	thermal convection
03 Jun	6,103,693	204,295	825,601	188,330	GB	D+N	cold front
21 Jul	5,541,425	150,363	943,644	142,023	GB	D+N	squall line, outflow boundary
31 Jul	4,885,532	114,133	391,602	106,142	GT	D	dry line, thermal convection
07 Aug	5,283,358	153,671	472,369	137,963	GB	D	thermal convection
13 Sep	1,015,483	28,301	61,124	21,168	GB	D	Hurricane Florence
TABLE 2. Comparison of distribution statistics for observed GLM data and the best generator for each target during the full test period. The recommended *linSVR*-based generator is shown in bold. Details about the target generator names are provided in the Appendix B.b.

Generator	Mean	Median	Minimum	Maximum	RMSE per flash	KS	CvM
			GLM flash	duration [s]			
Observed	0.43	0.31	0.00	16.44	0.00	0.00	0.0
linSVR num ext raw	0.46	0.30	0.00	9.41	0.77	0.15	656.5
$linSVR \ num \ ext(a) \ plus$	0.41	0.31	0.02	10.0	0.68	0.32	3770.3
		GL	M event nur	nber per flas	h [-]		
Observed	49.3	25.0	2	1395	0.0	0.00	0.0
linSVR num ext(a) raw plus	35.3	30.0	2	411	79.8	0.38	6687.6
$linSVR \ num \ ext(a) \ plus$	34.7	30.0	14	457	80.0	0.40	6989.5
			GLM flash	extent [km]			
Observed	32.9	27.5	0.0	277.0	0.0	0.00	0.0
$\begin{vmatrix} linSVR & num \\ ext(a2) \end{vmatrix}$	30.1	26.3	0.0	157.3	30.9	0.24	3479.2
$linSVR \ num \ ext(a) \ plus$	29.0	26.2	8.5	305.5	31.5	0.24	2738.4

TABLE 3. Comparison of  $D_{real}$  and  $D_{abs}$  in percent of observed value for the FED sum during the full test period. The best 20 and the worst 5 of the 196 generators (ranked by  $D_{abs}$ ) are included. The recommended *linSVR*-based generator is shown in bold. Details about the target generator names are provided in the Appendix B.b.

Generator	$D_{abs}$ [%]	$D_{real}$ [%]
linSVR num ext(a2) raw	22.2	2.3
$linSVR \ num \ ext(a) \ raw$	22.7	-22.5
$linSVR \ num \ ext(a)$	22.9	3.6
$linSVR \ num \ ext(a) \ plus$	24.9	9.8
linSVR num ext raw	25.7	11.4
linSVR num ext default	26.5	11.0
linSVR num ext(a2)	27.4	12.6
linSVR num ext(a) raw plus	28.8	15.4
linSVR plus num ext	29.6	17.0
$linSVR \ num(a) \ raw$	31.0	18.5
$linSVR \ num \ ext(a2) \ plus$	32.3	20.9
linSVR(a) raw	34.4	23.2
linSVR raw	35.1	24.2
linSVR num ext(a2) raw plus	35.6	24.9
linSVR num raw	36.0	25.4
linSVR default	36.1	25.3
linSVR num(a) raw plus	36.2	26.0
$linSVR \ num(a)$	36.4	25.6
linSVR(a)	36.7	26.0
linSVR num default	36.9	26.3
MLP alpha8 num ext(a) raw plus	95.0	93.6
$ETR \ num \ ext(a) \ raw$	95.3	93.8
MLP alpha8 num ext(a2) raw	96.7	95.6
ETR num ext(a)	97.8	96.3
MLP alpha8 num ext(a) raw	107.6	106.7

TABLE 4. Comparison of  $D_{real}$  and  $D_{abs}$  in percent of observed value for the electrified area during the full test period. The best 20 and the worst 5 of the 196 generators (ranked by  $D_{abs}$ ) are included. In addition, the recommended *linSVR*-based generator is shown in bold. Details about the target generator names are provided in the Appendix B.b.

Generator	$D_{abs}$ [%]	$D_{real}$ [%]
$HGBR \ num \ ext(a2) \ plus$	7.4	-2.3
$HGBR \ num \ ext(a2) \ raw \ plus$	7.4	-2.4
$HGBR \ num \ ext(a2) \ raw$	7.4	-3.0
$HGBR \ num \ ext(a2)$	7.5	-2.8
Poly plus num ext	7.5	-2.5
Poly num ext raw plus	7.5	-2.5
BAGR KNN dist raw plus	7.6	-1.4
BAGR KNN dist num raw plus	7.6	-1.5
BAGR KNN dist num(a) raw plus	7.6	-1.4
BAGR KNN dist(a) raw plus	7.6	-1.3
ETR plus num	7.7	-3.7
HGBR num ext default	7.7	-1.4
ETR plus	7.7	-3.7
ETR(a) plus	7.7	-3.5
MLP alpha8 num ext plus	7.7	-1.8
ETR raw plus	7.7	-3.9
$ETR \ num(a) \ plus$	7.7	-3.6
ETR num raw plus	7.7	-3.9
$BAGR \ KNN \ dist \ num(a)$	7.8	-2.1
MLP alpha8 num ext default	7.8	-4.0
linSVR num ext(a) plus	21.3	-21.3
Poly num ext raw	26.0	10.4
Poly num ext default	26.1	10.6
$linSVR \ num \ ext(a2) \ raw$	27.4	-27.4
$linSVR \ num \ ext(a)$	28.0	-28.0
$linSVR \ num \ ext(a) \ raw$	35.4	-35.4

ML model type	Abbreviation
Multivariate Linear Regression	LinReg
Multivariate Polynomial Regression	Poly
Random Forest Regressor <sup>1</sup>	RF
Random Forest Extra Trees Regressor	ETR
Bagging Regressor with k-Nearest Neighbor Regressor (distance weighting)	BAGN KNN dist
Multilayer Perceptron Neural Network	MLP
(Linear) Support Vector Regressor	$SVR \ (linSVR)$
Histogram-based Gradient Boosting Regression Tree	HGBR

Table B1. ML model types with abbreviation.

<sup>1</sup>This study uses ETR as a special form of RF.

Table B2. Naming conventions of used target generator configurations. The name extensions 1576 as of column 1 are used following the ML model type. The three columns indicate the utilized 1577 features during the ML training for each of the three targets GLM flash duration (Flash Duration), 1578 number of events per flash (Event Number), and GLM flash extent (Flash Extent). NLDN indicates 1579 that NLDN flash duration, the number of pulses/strokes per flash, NLDN flash extent, and the 1580 maximum LF amplitude are used as features. The GLM pseudo-features Flash Duration, Flash 1581 Extent and/or Event Number can complement the NLDN features for some configurations. Feature 1582 set selections define how one target (header) is generated, i.e., ST or multi-step approach. The 1583 attributes can or cannot be applied and may replace *default* in the generator name. Combinations 1584 of a feature set selection with 0, 1, or 2 attributes are possible. 1585

Name extension	Flash Duration	Event Number	Flash Extent
	Featur	e set selections	
default	NLDN	NLDN	NLDN
(a)	Training with default contraining uncertainty of the (Initial training step for	nfiguration. Model predict he default model applying the multi-step ap	ions within the pproach)
num	NLDN	NLDN + Flash Duration + Flash Extent	NLDN
num(a)	NLDN	NLDN + Flash Duration	NLDN
num ext	NLDN	NLDN + Flash Duration + Flash Extent	NLDN + Flash Duration + Event Number
$num \ ext(a)$	NLDN	NLDN + Flash Duration	NLDN + Flash Duration + Event Number
$num \ ext(a2)$	NLDN	NLDN + Flash Duration	NLDN + Flash Duration
	P	Attributes	
plus	NLDN with mean LF amplitude and CG fraction	NLDN with mean LF amplitude and CG fraction	NLDN with mean LF amplitude and CG fraction
raw	features and target not scaled	features and target not scaled 76	features and target not scaled

1586

Table D1. Comparison of distribution statistics for observed GLM data and the best generator for each target on 07 April 2018. The recommended *linSVR*-based generator is shown in bold. Details about the target generator names are provided in the Appendix B.b.

Generator	Mean	Median	Minimum	Maximum	RMSE per flash	KS	CvM
		G	LM flash du	ration [s]			
Observed	0.62	0.45	0.00	16.44	0.00	0.00	0.0
BAGR KNN dist num ext default	0.57	0.46	0.01	10.56	0.92	0.25	949.2
$linSVR \atop ext(a) \ plus \ num$	0.46	0.34	0.02	10.01	0.93	0.21	810.3
		GLM	event numb	er per flash [·	-]		
Observed	73.5	46.0	2	1395	0.0	0.00	0.0
BAGR KNN dist num raw	57.8	48.0	3	467	99.7	0.24	996.6
$linSVR \atop ext(a) \ plus \ num$	37.9	33.0	15	457	103.6	0.32	2066.6
		G	LM flash ex	tent [km]			
Observed	38.5	34.8	0.0	277.0	0.0	0.00	0.0
$\left  \begin{array}{c} BAGR \ KNN \ dist \\ num \ ext(a2) \ raw \\ plus \end{array} \right $	41.24	35.1	0.0	166.0	33.7	0.24	582.7
$linSVR \atop ext(a) \ plus$ num	31.1	26.3	8.7	182.6	34.6	0.27	1068.3

1590

Table D2. Comparison of distribution statistics for observed GLM data and the best generator for each target on 26 May 2018. The recommended *linSVR*-based generator is shown in bold. Details about the target generator names are provided in the Appendix B.b.

Generator	Mean	Median	Minimum	Maximum	RMSE per flash	KS	CvM
		C	LM flash du	ration [s]			
Observed	0.34	0.26	0.00	7.42	0.00	0.00	0.0
linSVR raw	0.41	0.25	0.01	4.73	0.56	0.21	599.9
$linSVR \atop ext(a) \ plus$ num	0.38	0.31	0.02	5.44	0.46	0.41	2451.3
		GLM	event numb	er per flash [	-]		
Observed	34.8	19.0	2	775	0.0	0.00	0.0
$ \begin{vmatrix} linSVR & num \\ ext(a) \ raw \ plus \end{vmatrix} $	32.2	29.0	3	341	54.0	0.45	3593.1
$linSVR \atop ext(a) \ plus \ num$	31.8	28.0	14	249	54.1	0.48	3670.5
		C	LM flash ex	tent [km]			
Observed	28.0	20.2	0.0	218.6	0.0	0.00	0.0
$\left \begin{array}{ccc} linSVR & num & ext\\ raw \end{array}\right $	27.4	26.1	0.0	154.8	27.8	0.28	1029.2
$linSVR \atop ext(a) \ plus$ num	26.7	26.1	8.5	157.6	27.2	0.29	1130.4

1594

Table D3. Comparison of distribution statistics for observed GLM data and the best generator for each target on 31 July 2018. The recommended *linSVR*-based generator is shown in bold. Details about the target generator names are provided in the Appendix B.b.

Generator	Mean	Median	Minimum	Maximum	RMSE per flash	KS	CvM
		G	LM flash du	ration [s]			
Observed	0.39	0.29	0.00	9.21	0.00	0.00	0.0
$linSVR \atop ext(a) \ plus$ num	0.39	0.30	0.02	5.34	0.58	0.32	1307.9
		GLM	event numb	er per flash [	-]		
Observed	45.7	23.0	2	883	0.0	0.00	0.0
$ \begin{array}{c} linSVR & num \\ ext(a) \ raw \ plus \end{array} $	33.9	30.0	2	316	76.4	0.40	2441.8
$linSVR \atop ext(a) \ plus$ num	34.4	30.0	16	315	76.1	0.42	2505.0
		G	LM flash ex	tent [km]			
Observed	33.8	27.5	0.0	242.2	0.0	0.00	0.0
linSVR raw	29.6	26.2	0.0	180.6	33.5	0.22	745.2
$linSVR \ num \ ext(a) \ plus$	29.5	26.2	8.5	305.5	32.6	0.24	871.4

## 1599 LIST OF FIGURES

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1658 1659 1660 1661 1662 1663	Fig. D1.	Normalized absolute difference of statistics and scores (titles) be- tween distributions of observed and simulated GLM flash duration (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator re- sults per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The barianted grant line give the median - Decults for the full test	
1658 1659 1660 1661 1662 1663 1664	Fig. D1.	Normalized absolute difference of statistics and scores (titles) be- tween distributions of observed and simulated GLM flash duration (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator re- sults per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The horizontal green line give the median. Results for the full test detect. ML type abbreviations provided in Table R1	02
1658 1659 1660 1661 1662 1663 1664 1665	Fig. D1.	Normalized absolute difference of statistics and scores (titles) be- tween distributions of observed and simulated GLM flash duration (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator re- sults per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The horizontal green line give the median. Results for the full test dataset. ML type abbreviations provided in Table B1	. 92
1658 1659 1660 1661 1662 1663 1664 1665	Fig. D1. Fig. D2.	Normalized absolute difference of statistics and scores (titles) be- tween distributions of observed and simulated GLM flash duration (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator re- sults per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The horizontal green line give the median. Results for the full test dataset. ML type abbreviations provided in Table B1	. 92
1658 1659 1660 1661 1662 1663 1664 1665 1666	Fig. D1. Fig. D2.	Normalized absolute difference of statistics and scores (titles) be- tween distributions of observed and simulated GLM flash duration (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator re- sults per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The horizontal green line give the median. Results for the full test dataset. ML type abbreviations provided in Table B1 As Figure D1 but for the normalized absolute difference of statistics and scores (titles) between distributions of observed and simulated	. 92
1658 1659 1660 1661 1662 1663 1664 1665 1666 1667 1668	Fig. D1. Fig. D2.	Normalized absolute difference of statistics and scores (titles) be- tween distributions of observed and simulated GLM flash duration (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator re- sults per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The horizontal green line give the median. Results for the full test dataset. ML type abbreviations provided in Table B1	. 92
1658 1659 1660 1661 1662 1663 1664 1665 1666 1667 1668 1669	Fig. D1. Fig. D2.	Normalized absolute difference of statistics and scores (titles) be- tween distributions of observed and simulated GLM flash duration (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator re- sults per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The horizontal green line give the median. Results for the full test dataset. ML type abbreviations provided in Table B1	. 92



FIG. 1. Relative flash detection efficiency per  $1^{\circ} \times 1^{\circ}$  pixel (color) for the full 10-day dataset. In (a) for GLM and in (b) for NLDN. Grey-scale lines contour the flash number at the 0th (1 flash), 50th, 80th, and 95th percentile of the flash number distribution per  $0.25^{\circ} \times 0.25^{\circ}$  pixel (only for pixels with flash activity). The corresponding percentile values are stated on the right-side color bar.



FIG. 2. Illustration of splitting the 10-day dataset with GLM and NLDN flashes in 7-day generator building (GB) and 3-day generator testing (GT) data. The GB data is further processed for the machine learning (ML) part.



FIG. 3. Flow chart of the multi-step approach illustrating the possible predictions of a given target using different combinations of features and pseudo-features (a, Training). The Application (b) shows the example of the *num ext(a)* configuration (Appendix B.b).



FIG. 4. An example of one simulated flash with corresponding GLM and NLDN observations on 26 May 2018. The final GEO lightning pseudo-observation generator is used including a linear SVR model, i.e., linSVR num ext(a) plus. Time series of latitudes (a), longitudes (b), and a map (c). The map (c) includes characteristics of the observed and simulated GLM flash. The time interval shown matches the simulated flash duration of 640 ms.



FIG. 5. Normalized absolute difference of statistics and scores (titles) between distributions of observed and simulated GLM flash extent (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator results per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The horizontal green line give the median. Results for the full test dataset. ML type abbreviations provided in Table B1.



FIG. 6. Normalized absolute difference of statistics and scores (titles) between distributions of observed and simulated GLM flash duration (a), event number per flash (b), and flash extent (c); y-range (0 to 1) as in Figures D1 (for a), D2 (for b), and 5 (for c). Boxplots (as in 5) represent the distribution for training the same model (x-axis) 10 times during the first step of the simulation. ML type abbreviations provided in Table B1.



FIG. 7. Observed (a) and simulated hourly FED using linSVR num ext(a) plus (b), MLP alpha8 num raw (c), and BAGR KNN dist num plus (d) generator on 26 May 2018, 20:00 to 21:00 UTC. The FED grid uses pixels of 5 km × 5 km. ML type abbreviations provided in Table B1.



FIG. 8. Pixel-to-pixel  $(5 \text{ km} \times 5 \text{ km})$  simulated versus observed hourly FED for the 3-day test period using the same linSVR (a), MLP (b), and BAGR KNN dist (c) based generators as in Figure 7. The gray box and white margins indicate the upper limits of distributions on each axis. ML type abbreviations provided in Table B1.



FIG. 9. Hourly sum of FED (a) and hourly electrified area (b) within the region of interest. Top (1): Absolute values and number of simulated flashes per hour. Bottom (2): Difference of simulation minus observation. The observation is plotted in blue, the remaining colors represent the 10 best generators for FED sum (a) and electrified area (b), respectively. The best generator of FED sum (a) is also included in (b) [orange], and the best generator from (b) is included in (a) [lime]. Results for 31 July 2018. Details about the generator names are provided in Appendix B.b.



FIG. 10. As Figure 9 with 10 repetitions of the recommended *linSVR num ext(a) plus* generator. Median (line) and range (shaded) of 10 generator repetitions for 31 July 2018.



FIG. D1. Normalized absolute difference of statistics and scores (titles) between distributions of observed and simulated GLM flash duration (0 means equal to observation, 1 represents the worst simulation). The boxplots represent the distributions of 28 target generator results per ML type (x-axis) including the Inter-Quartile-Range (IQR, blue box), 1.5 times the IQR (whiskers), and outliers (black cross). The horizontal green line give the median. Results for the full test dataset. ML type abbreviations provided in Table B1.



<sup>1718</sup> FIG. D2. As Figure D1 but for the normalized absolute difference of statistics and scores (titles) <sup>1719</sup> between distributions of observed and simulated GLM event number per flash (0 means equal to <sup>1720</sup> observation, 1 represents the worst simulation).